



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:50 AM UTC

PDB ID : 1FDU / pdb_00001fd
Title : HUMAN 17-BETA-HYDROXYSTEROID-DEHYDROGENASE TYPE 1
MUTANT H221L COMPLEXED WITH ESTRADIOL AND NADP+
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Deposited on : 1998-01-14
Resolution : 2.70 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

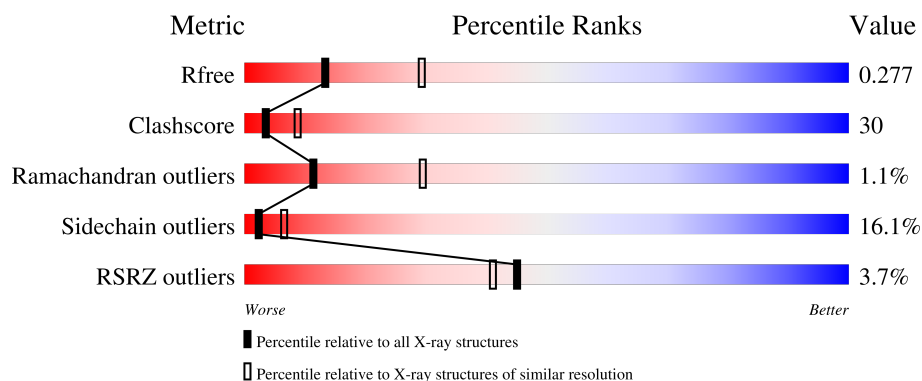
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	327	
1	B	327	
1	C	327	
1	D	327	

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	SO4	C	403	-	-	X	-
2	SO4	D	402	-	-	X	-
3	EST	A	351	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9114 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 17-BETA-HYDROXYSTEROID DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2148	1366	380	390	12			
1	B	280	Total	C	N	O	S	0	0	0
			2144	1364	379	389	12			
1	C	285	Total	C	N	O	S	0	0	0
			2179	1384	384	399	12			
1	D	281	Total	C	N	O	S	0	0	0
			2153	1369	380	392	12			

There are 8 discrepancies between the modelled and reference sequences:

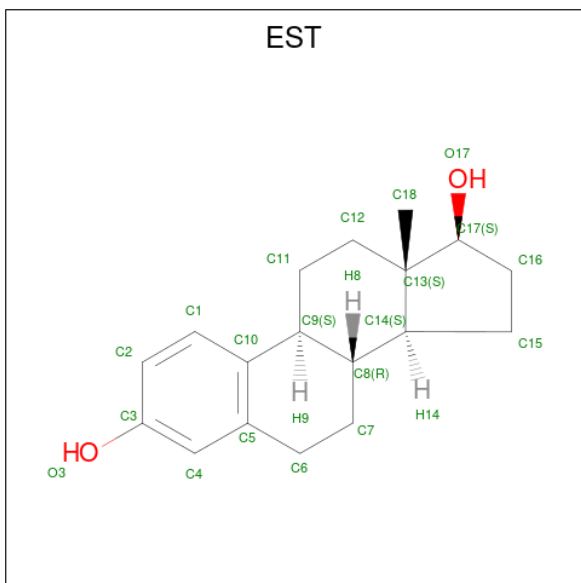
Chain	Residue	Modelled	Actual	Comment	Reference
A	221	LEU	HIS	engineered mutation	UNP P14061
A	301	ARG	ALA	conflict	UNP P14061
B	221	LEU	HIS	engineered mutation	UNP P14061
B	301	ARG	ALA	conflict	UNP P14061
C	221	LEU	HIS	engineered mutation	UNP P14061
C	301	ARG	ALA	conflict	UNP P14061
D	221	LEU	HIS	engineered mutation	UNP P14061
D	301	ARG	ALA	conflict	UNP P14061

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



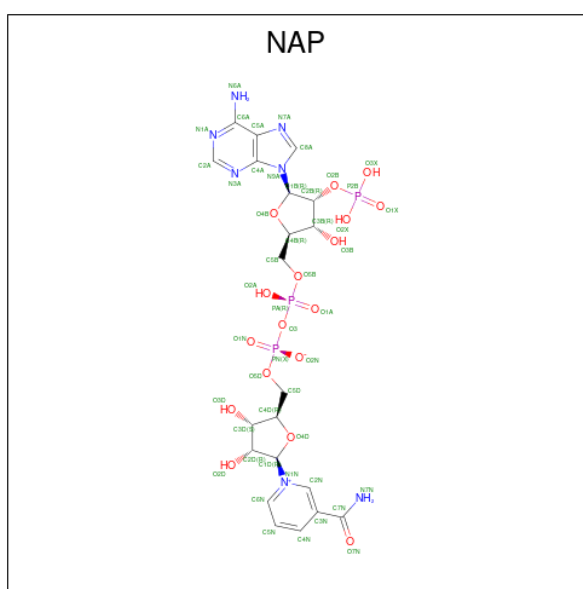
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ESTRADIOL (CCD ID: EST) (formula: $C_{18}H_{24}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 20	C 18	O 2	0	0
3	B	1	Total 20	C 18	O 2	0	0
3	C	1	Total 20	C 18	O 2	0	0
3	D	1	Total 20	C 18	O 2	0	0

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	51	Total O 51 51	0	0

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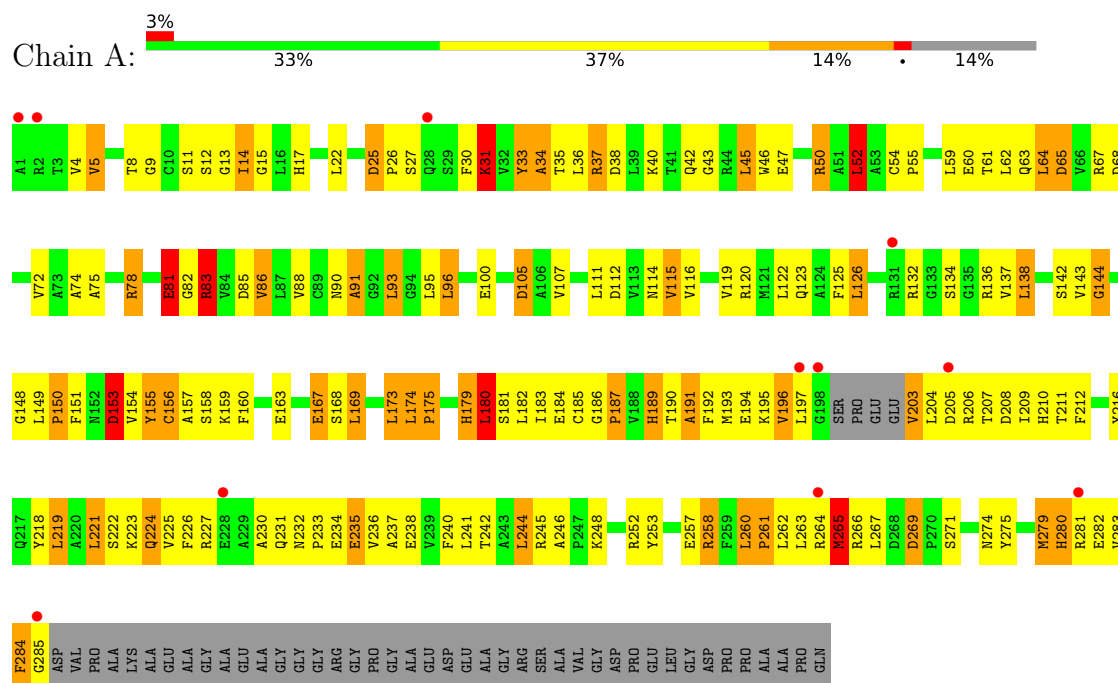
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	53	Total 53	O 53	0	0
5	C	48	Total 48	O 48	0	0
5	D	46	Total 46	O 46	0	0

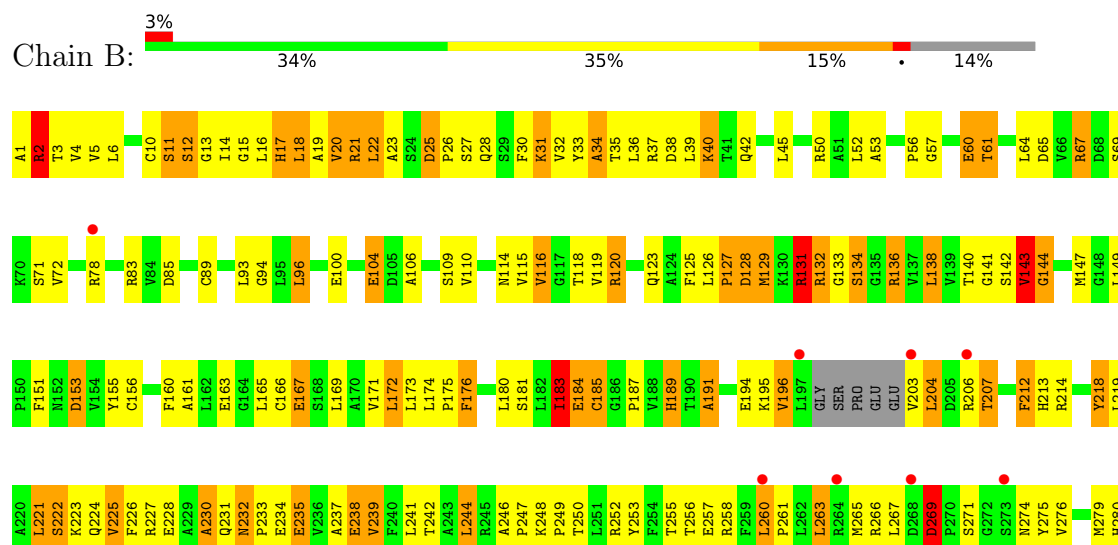
3 Residue-property plots

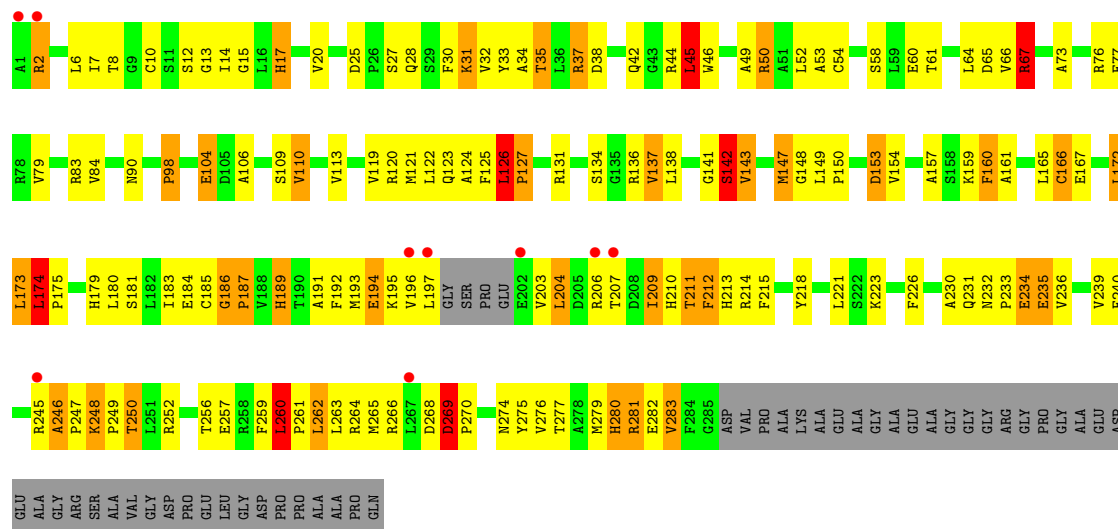
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 17-BETA-HYDROXYSTEROID DEHYDROGENASE



