



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 03:44 AM UTC

PDB ID : 2CJF / pdb_00002cjf
Title : TYPE II DEHYDROQUINASE INHIBITOR COMPLEX
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Deposited on : 2006-03-31
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

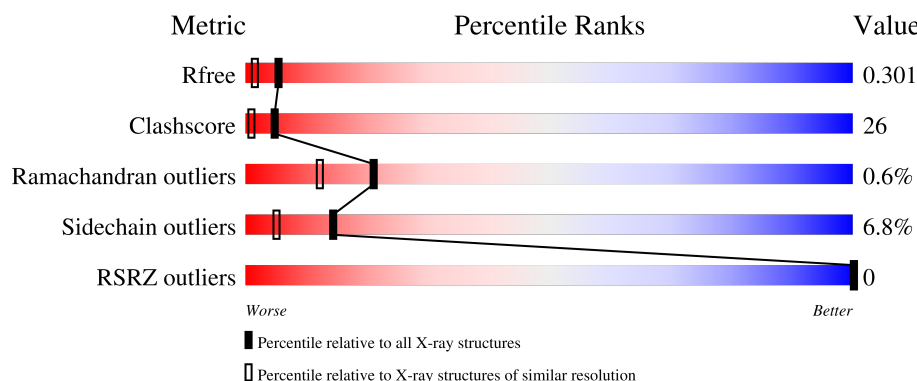
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



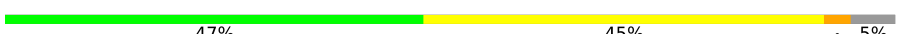
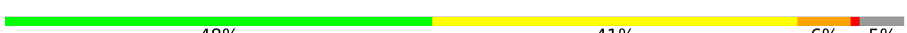
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	157	
1	B	157	
1	C	157	
1	D	157	
1	E	157	

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Mol	Chain	Length	Quality of chain
1	F	157	
1	G	157	
1	H	157	
1	I	157	
1	J	157	
1	K	157	
1	L	157	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	RP4	A	1151	-	-	X	-
3	GOL	A	1152	-	-	X	-
3	GOL	D	1753	-	-	X	-
3	GOL	E	1952	-	X	-	-
3	GOL	F	2153	-	-	X	-
3	GOL	G	2353	-	-	X	-
3	GOL	H	2552	-	-	X	-
3	GOL	J	2955	-	-	X	-
3	GOL	K	3153	-	-	X	-

2 Entry composition

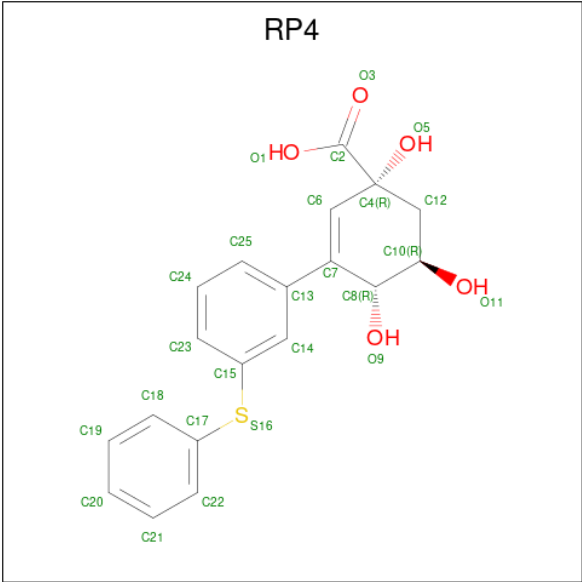
There are 6 unique types of molecules in this entry. The entry contains 15510 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-DEHYDROQUINATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	B	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	C	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	D	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	E	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	F	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	G	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	H	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	I	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			
1	J	149	Total	C	N	O	S	0	2	0
			1132	704	213	210	5			
1	K	149	Total	C	N	O	S	0	1	0
			1126	701	210	210	5			
1	L	149	Total	C	N	O	S	0	2	0
			1127	701	210	211	5			

- Molecule 2 is (1S,4S,5S)-1,4,5-TRIHIDROXY-3-[3-(PHENYLTHIO)PHENYL]CYCLOHE X-2-ENE-1-CARBOXYLIC ACID (CCD ID: RP4) (formula: C₁₉H₁₈O₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			25	19	5	1		
2	B	1	Total	C	O	S	0	0
			25	19	5	1		
2	C	1	Total	C	O	S	0	0
			25	19	5	1		
2	D	1	Total	C	O	S	0	0
			25	19	5	1		
2	E	1	Total	C	O	S	0	0
			25	19	5	1		
2	F	1	Total	C	O	S	0	0
			25	19	5	1		
2	G	1	Total	C	O	S	0	0
			25	19	5	1		
2	H	1	Total	C	O	S	0	0
			25	19	5	1		
2	I	1	Total	C	O	S	0	0
			25	19	5	1		
2	J	1	Total	C	O	S	0	0
			25	19	5	1		
2	K	1	Total	C	O	S	0	0
			25	19	5	1		
2	L	1	Total	C	O	S	0	0
			25	19	5	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



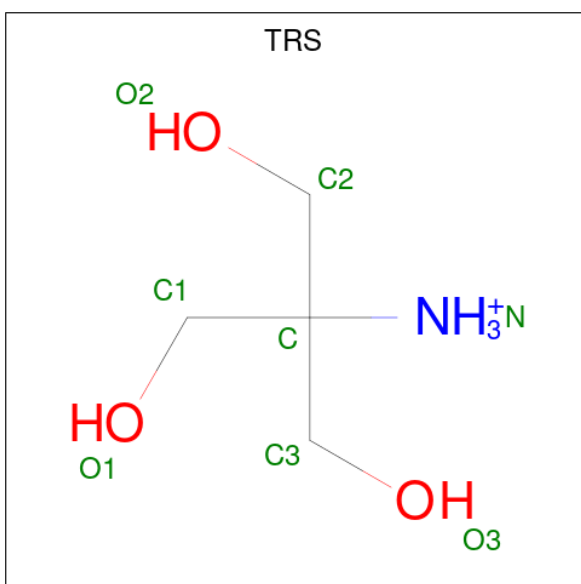
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		
4	J	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 8 4 1 3	0	0
5	D	1	Total C N O 8 4 1 3	0	0
5	I	1	Total C N O 8 4 1 3	0	0
5	J	1	Total C N O 8 4 1 3	0	0

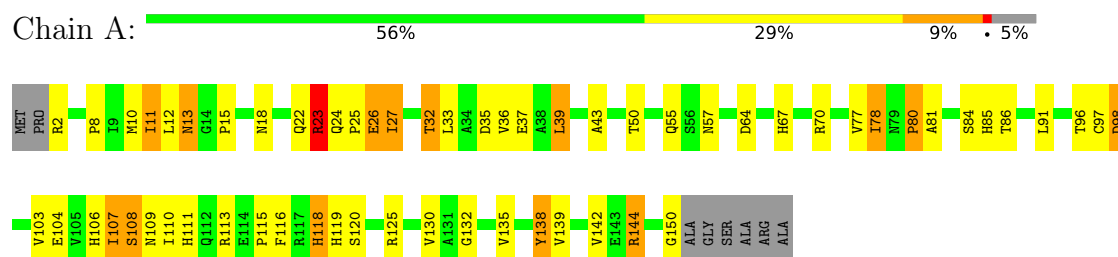
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	118	Total O 118 118	0	0
6	B	142	Total O 142 142	0	0
6	C	127	Total O 127 127	0	0
6	D	140	Total O 140 140	0	0
6	E	164	Total O 164 164	0	0
6	F	133	Total O 133 133	0	0
6	G	133	Total O 133 133	0	0
6	H	105	Total O 105 105	0	0
6	I	139	Total O 139 139	0	0
6	J	111	Total O 111 111	0	0
6	K	117	Total O 117 117	0	0
6	L	132	Total O 132 132	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

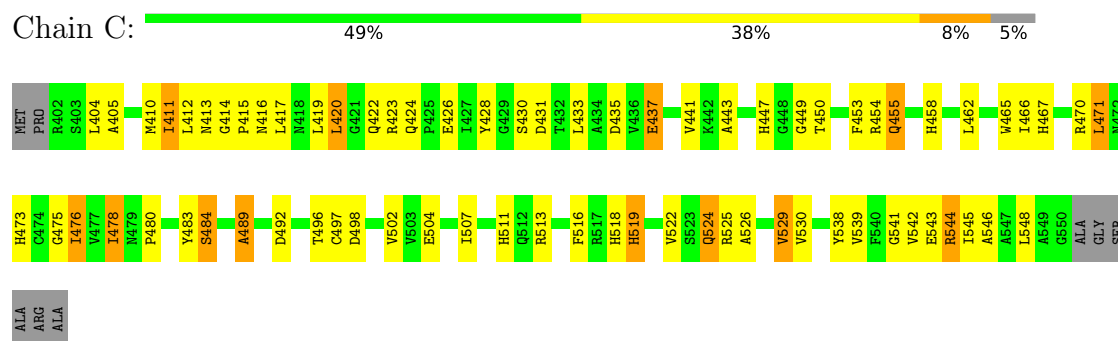
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

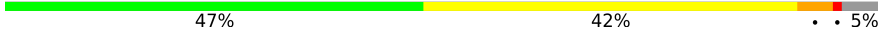


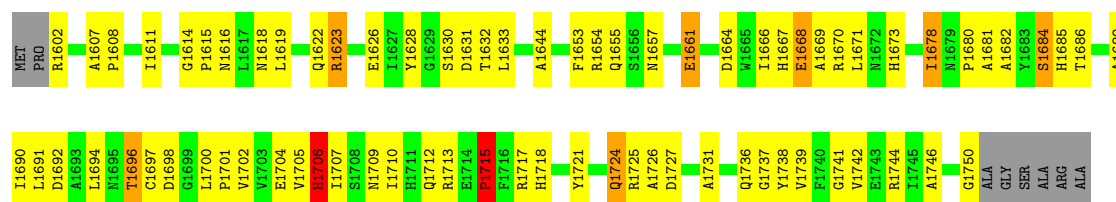
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

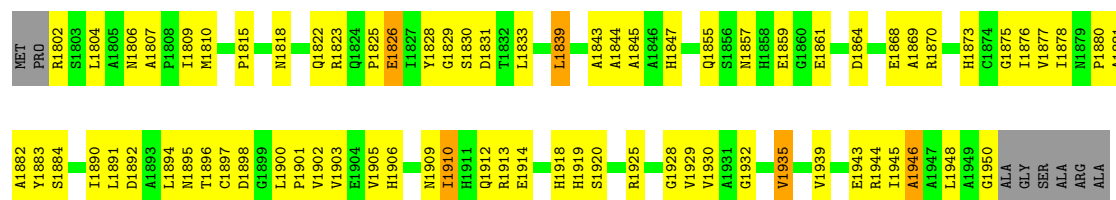


Chain I:  47% 42% 5%



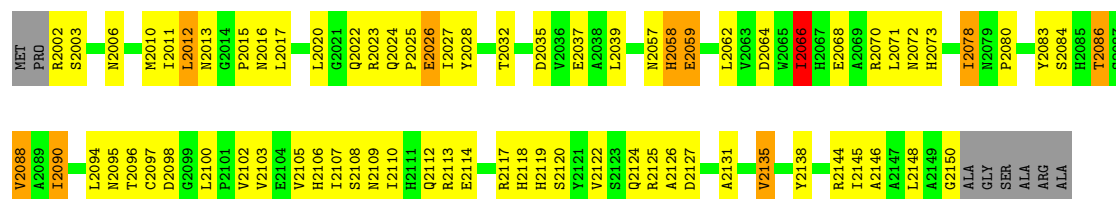
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain J:  47% 45% 5%



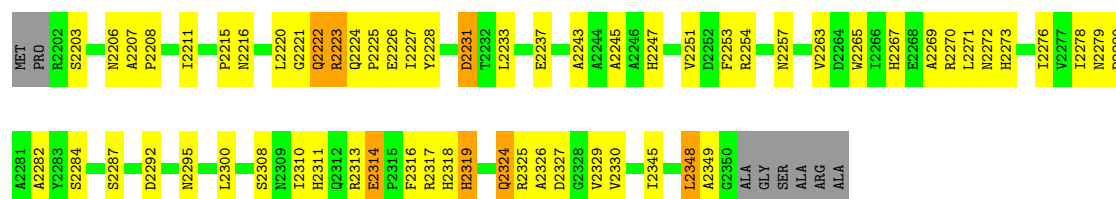
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain K:  48% 41% 6% 5%



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain L:  55% 35% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	195.75Å 195.73Å 239.68Å 65.84° 65.89° 89.97°	Depositor
Resolution (Å)	25.00 – 1.95 25.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	76.2 (25.00-1.95) 76.0 (25.00-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.274 , 0.334 0.298 , 0.301	Depositor DCC
R_{free} test set	80795 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.406 for k,-h,-h+1 0.406 for -k,h,-k+1 0.417 for -h,k,k-l 0.437 for h,-k,h-l 0.417 for -k,-h,-l 0.407 for k,h,h+k-l 0.416 for -h,-k,-h-k+1	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	15510	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, TRS, GOL, RP4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.36	7/1161 (0.6%)	1.37	10/1582 (0.6%)
1	B	1.33	1/1155 (0.1%)	1.46	11/1574 (0.7%)
1	C	1.21	1/1161 (0.1%)	1.38	9/1582 (0.6%)
1	D	1.40	5/1161 (0.4%)	1.39	10/1582 (0.6%)
1	E	1.35	5/1155 (0.4%)	1.41	12/1574 (0.8%)
1	F	1.24	4/1155 (0.3%)	1.31	9/1574 (0.6%)
1	G	1.41	5/1161 (0.4%)	1.46	12/1582 (0.8%)
1	H	1.23	2/1161 (0.2%)	1.32	8/1582 (0.5%)
1	I	1.35	5/1161 (0.4%)	1.41	11/1582 (0.7%)
1	J	1.24	4/1166 (0.3%)	1.38	9/1588 (0.6%)
1	K	1.32	4/1155 (0.3%)	1.33	3/1574 (0.2%)
1	L	1.37	2/1161 (0.2%)	1.42	6/1582 (0.4%)
All	All	1.32	45/13913 (0.3%)	1.39	110/18958 (0.6%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1090	ILE	CA-CB	-8.84	1.44	1.54
1	G	1305	VAL	CA-CB	7.87	1.64	1.54
1	G	1282	ALA	CA-C	7.30	1.63	1.52
1	I	1709	ASN	CA-C	7.23	1.61	1.53
1	L	2263	VAL	CA-CB	7.14	1.62	1.54
1	K	2105	VAL	CA-CB	6.90	1.62	1.54
1	D	705	VAL	C-O	-6.85	1.16	1.24
1	E	939	VAL	CA-CB	6.73	1.61	1.54
1	A	130	VAL	CA-CB	6.43	1.63	1.54
1	I	1707	ILE	CA-CB	6.41	1.62	1.54
1	D	666	ILE	CA-CB	6.37	1.62	1.54
1	E	881	ALA	CA-CB	6.34	1.64	1.53
1	H	1493	ALA	CA-CB	-6.29	1.43	1.53
1	K	2066	ILE	CA-CB	6.04	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	2107	ILE	CA-CB	6.00	1.62	1.54
1	F	1067	HIS	CA-C	5.90	1.60	1.52
1	D	710	ILE	CG1-CD1	5.89	1.74	1.51
1	A	32	THR	CA-CB	5.71	1.61	1.53
1	D	680	PRO	N-CA	-5.66	1.40	1.47
1	G	1251	VAL	CA-CB	5.62	1.62	1.54
1	G	1257	ASN	C-O	5.62	1.31	1.24
1	F	1126	ALA	CA-CB	-5.61	1.44	1.53
1	H	1463	VAL	CA-C	5.44	1.59	1.52
1	E	811	ILE	C-O	5.40	1.30	1.24
1	D	689	ALA	N-CA	5.38	1.52	1.46
1	I	1644	ALA	CA-CB	-5.38	1.45	1.53
1	K	2086	THR	CA-CB	5.37	1.63	1.54
1	J	1878	ILE	CA-CB	5.35	1.61	1.54
1	G	1329	VAL	CA-CB	5.33	1.61	1.54
1	A	130	VAL	C-O	-5.32	1.18	1.24
1	F	1082	ALA	CA-CB	-5.30	1.45	1.53
1	I	1689	ALA	CA-CB	-5.26	1.45	1.53
1	I	1686	THR	C-O	5.23	1.31	1.23
1	A	13	ASN	CA-C	-5.22	1.46	1.52
1	E	886	THR	CA-CB	5.15	1.61	1.53
1	C	489	ALA	C-O	5.13	1.29	1.24
1	J	1946	ALA	CA-CB	-5.13	1.45	1.53
1	A	86	THR	C-O	5.12	1.30	1.24
1	J	1890	ILE	CA-CB	-5.11	1.47	1.54
1	A	118	HIS	CA-C	5.10	1.59	1.52
1	B	279	ASN	N-CA	-5.09	1.40	1.46
1	E	927	ASP	N-CA	-5.07	1.40	1.46
1	L	2330	VAL	CA-CB	5.05	1.60	1.54
1	A	91	LEU	CA-C	5.05	1.59	1.52
1	J	1905	VAL	CA-CB	5.00	1.60	1.54

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	2295	ASN	N-CA-C	-9.08	101.64	112.89
1	G	1284	SER	N-CA-C	-7.95	101.58	111.75
1	D	690	ILE	N-CA-C	7.89	118.00	110.42
1	K	2078	ILE	N-CA-C	7.79	119.02	108.11
1	I	1696	THR	N-CA-C	-7.70	103.89	113.28
1	E	857	ASN	N-CA-C	7.68	121.75	112.38
1	G	1277	VAL	N-CA-C	-7.66	97.39	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	PRO	N-CA-C	-7.64	104.80	114.35
1	A	142	VAL	N-CA-C	-7.56	103.08	110.72
1	D	683	TYR	N-CA-C	-7.56	103.94	113.01
1	F	1078	ILE	N-CA-C	7.46	118.82	107.77
1	E	927	ASP	N-CA-C	-7.35	102.87	111.03
1	J	1861	GLU	N-CA-C	-6.92	102.96	111.40
1	D	711	HIS	N-CA-C	-6.88	104.62	113.16
1	E	894	LEU	N-CA-C	-6.84	103.90	111.36
1	B	277	VAL	N-CA-C	-6.67	98.85	108.53
1	C	478	ILE	N-CA-C	6.62	117.65	108.12
1	G	1233	LEU	N-CA-C	-6.53	104.24	111.36
1	D	721	TYR	N-CA-C	6.50	118.02	111.07
1	I	1706	HIS	CA-C-N	6.39	129.49	120.42
1	I	1706	HIS	C-N-CA	6.39	129.49	120.42
1	B	292	ASP	N-CA-C	6.38	118.32	111.36
1	B	249	GLY	N-CA-C	6.36	120.43	111.14
1	H	1466	ILE	N-CA-C	-6.35	104.30	110.72
1	I	1737	GLY	N-CA-C	6.33	120.55	112.83
1	G	1280	PRO	N-CD-CG	-6.28	93.78	103.20
1	H	1514	GLU	N-CA-C	6.27	116.81	109.60
1	I	1746	ALA	N-CA-C	-6.26	104.37	111.14
1	F	1098	ASP	N-CA-C	6.18	119.58	110.30
1	J	1900	LEU	N-CA-C	-6.15	101.82	110.31
1	E	852	ASP	N-CA-C	-6.15	97.17	107.80
1	C	475	GLY	N-CA-C	6.14	119.29	111.37
1	G	1212	LEU	N-CA-C	6.13	118.95	109.07
1	G	1204	LEU	N-CA-C	6.10	117.60	111.07
1	H	1482	ALA	N-CA-C	6.10	118.43	111.11
1	C	524	GLN	N-CA-C	-6.08	105.36	112.89
1	E	833	LEU	N-CA-C	-6.07	104.66	111.28
1	K	2059	GLU	N-CA-C	-6.06	104.79	111.82
1	I	1661	GLU	CA-C-N	6.03	128.28	120.44
1	I	1661	GLU	C-N-CA	6.03	128.28	120.44
1	B	322	VAL	N-CA-C	-5.99	104.67	110.72
1	E	856	SER	CA-C-N	5.99	130.18	120.60
1	E	856	SER	C-N-CA	5.99	130.18	120.60
1	D	688	VAL	N-CA-C	-5.96	103.63	111.09
1	C	455	GLN	N-CA-C	-5.93	100.04	109.23
1	J	1894	LEU	N-CA-C	-5.89	105.18	112.90
1	A	27	ILE	N-CA-C	5.89	116.67	111.90
1	I	1678	ILE	N-CA-C	5.84	116.28	107.75
1	G	1253	PHE	N-CA-C	5.83	118.17	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	729	VAL	CB-CA-C	-5.83	102.00	110.63
1	F	1041	VAL	CA-C-N	5.80	128.63	120.28
1	F	1041	VAL	C-N-CA	5.80	128.63	120.28
1	L	2282	ALA	N-CA-C	5.79	118.33	111.33
1	E	806	ASN	N-CA-C	5.78	119.52	112.23
1	E	929	VAL	CB-CA-C	-5.78	101.89	110.33
1	D	677	VAL	N-CA-C	-5.77	100.12	108.71
1	J	1929	VAL	CA-C-N	-5.71	115.74	123.10
1	J	1929	VAL	C-N-CA	-5.71	115.74	123.10
1	G	1339	VAL	N-CA-C	5.70	117.12	110.62
1	C	437	GLU	N-CA-C	-5.69	104.98	111.07
1	A	78	ILE	N-CA-C	5.67	116.91	108.46
1	A	138	TYR	N-CA-C	-5.67	105.09	112.23
1	B	330	VAL	N-CA-C	-5.66	99.39	107.77
1	H	1407	ALA	N-CA-C	5.66	113.22	108.13
1	G	1278	ILE	N-CA-C	5.63	116.39	108.17
1	D	607	ALA	N-CA-C	5.60	115.33	108.11
1	C	522	VAL	N-CA-C	5.58	116.31	110.62
1	G	1287	SER	N-CA-C	5.55	118.29	108.24
1	F	1067	HIS	N-CA-C	5.52	117.10	111.14
1	B	343	GLU	N-CA-C	5.49	117.97	111.33
1	B	240	CYS	N-CA-C	-5.42	105.02	111.69
1	J	1877	VAL	N-CA-C	-5.42	100.58	108.17
1	A	144	ARG	N-CA-C	5.41	117.61	111.11
1	G	1280	PRO	N-CA-C	-5.41	106.97	114.27
1	C	484	SER	N-CA-C	-5.35	105.61	111.82
1	F	1136	GLN	N-CA-C	-5.33	104.88	111.33
1	H	1468	GLU	N-CA-C	5.32	117.49	111.11
1	B	211	ILE	N-CA-C	5.31	116.16	107.24
1	J	1806	ASN	N-CA-C	5.30	117.13	111.36
1	B	284	SER	N-CA-C	-5.29	105.59	111.36
1	H	1548	LEU	N-CA-C	5.29	116.85	111.14
1	C	507	ILE	N-CA-C	5.27	115.48	110.42
1	J	1905	VAL	N-CA-C	5.27	115.45	107.75
1	K	2012	LEU	N-CA-C	5.27	118.40	109.76
1	E	880	PRO	N-CD-CG	-5.26	95.31	103.20
1	L	2326	ALA	N-CA-C	-5.24	102.63	110.23
1	E	882	ALA	N-CA-C	5.22	121.92	110.80
1	F	1149	ALA	N-CA-C	-5.18	106.91	113.18
1	I	1715	PRO	N-CA-C	5.18	123.13	112.47
1	C	450	THR	N-CA-C	5.17	116.85	109.14
1	D	615	PRO	N-CA-C	5.14	119.38	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1541	GLY	N-CA-C	-5.13	106.43	112.64
1	B	287	SER	N-CA-C	5.13	117.52	107.57
1	I	1710	ILE	N-CA-C	5.13	116.46	110.62
1	L	2329	VAL	N-CA-C	-5.13	100.86	108.45
1	E	885	HIS	N-CA-C	-5.12	107.08	113.38
1	A	23	ARG	N-CA-C	5.11	116.75	109.14
1	I	1739	VAL	N-CA-C	-5.10	105.57	110.72
1	B	264	ASP	N-CA-C	-5.09	105.62	111.07
1	H	1412	LEU	N-CA-C	5.09	117.20	108.90
1	A	108	SER	CA-C-N	-5.08	113.94	122.17
1	A	108	SER	C-N-CA	-5.08	113.94	122.17
1	J	1898	ASP	N-CA-C	5.07	117.91	110.30
1	F	1127	ASP	N-CA-C	-5.06	105.76	111.28
1	A	107	ILE	N-CA-C	5.04	115.27	110.53
1	L	2279	ASN	CA-C-O	-5.03	115.61	119.99
1	G	1282	ALA	N-CA-C	5.02	119.28	113.20
1	F	1010	MET	N-CA-C	5.02	117.44	109.96
1	D	606	ASN	N-CA-C	5.02	119.45	113.23
1	L	2287	SER	N-CA-C	5.01	117.07	107.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1127	0	1093	54	0
1	B	1126	0	1092	54	0
1	C	1127	0	1093	63	0
1	D	1127	0	1093	66	0
1	E	1126	0	1092	61	0
1	F	1126	0	1092	60	0
1	G	1127	0	1093	57	0
1	H	1127	0	1093	53	0
1	I	1127	0	1093	55	0
1	J	1132	0	1102	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1126	0	1092	71	0
1	L	1127	0	1093	56	0
2	A	25	0	17	10	0
2	B	25	0	17	2	0
2	C	25	0	17	2	0
2	D	25	0	17	0	0
2	E	25	0	17	2	0
2	F	25	0	17	2	0
2	G	25	0	17	1	0
2	H	25	0	17	2	0
2	I	25	0	17	1	0
2	J	25	0	18	0	0
2	K	25	0	17	4	0
2	L	25	0	17	5	0
3	A	6	0	8	4	0
3	B	6	0	8	0	0
3	D	6	0	8	8	0
3	E	6	0	8	2	0
3	F	6	0	8	5	0
3	G	6	0	8	4	0
3	H	6	0	8	4	0
3	J	12	0	16	8	0
3	K	12	0	16	10	0
3	L	6	0	8	2	0
4	B	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	J	5	0	0	0	0
5	B	8	0	12	0	0
5	D	8	0	12	0	0
5	I	8	0	12	1	0
5	J	8	0	12	1	0
6	A	118	0	0	18	0
6	B	142	0	0	15	0
6	C	127	0	0	14	0
6	D	140	0	0	23	0
6	E	164	0	0	16	0
6	F	133	0	0	16	0
6	G	133	0	0	19	0
6	H	105	0	0	13	0
6	I	139	0	0	17	0
6	J	111	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	117	0	0	19	0
6	L	132	0	0	17	0
All	All	15510	0	13470	701	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (701) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:710:ILE:CD1	1:D:710:ILE:CG1	1.74	1.59
1:C:447:HIS:CD2	6:C:2051:HOH:O	1.84	1.28
3:K:3153:GOL:H32	6:K:7116:HOH:O	1.34	1.26
1:C:447:HIS:HD2	6:C:2051:HOH:O	1.16	1.19
1:G:1228:TYR:CE1	6:G:2032:HOH:O	1.96	1.17
1:L:2243:ALA:O	1:L:2247:HIS:HD2	1.27	1.14
3:G:2353:GOL:C3	6:G:2132:HOH:O	1.90	1.11
1:K:2002:ARG:NH1	6:K:7007:HOH:O	1.82	1.11
1:B:239:LEU:HD23	1:B:242:LYS:HE2	1.30	1.10
1:J:1918:HIS:HB3	3:J:2955:GOL:O2	1.52	1.09
3:D:1753:GOL:H32	6:D:2139:HOH:O	1.50	1.08
1:E:803:SER:HB2	6:E:2043:HOH:O	1.51	1.08
1:H:1525:ARG:HD2	6:H:2095:HOH:O	1.54	1.07
1:L:2319[B]:HIS:HD2	6:L:2086:HOH:O	1.34	1.06
1:G:1228:TYR:HE1	6:G:2032:HOH:O	1.33	1.04
1:D:602:ARG:HG2	1:D:602:ARG:HH21	1.22	1.00
1:I:1725:ARG:O	6:I:2124:HOH:O	1.81	0.99
1:L:2311:HIS:HB3	3:L:3352:GOL:H11	1.45	0.97
1:E:815:PRO:HD2	1:E:881:ALA:HB3	1.45	0.96
1:K:2020:LEU:O	6:K:7017:HOH:O	1.84	0.96
3:F:2153:GOL:H12	1:H:1519[A]:HIS:CD2	2.00	0.96
3:D:1753:GOL:O1	6:D:2140:HOH:O	1.81	0.95
1:L:2243:ALA:O	1:L:2247:HIS:CD2	2.19	0.95
1:D:602:ARG:HH21	1:D:602:ARG:CG	1.80	0.94
1:H:1527:ASP:OD1	6:H:2098:HOH:O	1.83	0.94
1:I:1750:GLY:HA3	6:I:2139:HOH:O	1.68	0.93
1:J:1822:GLN:HE22	1:K:2070:ARG:HH12	1.13	0.91
1:H:1498:ASP:OD2	6:H:2073:HOH:O	1.87	0.91
1:C:465:TRP:CH2	6:C:2069:HOH:O	2.23	0.91
1:F:1150:GLY:HA2	6:F:2129:HOH:O	1.70	0.91
1:L:2247:HIS:CE1	6:L:2058:HOH:O	2.25	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:GLN:HG3	6:C:2111:HOH:O	1.72	0.90
1:J:1868:GLU:OE1	6:J:2062:HOH:O	1.90	0.89
1:E:824:GLN:HE21	1:E:827:ILE:HD12	1.37	0.89
1:F:1004:LEU:HD11	1:F:1146:ALA:HA	1.54	0.89
1:G:1223:ARG:HG3	6:G:2027:HOH:O	1.72	0.89
1:F:1024:GLN:HE21	1:F:1027:ILE:HD13	1.36	0.87
1:K:2064:ASP:OD2	6:K:7054:HOH:O	1.93	0.87
1:E:806:ASN:O	6:E:2049:HOH:O	1.91	0.86
1:D:711:HIS:HB3	3:D:1753:GOL:H11	1.56	0.86
1:D:710:ILE:O	1:D:718:HIS:HD2	1.59	0.86
1:F:1023:ARG:NH1	6:F:2029:HOH:O	2.07	0.86
3:A:1152:GOL:O1	6:A:2118:HOH:O	1.93	0.85
1:J:1804:LEU:HD13	6:J:2106:HOH:O	1.76	0.85
1:J:1882:ALA:HB1	1:K:2088:VAL:HG12	1.59	0.85
1:L:2206:ASN:HB2	6:L:2021:HOH:O	1.76	0.84
1:L:2215:PRO:O	1:L:2216:ASN:HB2	1.78	0.84
2:A:1151:RP4:H21	6:A:2014:HOH:O	1.79	0.83
3:F:2153:GOL:H12	1:H:1519[A]:HIS:HD2	1.43	0.83
1:D:602:ARG:HG2	1:D:602:ARG:NH2	1.83	0.82
1:C:538:TYR:O	1:C:542:VAL:HG23	1.79	0.82
1:F:1024:GLN:HA	1:F:1026:GLU:OE2	1.78	0.82
1:E:867:HIS:O	1:E:870:ARG:HB3	1.79	0.81
1:A:24:GLN:HG2	1:A:27:ILE:HB	1.60	0.81
1:J:1843:ALA:O	1:J:1847:HIS:HD2	1.64	0.81
1:B:340:PHE:HA	1:B:343:GLU:HG3	1.61	0.81
1:L:2247:HIS:HE1	6:L:2058:HOH:O	1.61	0.80
1:H:1524:GLN:OE1	6:H:2094:HOH:O	1.98	0.80
1:C:539:VAL:O	1:C:543:GLU:HG3	1.82	0.80
1:H:1423:ARG:HD3	6:H:2024:HOH:O	1.83	0.79
1:J:1843:ALA:CB	1:J:1939:VAL:HG13	2.13	0.79
1:C:419:LEU:O	1:C:422:GLN:HG3	1.82	0.79
1:J:1822:GLN:HE21	1:K:2070:ARG:HH22	1.30	0.79
1:B:349:ALA:O	6:B:2138:HOH:O	1.99	0.79
1:K:2108:SER:HB2	6:K:7078:HOH:O	1.83	0.79
1:C:423:ARG:HG2	2:C:1551:RP4:H20	1.66	0.77
1:E:853:PHE:O	6:E:2095:HOH:O	2.02	0.77
1:A:23:ARG:H	2:A:1151:RP4:H20	1.49	0.77
1:B:331:ALA:HB2	6:B:2106:HOH:O	1.85	0.77
6:F:2103:HOH:O	3:H:2552:GOL:H2	1.84	0.76
1:J:1822:GLN:NE2	1:K:2070:ARG:HH12	1.84	0.76
1:L:2318:HIS:ND1	3:L:3352:GOL:H31	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:ALA:O	6:C:2051:HOH:O	2.04	0.76
1:I:1691:LEU:HD13	1:I:1721:TYR:O	1.86	0.76
1:G:1336:GLN:HB2	6:G:2123:HOH:O	1.84	0.75
1:E:878:ILE:HG12	1:E:880:PRO:HG3	1.69	0.75
1:I:1630[B]:SER:HB2	6:I:2035:HOH:O	1.87	0.75
1:D:698:ASP:HA	6:D:2104:HOH:O	1.87	0.74
1:C:412:LEU:HB2	1:C:478:ILE:HG13	1.69	0.74
1:D:710:ILE:O	1:D:718:HIS:CD2	2.40	0.74
1:E:815:PRO:HG3	1:E:883:TYR:CE1	2.23	0.74
1:H:1428:TYR:HE1	6:H:2030:HOH:O	1.71	0.74
1:K:2039:LEU:CD1	1:K:2135:VAL:HG23	2.18	0.74
1:B:216:ASN:OD1	1:C:467:HIS:NE2	2.18	0.74
1:G:1283:TYR:HB3	1:G:1287:SER:HB2	1.70	0.74
1:I:1664:ASP:O	1:I:1667:HIS:HB2	1.88	0.73
1:J:1876:ILE:O	1:J:1902:VAL:HA	1.89	0.73
1:H:1428:TYR:CE1	6:H:2030:HOH:O	2.39	0.73
1:J:1843:ALA:HB2	1:J:1939:VAL:HG13	1.69	0.73
1:E:847:HIS:CD2	6:E:2083:HOH:O	2.41	0.72
1:G:1252:ASP:OD1	6:G:2065:HOH:O	2.07	0.72
1:B:239:LEU:CD2	1:B:242:LYS:HE2	2.14	0.72
3:D:1753:GOL:H2	6:D:2109:HOH:O	1.89	0.72
1:D:716:PHE:HD2	6:D:2116:HOH:O	1.72	0.72
1:D:643:ALA:O	1:D:647:HIS:HD2	1.72	0.72
1:J:1855:GLN:OE1	6:J:2053:HOH:O	2.06	0.72
1:I:1669:ALA:HA	1:I:1673:HIS:ND1	2.05	0.72
1:F:1011:ILE:HG13	1:F:1077:VAL:HB	1.71	0.71
1:F:1022:GLN:O	1:F:1023:ARG:HG2	1.90	0.71
1:C:423:ARG:HG3	1:C:424:GLN:HG3	1.72	0.71
1:H:1424:GLN:HA	1:H:1426:GLU:OE2	1.90	0.71
1:L:2327:ASP:HA	6:L:2116:HOH:O	1.89	0.71
1:L:2325:ARG:O	1:L:2325:ARG:NH1	2.23	0.71
6:I:2114:HOH:O	3:K:3152:GOL:H11	1.90	0.70
1:D:721:TYR:O	1:D:724:GLN:HG3	1.90	0.70
6:A:2065:HOH:O	1:C:458:HIS:NE2	2.22	0.70
1:H:1538:TYR:O	1:H:1542:VAL:HG23	1.92	0.70
1:F:1022:GLN:O	1:F:1023:ARG:CB	2.40	0.70
1:F:1136:GLN:O	1:F:1139:VAL:HB	1.92	0.69
1:L:2222:GLN:O	1:L:2223:ARG:HB3	1.91	0.69
1:F:1069:ALA:HA	1:F:1073:HIS:ND1	2.08	0.69
1:J:1950:GLY:HA3	6:J:2106:HOH:O	1.91	0.69
1:E:823:ARG:NH1	1:E:824:GLN:OE1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1882:ALA:CB	1:K:2088:VAL:HG12	2.23	0.69
1:G:1270:ARG:NH1	6:G:2078:HOH:O	2.26	0.69
1:I:1736:GLN:OE1	1:K:2144:ARG:NH1	2.24	0.69
1:L:2203:SER:HB2	6:L:2130:HOH:O	1.92	0.69
1:J:1822:GLN:HE22	1:K:2070:ARG:NH1	1.91	0.68
1:J:1839:LEU:HD12	1:J:1935:VAL:HG23	1.74	0.68
1:K:2094:LEU:O	1:K:2097:CYS:HB2	1.94	0.67
1:C:437:GLU:OE1	6:C:2047:HOH:O	2.11	0.67
1:B:331:ALA:CB	6:B:2106:HOH:O	2.42	0.67
1:G:1298:ASP:OD1	1:I:1623:ARG:NE	2.24	0.67
3:G:2353:GOL:O1	6:G:2133:HOH:O	1.97	0.67
1:F:1095:ASN:HB2	6:F:2086:HOH:O	1.95	0.67
1:K:2028:TYR:HB2	2:K:3151:RP4:H21	1.76	0.67
1:H:1409:ILE:CD1	1:H:1542:VAL:HG13	2.24	0.67
1:B:339:VAL:O	1:B:343:GLU:HG2	1.94	0.66
1:C:415:PRO:O	1:C:416:ASN:HB2	1.95	0.66
1:J:1939:VAL:O	1:J:1943:GLU:HG3	1.95	0.66
1:B:346:ALA:HB1	6:B:2136:HOH:O	1.94	0.66
1:E:842:LYS:HG2	6:E:2080:HOH:O	1.94	0.66
1:F:1022:GLN:O	1:F:1023:ARG:HB3	1.96	0.66
1:H:1470:ARG:HA	1:H:1500:LEU:HD22	1.78	0.66
1:D:623:ARG:HB2	6:D:2040:HOH:O	1.96	0.66
1:F:1117:ARG:NH2	6:F:2101:HOH:O	2.28	0.66
1:B:243:ALA:O	1:B:247:HIS:HD2	1.79	0.66
1:I:1607:ALA:O	6:I:2018:HOH:O	2.13	0.66
1:C:423:ARG:HG2	2:C:1551:RP4:C20	2.27	0.65
1:L:2237:GLU:HB2	1:L:2253:PHE:CE2	2.31	0.65
1:B:239:LEU:HD23	1:B:242:LYS:CE	2.19	0.65
1:J:1918:HIS:HB3	3:J:2955:GOL:HO2	1.59	0.64
1:B:230:SER:O	6:B:2053:HOH:O	2.15	0.64
1:I:1725:ARG:O	1:I:1726:ALA:C	2.40	0.64
1:C:511:HIS:NE2	6:C:2100:HOH:O	2.29	0.64
3:K:3152:GOL:H2	6:K:7081:HOH:O	1.98	0.64
3:K:3153:GOL:C3	6:K:7116:HOH:O	2.10	0.63
1:A:108:SER:OG	2:A:1151:RP4:O3	2.08	0.63
1:J:1895:ASN:ND2	6:J:2070:HOH:O	2.25	0.63
3:D:1753:GOL:C1	6:D:2109:HOH:O	2.46	0.63
1:J:1823:ARG:HD3	1:K:2096:THR:HA	1.79	0.63
1:G:1292:ASP:OD1	1:I:1717:ARG:NH2	2.31	0.63
1:B:252:ASP:OD2	1:B:273:HIS:NE2	2.28	0.62
1:I:1618:ASN:HA	1:I:1633:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:O	1:A:138:TYR:HB2	1.99	0.62
1:C:413:ASN:ND2	1:C:454:ARG:O	2.32	0.62
1:I:1615:PRO:HA	1:I:1657:ASN:OD1	2.00	0.62
1:G:1336:GLN:CB	6:G:2123:HOH:O	2.44	0.62
3:J:2955:GOL:H2	6:J:2111:HOH:O	1.99	0.62
1:E:824:GLN:HE21	1:E:827:ILE:CD1	2.11	0.62
1:A:11:ILE:HG23	1:A:77:VAL:HB	1.81	0.61
1:D:698:ASP:N	1:D:698:ASP:OD2	2.32	0.61
1:L:2325:ARG:O	6:L:2116:HOH:O	2.16	0.61
1:A:2:ARG:NH1	6:A:2001:HOH:O	2.32	0.61
1:E:803:SER:CB	6:E:2043:HOH:O	2.27	0.61
1:A:70:ARG:HH22	1:C:422:GLN:HE21	1.47	0.61
1:D:717:ARG:NH2	1:E:892:ASP:OD1	2.23	0.61
1:J:1919[A]:HIS:HD2	3:J:2954:GOL:H2	1.65	0.61
1:J:1839:LEU:CD1	1:J:1935:VAL:HG23	2.30	0.61
1:B:243:ALA:CB	1:B:339:VAL:HG13	2.30	0.61
1:E:825:PRO:HD3	6:E:2061:HOH:O	2.01	0.61
1:B:203:SER:HA	6:B:2138:HOH:O	2.01	0.61
1:A:67:HIS:O	1:A:70:ARG:HB3	2.01	0.60
1:K:2002:ARG:NH2	1:K:2071:LEU:O	2.33	0.60
1:C:465:TRP:HH2	6:C:2069:HOH:O	1.72	0.60
2:E:1951:RP4:H21	6:E:2064:HOH:O	1.99	0.60
1:D:602:ARG:HH21	1:D:602:ARG:CB	2.14	0.60
1:D:618:ASN:HB3	1:D:655:GLN:OE1	2.01	0.60
3:A:1152:GOL:H12	6:D:2120:HOH:O	2.00	0.60
1:E:832:THR:HB	6:E:2072:HOH:O	2.02	0.60
1:K:2102:VAL:O	1:K:2127:ASP:N	2.33	0.60
1:B:223:ARG:NH1	6:B:2045:HOH:O	2.16	0.60
1:I:1614:GLY:O	1:I:1655:GLN:NE2	2.31	0.60
3:K:3153:GOL:C1	6:K:7097:HOH:O	2.50	0.60
1:A:24:GLN:HE21	1:A:27:ILE:HD13	1.67	0.60
1:H:1404:LEU:CD2	1:H:1546:ALA:HA	2.31	0.60
1:K:2117:ARG:NH1	2:K:3151:RP4:O11	2.34	0.60
1:L:2216:ASN:O	2:L:3351:RP4:H18	2.01	0.59
1:C:462:LEU:O	1:C:466:ILE:HG13	2.01	0.59
1:E:824:GLN:NE2	1:E:827:ILE:HD12	2.14	0.59
1:H:1500:LEU:O	1:H:1525:ARG:NH2	2.36	0.59
1:I:1712:GLN:NE2	6:I:2104:HOH:O	2.34	0.59
1:G:1204:LEU:HD12	1:G:1349:ALA:HB3	1.84	0.59
1:A:70:ARG:HH22	1:C:422:GLN:NE2	2.00	0.59
1:H:1518:HIS:HB3	3:H:2552:GOL:O2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:3153:GOL:H11	6:K:7097:HOH:O	2.01	0.59
1:L:2223:ARG:HA	6:L:2035:HOH:O	2.02	0.59
1:A:98:ASP:HA	6:A:2083:HOH:O	2.02	0.59
1:J:1828:TYR:OH	1:J:1913:ARG:NH2	2.35	0.59
1:B:261:GLU:O	1:B:264:ASP:HB2	2.02	0.59
1:F:1144:ARG:NH2	6:F:2123:HOH:O	2.33	0.59
1:C:541:GLY:O	1:C:545:ILE:HG12	2.02	0.59
1:A:23:ARG:N	2:A:1151:RP4:H20	2.18	0.59
1:K:2015:PRO:HA	1:K:2057:ASN:OD1	2.02	0.59
1:K:2106:HIS:O	1:K:2131:ALA:HA	2.03	0.59
1:D:715:PRO:O	1:D:718:HIS:HB2	2.03	0.58
1:B:223:ARG:HD3	1:C:496:THR:HA	1.84	0.58
1:D:643:ALA:O	1:D:647:HIS:CD2	2.55	0.58
1:B:235:ASP:OD2	6:B:2061:HOH:O	2.17	0.58
1:B:280:PRO:O	1:B:281:ALA:C	2.47	0.58
1:J:1828:TYR:OH	1:J:1913:ARG:NH1	2.36	0.58
1:C:405:ALA:HA	6:C:2054:HOH:O	2.04	0.58
1:D:639:LEU:HD12	1:D:735:VAL:HG23	1.85	0.58
1:K:2080:PRO:HG2	1:K:2084:SER:OG	2.02	0.58
1:E:815:PRO:CD	1:E:881:ALA:HB3	2.29	0.58
1:F:1043:ALA:O	1:F:1047:HIS:HD2	1.87	0.57
1:J:1822:GLN:NE2	1:K:2070:ARG:HH22	2.01	0.57
1:D:623:ARG:HD3	6:D:2039:HOH:O	2.03	0.57
1:E:898:ASP:O	6:E:2128:HOH:O	2.17	0.57
1:F:1009:ILE:O	1:F:1011:ILE:HD12	2.05	0.57
1:G:1344:ARG:NH2	6:G:2128:HOH:O	2.15	0.57
1:H:1491:LEU:HD13	1:H:1521:TYR:O	2.04	0.57
1:B:223:ARG:NE	1:C:498:ASP:OD2	2.35	0.57
1:F:1022:GLN:O	1:F:1023:ARG:CG	2.51	0.57
1:K:2006:ASN:HB2	6:K:7011:HOH:O	2.05	0.57
1:G:1205:ALA:HB2	6:G:2018:HOH:O	2.05	0.57
1:H:1415:PRO:HA	1:H:1457:ASN:OD1	2.05	0.57
2:B:1351:RP4:H24	6:B:2046:HOH:O	2.03	0.57
1:G:1225:PRO:O	1:G:1229:GLY:N	2.31	0.57
1:H:1418:ASN:HD21	1:I:1667:HIS:CE1	2.23	0.57
1:I:1750:GLY:HA2	6:I:2138:HOH:O	2.05	0.57
1:K:2150:GLY:HA3	6:K:7113:HOH:O	2.05	0.57
1:E:921:TYR:O	1:E:924:GLN:HB2	2.04	0.56
1:B:288:VAL:HG22	1:B:321:TYR:CE2	2.40	0.56
1:D:719[A]:HIS:HD2	6:D:2115:HOH:O	1.87	0.56
1:H:1422:GLN:O	1:H:1423:ARG:HB3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1892:ASP:O	1:J:1896:THR:HG23	2.05	0.56
1:I:1602:ARG:N	6:I:2014:HOH:O	2.38	0.56
1:I:1616:ASN:O	1:I:1619:LEU:HB2	2.05	0.56
1:J:1864:ASP:OD1	1:L:2257:ASN:ND2	2.38	0.56
1:A:104:GLU:OE1	1:A:120:SER:OG	2.22	0.56
1:C:404:LEU:HG	1:C:449:GLY:HA3	1.88	0.56
1:A:116:PHE:HB3	6:A:2040:HOH:O	2.05	0.56
1:I:1694:LEU:O	1:I:1697:CYS:HB2	2.05	0.56
1:J:1880:PRO:HD2	1:J:1906:HIS:CE1	2.41	0.55
1:E:883:TYR:HB3	1:E:887:SER:HB2	1.87	0.55
1:K:2119[A]:HIS:CD2	3:K:3153:GOL:H12	2.41	0.55
1:D:642:LYS:HE2	6:D:2060:HOH:O	2.06	0.55
3:F:2153:GOL:O1	6:F:2133:HOH:O	2.01	0.55
1:I:1602:ARG:HD3	1:I:1607:ALA:HB2	1.87	0.55
1:A:107:ILE:O	1:A:132:GLY:HA2	2.06	0.55
1:D:638:ALA:HB3	6:D:2054:HOH:O	2.06	0.55
6:B:2010:HOH:O	1:C:471:LEU:HD21	2.04	0.55
1:E:879:ASN:OD1	1:E:879:ASN:C	2.49	0.55
1:J:1880:PRO:HD2	1:J:1906:HIS:HE1	1.72	0.55
1:A:23:ARG:O	2:A:1151:RP4:H21	2.06	0.55
1:A:33:LEU:C	6:A:2030:HOH:O	2.50	0.55
1:D:647:HIS:NE2	6:D:2066:HOH:O	1.82	0.55
1:G:1270:ARG:HD2	1:G:1296:THR:O	2.06	0.55
1:H:1423:ARG:HG3	2:H:2551:RP4:H20	1.88	0.55
1:J:1804:LEU:HD11	1:J:1946:ALA:HA	1.88	0.55
1:F:1097:CYS:HA	6:F:2091:HOH:O	2.06	0.54
1:G:1296:THR:HA	1:I:1623:ARG:HD2	1.89	0.54
6:I:2114:HOH:O	3:K:3152:GOL:C1	2.53	0.54
1:E:842:LYS:HE3	6:E:2080:HOH:O	2.06	0.54
1:K:2086:THR:O	6:K:7066:HOH:O	2.18	0.54
1:D:687:SER:OG	1:D:690:ILE:HG13	2.08	0.54
1:B:224:GLN:CD	1:B:227:ILE:HD12	2.33	0.54
1:K:2072:ASN:ND2	6:K:7061:HOH:O	2.41	0.54
1:C:497:CYS:O	1:C:498:ASP:C	2.51	0.54
1:K:2150:GLY:C	6:K:7113:HOH:O	2.49	0.54
1:J:1828:TYR:HE1	6:J:2026:HOH:O	1.89	0.54
1:K:2039:LEU:HD12	1:K:2135:VAL:HG23	1.90	0.54
1:C:411:ILE:HG21	1:C:453:PHE:CE1	2.43	0.54
1:C:545:ILE:O	1:C:548:LEU:N	2.40	0.54
1:E:823:ARG:NH2	1:F:1098:ASP:OD1	2.40	0.54
1:J:1822:GLN:NE2	1:K:2070:ARG:NH1	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1833:LEU:HD23	6:J:2005:HOH:O	2.07	0.54
1:K:2058:HIS:N	1:K:2058:HIS:CD2	2.76	0.54
1:A:24:GLN:HA	1:A:26:GLU:OE2	2.08	0.53
1:A:96:THR:HA	1:C:423:ARG:HD3	1.89	0.53
1:F:1024:GLN:HE21	1:F:1027:ILE:CD1	2.16	0.53
1:C:492:ASP:O	1:C:496:THR:HG23	2.08	0.53
1:H:1423:ARG:HG3	2:H:2551:RP4:C20	2.38	0.53
1:G:1223:ARG:NH1	6:G:2027:HOH:O	2.42	0.53
1:J:1818:ASN:HA	1:J:1833:LEU:HD22	1.91	0.53
1:A:15:PRO:HA	1:A:57:ASN:OD1	2.09	0.53