• Molecule 1: 17-BETA-HYDROXYSTEROID DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.80Å 78.78Å 121.19Å 90.00° 92.91° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 10.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 87.7 (10.00-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.33 (at 2.71Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.295 0.212 , 0.277	Depositor DCC
R_{free} test set	2691 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 79.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.011 for h,-k,-l 0.109 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9114	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: NAP, EST, SO4

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	1.02	1/2186 (0.0%)	2.07	79/2963 (2.7%)
1	B	0.94	0/2182	2.05	75/2958 (2.5%)
1	C	1.01	1/2219 (0.0%)	2.20	112/3010 (3.7%)
1	D	1.00	0/2191	2.10	83/2970 (2.8%)
All	All	0.99	2/8778 (0.0%)	2.11	349/11901 (2.9%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	190	THR	C-O	5.11	1.29	1.23
1	A	186	GLY	N-CA	5.11	1.51	1.44

All (349) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	ARG	CD-NE-CZ	11.85	140.99	124.40
1	A	114	ASN	CA-CB-CG	10.42	123.02	112.60
1	B	176	PHE	CA-CB-CG	9.64	123.44	113.80
1	B	160	PHE	CA-CB-CG	9.48	123.28	113.80
1	B	25	ASP	CA-CB-CG	-9.22	103.38	112.60
1	C	50	ARG	N-CA-CB	9.06	123.44	110.12
1	C	114	ASN	CA-CB-CG	9.04	121.64	112.60
1	A	216	TYR	CA-CB-CG	-9.01	97.68	113.90
1	A	37	ARG	NE-CZ-NH1	-8.98	112.52	121.50
1	C	245	ARG	CD-NE-CZ	8.72	136.61	124.40
1	C	204	LEU	CA-C-N	8.59	132.48	120.29
1	C	204	LEU	C-N-CA	8.59	132.48	120.29
1	A	50	ARG	CD-NE-CZ	8.39	136.15	124.40
1	D	212	PHE	CA-CB-CG	-8.31	105.49	113.80
1	C	216	TYR	CB-CA-C	8.25	124.49	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	184	GLU	CB-CG-CD	8.16	126.47	112.60
1	B	239	VAL	N-CA-CB	8.15	121.00	110.57
1	C	37	ARG	NE-CZ-NH1	-8.11	113.39	121.50
1	D	2	ARG	N-CA-C	8.09	123.58	111.04
1	B	119	VAL	CA-C-O	-8.08	112.86	121.27
1	D	143	VAL	CA-C-O	8.04	129.17	120.57
1	D	274	ASN	O-C-N	7.96	130.27	122.07
1	B	232	ASN	CA-CB-CG	-7.89	104.71	112.60
1	C	125	PHE	CA-C-O	-7.78	112.63	120.80
1	D	37	ARG	CD-NE-CZ	-7.73	113.58	124.40
1	B	12	SER	N-CA-C	7.71	118.13	108.19
1	A	134	SER	CA-C-O	7.62	129.92	120.54
1	C	265	MET	CB-CA-C	7.59	123.38	110.79
1	B	250	THR	CA-C-O	-7.56	114.07	122.01
1	C	54	CYS	CA-C-N	7.53	125.08	119.66
1	C	54	CYS	C-N-CA	7.53	125.08	119.66
1	D	147	MET	O-C-N	-7.52	115.06	123.48
1	D	195	LYS	N-CA-C	7.52	119.48	111.28
1	D	260	LEU	CA-C-N	7.50	126.77	118.97
1	D	260	LEU	C-N-CA	7.50	126.77	118.97
1	D	269	ASP	CA-C-N	7.47	127.50	119.28
1	D	269	ASP	C-N-CA	7.47	127.50	119.28
1	C	2	ARG	N-CA-C	7.46	123.06	113.88
1	D	31	LYS	N-CA-C	-7.40	96.46	108.52
1	C	142	SER	O-C-N	7.39	131.91	123.48
1	D	269	ASP	CA-CB-CG	7.39	119.99	112.60
1	C	83	ARG	CD-NE-CZ	7.35	134.69	124.40
1	D	143	VAL	O-C-N	-7.32	114.48	121.87
1	D	153	ASP	CA-CB-CG	7.30	119.90	112.60
1	A	31	LYS	N-CA-C	-7.29	97.86	109.59
1	A	179	HIS	CA-CB-CG	-7.27	106.53	113.80
1	C	206	ARG	CD-NE-CZ	7.27	134.58	124.40
1	C	284	PHE	CA-CB-CG	-7.27	106.53	113.80
1	B	183	ILE	CA-C-O	-7.25	112.34	120.97
1	C	192	PHE	N-CA-C	-7.23	102.44	111.11
1	A	160	PHE	CA-CB-CG	7.22	121.02	113.80
1	C	39	LEU	N-CA-CB	-7.22	98.73	110.14
1	C	281	ARG	CD-NE-CZ	7.18	134.45	124.40
1	C	190	THR	O-C-N	-7.15	114.48	121.85
1	B	237	ALA	CA-C-O	7.13	128.11	120.55
1	D	165	LEU	CA-C-O	7.12	128.10	120.55
1	C	185	CYS	N-CA-C	7.09	121.58	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	PHE	CA-CB-CG	-7.07	106.73	113.80
1	C	16	LEU	N-CA-C	-6.97	103.61	111.07
1	A	153	ASP	CA-CB-CG	6.96	119.56	112.60
1	D	79	VAL	CB-CA-C	-6.90	104.81	112.68
1	B	269	ASP	CA-C-N	6.89	127.18	119.32
1	B	269	ASP	C-N-CA	6.89	127.18	119.32
1	C	142	SER	CA-C-O	-6.88	112.32	120.43
1	A	64	LEU	CA-C-N	-6.83	113.96	122.84
1	A	64	LEU	C-N-CA	-6.83	113.96	122.84
1	B	214	ARG	NE-CZ-NH2	-6.80	113.08	119.20
1	D	166	CYS	CA-C-O	-6.79	113.91	120.90
1	B	132	ARG	CD-NE-CZ	6.75	133.85	124.40
1	D	17	HIS	N-CA-C	6.74	119.48	111.33
1	D	32	VAL	N-CA-C	6.74	117.54	108.11
1	D	30	PHE	CA-CB-CG	-6.73	107.07	113.80
1	C	126	LEU	N-CA-C	6.73	124.69	109.81
1	C	197	LEU	CA-C-N	6.72	130.11	120.56
1	C	197	LEU	C-N-CA	6.72	130.11	120.56
1	D	206	ARG	N-CA-C	6.71	121.76	113.50
1	A	185	CYS	N-CA-C	6.71	120.17	109.24
1	C	269	ASP	CA-CB-CG	6.70	119.30	112.60
1	C	93	LEU	N-CA-CB	-6.66	100.85	111.43
1	B	185	CYS	CB-CA-C	-6.64	96.24	109.33
1	D	131	ARG	CD-NE-CZ	6.64	133.70	124.40
1	C	125	PHE	CB-CA-C	6.61	121.77	110.86
1	A	187	PRO	O-C-N	-6.58	114.54	122.89
1	A	125	PHE	CA-C-N	6.56	130.68	120.97
1	A	125	PHE	C-N-CA	6.56	130.68	120.97
1	A	95	LEU	O-C-N	6.53	130.86	123.42
1	A	95	LEU	CA-C-O	-6.52	112.19	120.14
1	C	96	LEU	N-CA-C	6.51	119.42	108.02
1	C	17	HIS	CA-CB-CG	6.50	120.30	113.80
1	C	93	LEU	CA-C-O	-6.49	114.05	121.58
1	C	50	ARG	CA-C-O	-6.48	113.68	120.55
1	B	17	HIS	N-CA-C	6.41	118.27	111.28
1	A	68	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	185	CYS	CB-CA-C	-6.38	99.22	109.75
1	A	168	SER	CA-C-O	-6.38	114.12	120.82
1	D	173	LEU	N-CA-C	6.37	119.03	111.33
1	D	126	LEU	CA-C-N	6.35	127.78	119.84
1	D	126	LEU	C-N-CA	6.35	127.78	119.84
1	B	143	VAL	O-C-N	-6.35	114.62	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	HIS	CA-CB-CG	-6.31	107.49	113.80
1	B	227	ARG	CA-CB-CG	6.30	126.69	114.10
1	D	110	VAL	CA-C-O	-6.27	114.52	121.17
1	C	138	LEU	CA-C-O	-6.26	113.60	120.36
1	B	125	PHE	N-CA-C	6.25	121.57	113.88
1	C	44	ARG	CA-C-O	-6.24	112.79	119.97
1	C	248	LYS	O-C-N	6.24	126.26	121.27
1	D	31	LYS	CA-C-O	-6.24	113.46	120.32
1	C	119	VAL	CA-C-O	-6.23	114.80	121.27
1	B	213	HIS	O-C-N	-6.21	115.54	122.12
1	C	269	ASP	CA-C-N	6.20	127.59	119.84
1	C	269	ASP	C-N-CA	6.20	127.59	119.84
1	D	280	HIS	CA-C-N	6.20	128.91	120.54
1	D	280	HIS	C-N-CA	6.20	128.91	120.54
1	B	147	MET	O-C-N	-6.20	116.33	123.33
1	B	11	SER	CB-CA-C	-6.19	100.52	110.79
1	B	218	TYR	CA-C-O	6.18	127.49	121.00
1	C	114	ASN	O-C-N	-6.11	115.54	122.08
1	A	93	LEU	O-C-N	6.08	130.53	123.17
1	D	125	PHE	CA-C-O	-6.08	112.24	119.35
1	A	83	ARG	CA-C-N	-6.06	115.03	123.10
1	A	83	ARG	C-N-CA	-6.06	115.03	123.10
1	D	214	ARG	NH1-CZ-NH2	6.04	127.15	119.30
1	C	247	PRO	CA-C-N	-6.01	115.03	122.42
1	C	247	PRO	C-N-CA	-6.01	115.03	122.42
1	B	93	LEU	CA-C-O	-6.01	114.41	121.44
1	B	163	GLU	N-CA-C	-6.00	104.65	111.07
1	D	246	ALA	CA-C-N	6.00	126.43	119.47
1	D	246	ALA	C-N-CA	6.00	126.43	119.47
1	A	65	ASP	CA-C-O	6.00	126.78	120.54
1	D	214	ARG	NE-CZ-NH2	-6.00	113.80	119.20
1	A	205	ASP	CB-CA-C	-5.99	101.48	110.88
1	C	25	ASP	CA-C-N	5.98	125.46	119.24
1	C	25	ASP	C-N-CA	5.98	125.46	119.24
1	B	239	VAL	CA-C-O	-5.98	114.42	121.05
1	A	34	ALA	CA-C-O	-5.98	113.74	120.43
1	C	266	ARG	NE-CZ-NH1	-5.95	115.55	121.50
1	C	67	ARG	NE-CZ-NH2	5.95	124.55	119.20
1	C	96	LEU	N-CA-CB	-5.94	101.27	110.65
1	D	160	PHE	CA-CB-CG	5.93	119.73	113.80
1	B	143	VAL	CA-C-O	5.91	126.85	120.47
1	B	223	LYS	CA-C-O	-5.91	114.58	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	GLY	CA-C-N	5.90	132.97	121.41
1	A	144	GLY	C-N-CA	5.90	132.97	121.41
1	A	138	LEU	O-C-N	5.89	130.89	123.23
1	D	248	LYS	CA-C-N	5.89	125.65	119.76
1	D	248	LYS	C-N-CA	5.89	125.65	119.76
1	B	247	PRO	N-CA-C	-5.89	105.51	113.40
1	B	140	THR	CA-C-O	5.88	127.62	120.62
1	C	17	HIS	O-C-N	-5.88	115.89	122.12
1	A	93	LEU	CA-C-O	-5.87	114.76	121.40
1	B	61	THR	CA-C-O	-5.87	114.36	120.70
1	D	214	ARG	CD-NE-CZ	-5.87	116.19	124.40
1	A	5	VAL	CA-C-O	-5.87	114.03	120.84
1	D	172	LEU	CA-C-N	5.86	128.41	120.38
1	D	172	LEU	C-N-CA	5.86	128.41	120.38
1	D	185	CYS	CB-CA-C	-5.85	100.14	109.80
1	B	253	TYR	CA-C-O	-5.84	114.05	120.36
1	C	93	LEU	CB-CA-C	-5.84	98.74	110.30
1	D	266	ARG	O-C-N	5.83	128.30	122.12
1	B	189	HIS	CA-CB-CG	-5.83	107.97	113.80
1	C	63	GLN	OE1-CD-NE2	5.82	128.42	122.60
1	B	172	LEU	CA-C-N	5.82	129.92	120.60
1	B	172	LEU	C-N-CA	5.82	129.92	120.60
1	D	45	LEU	O-C-N	5.82	128.15	122.09
1	A	96	LEU	N-CA-CB	-5.81	100.74	110.80
1	C	177	GLY	N-CA-C	-5.80	106.73	115.32