1:B:221:GLY:HA2	6:B:2042:HOH:O	2.08	0.53
1:D:623:ARG:NH1	1:E:895:ASN:O	2.39	0.53
1:D:628:TYR:OH	1:D:713:ARG:NH1	2.35	0.53
1:I:1608:PRO:HA	6:I:2018:HOH:O	2.08	0.53
1:B:276:ILE:O	1:B:302:VAL:HA	2.09	0.53
1:B:309:ASN:O	1:B:313:ARG:HG3	2.09	0.53
1:D:625:PRO:HA	1:D:629:GLY:O	2.09	0.53
1:G:1215:PRO:HD2	1:G:1281:ALA:HB3	1.90	0.53
1:K:2035:ASP:OD1	6:K:7032:HOH:O	2.19	0.53
1:F:1036:VAL:CG2	1:F:1135:VAL:HG11	2.38	0.53
1:G:1283:TYR:C	1:G:1285:HIS:N	2.66	0.53
1:A:64:ASP:OD2	6:A:2065:HOH:O	2.19	0.52
1:G:1297:CYS:O	1:G:1325:ARG:NH2	2.42	0.52
1:H:1482:ALA:HB2	6:I:2091:HOH:O	2.09	0.52
1:K:2110:ILE:CG2	2:K:3151:RP4:H122	2.39	0.52
1:L:2215:PRO:O	1:L:2216:ASN:CB	2.51	0.52
1:C:428:TYR:OH	1:C:513:ARG:NH1	2.42	0.52
1:C:435:ASP:OD2	6:C:2045:HOH:O	2.19	0.52
1:K:2039:LEU:HD11	1:K:2135:VAL:HG23	1.90	0.52
1:L:2223:ARG:NH1	6:L:2032:HOH:O	2.36	0.52
1:A:106:HIS:HD1	2:A:1151:RP4:H5	1.58	0.52
1:G:1218:ASN:HA	1:G:1233:LEU:HD22	1.91	0.52
1:C:414:GLY:O	1:C:455:GLN:NE2	2.38	0.52
1:A:39:LEU:HD12	6:A:2032:HOH:O	2.10	0.52
1:C:419:LEU:O	1:C:420:LEU:C	2.53	0.52
1:E:907:ILE:HG23	1:E:934:GLY:HA2	1.91	0.52
1:K:2010:MET:HE2	1:K:2073:HIS:CE1	2.45	0.52
1:A:32:THR:O	1:A:36:VAL:HG23	2.10	0.52
1:I:1727:ASP:CG	6:I:2126:HOH:O	2.52	0.52
1:J:1843:ALA:HB1	1:J:1939:VAL:HG13	1.88	0.52
1:G:1299:GLY:HA2	6:G:2092:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:604:LEU:HD13	1:D:746:ALA:HA	1.92	0.51
1:A:23:ARG:HG3	2:A:1151:RP4:H20	1.91	0.51
1:G:1204:LEU:CD1	1:G:1346:ALA:HA	2.40	0.51
1:F:1085:HIS:CE1	1:F:1117:ARG:O	2.64	0.51
1:F:1150:GLY:CA	6:F:2129:HOH:O	2.44	0.51
1:L:2208:PRO:HG3	6:L:2062:HOH:O	2.11	0.51
1:L:2348:LEU:HD23	6:L:2129:HOH:O	2.10	0.51
3:D:1753:GOL:C2	6:D:2109:HOH:O	2.53	0.51
1:K:2135:VAL:O	1:K:2138:TYR:HB2	2.11	0.51
1:C:518:HIS:HB3	3:J:2954:GOL:H32	1.93	0.51
1:E:906:HIS:HB3	2:E:1951:RP4:C2	2.41	0.51
6:E:2037:HOH:O	1:L:2327:ASP:HB3	2.10	0.51
1:H:1422:GLN:NE2	1:I:1670:ARG:HH22	2.09	0.51
1:A:119[A]:HIS:HD2	3:D:1753:GOL:H31	1.75	0.51
1:D:698:ASP:CG	1:F:1023:ARG:HE	2.18	0.51
1:J:1859:GLU:OE1	5:J:2953:TRS:N	2.43	0.51
3:J:2954:GOL:C1	6:J:2085:HOH:O	2.59	0.51
1:K:2002:ARG:O	1:K:2002:ARG:HG2	2.10	0.51
2:A:1151:RP4:C21	6:A:2014:HOH:O	2.47	0.51
1:L:2237:GLU:HB2	1:L:2253:PHE:CD2	2.46	0.51
1:E:822:GLN:O	1:E:823:ARG:HB3	2.10	0.50
1:B:215:PRO:HD3	1:B:283:TYR:CD1	2.46	0.50
1:K:2024:GLN:N	1:K:2025:PRO:HD3	2.26	0.50
1:E:866:ILE:HG21	1:E:893:ALA:HB1	1.93	0.50
1:F:1004:LEU:HD23	1:F:1049:GLY:HA3	1.94	0.50
1:I:1666:ILE:HG21	1:I:1694:LEU:HD23	1.91	0.50
1:A:85:HIS:HB3	6:A:2096:HOH:O	2.11	0.50
1:B:223:ARG:CD	1:C:496:THR:HA	2.41	0.50
1:C:404:LEU:CD2	1:C:447:HIS:O	2.59	0.50
1:D:695:ASN:HB2	6:D:2099:HOH:O	2.11	0.50
1:G:1204:LEU:HD13	1:G:1346:ALA:HA	1.94	0.50
1:L:2223:ARG:CG	2:L:3351:RP4:H20	2.41	0.50
1:A:150:GLY:HA3	6:A:2114:HOH:O	2.11	0.50
1:C:467:HIS:O	1:C:470:ARG:HB3	2.11	0.50
1:D:639:LEU:CD1	1:D:735:VAL:HG23	2.41	0.50
3:D:1753:GOL:H12	6:D:2109:HOH:O	2.09	0.50
1:F:1114:GLU:CD	6:F:2097:HOH:O	2.55	0.50
1:J:1825:PRO:HD2	1:J:1826:GLU:OE2	2.11	0.50
1:B:243:ALA:HB2	1:B:339:VAL:HG13	1.93	0.50
1:B:286:THR:O	6:B:2098:HOH:O	2.19	0.50
1:E:901:PRO:HD3	6:E:2163:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1124:GLN:HA	1:H:1512:GLN:HG2	1.94	0.50
1:B:202:ARG:HD3	1:B:207:ALA:HB2	1.93	0.50
1:B:219:LEU:O	1:B:220:LEU:C	2.54	0.50
1:D:692:ASP:HB3	1:F:1016:ASN:ND2	2.27	0.50
1:D:695:ASN:CB	6:D:2099:HOH:O	2.60	0.50
1:H:1441:VAL:HG22	6:H:2047:HOH:O	2.11	0.50
1:F:1080:PRO:HG2	1:F:1084:SER:HB3	1.94	0.49
1:J:1870:ARG:HB2	1:J:1897:CYS:SG	2.52	0.49
1:J:1884:SER:OG	1:J:1906:HIS:HE1	1.93	0.49
1:B:224:GLN:HG2	1:B:226:GLU:OE1	2.11	0.49
1:G:1348:LEU:O	1:G:1350:GLY:N	2.40	0.49
1:K:2119[A]:HIS:HD2	3:K:3153:GOL:H12	1.77	0.49
1:L:2222:GLN:O	1:L:2223:ARG:CB	2.60	0.49
1:I:1667:HIS:O	1:I:1670:ARG:HB3	2.11	0.49
1:J:1884:SER:OG	1:J:1906:HIS:CE1	2.65	0.49
1:J:1896:THR:HA	1:L:2223:ARG:HD3	1.95	0.49
1:J:1901:PRO:HB2	1:J:1945:ILE:HD13	1.94	0.49
1:B:231:ASP:OD2	1:B:235:ASP:HB3	2.13	0.49
1:B:280:PRO:HG2	1:B:322:VAL:HG21	1.95	0.49
1:D:679:ASN:OD1	1:D:679:ASN:C	2.55	0.49
1:G:1287:SER:OG	1:G:1290:ILE:HB	2.12	0.49
1:L:2308:SER:OG	2:L:3351:RP4:O3	2.29	0.49
1:E:903:VAL:HG21	1:E:944:ARG:HB3	1.93	0.49
1:G:1211:ILE:HD13	1:G:1240:CYS:SG	2.52	0.49
1:J:1810:MET:HE2	1:J:1873:HIS:CE1	2.48	0.49
1:H:1522:VAL:HG12	1:H:1526:ALA:HB2	1.94	0.49
1:E:906:HIS:O	1:E:931:ALA:HA	2.13	0.49
1:J:1843:ALA:O	1:J:1847:HIS:CD2	2.56	0.49
1:L:2345:ILE:O	1:L:2349:ALA:N	2.44	0.49
1:A:24:GLN:NE2	1:A:27:ILE:HD13	2.28	0.49
1:G:1318:HIS:ND1	6:G:2105:HOH:O	2.16	0.49
1:K:2150:GLY:CA	6:K:7113:HOH:O	2.60	0.49
1:D:693:ALA:O	1:D:696:THR:OG1	2.29	0.49
1:G:1223:ARG:CG	6:G:2027:HOH:O	2.42	0.49
1:F:1036:VAL:HG22	1:F:1135:VAL:HG11	1.95	0.48
1:I:1715:PRO:O	1:I:1718:HIS:HB2	2.13	0.48
1:G:1294:LEU:HD22	1:G:1302:VAL:HG11	1.94	0.48
1:J:1914:GLU:H	1:J:1914:GLU:CD	2.20	0.48
1:A:13:ASN:HB2	1:A:55:GLN:HA	1.96	0.48
1:A:77:VAL:HA	1:A:103:VAL:O	2.13	0.48
1:J:1897:CYS:O	1:J:1925:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:2013:ASN:HB3	1:K:2017:LEU:HD13	1.95	0.48
1:G:1304:GLU:O	1:G:1329:VAL:HA	2.13	0.48
1:D:671:LEU:HB3	6:D:2095:HOH:O	2.12	0.48
2:G:2351:RP4:C20	6:G:2027:HOH:O	2.61	0.48
1:K:2148:LEU:C	1:K:2150:GLY:H	2.22	0.48
1:L:2314:GLU:H	1:L:2314:GLU:CD	2.21	0.48
1:B:252:ASP:CG	1:B:273:HIS:HE2	2.19	0.48
1:B:290:ILE:O	1:B:291:LEU:C	2.56	0.48
1:C:431:ASP:O	6:C:2040:HOH:O	2.20	0.48
1:G:1283:TYR:HB3	1:G:1287:SER:CB	2.41	0.48
1:B:223:ARG:HD2	1:C:496:THR:O	2.14	0.48
1:H:1423:ARG:NE	1:I:1698:ASP:OD2	2.47	0.48
1:H:1430[B]:SER:OG	6:H:2032:HOH:O	2.19	0.48
1:K:2095:ASN:C	1:K:2097:CYS:H	2.22	0.48
6:A:2065:HOH:O	1:C:458:HIS:CD2	2.65	0.48
1:B:282:ALA:CB	1:C:489:ALA:HA	2.45	0.47
1:E:857:ASN:ND2	1:F:1064:ASP:OD1	2.43	0.47
1:E:920:SER:HB3	1:E:923:SER:OG	2.13	0.47
1:F:1125:ARG:O	1:F:1126:ALA:C	2.57	0.47
1:J:1883:TYR:O	1:J:1884:SER:C	2.57	0.47
1:A:32:THR:O	1:A:35:ASP:HB2	2.14	0.47
1:E:836:VAL:O	1:E:839:LEU:HB2	2.14	0.47
1:E:839:LEU:HD11	6:E:2069:HOH:O	2.14	0.47
1:C:498:ASP:N	6:C:2094:HOH:O	2.38	0.47
1:E:901:PRO:HB2	1:E:945:ILE:HD13	1.97	0.47
1:F:1117:ARG:HD3	2:F:2151:RP4:O11	2.13	0.47
1:G:1294:LEU:O	1:G:1297:CYS:HB2	2.13	0.47
1:H:1445:ALA:C	1:H:1447:HIS:H	2.22	0.47
1:F:1114:GLU:OE1	6:F:2097:HOH:O	2.20	0.47
1:K:2032:THR:O	1:K:2035:ASP:HB2	2.13	0.47
1:D:680:PRO:HB2	1:D:684:SER:OG	2.13	0.47
1:F:1144:ARG:NH2	1:F:1148:LEU:HD21	2.29	0.47
3:K:3153:GOL:H2	6:K:7117:HOH:O	2.12	0.47
1:C:476:ILE:HB	1:C:502:VAL:HG13	1.96	0.47
1:D:654:ARG:HH11	1:D:665:TRP:CD1	2.32	0.47
1:E:818:ASN:HA	1:E:833:LEU:HD22	1.97	0.47
1:E:918:HIS:HB3	3:E:1952:GOL:H32	1.97	0.47
1:G:1204:LEU:HD23	1:G:1249:GLY:HA3	1.96	0.47
1:G:1325:ARG:O	1:G:1326:ALA:C	2.57	0.47
1:I:1681:ALA:O	1:I:1684:SER:OG	2.31	0.47
1:J:1823:ARG:HE	1:K:2098:ASP:CG	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:2012:LEU:HB2	1:K:2078:ILE:HG13	1.96	0.47
1:K:2103:VAL:HG21	1:K:2144:ARG:HB3	1.96	0.47
1:E:925:ARG:O	1:E:926:ALA:C	2.57	0.47
6:H:2010:HOH:O	1:I:1724:GLN:HG3	2.14	0.47
1:L:2310:ILE:HB	1:L:2317:ARG:O	2.15	0.47
1:D:739:VAL:HG11	6:D:2135:HOH:O	2.14	0.47
1:I:1704:GLU:OE1	1:I:1706:HIS:CE1	2.68	0.47
1:J:1815:PRO:HD2	1:J:1881:ALA:HB3	1.97	0.47
1:K:2118:HIS:HB2	1:K:2119[B]:HIS:CE1	2.50	0.47
1:A:10:MET:CG	1:A:12:LEU:HD21	2.45	0.47
1:E:903:VAL:HG11	1:E:941:GLY:HA2	1.97	0.47
1:I:1706:HIS:O	1:I:1731:ALA:HA	2.13	0.47
1:L:2207:ALA:HB1	1:L:2273:HIS:HA	1.97	0.47
1:H:1544:ARG:O	1:H:1545:ILE:C	2.58	0.46
1:I:1741:GLY:O	1:I:1742:VAL:C	2.58	0.46
1:K:2125:ARG:O	1:K:2126:ALA:C	2.57	0.46
1:L:2267:HIS:O	1:L:2270:ARG:HB3	2.15	0.46
1:G:1311:HIS:ND1	3:G:2353:GOL:O2	2.36	0.46
1:I:1661:GLU:O	1:I:1664:ASP:HB2	2.16	0.46
1:J:1875:GLY:HA3	1:J:1945:ILE:HD12	1.96	0.46
1:B:243:ALA:HB1	1:B:339:VAL:HG13	1.96	0.46
1:E:845:ALA:C	1:E:847:HIS:H	2.24	0.46
1:F:1002:ARG:NE	6:F:2017:HOH:O	2.48	0.46
1:K:2028:TYR:OH	1:K:2113:ARG:NH2	2.49	0.46
1:K:2059:GLU:OE1	6:K:7051:HOH:O	2.21	0.46
1:L:2245:ALA:C	1:L:2247:HIS:H	2.23	0.46
1:F:1119[A]:HIS:HD2	3:H:2552:GOL:H12	1.80	0.46
1:H:1404:LEU:HD21	1:H:1546:ALA:HA	1.95	0.46
1:J:1910:ILE:C	1:J:1912:GLN:H	2.23	0.46
1:K:2090:ILE:HG22	1:K:2122:VAL:HG22	1.98	0.46
1:C:423:ARG:NH1	1:C:424:GLN:OE1	2.48	0.46
1:I:1602:ARG:HD3	1:I:1607:ALA:CB	2.46	0.46
1:A:144:ARG:HD2	1:D:736:GLN:OE1	2.15	0.46
1:B:310:ILE:HB	1:B:317:ARG:O	2.16	0.46
1:D:656:SER:HB2	1:D:665:TRP:CH2	2.50	0.46
1:D:610:MET:O	1:D:676:ILE:HA	2.16	0.46
1:C:504:GLU:HB3	1:C:529:VAL:HG13	1.97	0.46
1:I:1653:PHE:C	1:I:1653:PHE:CD2	2.94	0.46
1:A:113:ARG:HG2	6:A:2091:HOH:O	2.15	0.46
1:C:410:MET:HB2	1:C:473:HIS:CD2	2.51	0.46
1:D:657:ASN:ND2	1:E:864:ASP:OD1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1809:ILE:HG12	1:J:1945:ILE:HG21	1.98	0.46
1:J:1950:GLY:CA	6:J:2106:HOH:O	2.59	0.46
1:L:2225:PRO:HD3	6:L:2035:HOH:O	2.16	0.46
1:D:613:ASN:OD1	1:D:617:LEU:HD13	2.16	0.45
1:F:1067:HIS:O	1:F:1070:ARG:HB3	2.15	0.45
1:G:1287:SER:OG	1:G:1290:ILE:HD12	2.16	0.45
1:K:2145:ILE:O	1:K:2146:ALA:C	2.56	0.45
1:C:415:PRO:HD3	1:C:483:TYR:CE1	2.52	0.45
1:G:1224:GLN:NE2	1:G:1227:ILE:HD12	2.31	0.45
1:I:1678:ILE:O	1:I:1680:PRO:HD3	2.17	0.45
1:L:2228:TYR:OH	1:L:2313:ARG:NH1	2.50	0.45
1:L:2272:ASN:ND2	6:L:2083:HOH:O	2.46	0.45
1:D:672:ASN:ND2	6:D:2091:HOH:O	2.30	0.45
1:D:680:PRO:HG2	1:D:684:SER:OG	2.16	0.45
1:F:1004:LEU:HD12	1:F:1004:LEU:H	1.81	0.45
1:F:1136:GLN:O	1:F:1139:VAL:N	2.38	0.45
1:K:2124:GLN:HG2	6:K:7097:HOH:O	2.16	0.45
1:K:2097:CYS:O	1:K:2125:ARG:NH2	2.49	0.45
1:K:2117:ARG:NH1	2:K:3151:RP4:H8	2.32	0.45
1:A:109:ASN:HB2	1:A:132:GLY:HA3	1.99	0.45
1:C:530:VAL:HG13	1:J:1930:VAL:HG22	1.99	0.45
1:E:822:GLN:O	1:E:823:ARG:CB	2.64	0.45
1:G:1256:SER:HB2	1:G:1265:TRP:CH2	2.51	0.45
1:H:1436:VAL:O	1:H:1439:LEU:HB2	2.16	0.45
1:A:24:GLN:N	1:A:25:PRO:CD	2.80	0.45
1:E:919[B]:HIS:HB2	6:E:2145:HOH:O	2.17	0.45
1:L:2231:ASP:N	1:L:2231:ASP:OD1	2.50	0.45
1:D:624:GLN:HE21	1:D:624:GLN:HA	1.82	0.45
1:D:710:ILE:CD1	1:D:710:ILE:CB	2.81	0.45
1:J:1903:VAL:HA	1:J:1928:GLY:O	2.17	0.45
1:F:1010:MET:HB2	1:F:1073:HIS:CD2	2.52	0.45
1:K:2023:ARG:NH1	1:K:2024:GLN:OE1	2.50	0.45
6:I:2124:HOH:O	1:K:2112:GLN:NE2	2.50	0.44
1:J:1914:GLU:O	1:J:1918:HIS:CD2	2.70	0.44
1:C:525:ARG:O	1:C:526:ALA:C	2.60	0.44
1:E:845:ALA:C	1:E:847:HIS:N	2.74	0.44
1:E:866:ILE:HG12	1:E:894:LEU:CD2	2.47	0.44
1:H:1423:ARG:HD2	1:I:1696:THR:HA	1.99	0.44
1:I:1619:LEU:HD22	1:I:1622:GLN:HE22	1.82	0.44
1:C:516:PHE:CD1	1:C:516:PHE:C	2.96	0.44
1:D:624:GLN:HB3	1:D:627:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1952:GOL:H11	6:L:2114:HOH:O	2.16	0.44
1:F:1026:GLU:HB2	1:F:1027:ILE:HD12	1.98	0.44
1:F:1109:ASN:ND2	1:H:1523:SER:O	2.49	0.44
1:F:1116:PHE:HD2	6:F:2099:HOH:O	2.00	0.44
1:K:2024:GLN:HA	1:K:2026:GLU:OE2	2.17	0.44
1:L:2220:LEU:O	6:L:2030:HOH:O	2.20	0.44
1:L:2223:ARG:HG3	2:L:3351:RP4:H20	1.98	0.44
1:H:1504:GLU:OE1	1:H:1520:SER:OG	2.29	0.44
1:I:1741:GLY:O	1:I:1744:ARG:N	2.50	0.44
1:G:1301:PRO:HB2	1:G:1345:ILE:HD12	2.00	0.44
1:B:323:SER:HB2	6:B:2116:HOH:O	2.17	0.44
1:D:698:ASP:OD2	1:F:1023:ARG:NE	2.48	0.44
1:F:1085:HIS:HB3	6:F:2100:HOH:O	2.17	0.44
1:F:1135:VAL:O	1:F:1136:GLN:C	2.60	0.44
1:G:1215:PRO:HA	1:G:1257:ASN:OD1	2.16	0.44
1:I:1631:ASP:HB2	6:I:2038:HOH:O	2.18	0.44
1:J:1891:LEU:CD1	1:J:1895:ASN:HD21	2.31	0.44
1:K:2114:GLU:H	1:K:2114:GLU:CD	2.25	0.44
1:I:1694:LEU:HD13	1:I:1702:VAL:HG11	1.99	0.44
1:C:511:HIS:CE1	6:C:2100:HOH:O	2.71	0.44
1:K:2022:GLN:NE2	1:L:2270:ARG:HH12	2.15	0.44
1:L:2233:LEU:N	6:L:2030:HOH:O	2.41	0.44
1:A:23:ARG:NH1	1:A:24:GLN:OE1	2.50	0.44
1:C:544:ARG:O	1:C:545:ILE:C	2.61	0.44
1:A:115:PRO:HD2	6:A:2095:HOH:O	2.16	0.43
1:C:480:PRO:HB2	1:C:484:SER:OG	2.18	0.43
1:E:822:GLN:HE21	1:F:1070:ARG:HH22	1.65	0.43
1:F:1080:PRO:HB2	1:F:1084:SER:HB3	2.00	0.43
1:J:1823:ARG:NH2	1:K:2098:ASP:OD1	2.46	0.43
1:A:110:ILE:HA	1:A:113:ARG:HG3	2.00	0.43
1:J:1828:TYR:OH	1:J:1913:ARG:CZ	2.65	0.43
1:F:1043:ALA:HB2	6:F:2045:HOH:O	2.18	0.43
1:H:1432:THR:O	1:H:1435:ASP:HB2	2.18	0.43
1:H:1517:ARG:NH2	1:I:1692:ASP:OD1	2.47	0.43
1:L:2278:ILE:HG12	1:L:2280:PRO:HG3	2.01	0.43
1:B:224:GLN:NE2	1:B:227:ILE:HD12	2.33	0.43
1:D:654:ARG:NH1	1:D:665:TRP:CD1	2.86	0.43
1:D:725:ARG:O	1:D:726:ALA:C	2.61	0.43
1:D:623:ARG:NE	1:E:898:ASP:OD1	2.51	0.43
1:F:1002:ARG:NH1	1:F:1071:LEU:O	2.51	0.43
1:F:1024:GLN:NE2	1:F:1027:ILE:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1654:ARG:NH2	1:I:1668:GLU:OE2	2.48	0.43
1:C:411:ILE:HB	1:C:453:PHE:CD1	2.53	0.43
1:C:519[B]:HIS:ND1	6:C:2108:HOH:O	2.22	0.43
1:I:1721:TYR:O	1:I:1724:GLN:HB2	2.17	0.43
1:J:1844:ALA:O	1:J:1845:ALA:C	2.61	0.43
1:K:2015:PRO:HD3	1:K:2083:TYR:CE1	2.54	0.43
1:G:1286:THR:HB	5:I:2752:TRS:H12	2.01	0.43
1:D:602:ARG:HH21	1:D:602:ARG:HB3	1.83	0.43
1:F:1094:LEU:O	1:F:1097:CYS:HB2	2.18	0.43
1:K:2098:ASP:O	1:K:2100:LEU:N	2.48	0.43
1:L:2223:ARG:HG2	2:L:3351:RP4:H20	2.01	0.43
1:L:2224:GLN:NE2	1:L:2227:ILE:HG13	2.33	0.43
1:C:417:LEU:O	1:C:433:LEU:HD13	2.19	0.43
1:H:1404:LEU:H	1:H:1404:LEU:HG	1.32	0.43
1:I:1628:TYR:OH	1:I:1713:ARG:NH1	2.45	0.43
1:I:1715:PRO:HB2	6:I:2111:HOH:O	2.19	0.43
1:J:1857:ASN:ND2	1:K:2064:ASP:OD1	2.39	0.43
2:A:1151:RP4:H24	6:B:2099:HOH:O	2.17	0.43
1:F:1118:HIS:CG	3:F:2153:GOL:O2	2.71	0.43
1:H:1536:GLN:O	1:H:1539:VAL:HB	2.18	0.43
1:A:84:SER:OG	1:A:106:HIS:HE1	2.02	0.42
1:I:1685:HIS:HB3	6:I:2112:HOH:O	2.19	0.42
1:L:2211:ILE:HD12	1:L:2251:VAL:HB	2.00	0.42
1:L:2324:GLN:HE21	1:L:2324:GLN:N	2.17	0.42
1:A:118:HIS:HB3	3:A:1152:GOL:O2	2.18	0.42
1:D:660:GLY:O	1:D:663:VAL:HB	2.19	0.42
1:E:808:PRO:O	1:E:874:CYS:N	2.40	0.42
1:G:1223:ARG:CD	1:H:1496:THR:HA	2.49	0.42
1:H:1419:LEU:O	1:H:1420:LEU:C	2.61	0.42
1:J:1909:ASN:HB2	1:J:1932:GLY:HA3	2.01	0.42
1:K:2109:ASN:HD22	1:K:2112:GLN:NE2	2.16	0.42
1:L:2314:GLU:HB3	1:L:2316:PHE:CD2	2.54	0.42
1:B:220:LEU:O	1:B:232:THR:HA	2.19	0.42
1:B:232:THR:O	1:B:236:VAL:HG23	2.20	0.42
1:A:18:ASN:HD21	1:B:267:HIS:CE1	2.37	0.42
1:D:602:ARG:HH11	1:D:672:ASN:HA	1.85	0.42
1:H:1423:ARG:O	1:H:1424:GLN:C	2.62	0.42
1:J:1895:ASN:OD1	1:J:1925:ARG:HB2	2.20	0.42
1:C:423:ARG:O	1:C:424:GLN:C	2.63	0.42
1:E:879:ASN:HA	1:E:880:PRO:HD3	1.81	0.42
1:H:1413:ASN:ND2	1:H:1454:ARG:O	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2220:LEU:HG	1:L:2221:GLY:N	2.34	0.42
1:A:111:HIS:HB3	3:A:1152:GOL:H11	2.02	0.42
1:B:228:TYR:CD1	2:B:1351:RP4:C21	3.02	0.42
1:L:2215:PRO:HB3	1:L:2257:ASN:HA	2.02	0.42
1:L:2269:ALA:O	1:L:2270:ARG:C	2.61	0.42
1:G:1285:HIS:HB3	6:G:2082:HOH:O	2.20	0.42
1:J:1910:ILE:H	1:J:1910:ILE:HG13	1.54	0.42
1:A:22:GLN:NE2	6:A:2017:HOH:O	2.53	0.42
1:D:694:LEU:HD13	1:D:702:VAL:HG11	2.01	0.42
1:E:853:PHE:HD2	6:E:2095:HOH:O	2.03	0.42
1:F:1026:GLU:OE1	1:F:1027:ILE:CD1	2.68	0.42
1:G:1292:ASP:O	1:G:1296:THR:HG23	2.19	0.42
1:J:1822:GLN:NE2	1:K:2070:ARG:NH2	2.66	0.42
1:A:78:ILE:HG12	1:A:80:PRO:HG3	2.02	0.41
1:E:859:GLU:OE2	1:E:887:SER:OG	2.26	0.41
1:G:1216:ASN:O	1:G:1219:LEU:HB2	2.20	0.41
1:H:1409:ILE:HD12	1:H:1542:VAL:HG13	1.99	0.41
1:J:1802[B]:ARG:HG2	1:J:1807:ALA:CB	2.50	0.41
1:G:1285:HIS:CE1	1:G:1317:ARG:HA	2.55	0.41
1:G:1292:ASP:OD2	1:I:1682:ALA:HB2	2.20	0.41
1:J:1828:TYR:HH	1:J:1913:ARG:HH22	1.66	0.41
1:K:2016:ASN:ND2	1:L:2292:ASP:HB2	2.35	0.41
1:K:2062:LEU:O	1:K:2066:ILE:HD12	2.20	0.41
1:D:645:ALA:C	1:D:647:HIS:H	2.28	0.41
1:E:815:PRO:O	1:E:816:ASN:HB2	2.20	0.41
1:E:870:ARG:NH1	1:E:871:LEU:HD21	2.35	0.41
1:F:1016:ASN:O	2:F:2151:RP4:S16	2.78	0.41
1:H:1413:ASN:O	1:H:1455:GLN:HA	2.21	0.41
1:I:1705:VAL:HG21	1:I:1738:TYR:HA	2.02	0.41
1:A:97:CYS:O	1:A:125:ARG:NH2	2.50	0.41
1:H:1422:GLN:O	1:H:1423:ARG:CB	2.66	0.41
1:H:1519[A]:HIS:NE2	6:H:2094:HOH:O	2.19	0.41
1:J:1869:ALA:HA	1:J:1873:HIS:ND1	2.35	0.41
1:K:2068:GLU:O	1:K:2072:ASN:HB2	2.19	0.41
1:A:43:ALA:CB	1:A:139:VAL:HG13	2.51	0.41
1:D:735:VAL:HG13	6:D:2132:HOH:O	2.19	0.41
1:B:319[A]:HIS:HD2	3:G:2353:GOL:H12	1.84	0.41
1:C:545:ILE:O	1:C:546:ALA:C	2.62	0.41
1:H:1404:LEU:HD21	1:H:1549:ALA:HB3	2.01	0.41
1:I:1700:LEU:HD12	1:I:1701:PRO:HD2	2.03	0.41
1:J:1944:ARG:O	1:J:1948:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:PRO:O	1:A:81:ALA:C	2.64	0.41
1:C:519[B]:HIS:HD2	3:J:2955:GOL:H12	1.86	0.41
1:D:612:LEU:HB2	1:D:678:ILE:HG13	2.02	0.41
1:A:15:PRO:HA	1:A:57:ASN:HA	2.02	0.41
1:A:43:ALA:HB2	1:A:139:VAL:HG13	2.03	0.41
1:B:215:PRO:HD3	1:B:283:TYR:CE1	2.56	0.41
1:F:1118:HIS:HB3	3:F:2153:GOL:O2	2.21	0.41
1:I:1618:ASN:OD1	1:I:1618:ASN:N	2.53	0.41
1:B:217:LEU:O	1:B:218:ASN:C	2.61	0.41
1:B:223:ARG:NH2	6:B:2047:HOH:O	2.44	0.41
1:E:811:ILE:CD1	1:E:840:CYS:HB3	2.51	0.41
1:F:1095:ASN:HA	6:F:2089:HOH:O	2.21	0.41
1:G:1211:ILE:HG12	1:G:1277:VAL:HB	2.03	0.41
1:G:1335:VAL:HG22	6:G:2121:HOH:O	2.21	0.41
1:K:2086:THR:HG22	6:L:2087:HOH:O	2.20	0.41
1:L:2245:ALA:O	1:L:2247:HIS:N	2.54	0.41
1:A:8:PRO:HA	1:A:50:THR:O	2.21	0.40
1:A:36:VAL:O	1:A:37:GLU:C	2.63	0.40
2:A:1151:RP4:H24	1:B:292:ASP:HB3	2.03	0.40
1:B:270:ARG:HG3	1:B:297:CYS:HA	2.02	0.40
1:D:739:VAL:CG1	6:D:2135:HOH:O	2.68	0.40
1:E:815:PRO:HG3	1:E:883:TYR:CZ	2.56	0.40
1:G:1258:HIS:ND1	1:H:1460:GLY:HA3	2.35	0.40
1:G:1279:ASN:HA	1:G:1280:PRO:HD3	1.76	0.40
1:L:2254:ARG:HB3	1:L:2265:TRP:CZ3	2.55	0.40
1:D:694:LEU:O	1:D:695:ASN:C	2.61	0.40
1:G:1223:ARG:CD	6:G:2027:HOH:O	2.69	0.40
1:G:1253:PHE:CD2	1:G:1253:PHE:C	2.98	0.40
1:H:1445:ALA:C	1:H:1447:HIS:N	2.79	0.40
1:D:682:ALA:C	1:D:684:SER:N	2.79	0.40
1:E:820:LEU:HD12	1:E:820:LEU:HA	1.88	0.40
1:F:1015:PRO:HD3	1:F:1083:TYR:CE1	2.56	0.40
1:F:1119[A]:HIS:CD2	3:H:2552:GOL:H12	2.56	0.40
1:H:1490:ILE:O	1:H:1493:ALA:HB3	2.21	0.40
1:I:1654:ARG:HH22	1:I:1668:GLU:CD	2.29	0.40
1:I:1681:ALA:HA	2:I:2751:RP4:O5	2.21	0.40
1:J:1802[B]:ARG:HG2	1:J:1807:ALA:HB2	2.04	0.40
1:J:1825:PRO:O	1:J:1829:GLY:HA2	2.21	0.40
1:A:144:ARG:NH2	6:A:2113:HOH:O	2.52	0.40
1:B:343:GLU:OE1	1:G:1343:GLU:OE1	2.39	0.40
1:D:719[B]:HIS:ND1	6:D:2117:HOH:O	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:741:GLY:O	1:D:745:ILE:HG12	2.21	0.40
1:G:1243:ALA:HB2	1:G:1339:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	149/157 (95%)	138 (93%)	11 (7%)	0	100	100
1	B	148/157 (94%)	140 (95%)	8 (5%)	0	100	100
1	C	149/157 (95%)	133 (89%)	15 (10%)	1 (1%)	18	10
1	D	149/157 (95%)	138 (93%)	9 (6%)	2 (1%)	9	3
1	E	148/157 (94%)	137 (93%)	10 (7%)	1 (1%)	18	10
1	F	148/157 (94%)	138 (93%)	8 (5%)	2 (1%)	9	3
1	G	149/157 (95%)	138 (93%)	9 (6%)	2 (1%)	9	3
1	H	149/157 (95%)	140 (94%)	9 (6%)	0	100	100
1	I	149/157 (95%)	133 (89%)	16 (11%)	0	100	100
1	J	148/157 (94%)	135 (91%)	13 (9%)	0	100	100
1	K	148/157 (94%)	134 (90%)	14 (10%)	0	100	100
1	L	149/157 (95%)	140 (94%)	6 (4%)	3 (2%)	6	1
All	All	1783/1884 (95%)	1644 (92%)	128 (7%)	11 (1%)	21	12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	1023	ARG
1	E	949	ALA