1	D	50	ARG	CD-NE-CZ	-5.80	116.28	124.40
1	A	191	ALA	CA-C-O	5.79	126.04	119.27
1	C	39	LEU	CA-C-O	5.75	126.64	120.20
1	C	153	ASP	CA-CB-CG	5.75	118.35	112.60
1	D	280	HIS	N-CA-C	-5.74	104.92	111.07
1	B	144	GLY	CA-C-N	5.74	132.65	121.41
1	B	144	GLY	C-N-CA	5.74	132.65	121.41
1	C	32	VAL	N-CA-C	5.73	116.19	108.17
1	C	179	HIS	N-CA-C	5.73	117.85	108.52
1	B	56	PRO	N-CA-CB	5.72	108.26	103.17
1	A	248	LYS	O-C-N	5.72	126.52	121.32
1	A	31	LYS	CA-C-O	-5.71	114.66	120.71
1	C	73	ALA	CA-C-O	-5.70	115.02	121.00
1	B	185	CYS	N-CA-C	5.69	118.83	109.72
1	B	22	LEU	CA-C-O	-5.69	114.84	120.70
1	A	144	GLY	N-CA-C	-5.68	108.26	115.31
1	A	280	HIS	CA-CB-CG	-5.68	108.12	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	MET	CA-C-O	5.67	126.56	120.55
1	C	95	LEU	CA-C-N	5.66	131.34	123.07
1	C	95	LEU	C-N-CA	5.66	131.34	123.07
1	C	118	THR	CA-C-N	-5.65	113.31	120.60
1	C	118	THR	C-N-CA	-5.65	113.31	120.60
1	C	56	PRO	N-CA-CB	5.65	108.28	103.19
1	C	67	ARG	CD-NE-CZ	-5.64	116.50	124.40
1	B	85	ASP	N-CA-C	-5.64	105.18	112.68
1	D	148	GLY	CA-C-O	-5.62	116.52	121.58
1	B	14	ILE	N-CA-C	5.62	115.81	110.42
1	B	128	ASP	O-C-N	-5.62	115.65	122.22
1	B	93	LEU	CB-CA-C	-5.61	98.30	109.79
1	B	256	THR	CA-C-O	-5.60	115.24	121.23
1	D	25	ASP	CA-CB-CG	-5.60	107.00	112.60
1	A	55	PRO	N-CA-CB	5.58	108.49	103.08
1	A	150	PRO	N-CA-CB	5.57	109.10	103.25
1	C	47	GLU	CA-C-N	5.57	127.74	120.28
1	C	47	GLU	C-N-CA	5.57	127.74	120.28
1	C	114	ASN	CA-C-O	5.57	127.19	121.07
1	B	238	GLU	CB-CG-CD	5.56	122.05	112.60
1	D	137	VAL	N-CA-C	-5.56	99.14	107.37
1	D	84	VAL	N-CA-CB	5.55	118.86	111.64
1	B	230	ALA	CA-C-O	-5.55	115.66	120.88
1	B	32	VAL	N-CA-C	5.55	115.85	107.80
1	B	184	GLU	CA-C-N	5.55	131.52	122.81
1	B	184	GLU	C-N-CA	5.55	131.52	122.81
1	B	235	GLU	CA-C-O	5.55	126.30	120.42
1	D	211	THR	N-CA-C	-5.54	105.24	111.28
1	D	274	ASN	CB-CA-C	-5.53	102.19	110.88
1	B	120	ARG	N-CA-C	5.53	117.31	111.28
1	D	98	PRO	N-CA-C	-5.53	102.52	111.03
1	C	225	VAL	CB-CA-C	-5.53	104.68	112.14
1	D	259	PHE	CA-CB-CG	5.53	119.33	113.80
1	C	278	ALA	CA-C-O	5.52	126.80	121.00
1	B	25	ASP	CA-C-O	5.51	124.93	119.75
1	D	213	HIS	O-C-N	-5.50	116.29	122.12
1	D	186	GLY	N-CA-C	-5.49	101.15	112.34
1	A	37	ARG	NH1-CZ-NH2	5.48	126.43	119.30
1	C	54	CYS	N-CA-C	-5.48	101.44	109.50
1	D	160	PHE	N-CA-C	-5.48	105.22	111.14
1	C	188	VAL	CB-CA-C	-5.48	102.06	110.50
1	D	119	VAL	N-CA-C	-5.48	104.99	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	THR	CA-CB-OG1	-5.47	101.39	109.60
1	D	90	ASN	CA-C-O	-5.47	113.12	118.97
1	A	105	ASP	N-CA-CB	5.46	119.30	110.40
1	A	96	LEU	CA-C-O	-5.45	114.27	120.32
1	C	252	ARG	N-CA-C	5.45	118.28	109.40
1	A	284	PHE	CA-CB-CG	5.44	119.24	113.80
1	C	136	ARG	O-C-N	5.44	129.67	123.31
1	A	120	ARG	CA-C-N	5.43	128.02	120.63
1	A	120	ARG	C-N-CA	5.43	128.02	120.63
1	C	264	ARG	CA-C-O	5.43	126.71	120.90
1	D	189	HIS	CA-C-N	5.43	130.26	122.23
1	D	189	HIS	C-N-CA	5.43	130.26	122.23
1	D	150	PRO	N-CA-CB	5.42	107.88	103.32
1	B	252	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	D	37	ARG	NH1-CZ-NH2	5.41	126.34	119.30
1	C	11	SER	O-C-N	5.40	130.08	122.41
1	A	265	MET	CA-C-N	5.40	127.95	120.29
1	A	265	MET	C-N-CA	5.40	127.95	120.29
1	B	131	ARG	CD-NE-CZ	5.39	131.95	124.40
1	B	252	ARG	CA-C-O	5.39	126.30	120.32
1	C	215	PHE	CA-CB-CG	-5.39	108.41	113.80
1	C	68	ASP	CA-C-N	5.37	127.74	120.38
1	C	68	ASP	C-N-CA	5.37	127.74	120.38
1	B	5	VAL	CA-C-O	-5.36	114.59	121.40
1	A	126	LEU	CA-C-N	5.36	126.53	119.84
1	A	126	LEU	C-N-CA	5.36	126.53	119.84
1	B	260	LEU	CA-C-N	5.35	124.80	119.24
1	B	260	LEU	C-N-CA	5.35	124.80	119.24
1	C	236	VAL	CB-CA-C	-5.35	105.03	112.04
1	D	67	ARG	NE-CZ-NH1	5.34	126.84	121.50
1	A	14	ILE	O-C-N	-5.33	116.70	121.87
1	D	223	LYS	CA-C-O	-5.33	115.20	120.90
1	C	90	ASN	N-CA-CB	-5.32	103.82	110.90
1	B	31	LYS	N-CA-C	-5.32	99.86	108.52
1	A	52	LEU	N-CA-C	-5.31	106.03	112.88
1	D	235	GLU	CA-C-O	5.31	126.14	120.24
1	B	191	ALA	CA-C-N	5.30	129.62	121.19
1	B	191	ALA	C-N-CA	5.30	129.62	121.19
1	A	112	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	261	PRO	N-CA-C	-5.30	106.30	113.40
1	D	187	PRO	CA-C-O	5.30	127.34	121.36
1	A	180	LEU	CA-C-O	-5.29	114.64	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	ALA	N-CA-CB	5.29	117.90	110.12
1	A	91	ALA	CA-C-N	5.29	128.81	121.09
1	A	91	ALA	C-N-CA	5.29	128.81	121.09
1	A	160	PHE	N-CA-C	-5.29	106.09	112.54
1	D	121	MET	N-CA-C	-5.28	105.42	111.07
1	D	113	VAL	N-CA-C	5.27	116.75	111.00
1	C	157	ALA	N-CA-C	-5.27	105.61	111.36
1	C	163	GLU	CA-C-N	5.27	125.80	120.00
1	C	163	GLU	C-N-CA	5.27	125.80	120.00
1	B	184	GLU	CB-CG-CD	5.27	121.55	112.60
1	D	124	ALA	CA-C-O	5.27	126.13	120.55
1	A	235	GLU	N-CA-C	-5.25	105.47	111.14
1	A	85	ASP	CB-CA-C	5.24	120.01	110.11
1	D	194	GLU	CA-C-N	5.24	127.30	120.28
1	D	194	GLU	C-N-CA	5.24	127.30	120.28
1	B	207	THR	CA-C-O	-5.24	115.33	121.46
1	A	25	ASP	CA-C-N	5.23	124.68	119.24
1	A	25	ASP	C-N-CA	5.23	124.68	119.24
1	C	138	LEU	O-C-N	5.22	129.51	123.30
1	D	194	GLU	N-CA-C	-5.22	104.84	111.11
1	D	245	ARG	N-CA-C	-5.22	105.65	112.23
1	B	57	GLY	N-CA-C	-5.22	108.14	114.92
1	C	156	CYS	CA-C-N	-5.21	112.89	120.29
1	C	156	CYS	C-N-CA	-5.21	112.89	120.29
1	C	228	GLU	CA-C-O	-5.21	113.12	119.43
1	C	100	GLU	CA-C-N	5.21	131.42	122.09
1	C	100	GLU	C-N-CA	5.21	131.42	122.09
1	B	153	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	269	ASP	CA-C-N	5.20	124.38	118.97
1	A	269	ASP	C-N-CA	5.20	124.38	118.97
1	A	65	ASP	CB-CA-C	5.19	119.09	110.78
1	A	148	GLY	N-CA-C	5.19	120.28	111.15
1	C	275	TYR	CB-CA-C	-5.18	102.14	110.74
1	C	179	HIS	CA-CB-CG	-5.18	108.62	113.80
1	B	67	ARG	CD-NE-CZ	5.17	131.65	124.40
1	C	107	VAL	CB-CA-C	-5.17	105.16	112.14
1	D	142	SER	CA-C-O	-5.16	114.19	120.54
1	D	58	SER	N-CA-C	-5.16	106.94	113.18
1	D	79	VAL	N-CA-CB	-5.16	107.06	112.06
1	C	271	SER	CA-C-N	5.15	131.51	121.41
1	C	271	SER	C-N-CA	5.15	131.51	121.41
1	B	60	GLU	CA-C-O	-5.14	114.22	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	TYR	N-CA-C	-5.14	105.57	111.07
1	A	81	GLU	CA-CB-CG	5.14	124.38	114.10
1	C	160	PHE	N-CA-C	-5.14	105.76	111.36
1	B	167	GLU	CB-CG-CD	-5.13	103.87	112.60
1	C	13	GLY	N-CA-C	5.13	120.61	111.73
1	B	125	PHE	CA-C-O	-5.13	113.44	119.24
1	C	126	LEU	CA-C-N	5.13	126.25	119.84
1	C	126	LEU	C-N-CA	5.13	126.25	119.84
1	C	186	GLY	N-CA-C	-5.13	101.87	112.34
1	A	253	TYR	CA-C-O	-5.13	114.81	120.24
1	A	30	PHE	N-CA-C	5.12	118.41	110.17
1	B	17	HIS	O-C-N	-5.12	116.69	122.12
1	C	238	GLU	CB-CA-C	5.12	120.68	109.99
1	A	173	LEU	CA-C-O	-5.11	114.33	120.10
1	A	54	CYS	CA-C-N	5.10	125.64	120.38
1	A	54	CYS	C-N-CA	5.10	125.64	120.38
1	C	125	PHE	O-C-N	-5.10	116.19	122.11
1	C	55	PRO	O-C-N	5.10	123.55	121.15
1	A	260	LEU	CB-CA-C	5.10	120.21	110.17
1	B	22	LEU	O-C-N	5.09	127.59	122.09
1	C	74	ALA	CA-C-O	-5.08	115.48	121.07
1	A	156	CYS	O-C-N	-5.07	116.75	122.12
1	C	107	VAL	CA-C-N	-5.07	113.73	120.63
1	C	107	VAL	C-N-CA	-5.07	113.73	120.63
1	C	206	ARG	N-CA-C	5.07	119.44	113.16
1	C	263	LEU	N-CA-C	-5.05	105.42	111.03
1	A	167	GLU	CA-C-O	5.05	125.85	120.24
1	C	64	LEU	CA-C-N	-5.05	115.70	122.42
1	C	64	LEU	C-N-CA	-5.05	115.70	122.42
1	B	225	VAL	N-CA-C	5.05	115.82	110.72
1	A	175	PRO	O-C-N	-5.04	115.83	122.64
1	C	73	ALA	N-CA-C	-5.03	105.48	110.97
1	A	33	TYR	CA-C-O	-5.02	115.41	120.84
1	C	55	PRO	CA-C-N	5.02	125.30	119.93
1	C	55	PRO	C-N-CA	5.02	125.30	119.93
1	D	17	HIS	CA-CB-CG	-5.01	108.78	113.80
1	A	155	TYR	N-CA-CB	5.01	117.28	110.01
1	D	179	HIS	N-CA-C	5.01	117.06	108.90
1	D	12	SER	CA-C-N	5.00	131.21	121.41
1	D	12	SER	C-N-CA	5.00	131.21	121.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2148	0	2200	139	0
1	B	2144	0	2197	123	0
1	C	2179	0	2225	144	0
1	D	2153	0	2203	127	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	2	0
2	D	5	0	0	2	0
3	A	20	0	24	10	0
3	B	20	0	24	7	0
3	C	20	0	23	3	0
3	D	20	0	23	6	0
4	A	48	0	25	6	0
4	B	48	0	25	6	0
4	C	48	0	25	5	0
4	D	48	0	25	5	0
5	A	51	0	0	9	0
5	B	53	0	0	3	0
5	C	48	0	0	2	0
5	D	46	0	0	3	0
All	All	9114	0	9019	520	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 30.

All (520) 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:C:193:MET:HA	1:C:196:VAL:HG23	1.38	1.01
1:D:174:LEU:HB3	1:D:175:PRO:HD3	1.41	0.99
1:D:174:LEU:HB3	1:D:175:PRO:CD	1.95	0.97
1:C:100:GLU:HA	1:D:123:GLN:HG2	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HA	1:A:267:LEU:HD12	1.51	0.93
1:A:232:ASN:HB2	1:A:235:GLU:HG3	1.54	0.87
1:A:262:LEU:HD12	1:A:265:MET:HG2	1.57	0.86
1:B:232:ASN:HB2	1:B:235:GLU:HG3	1.59	0.85
1:A:260:LEU:N	1:A:261:PRO:HD2	1.94	0.82
1:C:35:THR:HG22	1:C:62:LEU:HB2	1.61	0.82
1:A:100:GLU:HA	1:B:123:GLN:HG2	1.61	0.82
1:D:166:CYS:HB3	1:D:180:LEU:HD21	1.62	0.81
1:C:260:LEU:N	1:C:261:PRO:HD2	1.96	0.80
1:C:76:ARG:HG3	1:C:125:PHE:CE2	2.18	0.79
1:D:35:THR:HG23	1:D:64:LEU:HB3	1.64	0.78
1:A:203:VAL:O	1:A:207:THR:HG22	1.83	0.78
1:C:190:THR:O	1:C:191:ALA:HB3	1.84	0.77
1:C:44:ARG:NH2	2:C:403:SO4:O2	2.18	0.77
1:D:193:MET:SD	1:D:196:VAL:HG21	2.25	0.76
1:B:31:LYS:NZ	1:B:60:GLU:HG3	2.00	0.76
1:C:219:LEU:O	1:C:223:LYS:HG3	1.85	0.76
1:C:174:LEU:HB3	1:C:175:PRO:HD3	1.65	0.75
1:B:34:ALA:HB3	1:B:61:THR:HG22	1.66	0.75
1:B:138:LEU:HD22	1:B:181:SER:HB2	1.70	0.74
1:C:64:LEU:HD21	1:C:72:VAL:HG22	1.70	0.74
1:D:142:SER:HB2	4:D:362:NAP:H6N	1.69	0.73
1:B:142:SER:HB2	4:B:364:NAP:H6N	1.70	0.73
1:A:107:VAL:HG13	1:A:154:VAL:HG11	1.69	0.73
1:B:165:LEU:O	1:B:169:LEU:HD12	1.88	0.73
1:C:189:HIS:CE1	1:C:230:ALA:HB3	2.24	0.73
1:A:111:LEU:HD23	1:A:158:SER:HB3	1.70	0.72
1:B:174:LEU:HB3	1:B:175:PRO:CD	2.19	0.72
1:C:193:MET:HA	1:C:196:VAL:CG2	2.17	0.72
1:A:42:GLN:NE2	1:A:46:TRP:HE1	1.88	0.72
1:C:13:GLY:HA2	1:C:190:THR:HG22	1.70	0.72
1:D:7:ILE:O	1:D:35:THR:HB	1.89	0.72
1:C:5:VAL:HG22	1:C:86:VAL:HB	1.70	0.72
1:D:203:VAL:O	1:D:207:THR:HG22	1.89	0.71
1:A:119:VAL:O	1:A:123:GLN:HG3	1.91	0.71
1:C:45:LEU:HD11	1:C:59:LEU:HD21	1.73	0.71
1:A:45:LEU:HD11	1:A:59:LEU:HD21	1.70	0.71
1:D:143:VAL:HB	3:D:352:EST:H121	1.71	0.70
1:B:96:LEU:HD23	1:B:196:VAL:CG1	2.22	0.70
1:D:260:LEU:N	1:D:261:PRO:HD2	2.07	0.70
1:A:8:THR:O	1:A:90:ASN:HB3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:VAL:O	1:C:197:LEU:HB2	1.91	0.70
1:A:266:ARG:HH21	1:B:167:GLU:CD	2.00	0.70
1:B:128:ASP:O	1:B:132:ARG:HG2	1.92	0.69
1:C:219:LEU:HD22	1:C:223:LYS:HE2	1.74	0.69
1:D:65:ASP:OD2	1:D:67:ARG:NH1	2.24	0.69
1:B:65:ASP:OD1	1:B:67:ARG:HG2	1.93	0.69
1:C:174:LEU:HB3	1:C:175:PRO:CD	2.23	0.69
1:B:20:VAL:HG23	1:B:52:LEU:HD22	1.73	0.69
1:A:43:GLY:O	1:A:47:GLU:HG3	1.93	0.68
1:A:42:GLN:HE21	1:A:46:TRP:HE1	1.40	0.68
1:C:78:ARG:NH1	1:C:78:ARG:HB3	2.09	0.68
1:D:42:GLN:NE2	1:D:46:TRP:HE1	1.92	0.67
1:B:174:LEU:HB3	1:B:175:PRO:HD3	1.75	0.67
1:C:199:SER:OG	1:C:202:GLU:HB2	1.94	0.67
1:C:187:PRO:HD3	3:C:353:EST:H122	1.76	0.67
1:B:221:LEU:HD22	1:B:225:VAL:HG23	1.75	0.67
1:B:149:LEU:HD11	3:B:354:EST:H121	1.76	0.67
1:D:142:SER:HB2	4:D:362:NAP:C6N	2.25	0.67
1:D:13:GLY:O	1:D:17:HIS:HD2	1.78	0.66
1:A:240:PHE:O	1:A:244:LEU:HD23	1.95	0.66
1:D:143:VAL:HB	3:D:352:EST:C12	2.25	0.66
1:C:266:ARG:NH2	1:D:167:GLU:OE2	2.23	0.65
1:A:150:PRO:HD3	1:B:171:VAL:HG11	1.78	0.65
1:D:50:ARG:NH1	5:D:594:HOH:O	2.29	0.65
1:C:190:THR:O	1:C:191:ALA:CB	2.43	0.65
1:C:239:VAL:HG21	1:C:255:THR:HG22	1.78	0.65
1:A:260:LEU:N	1:A:261:PRO:CD	2.60	0.64
1:C:116:VAL:HG12	1:C:120:ARG:NH1	2.12	0.64
1:B:27:SER:O	1:B:28:GLN:HB2	1.97	0.64
1:B:191:ALA:O	1:B:194:GLU:HG2	1.96	0.64
1:C:42:GLN:NE2	1:C:46:TRP:HE1	1.95	0.64
1:C:260:LEU:HA	1:C:263:LEU:HB2	1.80	0.64
1:C:119:VAL:O	1:C:123:GLN:HG2	1.98	0.63
1:A:142:SER:HB2	4:A:361:NAP:H6N	1.80	0.63
1:C:240:PHE:O	1:C:244:LEU:HD23	1.98	0.63
1:D:260:LEU:HB3	1:D:264:ARG:NH2	2.13	0.63
1:A:174:LEU:C	1:A:174:LEU:HD12	2.25	0.62
1:A:31:LYS:HE2	1:A:33:TYR:CE1	2.35	0.62
1:B:174:LEU:N	1:B:175:PRO:HD2	2.15	0.62
1:D:66:VAL:HG22	4:D:362:NAP:N1A	2.14	0.61
1:A:262:LEU:CD1	1:A:265:MET:HG2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:HIS:CE1	1:A:230:ALA:HB3	2.35	0.61
1:B:187:PRO:HB3	1:B:226:PHE:CD2	2.35	0.60
1:C:221:LEU:HD13	1:C:221:LEU:C	2.26	0.60
1:B:31:LYS:HZ1	1:B:60:GLU:HG3	1.65	0.60
1:C:81:GLU:CD	1:C:81:GLU:H	2.10	0.59
1:A:244:LEU:HA	5:A:556:HOH:O	2.02	0.59
1:D:189:HIS:CE1	1:D:230:ALA:HB3	2.37	0.59
1:C:42:GLN:HE21	1:C:46:TRP:HE1	1.50	0.59
1:C:260:LEU:N	1:C:261:PRO:CD	2.65	0.59
1:C:191:ALA:O	1:C:195:LYS:HG3	2.03	0.59
1:A:175:PRO:HG3	1:B:280:HIS:CE1	2.38	0.58
1:A:232:ASN:HB3	1:A:234:GLU:OE1	2.03	0.58
1:A:266:ARG:NH2	1:B:167:GLU:OE2	2.35	0.58
1:C:222:SER:HB3	3:C:353:EST:H61	1.84	0.58
1:C:202:GLU:HB3	1:C:206:ARG:HH21	1.68	0.58
1:C:116:VAL:HG12	1:C:120:ARG:CZ	2.33	0.58
1:C:232:ASN:HB3	1:C:234:GLU:HG2	1.84	0.58
1:D:279:MET:O	1:D:283:VAL:HG23	2.04	0.58
1:A:83:ARG:HG2	1:A:83:ARG:HH11	1.68	0.58
1:B:141:GLY:HA3	1:B:184:GLU:HA	1.86	0.58
1:C:257:GLU:HA	1:C:260:LEU:HD13	1.86	0.58
1:B:13:GLY:HA3	4:B:364:NAP:O2N	2.03	0.58
1:D:83:ARG:HG2	1:D:83:ARG:HH11	1.69	0.58
1:D:38:ASP:OD1	1:D:38:ASP:C	2.46	0.58
1:B:131:ARG:HH12	1:B:132:ARG:NH2	2.02	0.57
1:A:82:GLY:O	1:A:83:ARG:HB3	2.03	0.57
1:C:137:VAL:O	1:C:180:LEU:HA	2.05	0.57
1:D:149:LEU:CD1	3:D:352:EST:H182	2.35	0.57
1:B:65:ASP:OD2	1:B:67:ARG:NH1	2.38	0.57
1:D:207:THR:OG1	1:D:211:THR:HB	2.05	0.56
1:B:172:LEU:HD12	1:B:172:LEU:O	2.05	0.56
1:C:35:THR:HA	1:C:62:LEU:O	2.05	0.56
1:B:233:PRO:HD2	1:B:234:GLU:OE2	2.06	0.56
1:C:188:VAL:HG21	1:C:236:VAL:HG21	1.86	0.56
1:D:73:ALA:O	1:D:77:GLU:HG2	2.05	0.56
1:D:98:PRO:HG2	1:D:203:VAL:HG13	1.87	0.56
1:C:96:LEU:HB2	1:C:196:VAL:HG12	1.87	0.56
1:D:173:LEU:O	1:D:174:LEU:C	2.48	0.56
1:C:45:LEU:HD13	1:C:45:LEU:C	2.30	0.56
1:D:27:SER:O	1:D:28:GLN:HB2	2.04	0.56
1:D:257:GLU:HG2	1:D:260:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD11	5:A:696:HOH:O	2.04	0.56
1:C:13:GLY:O	1:C:17:HIS:HD2	1.89	0.56
1:D:8:THR:HA	1:D:35:THR:CG2	2.36	0.56
1:D:154:VAL:N	5:D:603:HOH:O	2.38	0.56
1:A:65:ASP:CG	1:A:67:ARG:HH21	2.14	0.56
1:B:13:GLY:O	1:B:17:HIS:HD2	1.87	0.56
1:C:160:PHE:HB3	1:D:160:PHE:HB3	1.86	0.56
1:D:8:THR:HA	1:D:35:THR:HG22	1.88	0.56
1:D:203:VAL:HG21	1:D:215:PHE:HE2	1.72	0.55
1:A:9:GLY:O	1:A:15:GLY:HA3	2.06	0.55
1:A:8:THR:HA	1:A:35:THR:OG1	2.06	0.55
1:D:31:LYS:NZ	1:D:60:GLU:HG3	2.21	0.55
1:D:34:ALA:HB3	1:D:61:THR:HG22	1.88	0.55
1:B:52:LEU:O	1:B:53:ALA:HB3	2.05	0.55
1:D:65:ASP:OD1	1:D:67:ARG:HG2	2.06	0.55
1:A:31:LYS:HE2	1:A:33:TYR:CZ	2.42	0.54
1:A:187:PRO:HG3	3:A:351:EST:H9	1.88	0.54
1:B:96:LEU:HD23	1:B:196:VAL:HG11	1.89	0.54
1:B:136:ARG:NH1	1:B:249:PRO:HG3	2.22	0.54
1:D:232:ASN:HB2	1:D:235:GLU:HG3	1.89	0.54
1:B:31:LYS:HZ2	1:B:60:GLU:HG3	1.71	0.54
1:D:233:PRO:HD2	1:D:234:GLU:OE2	2.06	0.54
1:A:26:PRO:O	1:A:27:SER:C	2.49	0.54
1:B:166:CYS:HB3	1:B:180:LEU:HD21	1.87	0.54
1:B:224:GLN:O	1:B:228:GLU:HG3	2.06	0.54
1:C:42:GLN:HE21	1:C:61:THR:HG21	1.72	0.54
1:B:104:GLU:HG3	5:B:679:HOH:O	2.06	0.54
1:B:187:PRO:HB3	1:B:226:PHE:CE2	2.43	0.54
1:A:90:ASN:O	1:A:91:ALA:C	2.51	0.54
1:A:231:GLN:NE2	5:A:571:HOH:O	2.28	0.54
1:B:138:LEU:CD2	1:B:181:SER:HB2	2.37	0.54
1:B:263:LEU:O	1:B:266:ARG:HB3	2.07	0.54
1:A:13:GLY:HA2	1:A:190:THR:HG22	1.90	0.54
1:B:1:ALA:HB1	1:B:2:ARG:NH2	2.23	0.53
1:C:14:ILE:HG12	1:C:236:VAL:HG11	1.91	0.53
1:C:96:LEU:HB2	1:C:196:VAL:CG1	2.39	0.53
1:C:221:LEU:O	1:C:225:VAL:HG23	2.09	0.53
1:C:245:ARG:O	1:C:246:ALA:C	2.51	0.53
1:C:114:ASN:O	1:C:162:LEU:HD21	2.08	0.53
1:D:193:MET:HA	1:D:196:VAL:HG23	1.91	0.53
1:C:119:VAL:HG22	1:C:165:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:PRO:HB3	1:D:226:PHE:CE1	2.43	0.53
1:C:196:VAL:O	1:C:197:LEU:CB	2.57	0.53
1:D:122:LEU:O	1:D:126:LEU:HB2	2.09	0.53
1:C:216:TYR:CD1	1:C:219:LEU:HD12	2.43	0.53
1:D:212:PHE:O	1:D:215:PHE:HB3	2.09	0.53
1:A:64:LEU:HD21	1:A:72:VAL:HG22	1.91	0.52
1:A:163:GLU:OE2	1:A:184:GLU:OE2	2.27	0.52
1:C:281:ARG:NH1	1:C:282:GLU:OE2	2.42	0.52