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Mol	Chain	Res	Type
1	G	1349	ALA
1	L	2223	ARG
1	C	420	LEU
1	D	646	ALA
1	L	2222	GLN
1	D	618	ASN
1	F	1068	GLU
1	G	1216	ASN
1	L	2314	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	119/121 (98%)	114 (96%)	5 (4%)	26	16
1	B	118/121 (98%)	111 (94%)	7 (6%)	18	7
1	C	119/121 (98%)	108 (91%)	11 (9%)	8	2
1	D	119/121 (98%)	108 (91%)	11 (9%)	8	2
1	E	118/121 (98%)	112 (95%)	6 (5%)	21	10
1	F	118/121 (98%)	112 (95%)	6 (5%)	21	10
1	G	119/121 (98%)	110 (92%)	9 (8%)	12	4
1	H	119/121 (98%)	113 (95%)	6 (5%)	22	11
1	I	119/121 (98%)	108 (91%)	11 (9%)	8	2
1	J	119/121 (98%)	112 (94%)	7 (6%)	18	7
1	K	118/121 (98%)	107 (91%)	11 (9%)	8	2
1	L	119/121 (98%)	109 (92%)	10 (8%)	10	3
All	All	1424/1452 (98%)	1324 (93%)	100 (7%)	14	4

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE

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Mol	Chain	Res	Type
1	A	23	ARG
1	A	26	GLU
1	A	39	LEU
1	A	98	ASP
1	B	226	GLU
1	B	241	VAL
1	B	242	LYS
1	B	271	LEU
1	B	313	ARG
1	B	342	VAL
1	B	343	GLU
1	C	411	ILE
1	C	426	GLU
1	C	430[A]	SER
1	C	430[B]	SER
1	C	441	VAL
1	C	471	LEU
1	C	476	ILE
1	C	519[A]	HIS
1	C	519[B]	HIS
1	C	529	VAL
1	C	544	ARG
1	D	602	ARG
1	D	624	GLN
1	D	626	GLU
1	D	666	ILE
1	D	698	ASP
1	D	712	GLN
1	D	719[A]	HIS
1	D	719[B]	HIS
1	D	724	GLN
1	D	729	VAL
1	D	735	VAL
1	E	804	LEU
1	E	822	GLN
1	E	823	ARG
1	E	866	ILE
1	E	898	ASP
1	E	945	ILE
1	F	1026	GLU
1	F	1031	ASP
1	F	1042	LYS