1:D:10:CYS:HA	1:D:15:GLY:HA3	1.90	0.52
1:B:89:CYS:HB3	1:B:118:THR:HG23	1.91	0.52
1:D:76:ARG:NH1	1:D:76:ARG:HG2	2.25	0.52
1:D:204:LEU:HD23	1:D:212:PHE:CE1	2.44	0.52
1:D:187:PRO:HB3	1:D:226:PHE:CD1	2.44	0.52
1:C:136:ARG:NH2	1:C:246:ALA:O	2.40	0.52
1:B:37:ARG:HH21	4:B:364:NAP:P2B	2.33	0.52
1:D:154:VAL:O	1:D:157:ALA:HB3	2.10	0.52
1:D:174:LEU:CB	1:D:175:PRO:CD	2.72	0.52
1:C:142:SER:HB2	4:C:363:NAP:H6N	1.90	0.52
1:B:37:ARG:NH2	4:B:364:NAP:O2X	2.43	0.52
1:B:221:LEU:HD22	1:B:225:VAL:CG2	2.37	0.52
1:D:143:VAL:CB	3:D:352:EST:H121	2.40	0.52
1:A:11:SER:O	1:A:12:SER:HB3	2.10	0.52
1:D:141:GLY:N	1:D:183:ILE:O	2.42	0.52
1:C:39:LEU:HB2	5:C:591:HOH:O	2.10	0.51
1:C:44:ARG:NH2	2:C:403:SO4:S	2.83	0.51
1:B:128:ASP:OD2	1:B:131:ARG:NH1	2.43	0.51
1:C:96:LEU:CB	1:C:196:VAL:HG12	2.40	0.51
1:D:236:VAL:HG12	1:D:240:PHE:HE1	1.75	0.51
1:D:34:ALA:CB	1:D:45:LEU:HD11	2.41	0.51
1:D:262:LEU:O	1:D:265:MET:HB3	2.11	0.51
1:C:11:SER:CB	1:C:36:LEU:HD23	2.40	0.51
1:D:231:GLN:NE2	5:D:541:HOH:O	2.43	0.51
1:D:204:LEU:HD23	1:D:212:PHE:CZ	2.46	0.51
1:C:184:GLU:OE1	1:C:184:GLU:HA	2.10	0.51
1:C:183:ILE:HG13	1:C:240:PHE:CD2	2.46	0.51
5:C:569:HOH:O	1:D:104:GLU:HG3	2.10	0.51
1:C:271:SER:HB2	1:D:250:THR:CG2	2.41	0.50
1:D:126:LEU:N	1:D:127:PRO:HD2	2.27	0.50
1:A:257:GLU:HA	1:A:260:LEU:HD13	1.93	0.50
1:B:189:HIS:O	1:B:233:PRO:HG3	2.11	0.50
1:A:174:LEU:CB	1:A:175:PRO:CD	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:HIS:O	1:B:21:ARG:HB2	2.11	0.50
1:D:73:ALA:O	1:D:76:ARG:HB3	2.11	0.50
1:A:149:LEU:HD23	1:A:279:MET:HE3	1.93	0.50
1:A:264:ARG:CA	1:A:267:LEU:HD12	2.34	0.50
1:B:221:LEU:O	1:B:225:VAL:HG23	2.11	0.50
1:C:16:LEU:O	1:C:19:ALA:HB3	2.12	0.50
1:C:225:VAL:O	1:C:229:ALA:HB3	2.11	0.50
1:B:21:ARG:HD2	1:B:21:ARG:O	2.11	0.50
1:B:279:MET:HG3	1:B:279:MET:O	2.12	0.50
1:B:232:ASN:CB	1:B:235:GLU:HG3	2.38	0.50
1:B:260:LEU:N	1:B:261:PRO:HD2	2.27	0.50
1:C:2:ARG:HH21	1:C:83:ARG:NH2	2.10	0.50
1:D:126:LEU:N	1:D:127:PRO:CD	2.74	0.50
1:C:140:THR:HG21	4:C:363:NAP:O4D	2.11	0.50
1:D:203:VAL:HG11	1:D:215:PHE:CD2	2.47	0.50
1:A:136:ARG:HD3	5:A:556:HOH:O	2.11	0.49
1:D:147:MET:HE3	1:D:279:MET:HE3	1.94	0.49
1:C:2:ARG:HH21	1:C:83:ARG:HH22	1.59	0.49
1:A:241:LEU:N	1:A:241:LEU:HD12	2.27	0.49
1:B:38:ASP:OD1	1:B:40:LYS:HG2	2.12	0.49
1:A:33:TYR:HD2	1:A:62:LEU:HD11	1.77	0.49
1:C:239:VAL:O	1:C:240:PHE:C	2.54	0.49
1:C:122:LEU:O	1:C:123:GLN:C	2.55	0.49
1:B:10:CYS:HA	1:B:15:GLY:HA3	1.94	0.49
1:D:137:VAL:O	1:D:180:LEU:HA	2.13	0.49
1:D:65:ASP:CG	1:D:67:ARG:HH11	2.20	0.49
1:D:66:VAL:HG22	4:D:362:NAP:C6A	2.43	0.49
1:A:4:VAL:HG21	1:A:81:GLU:HG2	1.94	0.49
1:C:202:GLU:HB3	1:C:206:ARG:HE	1.77	0.49
1:B:21:ARG:HD2	1:B:21:ARG:C	2.38	0.49
1:C:203:VAL:O	1:C:207:THR:HG22	2.13	0.49
1:A:37:ARG:HG3	4:A:361:NAP:N1A	2.28	0.49
3:A:351:EST:H17	4:A:361:NAP:C4N	2.43	0.49
3:A:351:EST:H17	4:A:361:NAP:H4N	1.94	0.49
1:B:231:GLN:HG3	5:B:649:HOH:O	2.12	0.49
1:B:143:VAL:CG1	3:B:354:EST:H122	2.44	0.48
1:C:37:ARG:NH1	4:C:363:NAP:O3X	2.46	0.48
1:B:126:LEU:N	1:B:127:PRO:HD2	2.28	0.48
1:C:37:ARG:HG3	4:C:363:NAP:N1A	2.28	0.48
1:C:148:GLY:HA3	1:D:167:GLU:HB3	1.95	0.48
1:D:239:VAL:O	1:D:240:PHE:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:HG13	1:A:86:VAL:HG12	1.94	0.48
1:C:75:ALA:O	1:C:76:ARG:C	2.54	0.48
1:C:147:MET:HE3	1:C:149:LEU:HD21	1.94	0.48
1:C:38:ASP:OD1	1:C:40:LYS:HB2	2.13	0.48
1:C:149:LEU:HD23	1:C:279:MET:HE2	1.95	0.48
1:A:37:ARG:NH1	4:A:361:NAP:O3X	2.46	0.48
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.78	0.48
1:A:45:LEU:CD1	1:A:59:LEU:HD21	2.40	0.48
1:A:281:ARG:HA	1:A:285:GLY:O	2.14	0.48
1:B:1:ALA:O	1:B:2:ARG:HB2	2.14	0.48
1:B:173:LEU:O	1:B:174:LEU:C	2.57	0.48
1:C:200:PRO:O	1:C:204:LEU:HB2	2.13	0.48
1:B:195:LYS:NZ	4:B:364:NAP:O1A	2.40	0.48
1:B:275:TYR:O	1:B:276:VAL:C	2.55	0.48
1:C:31:LYS:HD3	1:C:81:GLU:OE2	2.14	0.48
1:C:174:LEU:CB	1:C:175:PRO:CD	2.87	0.48
1:D:37:ARG:NH1	4:D:362:NAP:O3X	2.46	0.48
1:B:65:ASP:OD1	1:B:65:ASP:C	2.55	0.48
1:D:281:ARG:O	1:D:282:GLU:C	2.53	0.48
1:A:45:LEU:HD13	1:A:45:LEU:C	2.38	0.48
1:C:126:LEU:HB2	1:C:127:PRO:HD3	1.96	0.48
1:C:174:LEU:C	1:C:174:LEU:HD12	2.39	0.48
3:C:353:EST:H17	4:C:363:NAP:H4N	1.95	0.47
1:A:183:ILE:HG13	1:A:240:PHE:CD2	2.49	0.47
1:B:11:SER:HB2	4:B:364:NAP:O3B	2.14	0.47
1:C:95:LEU:HD11	1:C:102:LEU:HD22	1.96	0.47
1:C:216:TYR:CE1	1:C:219:LEU:HD12	2.49	0.47
1:A:155:TYR:CE1	1:A:192:PHE:HZ	2.32	0.47
1:D:189:HIS:O	1:D:233:PRO:HG3	2.13	0.47
1:A:264:ARG:O	1:A:265:MET:C	2.57	0.47
1:B:25:ASP:OD1	1:B:26:PRO:HD2	2.14	0.47
1:B:226:PHE:HE2	3:B:354:EST:H151	1.79	0.47
1:D:20:VAL:HG12	1:D:49:ALA:HB2	1.96	0.47
1:D:52:LEU:O	1:D:53:ALA:HB3	2.14	0.47
1:C:11:SER:HB2	1:C:36:LEU:HD23	1.97	0.47
1:C:45:LEU:HD13	1:C:45:LEU:O	2.14	0.47
1:D:34:ALA:HB1	1:D:45:LEU:HD11	1.96	0.47
1:D:209:ILE:HG23	1:D:210:HIS:N	2.29	0.47
1:A:78:ARG:HE	1:A:78:ARG:HB3	1.52	0.47
1:A:193:MET:HE3	1:A:193:MET:HB3	1.73	0.47
4:A:361:NAP:H2N	4:A:361:NAP:O1N	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:HB3	1:C:78:ARG:HH11	1.80	0.47
1:D:31:LYS:HE2	1:D:33:TYR:CE1	2.50	0.47
1:D:76:ARG:HG2	1:D:76:ARG:HH11	1.79	0.47
1:B:18:LEU:HD11	1:B:22:LEU:HD11	1.96	0.47
1:B:185:CYS:HA	1:B:255:THR:OG1	2.15	0.47
1:D:13:GLY:N	2:D:402:SO4:O2	2.41	0.47
1:D:269:ASP:HA	1:D:270:PRO:HD2	1.69	0.47
1:B:17:HIS:CD2	1:B:233:PRO:HB2	2.50	0.47
1:C:187:PRO:HB3	1:C:226:PHE:CE1	2.50	0.47
1:A:174:LEU:HB3	1:A:175:PRO:CD	2.45	0.47
1:B:129:MET:HB3	1:B:134:SER:O	2.15	0.47
1:C:269:ASP:HA	1:C:270:PRO:HD2	1.54	0.47
1:D:187:PRO:HB2	1:D:230:ALA:HA	1.97	0.46
1:B:138:LEU:HD13	1:B:183:ILE:HD11	1.97	0.46
1:A:50:ARG:HG2	1:A:50:ARG:HH11	1.80	0.46
1:A:149:LEU:CD1	3:A:351:EST:H182	2.46	0.46
1:A:156:CYS:O	1:A:157:ALA:C	2.57	0.46
1:A:236:VAL:O	1:A:237:ALA:C	2.54	0.46
1:D:265:MET:HE3	1:D:265:MET:HB2	1.69	0.46
1:A:5:VAL:HG13	1:A:86:VAL:CG1	2.46	0.46
1:A:81:GLU:H	1:A:81:GLU:CD	2.23	0.46
1:D:215:PHE:O	1:D:218:TYR:HB3	2.15	0.46
1:A:167:GLU:CD	1:B:266:ARG:HH21	2.23	0.46
1:A:279:MET:O	1:A:283:VAL:HG23	2.16	0.46
1:C:271:SER:HB2	1:D:250:THR:HG21	1.98	0.46
1:D:275:TYR:O	1:D:276:VAL:C	2.58	0.46
1:A:144:GLY:H	3:A:351:EST:H183	1.81	0.46
1:A:219:LEU:O	1:A:223:LYS:HG3	2.16	0.46
1:A:241:LEU:HA	1:A:244:LEU:CD2	2.45	0.46
1:A:245:ARG:O	1:A:246:ALA:C	2.58	0.46
1:A:173:LEU:O	1:A:174:LEU:C	2.59	0.46
1:B:94:GLY:HA2	1:B:155:TYR:CD1	2.51	0.46
1:A:174:LEU:HG	1:A:175:PRO:HD3	1.96	0.46
1:B:64:LEU:HD21	1:B:72:VAL:HG22	1.98	0.46
1:B:189:HIS:CE1	1:B:230:ALA:HB3	2.51	0.46
1:C:74:ALA:O	1:C:75:ALA:C	2.57	0.46
1:D:122:LEU:HD21	1:D:137:VAL:HG11	1.97	0.46
1:A:122:LEU:O	1:A:123:GLN:C	2.58	0.46
1:A:144:GLY:N	3:A:351:EST:H183	2.30	0.46
1:A:149:LEU:CD2	1:A:279:MET:HE3	2.45	0.46
1:D:14:ILE:HD13	1:D:236:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:PHE:CE2	3:B:354:EST:H151	2.51	0.46
1:C:172:LEU:O	1:C:175:PRO:HD2	2.16	0.46
1:A:275:TYR:CD1	1:A:275:TYR:C	2.94	0.45
1:A:280:HIS:CD2	1:A:280:HIS:C	2.93	0.45
1:C:221:LEU:HD13	1:C:221:LEU:O	2.17	0.45
1:D:31:LYS:HE2	1:D:33:TYR:CZ	2.51	0.45
1:D:35:THR:HG23	1:D:64:LEU:CB	2.41	0.45
1:D:123:GLN:HE21	1:D:123:GLN:HB2	1.50	0.45
1:B:143:VAL:HG12	3:B:354:EST:H122	1.99	0.45
1:A:174:LEU:HB3	1:A:175:PRO:HD3	1.99	0.45
1:D:193:MET:HA	1:D:196:VAL:CG2	2.47	0.45
1:C:214:ARG:HB3	1:C:284:PHE:CE1	2.51	0.45
1:D:31:LYS:HZ2	1:D:60:GLU:HG3	1.80	0.45
1:A:167:GLU:OE1	1:B:266:ARG:NH2	2.45	0.45
1:B:4:VAL:HG11	1:B:83:ARG:O	2.17	0.45
1:B:115:VAL:O	1:B:116:VAL:C	2.58	0.45
1:D:149:LEU:HD13	3:D:352:EST:H182	1.98	0.45
1:D:191:ALA:O	1:D:194:GLU:HB2	2.16	0.45
1:D:246:ALA:HA	1:D:247:PRO:HD2	1.86	0.45
1:B:244:LEU:HD12	1:B:244:LEU:C	2.41	0.45
1:C:131:ARG:HA	1:C:131:ARG:HD3	1.74	0.45
1:D:203:VAL:HG12	1:D:207:THR:HG21	1.98	0.45