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Mol	Chain	Res	Type
1	F	1050	THR
1	F	1124	GLN
1	F	1139	VAL
1	G	1202	ARG
1	G	1204	LEU
1	G	1220	LEU
1	G	1222	GLN
1	G	1223	ARG
1	G	1270	ARG
1	G	1290	ILE
1	G	1319[A]	HIS
1	G	1319[B]	HIS
1	H	1404	LEU
1	H	1411	ILE
1	H	1423	ARG
1	H	1426	GLU
1	H	1466	ILE
1	H	1498	ASP
1	I	1611	ILE
1	I	1623	ARG
1	I	1626	GLU
1	I	1632	THR
1	I	1668	GLU
1	I	1671	LEU
1	I	1684	SER
1	I	1690	ILE
1	I	1706	HIS
1	I	1715	PRO
1	I	1724	GLN
1	J	1826	GLU
1	J	1830	SER
1	J	1831	ASP
1	J	1839	LEU
1	J	1910	ILE
1	J	1920	SER
1	J	1935	VAL
1	K	2003	SER
1	K	2011	ILE
1	K	2026	GLU
1	K	2027	ILE
1	K	2037	GLU
1	K	2058	HIS

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Mol	Chain	Res	Type
1	K	2066	ILE
1	K	2088	VAL
1	K	2090	ILE
1	K	2120	SER
1	K	2135	VAL
1	L	2226	GLU
1	L	2231	ASP
1	L	2271	LEU
1	L	2276	ILE
1	L	2284	SER
1	L	2300	LEU
1	L	2319[A]	HIS
1	L	2319[B]	HIS
1	L	2324	GLN
1	L	2348	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	47	HIS
1	A	136	GLN
1	B	224	GLN
1	B	247	HIS
1	B	324	GLN
1	C	406	ASN
1	C	422	GLN
1	C	447	HIS
1	D	624	GLN
1	D	718	HIS
1	D	724	GLN
1	E	822	GLN
1	F	1016	ASN
1	F	1072	ASN
1	F	1124	GLN
1	G	1206	ASN
1	G	1222	GLN
1	G	1324	GLN
1	H	1422	GLN
1	H	1447	HIS
1	H	1458	HIS
1	H	1509	ASN

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Mol	Chain	Res	Type
1	H	1524	GLN
1	I	1622	GLN
1	I	1647	HIS
1	I	1724	GLN
1	J	1822	GLN
1	J	1906	HIS
1	J	1912	GLN
1	K	2016	ASN
1	K	2022	GLN
1	K	2058	HIS
1	K	2112	GLN
1	L	2247	HIS
1	L	2312	GLN
1	L	2324	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	1152	-	5,5,5	0.60	0	5,5,5	0.46	0
4	PO4	J	2952	-	4,4,4	0.51	0	6,6,6	1.12	0
5	TRS	D	1752	-	7,7,7	0.60	0	9,9,9	0.91	0
3	GOL	L	3352	-	5,5,5	0.60	0	5,5,5	1.05	0
2	RP4	K	3151	-	25,27,27	1.86	3 (12%)	28,39,39	1.93	10 (35%)
2	RP4	F	2151	-	25,27,27	1.51	3 (12%)	28,39,39	1.48	3 (10%)
2	RP4	D	1751	-	25,27,27	1.79	3 (12%)	28,39,39	2.00	7 (25%)
3	GOL	F	2153	-	5,5,5	0.62	0	5,5,5	1.03	0
3	GOL	D	1753	-	5,5,5	0.64	0	5,5,5	1.29	0
3	GOL	H	2552	-	5,5,5	0.51	0	5,5,5	1.19	0
3	GOL	G	2353	-	5,5,5	0.65	0	5,5,5	0.56	0
3	GOL	K	3153	-	5,5,5	0.50	0	5,5,5	1.66	1 (20%)
3	GOL	J	2955	-	5,5,5	0.54	0	5,5,5	0.74	0
3	GOL	B	1354	-	5,5,5	0.66	0	5,5,5	0.74	0
5	TRS	I	2752	-	7,7,7	1.07	1 (14%)	9,9,9	1.71	2 (22%)
2	RP4	E	1951	-	25,27,27	1.60	4 (16%)	28,39,39	1.11	2 (7%)
5	TRS	J	2953	-	7,7,7	0.59	0	9,9,9	1.11	0
2	RP4	I	2751	-	25,27,27	1.52	3 (12%)	28,39,39	1.58	6 (21%)
3	GOL	J	2954	-	5,5,5	0.52	0	5,5,5	0.64	0
2	RP4	A	1151	-	25,27,27	1.63	3 (12%)	28,39,39	1.55	2 (7%)
5	TRS	B	1353	-	7,7,7	0.80	0	9,9,9	1.71	1 (11%)
2	RP4	B	1351	-	25,27,27	1.81	4 (16%)	28,39,39	1.71	6 (21%)
2	RP4	H	2551	-	25,27,27	1.65	2 (8%)	28,39,39	1.58	6 (21%)
4	PO4	G	2352	-	4,4,4	1.06	0	6,6,6	1.63	1 (16%)
4	PO4	B	1352	-	4,4,4	0.79	0	6,6,6	0.89	0
2	RP4	J	2951	-	25,27,27	1.77	2 (8%)	28,39,39	2.26	4 (14%)
3	GOL	K	3152	-	5,5,5	0.59	0	5,5,5	0.44	0
2	RP4	L	3351	-	25,27,27	2.24	6 (24%)	28,39,39	1.43	6 (21%)
2	RP4	G	2351	-	25,27,27	1.54	4 (16%)	28,39,39	1.60	5 (17%)
2	RP4	C	1551	-	25,27,27	1.64	3 (12%)	28,39,39	1.48	5 (17%)
3	GOL	E	1952	-	5,5,5	1.11	0	5,5,5	1.75	2 (40%)
4	PO4	F	2152	-	4,4,4	0.75	0	6,6,6	1.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1152	-	-	0/4/4/4	-
5	TRS	D	1752	-	-	0/9/9/9	-
3	GOL	L	3352	-	-	4/4/4/4	-
2	RP4	K	3151	-	-	1/14/32/32	0/3/3/3
2	RP4	F	2151	-	-	1/14/32/32	0/3/3/3
2	RP4	D	1751	-	-	2/14/32/32	0/3/3/3
3	GOL	F	2153	-	-	4/4/4/4	-
3	GOL	D	1753	-	-	2/4/4/4	-
3	GOL	H	2552	-	-	3/4/4/4	-
3	GOL	G	2353	-	-	1/4/4/4	-
3	GOL	K	3153	-	-	3/4/4/4	-
3	GOL	J	2955	-	-	3/4/4/4	-
3	GOL	B	1354	-	-	2/4/4/4	-
5	TRS	I	2752	-	-	4/9/9/9	-
2	RP4	E	1951	-	-	1/14/32/32	0/3/3/3
5	TRS	J	2953	-	-	1/9/9/9	-
2	RP4	I	2751	-	-	3/14/32/32	0/3/3/3
3	GOL	J	2954	-	-	2/4/4/4	-
2	RP4	A	1151	-	-	3/14/32/32	0/3/3/3
5	TRS	B	1353	-	-	2/9/9/9	-
2	RP4	B	1351	-	-	1/14/32/32	0/3/3/3
2	RP4	H	2551	-	-	2/14/32/32	0/3/3/3
2	RP4	J	2951	-	-	3/14/32/32	0/3/3/3
3	GOL	K	3152	-	-	4/4/4/4	-
2	RP4	L	3351	-	-	2/14/32/32	0/3/3/3
2	RP4	G	2351	-	-	2/14/32/32	0/3/3/3
2	RP4	C	1551	-	-	1/14/32/32	0/3/3/3
3	GOL	E	1952	-	-	4/4/4/4	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1751	RP4	C15-S16	-6.25	1.66	1.77
2	B	1351	RP4	C15-S16	-5.58	1.67	1.77
2	H	2551	RP4	C17-S16	-5.55	1.67	1.77
2	K	3151	RP4	C17-S16	-5.47	1.67	1.77
2	L	3351	RP4	C17-S16	-5.36	1.67	1.77
2	J	2951	RP4	C15-S16	-5.17	1.68	1.77
2	L	3351	RP4	C13-C7	4.97	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	3151	RP4	C15-S16	-4.90	1.68	1.77
2	L	3351	RP4	C6-C7	4.87	1.38	1.34
2	A	1151	RP4	C15-S16	-4.86	1.68	1.77
2	L	3351	RP4	O5-C4	4.80	1.50	1.42
2	C	1551	RP4	C15-S16	-4.79	1.68	1.77
2	J	2951	RP4	C17-S16	-4.65	1.69	1.77
2	E	1951	RP4	C17-S16	-4.30	1.69	1.77
2	H	2551	RP4	C15-S16	-4.26	1.69	1.77
2	I	2751	RP4	C15-S16	-4.22	1.70	1.77
2	A	1151	RP4	C17-S16	-4.21	1.70	1.77
2	F	2151	RP4	C17-S16	-4.21	1.70	1.77
2	E	1951	RP4	C15-S16	-4.19	1.70	1.77
2	I	2751	RP4	C17-S16	-4.16	1.70	1.77
2	D	1751	RP4	C17-S16	-3.99	1.70	1.77
2	B	1351	RP4	C17-S16	-3.94	1.70	1.77
2	G	2351	RP4	C15-S16	-3.78	1.70	1.77
2	G	2351	RP4	C17-S16	-3.75	1.70	1.77
2	F	2151	RP4	C15-S16	-3.65	1.71	1.77
2	B	1351	RP4	O5-C4	3.48	1.48	1.42
2	G	2351	RP4	O5-C4	3.40	1.47	1.42
2	B	1351	RP4	C6-C7	3.36	1.37	1.34
2	C	1551	RP4	C17-S16	-3.18	1.71	1.77
2	L	3351	RP4	C15-S16	-2.85	1.72	1.77
2	A	1151	RP4	C6-C7	2.66	1.36	1.34
2	K	3151	RP4	O5-C4	2.61	1.46	1.42
2	I	2751	RP4	C6-C7	2.41	1.36	1.34
5	I	2752	TRS	O3-C3	2.37	1.49	1.42
2	G	2351	RP4	C6-C7	2.37	1.36	1.34
2	E	1951	RP4	C13-C7	2.36	1.51	1.48
2	F	2151	RP4	O11-C10	-2.36	1.38	1.43
2	D	1751	RP4	C14-C13	-2.27	1.36	1.39
2	C	1551	RP4	C6-C7	2.26	1.36	1.34
2	E	1951	RP4	O5-C4	2.16	1.46	1.42
2	L	3351	RP4	C4-C6	2.09	1.54	1.50

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2951	RP4	O11-C10-C8	-9.99	93.07	109.80
2	A	1151	RP4	C17-S16-C15	5.80	115.75	103.13
2	I	2751	RP4	O11-C10-C8	-4.86	101.67	109.80
2	D	1751	RP4	O11-C10-C8	-4.71	101.92	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1751	RP4	O5-C4-C2	-4.70	99.25	108.52
2	G	2351	RP4	O9-C8-C10	-4.55	102.67	110.34
2	F	2151	RP4	O11-C10-C12	-4.37	99.82	109.97
2	H	2551	RP4	O11-C10-C8	-4.05	103.02	109.80
2	G	2351	RP4	C17-S16-C15	4.05	111.94	103.13
2	K	3151	RP4	O9-C8-C10	-4.01	103.58	110.34
2	D	1751	RP4	C23-C15-C14	4.00	125.25	119.79
2	B	1351	RP4	O11-C10-C8	-3.88	103.31	109.80
2	C	1551	RP4	C25-C13-C7	3.80	124.83	121.11
5	B	1353	TRS	C3-C-N	3.64	117.45	108.17
2	K	3151	RP4	O1-C2-O3	-3.54	112.55	123.86
2	F	2151	RP4	C25-C13-C7	3.38	124.42	121.11
2	E	1951	RP4	O5-C4-C6	3.38	116.50	109.10
2	K	3151	RP4	O9-C8-C7	-3.33	101.26	110.76
2	G	2351	RP4	O5-C4-C6	3.32	116.36	109.10
2	B	1351	RP4	O5-C4-C6	3.25	116.22	109.10
2	E	1951	RP4	C17-S16-C15	3.22	110.13	103.13
2	H	2551	RP4	C18-C17-C22	3.19	124.03	118.85
2	C	1551	RP4	O11-C10-C12	-3.13	102.69	109.97
2	B	1351	RP4	C25-C13-C14	3.12	122.86	119.25
4	G	2352	PO4	O3-P-O2	-3.03	98.50	107.91
2	K	3151	RP4	O11-C10-C12	3.02	116.99	109.97
2	K	3151	RP4	C17-S16-C15	2.97	109.59	103.13
2	F	2151	RP4	C13-C7-C6	-2.90	117.91	123.05
2	I	2751	RP4	C12-C4-C2	2.90	116.87	110.70
2	D	1751	RP4	C14-C15-S16	-2.88	111.39	119.75
2	B	1351	RP4	C12-C4-C2	2.88	116.83	110.70
2	B	1351	RP4	O9-C8-C7	-2.85	102.64	110.76
2	G	2351	RP4	O11-C10-C8	-2.83	105.06	109.80
2	J	2951	RP4	C12-C4-C2	2.81	116.67	110.70
2	L	3351	RP4	O11-C10-C12	-2.74	103.60	109.97
2	D	1751	RP4	C25-C13-C7	2.71	123.76	121.11
2	D	1751	RP4	C24-C25-C13	2.70	123.02	120.36
2	I	2751	RP4	C13-C14-C15	-2.68	117.41	119.97
2	K	3151	RP4	O11-C10-C8	-2.67	105.34	109.80
2	C	1551	RP4	C24-C25-C13	2.61	122.93	120.36
5	I	2752	TRS	O2-C2-C	2.58	118.07	110.88
2	L	3351	RP4	O1-C2-O3	-2.55	115.69	123.86
2	K	3151	RP4	C23-C15-C14	2.51	123.21	119.79
2	H	2551	RP4	C17-S16-C15	2.47	108.50	103.13
2	K	3151	RP4	O5-C4-C6	2.47	114.50	109.10
2	K	3151	RP4	C12-C4-C2	2.45	115.91	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2551	RP4	C12-C4-C2	2.43	115.86	110.70
2	J	2951	RP4	C17-S16-C15	2.43	108.40	103.13
2	I	2751	RP4	C13-C7-C6	-2.42	118.77	123.05
2	C	1551	RP4	C23-C15-C14	2.41	123.08	119.79
2	J	2951	RP4	C25-C13-C7	2.40	123.46	121.11
2	I	2751	RP4	C25-C13-C14	2.39	122.02	119.25
2	L	3351	RP4	C13-C14-C15	2.38	122.24	119.97
2	B	1351	RP4	C24-C25-C13	-2.37	118.03	120.36
3	K	3153	GOL	O2-C2-C3	2.37	118.99	109.18
2	H	2551	RP4	C13-C14-C15	-2.30	117.78	119.97
2	I	2751	RP4	O5-C4-C6	2.30	114.14	109.10
2	C	1551	RP4	C13-C7-C6	-2.23	119.11	123.05
2	K	3151	RP4	C24-C25-C13	2.21	122.54	120.36
2	L	3351	RP4	C25-C13-C14	-2.18	116.72	119.25
2	G	2351	RP4	O9-C8-C7	-2.17	104.59	110.76
2	A	1151	RP4	O5-C4-C6	2.17	113.84	109.10
5	I	2752	TRS	O1-C1-C	-2.16	104.86	110.88
2	L	3351	RP4	O5-C4-C6	2.12	113.75	109.10
3	E	1952	GOL	O1-C1-C2	2.09	119.77	110.38
2	H	2551	RP4	O1-C2-O3	-2.08	117.20	123.86
2	D	1751	RP4	C13-C14-C15	-2.06	118.01	119.97
2	L	3351	RP4	C18-C17-C22	2.06	122.19	118.85
3	E	1952	GOL	C3-C2-C1	2.03	119.23	111.80

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1551	RP4	O1-C2-C4-O5
2	I	2751	RP4	O3-C2-C4-C6
3	B	1354	GOL	O1-C1-C2-O2
3	B	1354	GOL	O1-C1-C2-C3
3	D	1753	GOL	C1-C2-C3-O3
3	E	1952	GOL	O1-C1-C2-C3
3	F	2153	GOL	O1-C1-C2-C3
3	F	2153	GOL	C1-C2-C3-O3
3	H	2552	GOL	O1-C1-C2-O2
3	H	2552	GOL	O1-C1-C2-C3
3	J	2954	GOL	C1-C2-C3-O3
3	J	2954	GOL	O2-C2-C3-O3
3	K	3152	GOL	O1-C1-C2-C3
3	K	3152	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	L	3352	GOL	O1-C1-C2-C3
3	L	3352	GOL	C1-C2-C3-O3
3	L	3352	GOL	O2-C2-C3-O3
5	I	2752	TRS	N-C-C3-O3
3	K	3152	GOL	O1-C1-C2-O2
3	K	3153	GOL	O1-C1-C2-C3
3	E	1952	GOL	O2-C2-C3-O3
3	F	2153	GOL	O1-C1-C2-O2
3	K	3152	GOL	O2-C2-C3-O3
3	K	3153	GOL	O1-C1-C2-O2
3	L	3352	GOL	O1-C1-C2-O2
3	F	2153	GOL	O2-C2-C3-O3
3	J	2955	GOL	O1-C1-C2-C3
3	E	1952	GOL	C1-C2-C3-O3
3	G	2353	GOL	O1-C1-C2-C3
3	D	1753	GOL	O2-C2-C3-O3
3	H	2552	GOL	O2-C2-C3-O3
5	B	1353	TRS	C2-C-C3-O3
5	J	2953	TRS	C2-C-C1-O1
2	I	2751	RP4	O3-C2-C4-O5
3	E	1952	GOL	O1-C1-C2-O2
5	I	2752	TRS	C1-C-C2-O2
5	I	2752	TRS	C2-C-C3-O3
3	J	2955	GOL	C1-C2-C3-O3
3	J	2955	GOL	O1-C1-C2-O2
3	K	3153	GOL	O2-C2-C3-O3
5	B	1353	TRS	C1-C-C3-O3
5	I	2752	TRS	C3-C-C1-O1
2	A	1151	RP4	O1-C2-C4-O5
2	B	1351	RP4	O1-C2-C4-O5
2	D	1751	RP4	O1-C2-C4-O5
2	E	1951	RP4	O1-C2-C4-O5
2	F	2151	RP4	O1-C2-C4-O5
2	G	2351	RP4	O1-C2-C4-O5
2	H	2551	RP4	O1-C2-C4-O5
2	I	2751	RP4	O1-C2-C4-O5
2	J	2951	RP4	O1-C2-C4-O5
2	K	3151	RP4	O1-C2-C4-O5
2	L	3351	RP4	O1-C2-C4-O5
2	A	1151	RP4	O1-C2-C4-C6
2	D	1751	RP4	O1-C2-C4-C6
2	G	2351	RP4	O1-C2-C4-C6

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Mol	Chain	Res	Type	Atoms
2	A	1151	RP4	O3-C2-C4-O5
2	H	2551	RP4	O3-C2-C4-O5
2	J	2951	RP4	O3-C2-C4-C12
2	J	2951	RP4	O1-C2-C4-C12
2	L	3351	RP4	O3-C2-C4-O5

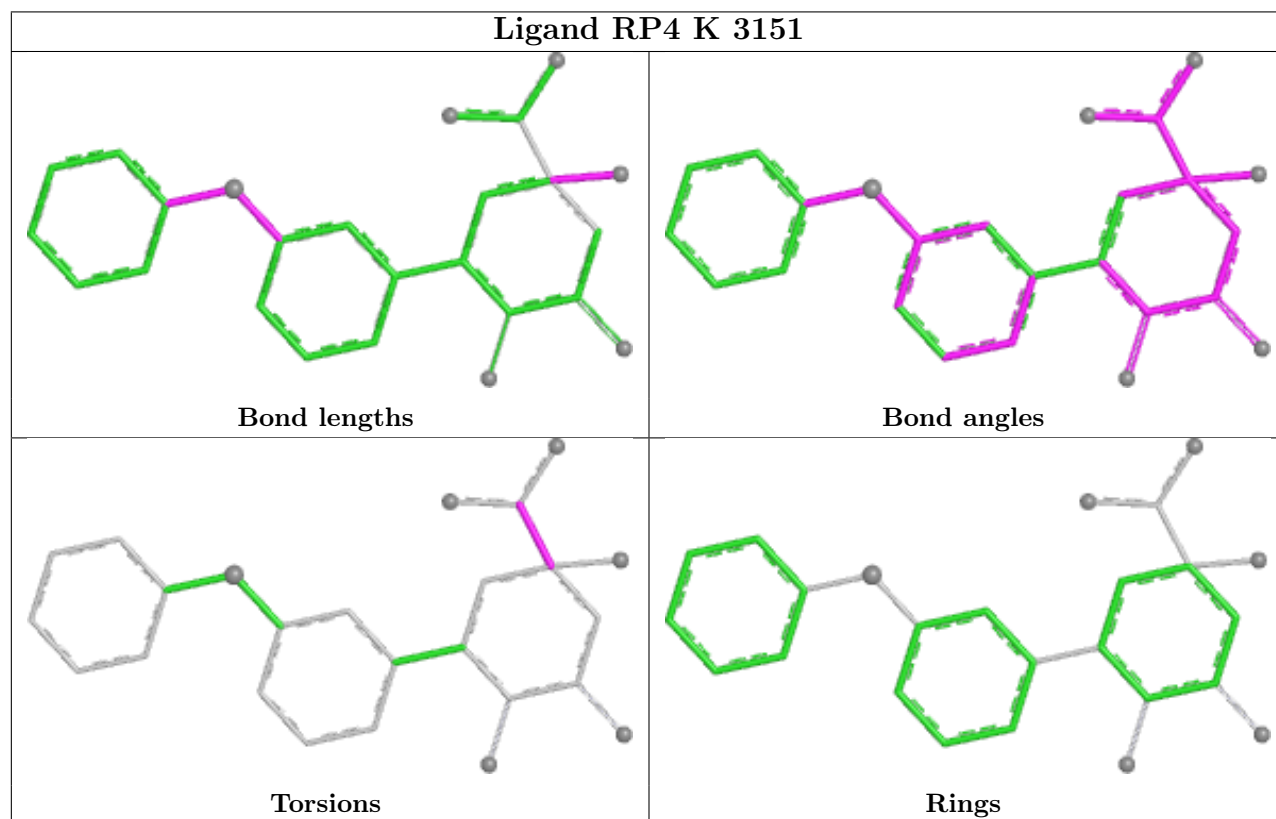
There are no ring outliers.

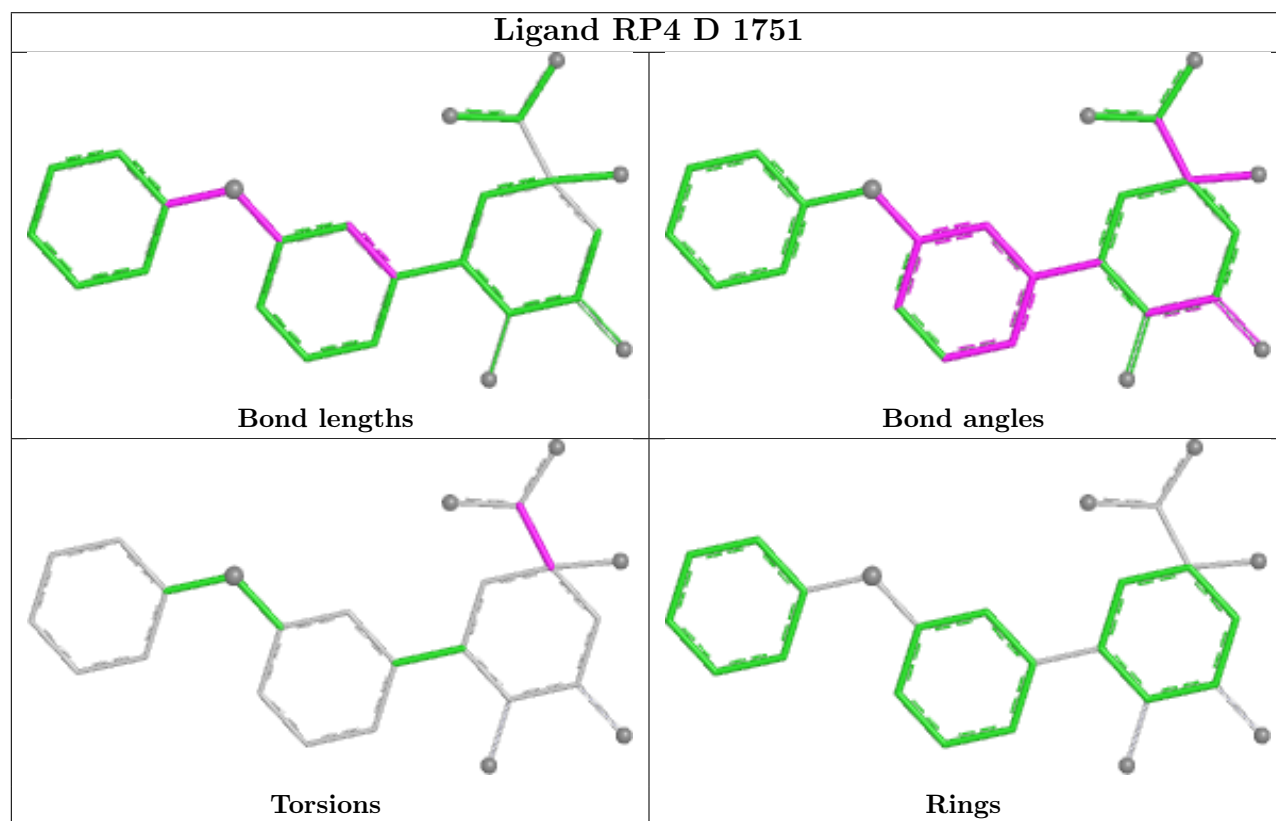
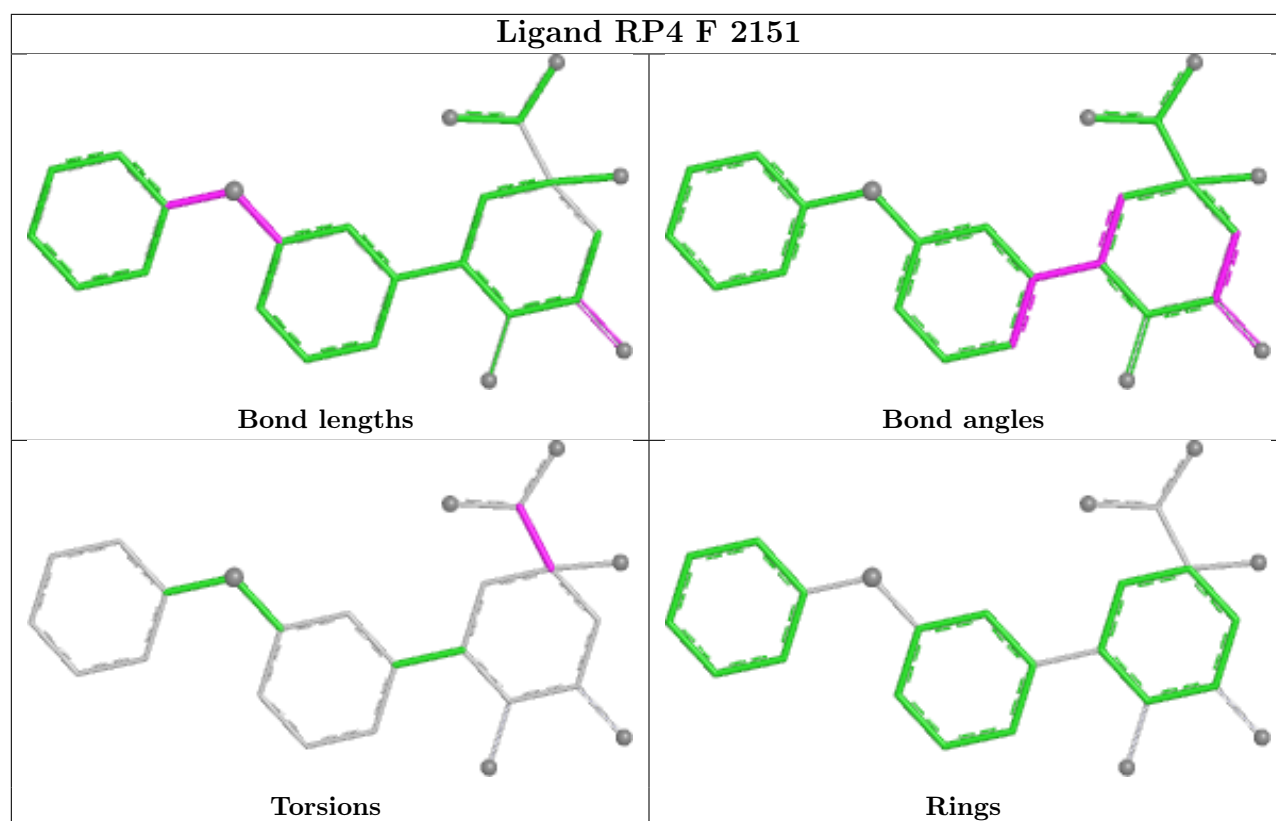
23 monomers are involved in 80 short contacts:

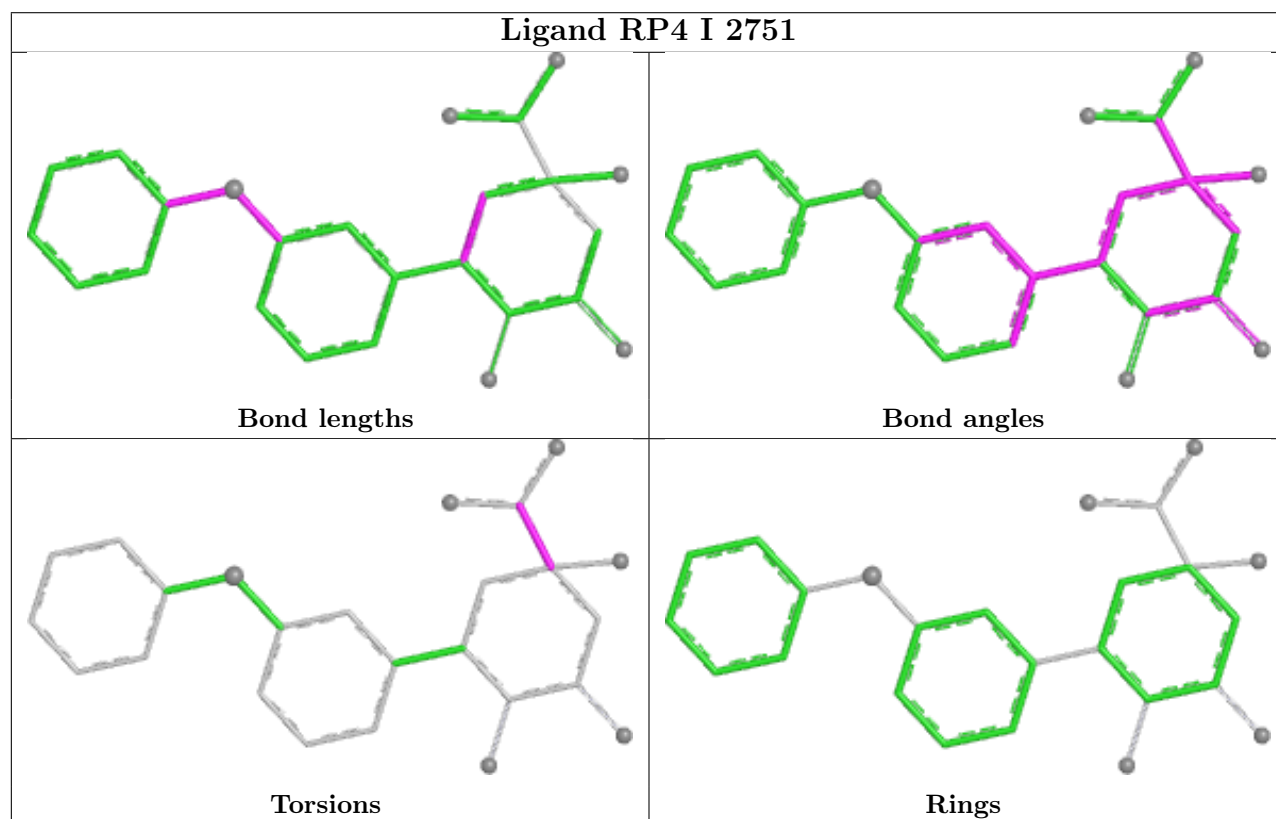
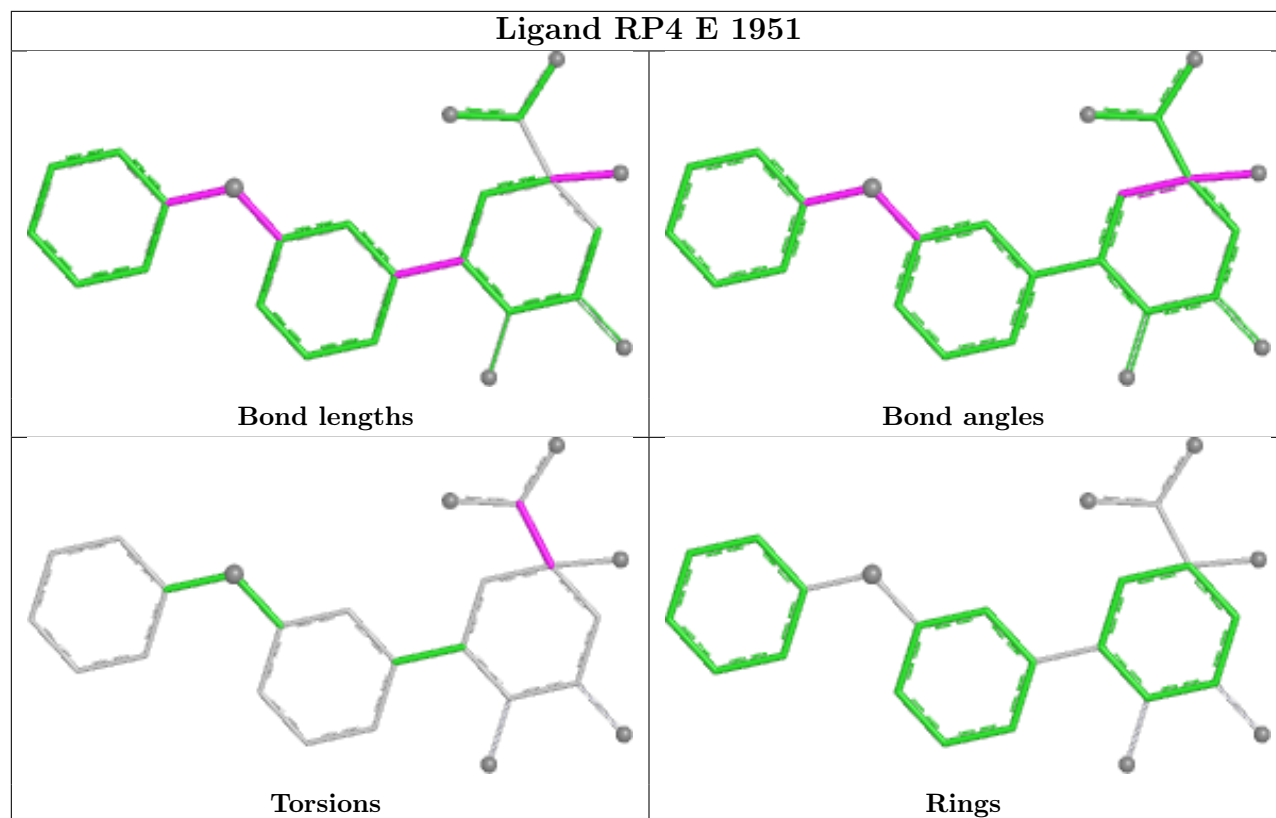
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1152	GOL	4	0
3	L	3352	GOL	2	0
2	K	3151	RP4	4	0
2	F	2151	RP4	2	0
3	F	2153	GOL	5	0
3	D	1753	GOL	8	0
3	H	2552	GOL	4	0
3	G	2353	GOL	4	0
3	K	3153	GOL	7	0
3	J	2955	GOL	5	0
5	I	2752	TRS	1	0
2	E	1951	RP4	2	0
5	J	2953	TRS	1	0
2	I	2751	RP4	1	0
3	J	2954	GOL	3	0
2	A	1151	RP4	10	0
2	B	1351	RP4	2	0
2	H	2551	RP4	2	0
3	K	3152	GOL	3	0
2	L	3351	RP4	5	0
2	G	2351	RP4	1	0
2	C	1551	RP4	2	0
3	E	1952	GOL	2	0

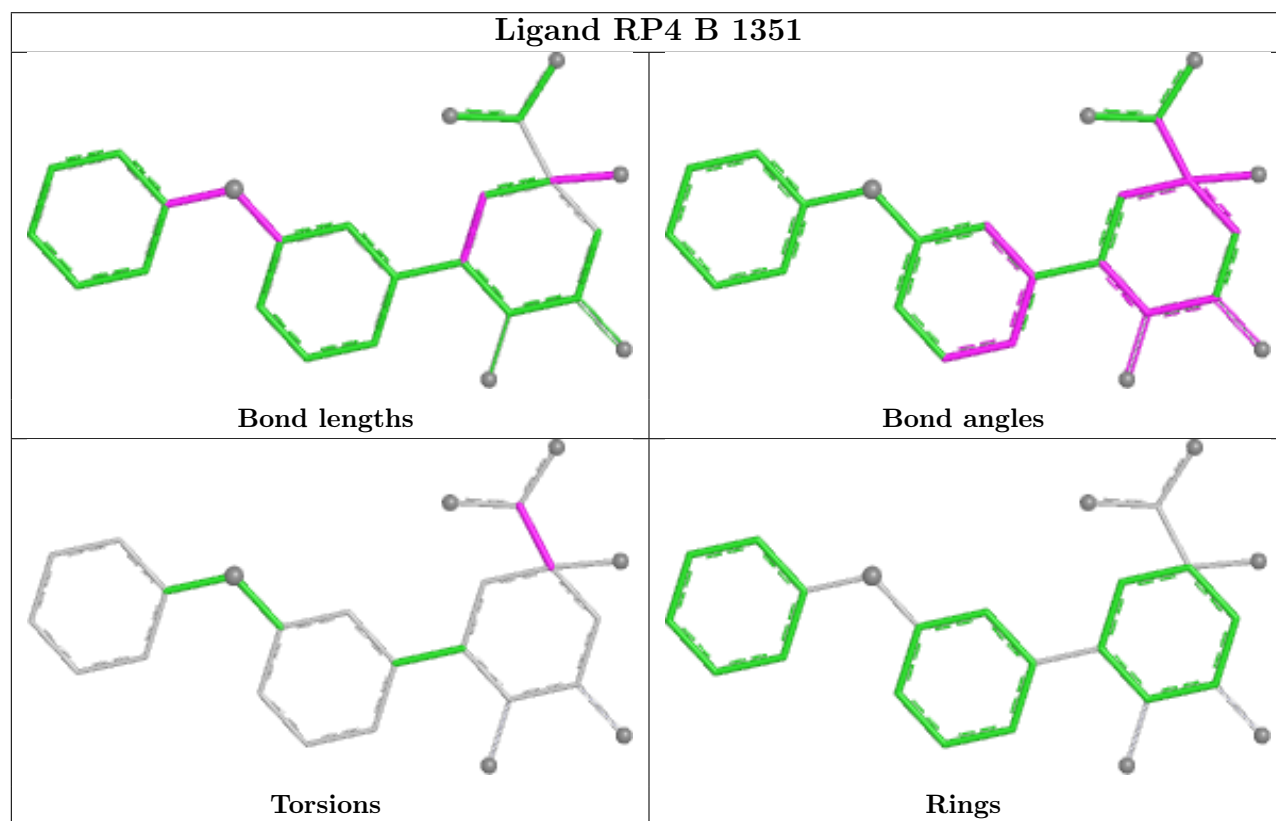
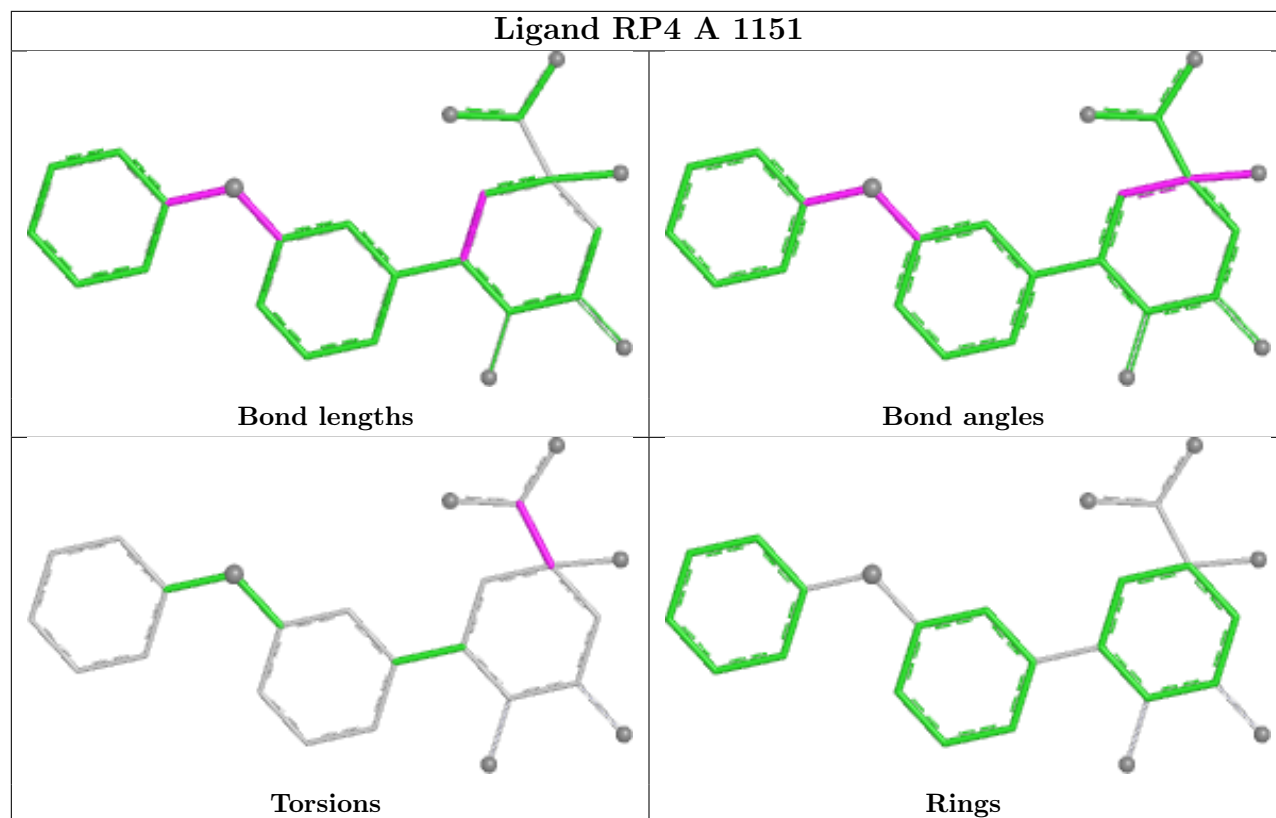
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