1:B:3:THR:HG21	1:B:30:PHE:CE1	2.52	0.45
1:B:218:TYR:O	1:B:219:LEU:C	2.58	0.45
1:C:129:MET:HG2	1:C:135:GLY:HA3	1.98	0.45
1:A:34:ALA:O	1:A:61:THR:HA	2.16	0.45
1:A:193:MET:O	1:A:194:GLU:C	2.57	0.44
1:A:163:GLU:OE2	1:A:182:LEU:HD13	2.18	0.44
1:B:269:ASP:OD2	1:B:274:ASN:HB2	2.17	0.44
1:A:252:ARG:HG3	1:A:252:ARG:NH1	2.32	0.44
1:B:180:LEU:C	1:B:180:LEU:HD23	2.42	0.44
1:B:6:LEU:C	1:B:6:LEU:HD23	2.42	0.44
1:B:231:GLN:HB3	1:B:235:GLU:OE2	2.18	0.44
1:C:90:ASN:O	1:C:91:ALA:C	2.59	0.44
1:A:14:ILE:HD12	1:A:14:ILE:H	1.81	0.44
1:C:115:VAL:HG22	1:C:161:ALA:HB3	2.00	0.44
1:D:49:ALA:HB1	1:D:54:CYS:SG	2.57	0.44
1:B:221:LEU:O	1:B:222:SER:C	2.61	0.44
1:B:263:LEU:O	1:B:267:LEU:HG	2.17	0.44
1:C:8:THR:HG23	1:C:121:MET:HE2	1.99	0.44
1:A:219:LEU:HB3	1:A:223:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:PHE:O	1:D:196:VAL:HG23	2.18	0.44
1:C:95:LEU:CD1	1:C:102:LEU:HD22	2.48	0.44
1:D:166:CYS:HB3	1:D:180:LEU:CD2	2.39	0.44
1:A:96:LEU:CB	1:A:196:VAL:HG13	2.48	0.44
1:A:126:LEU:HD11	1:A:169:LEU:HD11	1.99	0.44
1:A:142:SER:HB3	1:A:159:LYS:HD2	2.00	0.44
1:B:31:LYS:HE2	1:B:33:TYR:CE1	2.53	0.44
1:A:116:VAL:HG21	5:A:665:HOH:O	2.16	0.43
1:C:25:ASP:O	1:C:28:GLN:N	2.51	0.43
1:C:265:MET:HE2	1:C:265:MET:O	2.18	0.43
1:B:33:TYR:O	1:B:35:THR:HG23	2.18	0.43
1:A:86:VAL:HA	1:A:136:ARG:O	2.18	0.43
1:B:2:ARG:HA	1:B:83:ARG:NH2	2.34	0.43
1:B:279:MET:HE1	3:B:354:EST:C2	2.48	0.43
1:A:78:ARG:NH1	5:A:629:HOH:O	2.43	0.43
1:D:261:PRO:HA	1:D:264:ARG:HD2	2.00	0.43
1:A:241:LEU:O	1:A:242:THR:C	2.62	0.43
1:A:88:VAL:HA	1:A:138:LEU:O	2.19	0.43
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.71	0.43
1:A:203:VAL:HG12	1:A:212:PHE:CE1	2.54	0.43
1:C:17:HIS:CD2	1:C:233:PRO:HB2	2.53	0.43
1:C:42:GLN:NE2	1:C:61:THR:HG21	2.34	0.43
1:D:159:LYS:HA	1:D:159:LYS:HD3	1.81	0.43
1:A:38:ASP:OD1	1:A:40:LYS:N	2.50	0.43
1:C:154:VAL:O	1:C:155:TYR:C	2.62	0.43
1:C:199:SER:O	1:C:202:GLU:N	2.52	0.43
1:D:6:LEU:C	1:D:6:LEU:HD23	2.44	0.43
1:B:239:VAL:O	1:B:242:THR:HB	2.19	0.43
1:C:175:PRO:HG3	1:D:280:HIS:CE1	2.54	0.43
1:C:193:MET:CA	1:C:196:VAL:HG23	2.27	0.43
1:A:5:VAL:HG11	1:A:22:LEU:CD1	2.49	0.42
1:A:25:ASP:HA	1:A:26:PRO:HD3	1.85	0.42
1:C:45:LEU:C	1:C:45:LEU:CD1	2.91	0.42
1:A:33:TYR:HA	1:A:60:GLU:O	2.19	0.42
1:A:115:VAL:O	1:A:116:VAL:C	2.60	0.42
1:B:263:LEU:HD13	1:B:267:LEU:HD11	2.00	0.42
1:C:265:MET:SD	1:C:265:MET:C	3.02	0.42
1:A:38:ASP:OD1	1:A:38:ASP:C	2.63	0.42
1:A:224:GLN:HG2	1:A:227:ARG:NH2	2.35	0.42
1:B:136:ARG:NH2	1:B:246:ALA:O	2.52	0.42
1:C:4:VAL:HG21	1:C:81:GLU:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ARG:NH1	1:C:132:ARG:HG3	2.33	0.42
1:D:67:ARG:HA	1:D:120:ARG:NH1	2.35	0.42
1:D:160:PHE:O	1:D:161:ALA:C	2.61	0.42
1:A:52:LEU:HD12	1:A:52:LEU:N	2.35	0.42
1:A:116:VAL:HG11	5:A:665:HOH:O	2.18	0.42
1:A:157:ALA:HB1	1:B:161:ALA:HB1	2.01	0.42
1:C:2:ARG:HH22	1:C:81:GLU:CG	2.33	0.42
1:C:38:ASP:O	1:C:41:THR:OG1	2.38	0.42
1:A:25:ASP:OD1	1:A:27:SER:OG	2.33	0.42
1:B:16:LEU:O	1:B:19:ALA:HB3	2.19	0.42
1:B:39:LEU:HD22	1:B:42:GLN:NE2	2.34	0.42
1:B:132:ARG:HD2	5:B:506:HOH:O	2.19	0.42
1:C:8:THR:CG2	1:C:121:MET:HE2	2.49	0.42
1:C:145:GLY:O	1:C:163:GLU:HG3	2.20	0.42
1:D:186:GLY:O	1:D:187:PRO:C	2.61	0.42
1:A:122:LEU:HD21	1:A:137:VAL:HG11	2.02	0.42
1:A:231:GLN:HG3	5:A:571:HOH:O	2.20	0.42
1:B:33:TYR:O	1:B:34:ALA:C	2.61	0.42
1:C:22:LEU:CD2	1:C:241:LEU:HD11	2.49	0.42
1:C:202:GLU:O	1:C:205:ASP:HB3	2.19	0.42
1:D:138:LEU:CD2	1:D:181:SER:HB2	2.49	0.42
1:D:149:LEU:HD11	3:D:352:EST:H111	2.02	0.42
1:D:248:LYS:O	1:D:248:LYS:HG2	2.18	0.42
1:A:218:TYR:OH	3:A:351:EST:H62	2.20	0.42
1:A:221:LEU:HD13	1:A:225:VAL:HG23	2.02	0.42
1:B:126:LEU:O	1:B:127:PRO:C	2.60	0.42
1:B:100:GLU:HG3	1:B:206:ARG:O	2.20	0.42
1:A:174:LEU:CB	1:A:175:PRO:HD3	2.50	0.42
1:C:52:LEU:HD12	1:C:52:LEU:N	2.35	0.42
1:C:149:LEU:CD2	1:C:279:MET:HE2	2.50	0.42
1:D:37:ARG:HH11	1:D:37:ARG:HD3	1.39	0.42
1:A:132:ARG:HD2	5:A:635:HOH:O	2.20	0.41
1:A:149:LEU:HD11	3:A:351:EST:H182	2.01	0.41
1:C:136:ARG:NH1	1:C:244:LEU:HA	2.35	0.41
1:C:274:ASN:O	1:C:275:TYR:C	2.62	0.41
1:A:17:HIS:CD2	1:A:233:PRO:HB2	2.55	0.41
1:B:143:VAL:HG12	3:B:354:EST:C12	2.50	0.41
1:B:204:LEU:HD23	1:B:212:PHE:CE2	2.55	0.41
1:C:186:GLY:O	1:C:187:PRO:C	2.61	0.41
1:D:138:LEU:HD22	1:D:181:SER:HB2	2.02	0.41
1:A:14:ILE:O	1:A:15:GLY:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ARG:HH22	1:C:81:GLU:HG2	1.85	0.41
1:C:262:LEU:HD12	1:C:262:LEU:HA	1.92	0.41
1:A:33:TYR:CD2	1:A:62:LEU:HD11	2.53	0.41
1:A:67:ARG:HE	1:A:67:ARG:HB2	1.55	0.41
1:A:74:ALA:O	1:A:75:ALA:C	2.63	0.41
1:A:136:ARG:HA	1:A:179:HIS:O	2.21	0.41
1:B:34:ALA:O	1:B:61:THR:HA	2.19	0.41
1:B:204:LEU:HA	1:B:212:PHE:CE2	2.55	0.41
1:A:155:TYR:CE2	3:A:351:EST:H162	2.56	0.41
1:A:262:LEU:HD12	1:A:262:LEU:HA	1.84	0.41
1:B:39:LEU:O	1:B:42:GLN:HG2	2.20	0.41
1:D:106:ALA:O	1:D:110:VAL:HG23	2.20	0.41
1:D:232:ASN:HB2	1:D:235:GLU:CG	2.50	0.41
1:A:153:ASP:OD1	1:B:169:LEU:HG	2.21	0.41
1:B:12:SER:O	1:B:13:GLY:C	2.62	0.41
1:B:129:MET:O	1:B:133:GLY:N	2.54	0.41
1:C:256:THR:OG1	1:C:257:GLU:N	2.53	0.41
1:D:42:GLN:NE2	1:D:46:TRP:NE1	2.65	0.41
1:A:5:VAL:HG11	1:A:22:LEU:HD13	2.03	0.41
1:B:3:THR:HG21	1:B:30:PHE:HE1	1.85	0.41
1:B:239:VAL:HG21	1:B:255:THR:HA	2.03	0.41
1:B:126:LEU:HD13	1:B:173:LEU:HD21	2.03	0.41
1:C:188:VAL:CG2	1:C:236:VAL:HG21	2.49	0.41
1:D:44:ARG:O	1:D:45:LEU:C	2.62	0.41
1:D:77:GLU:HG2	1:D:77:GLU:H	1.71	0.41
1:D:166:CYS:CB	1:D:180:LEU:HD21	2.44	0.41
1:A:111:LEU:HD23	1:A:158:SER:CB	2.45	0.41
1:B:265:MET:HE3	1:B:265:MET:HB3	1.83	0.41
1:C:2:ARG:NH2	1:C:83:ARG:HH22	2.18	0.41
1:C:130:LYS:O	1:C:131:ARG:C	2.61	0.41
1:C:155:TYR:CE1	1:C:192:PHE:HZ	2.39	0.41
1:B:239:VAL:HG21	1:B:255:THR:HG22	2.03	0.41
1:A:96:LEU:HB3	1:A:196:VAL:HG13	2.03	0.40
1:A:187:PRO:HB3	1:A:226:PHE:CE1	2.56	0.40
1:A:208:ASP:OD1	1:A:211:THR:HB	2.21	0.40
1:A:257:GLU:O	1:A:258:ARG:C	2.64	0.40
1:D:35:THR:CG2	1:D:64:LEU:HB3	2.42	0.40
1:D:44:ARG:NH2	2:D:402:SO4:O1	2.54	0.40
1:D:218:TYR:HD1	1:D:283:VAL:CG1	2.34	0.40
1:A:150:PRO:O	1:A:151:PHE:C	2.65	0.40
1:B:144:GLY:O	1:B:156:CYS:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ILE:HG23	1:C:88:VAL:HB	2.02	0.40
1:C:25:ASP:HA	1:C:26:PRO:HD3	1.93	0.40
1:C:239:VAL:HG21	1:C:255:THR:CG2	2.49	0.40
1:C:252:ARG:NH1	1:C:252:ARG:HG3	2.36	0.40
1:D:136:ARG:NH1	1:D:249:PRO:HG3	2.36	0.40
1:D:172:LEU:O	1:D:175:PRO:HD2	2.21	0.40
1:A:191:ALA:O	1:A:192:PHE:C	2.63	0.40
1:B:106:ALA:O	1:B:110:VAL:HG23	2.21	0.40
1:C:15:GLY:O	1:C:16:LEU:C	2.62	0.40
1:C:188:VAL:HG12	1:C:190:THR:HG23	2.03	0.40
1:C:239:VAL:CG2	1:C:255:THR:HG22	2.50	0.40
1:D:35:THR:HG21	1:D:64:LEU:HD13	2.03	0.40
1:A:137:VAL:O	1:A:180:LEU:HA	2.20	0.40
1:B:204:LEU:HD23	1:B:212:PHE:CD2	2.57	0.40
1:C:16:LEU:HD21	1:C:48:ALA:CB	2.51	0.40
1:D:246:ALA:O	1:D:249:PRO:HD3	2.21	0.40
1:A:25:ASP:CG	1:A:26:PRO:HD2	2.47	0.40
1:A:192:PHE:CE2	3:A:351:EST:H161	2.56	0.40
1:A:269:ASP:OD2	1:A:274:ASN:HB2	2.21	0.40
1:B:141:GLY:N	1:B:183:ILE:O	2.51	0.40
1:B:166:CYS:HB3	1:B:180:LEU:CD2	2.51	0.40
1:C:87:LEU:HD22	1:C:125:PHE:HB2	2.02	0.40
1:C:271:SER:HA	1:D:252:ARG:HB2	2.04	0.40
1:D:180:LEU:HD23	1:D:180:LEU:O	2.21	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	277/327 (85%)	245 (88%)	31 (11%)	1 (0%)	30 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	276/327 (84%)	246 (89%)	25 (9%)	5 (2%)	6	18
1	C	283/327 (86%)	253 (89%)	25 (9%)	5 (2%)	6	18
1	D	277/327 (85%)	250 (90%)	26 (9%)	1 (0%)	30	54
All	All	1113/1308 (85%)	994 (89%)	107 (10%)	12 (1%)	11	29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	197	LEU
1	C	199	SER
1	C	271	SER
1	D	174	LEU
1	C	270	PRO
1	B	34	ALA
1	B	127	PRO
1	B	258	ARG
1	C	151	PHE
1	A	174	LEU
1	B	2	ARG
1	B	151	PHE