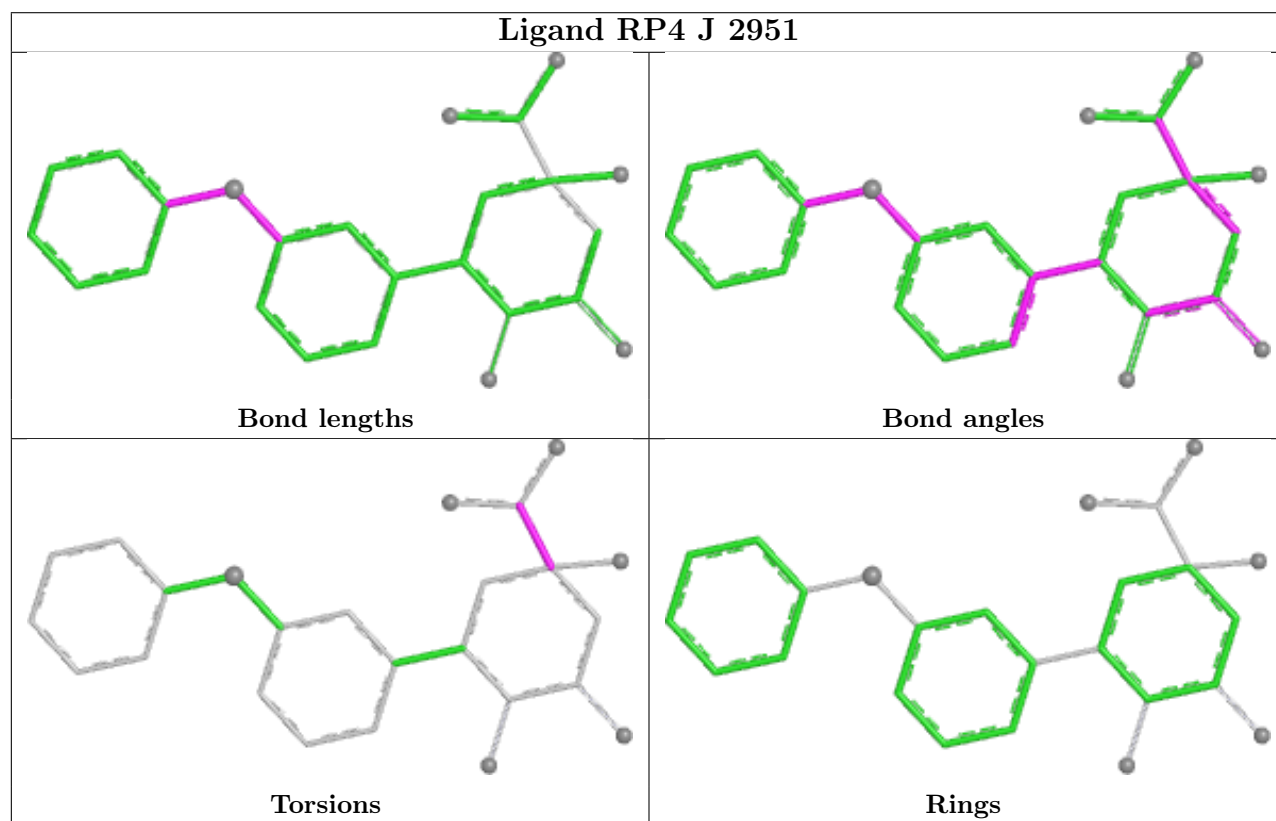
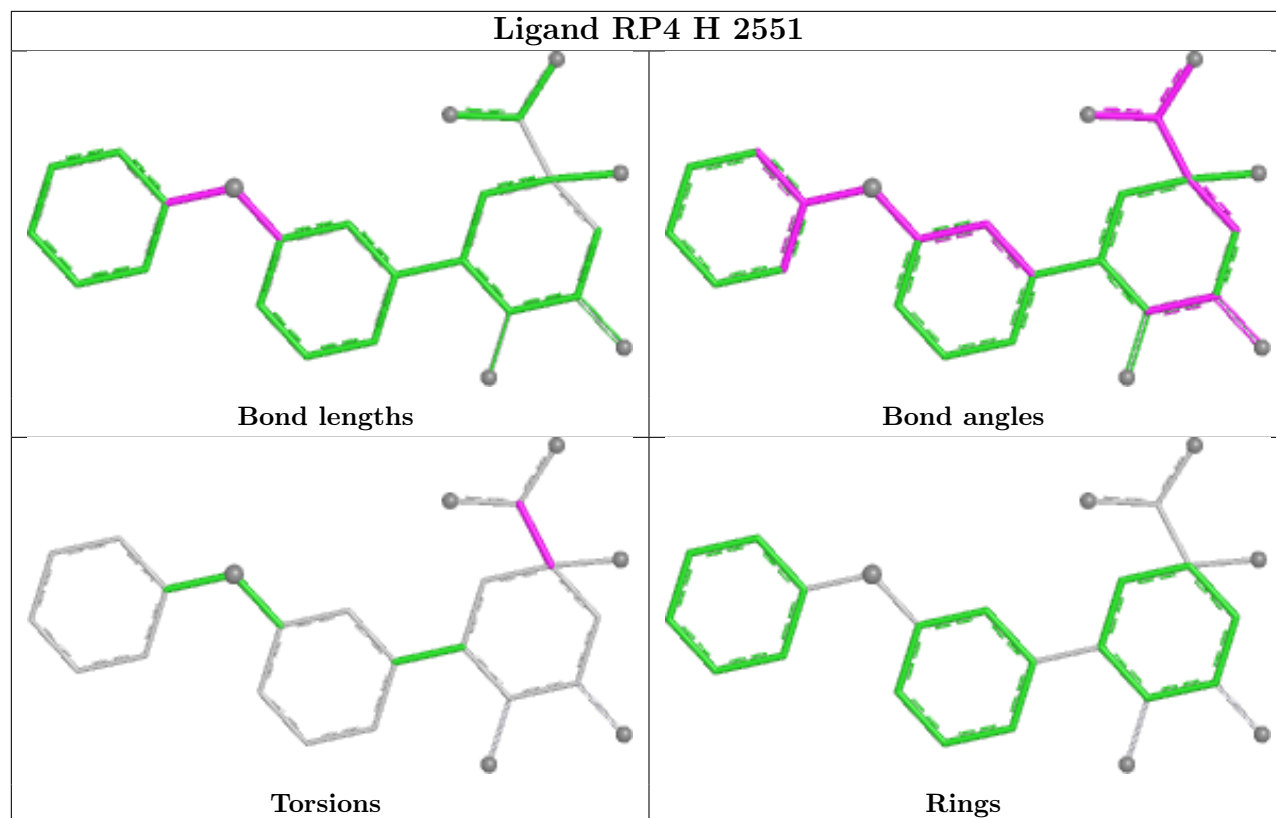
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

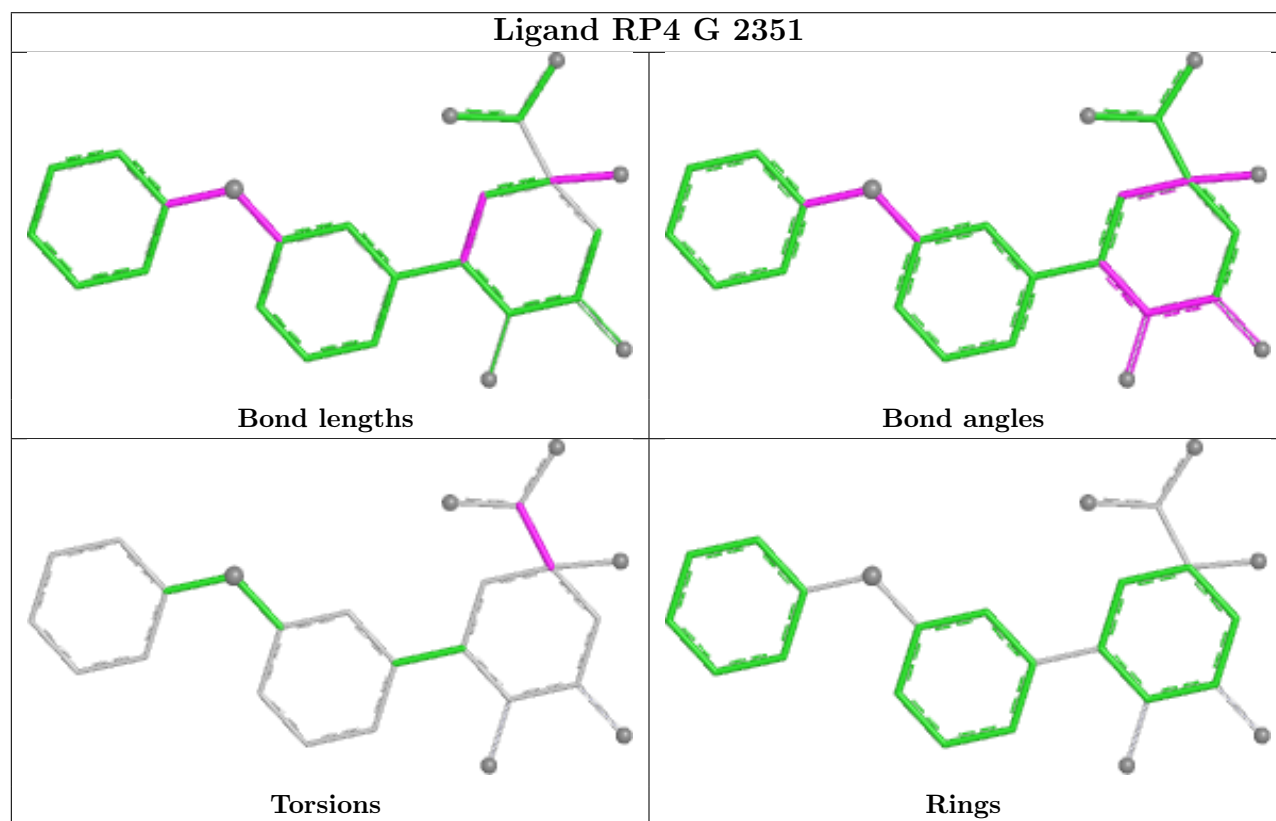
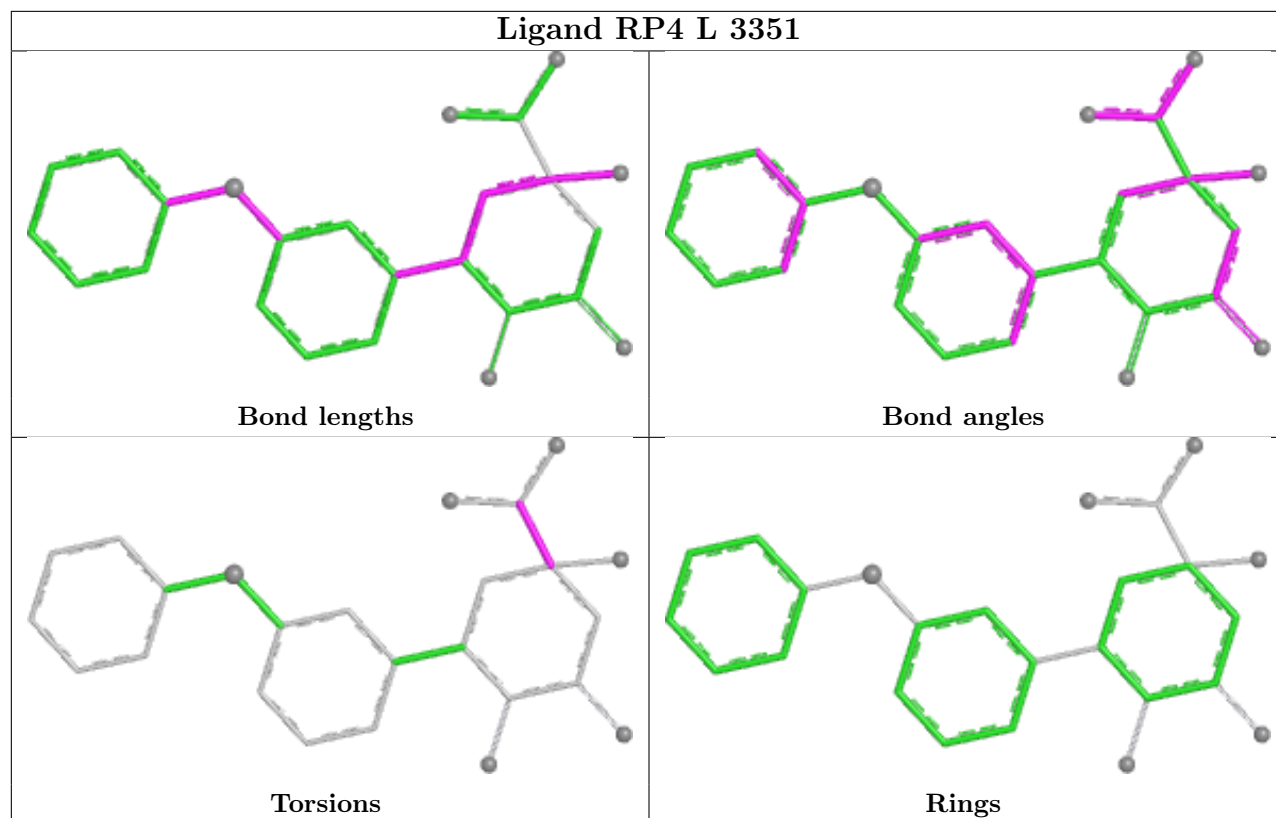


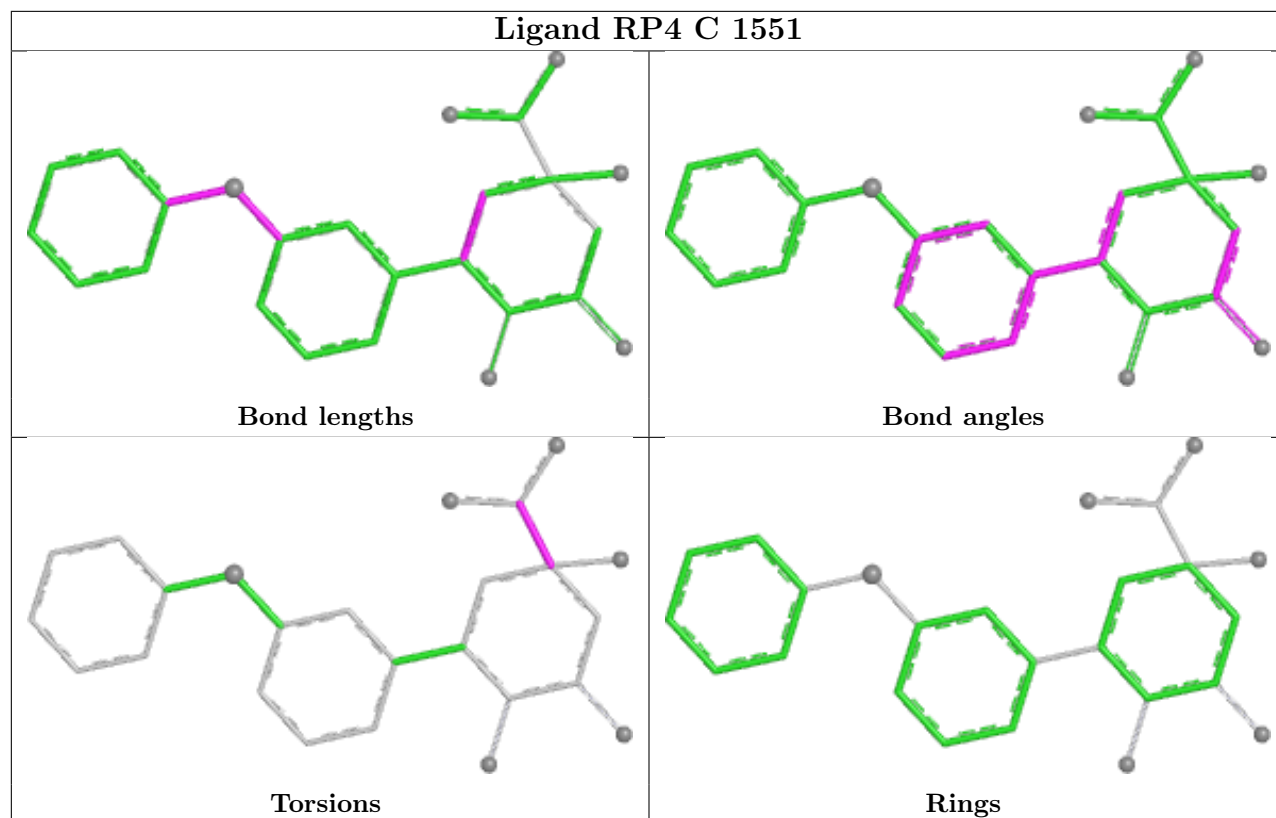












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	149/157 (94%)	-0.78	0 100 100	6, 20, 42, 51	2 (1%)
1	B	149/157 (94%)	-0.76	0 100 100	11, 21, 39, 48	1 (0%)
1	C	149/157 (94%)	-0.68	0 100 100	9, 24, 42, 56	2 (1%)
1	D	149/157 (94%)	-0.75	0 100 100	8, 21, 43, 54	2 (1%)
1	E	149/157 (94%)	-0.72	0 100 100	8, 20, 40, 48	1 (0%)
1	F	149/157 (94%)	-0.71	0 100 100	11, 25, 44, 52	1 (0%)
1	G	149/157 (94%)	-0.81	0 100 100	7, 19, 38, 47	2 (1%)
1	H	149/157 (94%)	-0.68	0 100 100	10, 25, 42, 55	2 (1%)
1	I	149/157 (94%)	-0.75	0 100 100	9, 21, 41, 49	2 (1%)
1	J	149/157 (94%)	-0.72	0 100 100	8, 25, 43, 46	2 (1%)
1	K	149/157 (94%)	-0.72	0 100 100	8, 22, 43, 51	1 (0%)
1	L	149/157 (94%)	-0.80	0 100 100	9, 20, 42, 56	2 (1%)
All	All	1788/1884 (94%)	-0.74	0 100 100	6, 22, 43, 56	20 (1%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

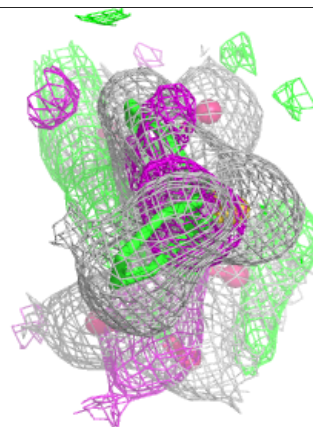
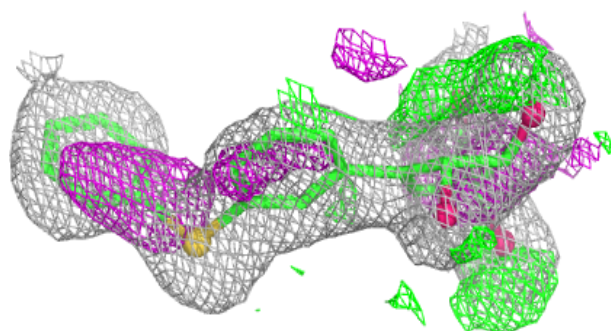
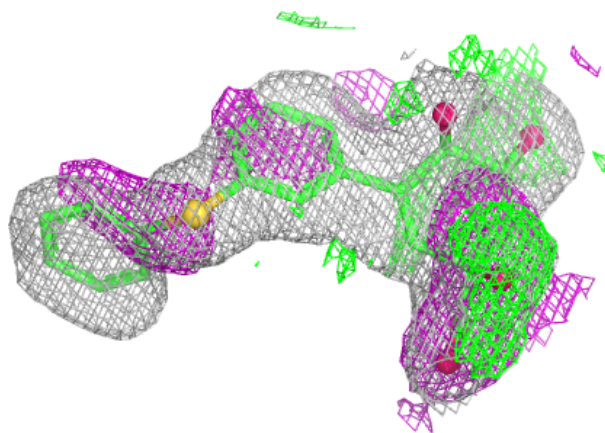
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	RP4	G	2351	25/25	0.97	0.08	14,30,33,35	0
3	GOL	D	1753	6/6	0.97	0.13	27,32,33,34	0
3	GOL	H	2552	6/6	0.97	0.12	41,44,49,53	0
3	GOL	J	2954	6/6	0.97	0.11	40,43,47,49	0
3	GOL	K	3152	6/6	0.97	0.13	39,44,45,47	0
5	TRS	B	1353	8/8	0.97	0.06	13,15,18,18	0
2	RP4	I	2751	25/25	0.98	0.08	24,32,35,38	0
2	RP4	J	2951	25/25	0.98	0.07	16,27,37,38	0
3	GOL	A	1152	6/6	0.98	0.11	31,39,42,45	0
3	GOL	B	1354	6/6	0.98	0.10	34,38,39,40	0
2	RP4	C	1551	25/25	0.98	0.05	18,29,32,33	0
3	GOL	F	2153	6/6	0.98	0.13	46,49,49,50	0
2	RP4	D	1751	25/25	0.98	0.06	21,26,28,30	0
2	RP4	E	1951	25/25	0.98	0.07	16,29,38,39	0
2	RP4	B	1351	25/25	0.98	0.07	16,35,39,39	0
3	GOL	K	3153	6/6	0.98	0.11	29,33,36,37	0
3	GOL	L	3352	6/6	0.98	0.07	33,38,41,42	0
4	PO4	J	2952	5/5	0.98	0.11	46,50,52,55	0
2	RP4	H	2551	25/25	0.98	0.06	15,29,37,38	0
2	RP4	F	2151	25/25	0.99	0.05	21,29,32,33	0
3	GOL	J	2955	6/6	0.99	0.10	44,45,46,47	0
2	RP4	K	3151	25/25	0.99	0.05	20,28,34,34	0
3	GOL	E	1952	6/6	0.99	0.08	20,31,35,35	0
2	RP4	L	3351	25/25	0.99	0.05	5,30,35,37	0
4	PO4	B	1352	5/5	0.99	0.06	60,62,64,64	0
4	PO4	F	2152	5/5	0.99	0.09	48,48,53,53	0
4	PO4	G	2352	5/5	0.99	0.04	41,41,42,46	0
3	GOL	G	2353	6/6	0.99	0.06	10,33,34,36	0
2	RP4	A	1151	25/25	0.99	0.06	14,38,45,46	0
5	TRS	D	1752	8/8	0.99	0.05	11,13,15,15	0
5	TRS	I	2752	8/8	0.99	0.04	4,6,9,13	0
5	TRS	J	2953	8/8	0.99	0.04	6,17,19,21	0