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	231/258 (90%)	194 (84%)	37 (16%)	2	6
1	B	231/258 (90%)	191 (83%)	40 (17%)	2	5
1	C	235/258 (91%)	189 (80%)	46 (20%)	1	4
1	D	232/258 (90%)	205 (88%)	27 (12%)	5	13
All	All	929/1032 (90%)	779 (84%)	150 (16%)	2	6

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	36	LEU
1	A	45	LEU
1	A	52	LEU
1	A	63	GLN
1	A	78	ARG
1	A	81	GLU
1	A	83	ARG
1	A	86	VAL
1	A	105	ASP
1	A	115	VAL
1	A	143	VAL
1	A	153	ASP
1	A	169	LEU
1	A	180	LEU
1	A	181	SER
1	A	195	LYS
1	A	196	VAL
1	A	197	LEU
1	A	203	VAL
1	A	204	LEU
1	A	206	ARG
1	A	209	ILE
1	A	210	HIS
1	A	219	LEU
1	A	221	LEU
1	A	222	SER
1	A	224	GLN
1	A	238	GLU
1	A	244	LEU
1	A	258	ARG
1	A	263	LEU
1	A	265	MET
1	A	271	SER
1	A	279	MET
1	A	282	GLU
1	A	284	PHE
1	B	2	ARG
1	B	18	LEU
1	B	20	VAL
1	B	21	ARG
1	B	36	LEU
1	B	40	LYS