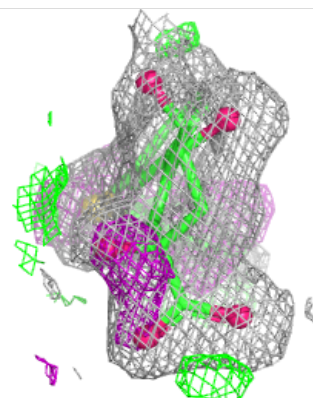
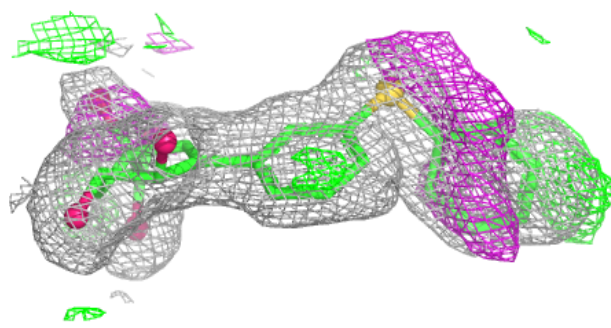
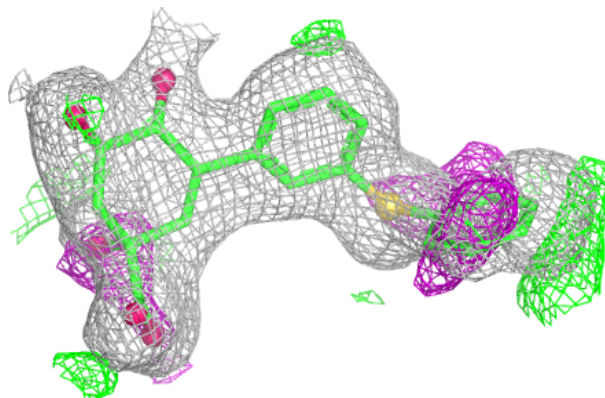
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around RP4 G 2351:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

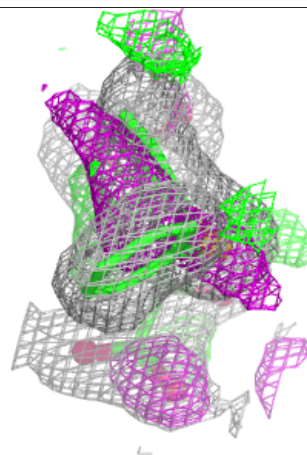
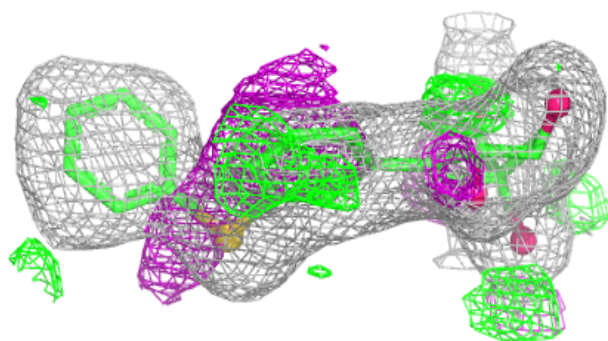
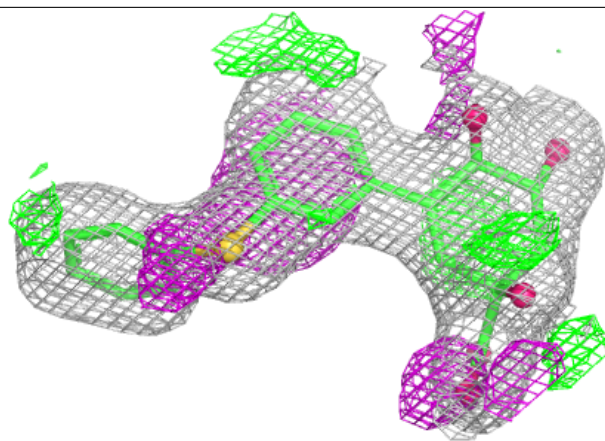
**Electron density around RP4 I 2751:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



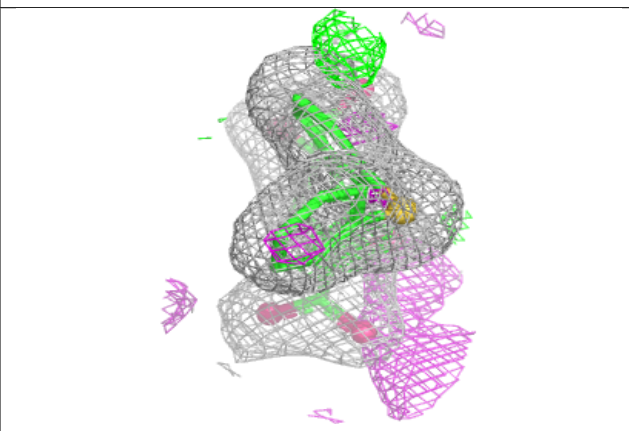
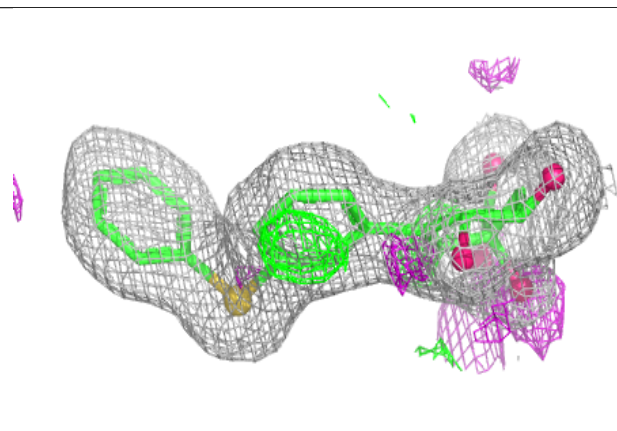
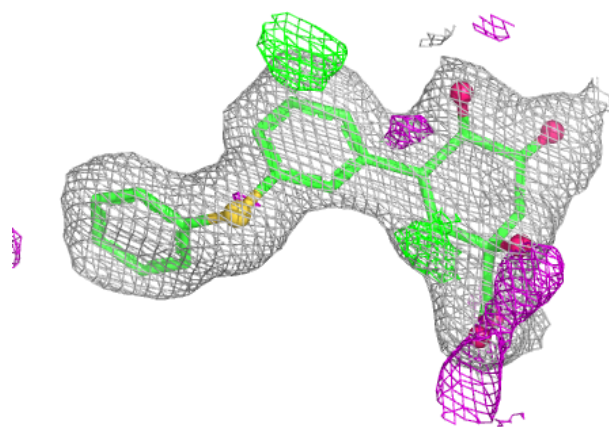
Electron density around RP4 J 2951:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



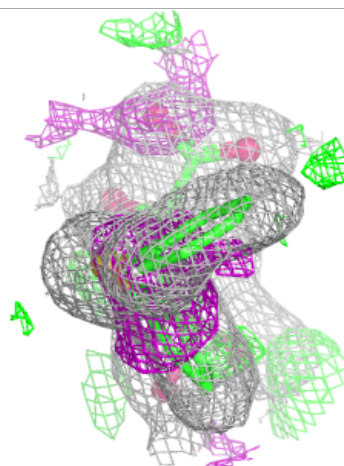
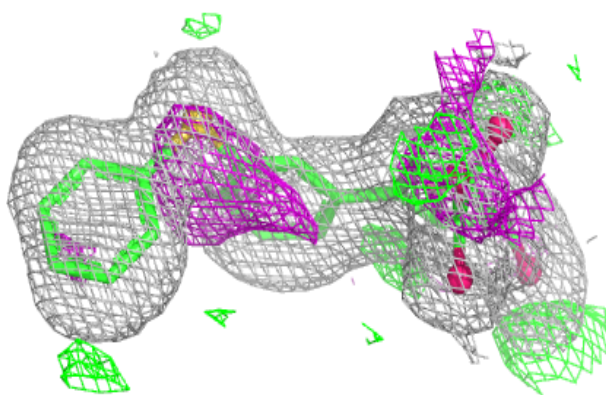
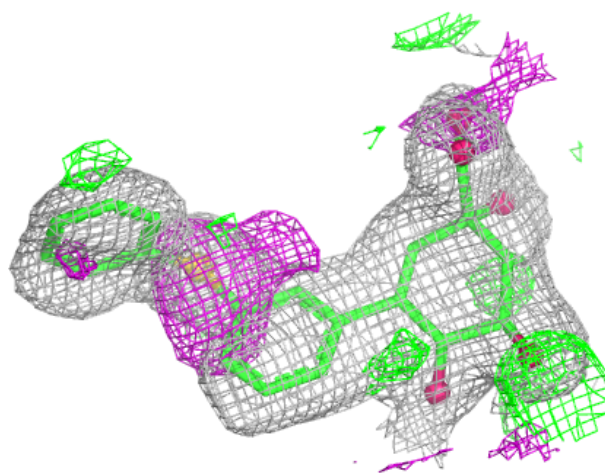
Electron density around RP4 C 1551:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



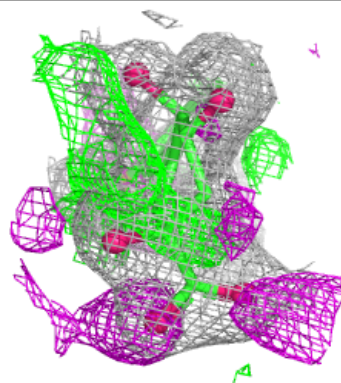
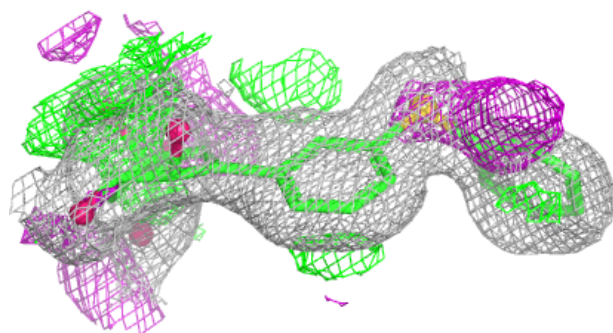
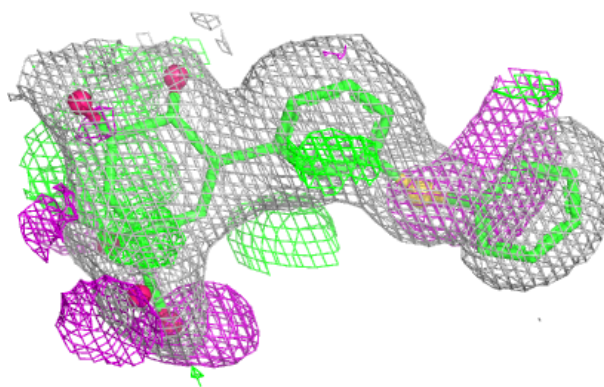
Electron density around RP4 D 1751:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

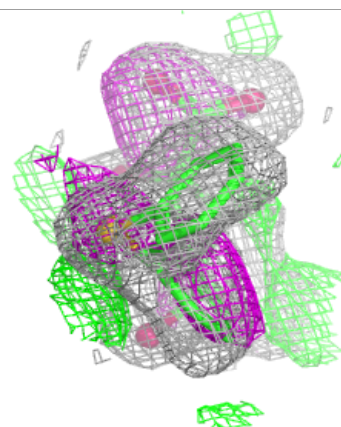
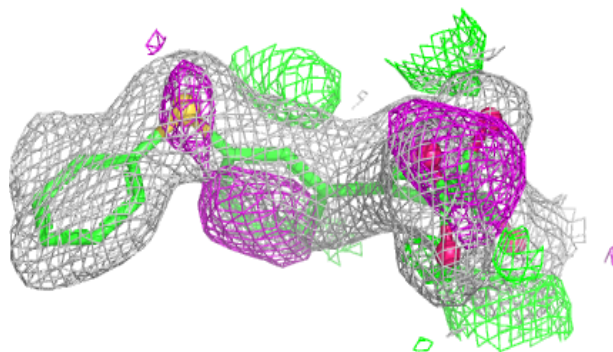
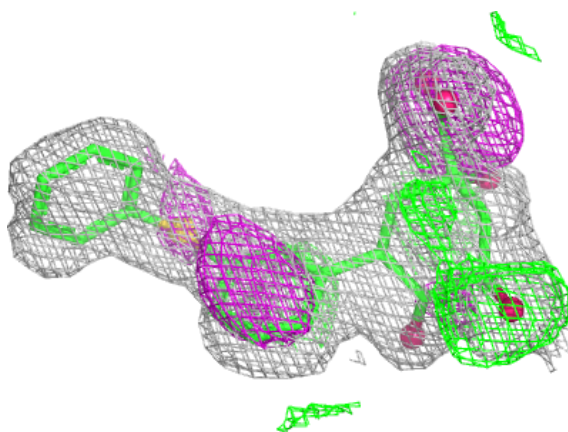


Electron density around RP4 E 1951:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

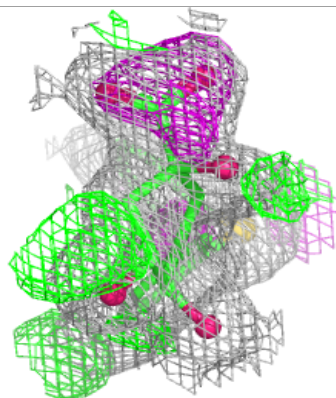
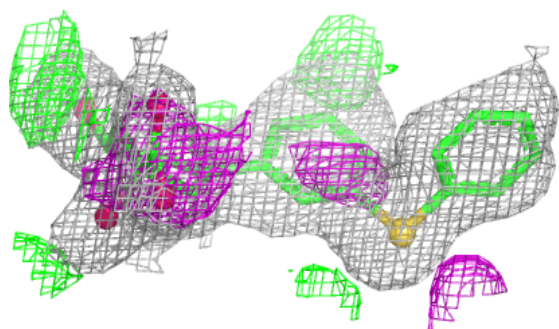
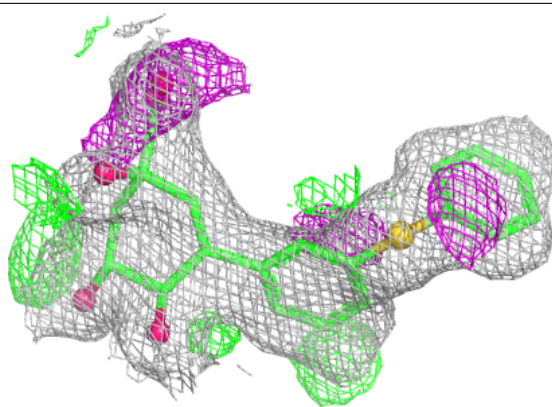
**Electron density around RP4 B 1351:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

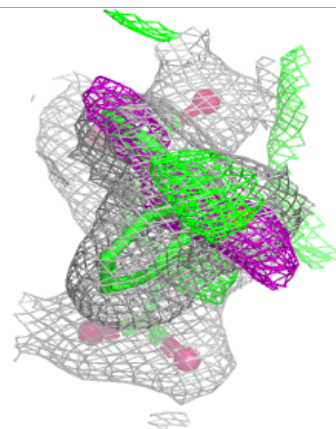
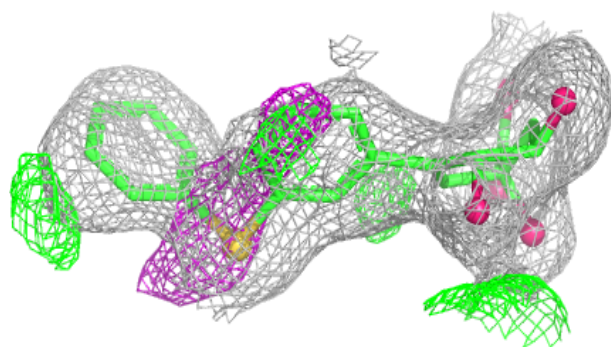
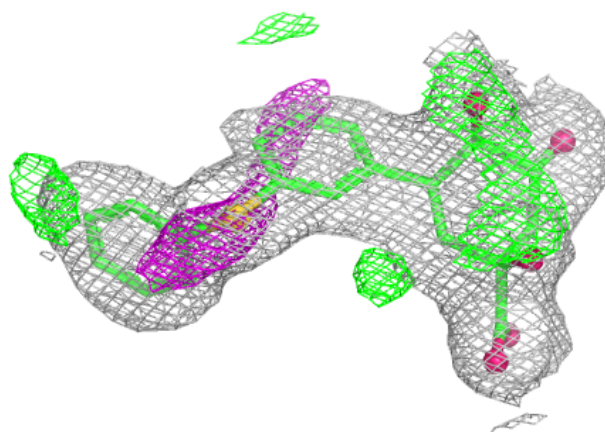


Electron density around RP4 H 2551:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

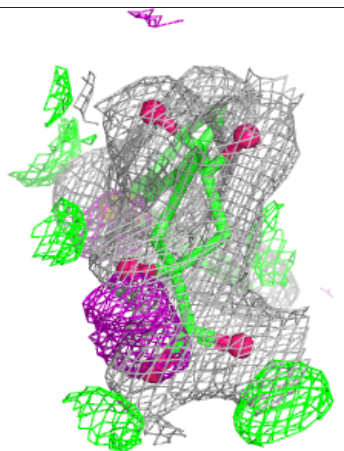
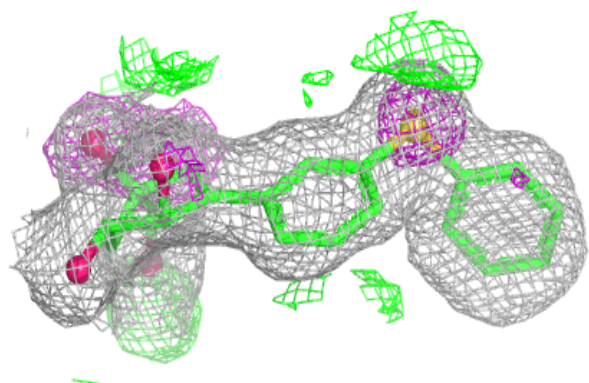
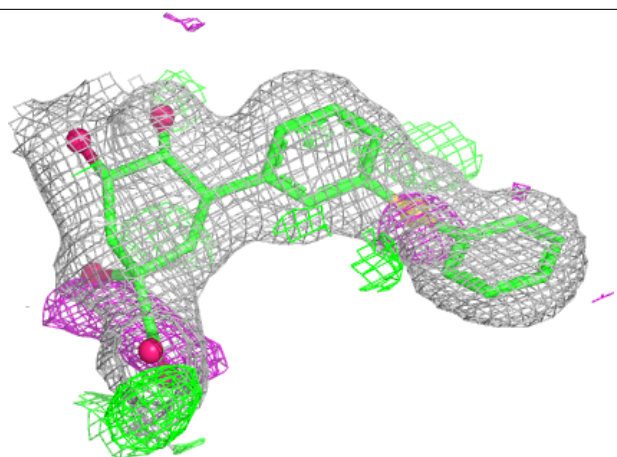
**Electron density around RP4 F 2151:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



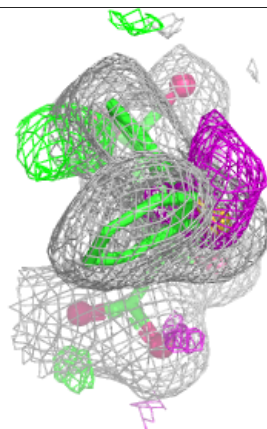
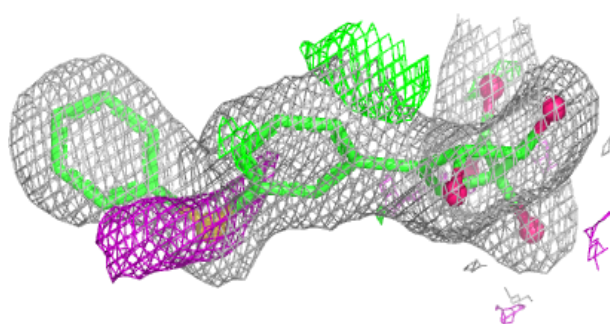
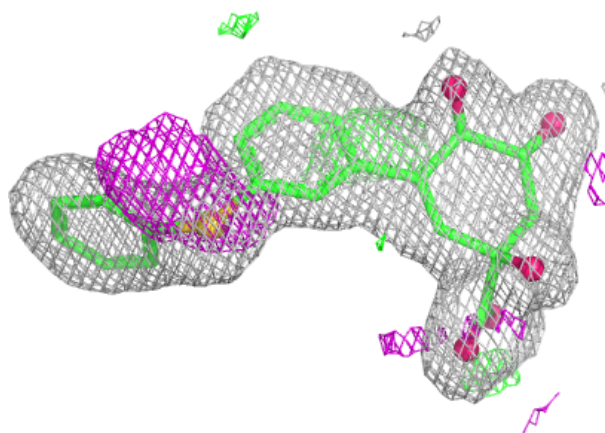
Electron density around RP4 K 3151:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

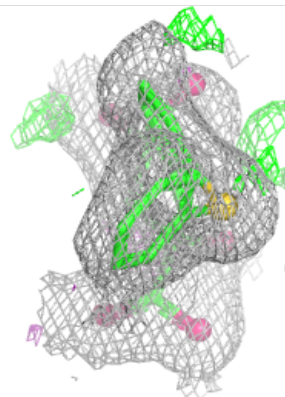
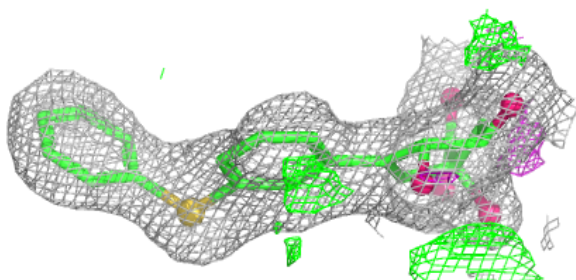
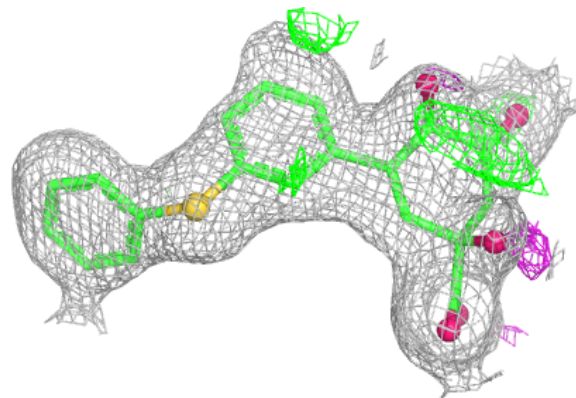


Electron density around RP4 L 3351:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around RP4 A 1151:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.