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Mol	Chain	Res	Type
1	B	45	LEU
1	B	50	ARG
1	B	69	SER
1	B	71	SER
1	B	78	ARG
1	B	96	LEU
1	B	104	GLU
1	B	109	SER
1	B	114	ASN
1	B	116	VAL
1	B	120	ARG
1	B	129	MET
1	B	131	ARG
1	B	134	SER
1	B	136	ARG
1	B	138	LEU
1	B	143	VAL
1	B	153	ASP
1	B	176	PHE
1	B	183	ILE
1	B	196	VAL
1	B	203	VAL
1	B	204	LEU
1	B	207	THR
1	B	221	LEU
1	B	222	SER
1	B	238	GLU
1	B	241	LEU
1	B	244	LEU
1	B	248	LYS
1	B	257	GLU
1	B	263	LEU
1	B	269	ASP
1	B	271	SER
1	C	2	ARG
1	C	3	THR
1	C	10	CYS
1	C	28	GLN
1	C	29	SER
1	C	31	LYS
1	C	39	LEU
1	C	45	LEU

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Mol	Chain	Res	Type
1	C	66	VAL
1	C	69	SER
1	C	81	GLU
1	C	83	ARG
1	C	109	SER
1	C	123	GLN
1	C	129	MET
1	C	131	ARG
1	C	132	ARG
1	C	143	VAL
1	C	153	ASP
1	C	162	LEU
1	C	173	LEU
1	C	174	LEU
1	C	182	LEU
1	C	193	MET
1	C	195	LYS
1	C	197	LEU
1	C	199	SER
1	C	204	LEU
1	C	206	ARG
1	C	209	ILE
1	C	222	SER
1	C	224	GLN
1	C	226	PHE
1	C	227	ARG
1	C	234	GLU
1	C	238	GLU
1	C	241	LEU
1	C	244	LEU
1	C	256	THR
1	C	257	GLU
1	C	262	LEU
1	C	263	LEU
1	C	265	MET
1	C	266	ARG
1	C	269	ASP
1	C	276	VAL
1	D	2	ARG
1	D	35	THR
1	D	45	LEU
1	D	67	ARG

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Mol	Chain	Res	Type
1	D	104	GLU
1	D	109	SER
1	D	126	LEU
1	D	127	PRO
1	D	134	SER
1	D	142	SER
1	D	153	ASP
1	D	174	LEU
1	D	197	LEU
1	D	204	LEU
1	D	209	ILE
1	D	221	LEU
1	D	234	GLU
1	D	250	THR
1	D	256	THR
1	D	260	LEU
1	D	262	LEU
1	D	263	LEU
1	D	268	ASP
1	D	269	ASP
1	D	277	THR
1	D	281	ARG
1	D	283	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	123	GLN
1	A	179	HIS
1	A	189	HIS
1	A	274	ASN
1	A	280	HIS
1	B	17	HIS
1	B	28	GLN
1	B	42	GLN
1	B	123	GLN
1	B	189	HIS
1	B	210	HIS
1	B	224	GLN
1	B	274	ASN
1	B	280	HIS

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Mol	Chain	Res	Type
1	C	17	HIS
1	C	42	GLN
1	C	123	GLN
1	C	152	ASN
1	C	179	HIS
1	C	189	HIS
1	C	217	GLN
1	C	224	GLN
1	C	231	GLN
1	C	274	ASN
1	D	17	HIS
1	D	42	GLN
1	D	123	GLN
1	D	189	HIS
1	D	213	HIS
1	D	224	GLN
1	D	231	GLN
1	D	280	HIS

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](#)

12 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	EST	A	351	-	23,23,23	0.83	1 (4%)	36,36,36	2.41	16 (44%)
4	NAP	A	361	-	50,52,52	2.10	8 (16%)	71,80,80	2.25	16 (22%)
2	SO4	A	401	-	4,4,4	0.80	0	6,6,6	0.88	0
4	NAP	C	363	-	50,52,52	2.14	12 (24%)	71,80,80	2.04	16 (22%)
3	EST	B	354	-	23,23,23	1.12	2 (8%)	36,36,36	2.61	12 (33%)
2	SO4	B	400	-	4,4,4	0.78	0	6,6,6	0.61	0
4	NAP	D	362	-	50,52,52	2.04	10 (20%)	71,80,80	2.06	13 (18%)
3	EST	D	352	-	23,23,23	1.15	1 (4%)	36,36,36	2.31	13 (36%)
2	SO4	D	402	-	4,4,4	0.67	0	6,6,6	0.73	0
4	NAP	B	364	-	50,52,52	1.92	10 (20%)	71,80,80	1.87	15 (21%)
3	EST	C	353	-	23,23,23	0.82	0	36,36,36	1.88	9 (25%)
2	SO4	C	403	-	4,4,4	0.68	0	6,6,6	0.61	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	EST	A	351	-	-	-	0/4/4/4
4	NAP	A	361	-	-	13/35/67/67	0/5/5/5
4	NAP	C	363	-	-	11/35/67/67	0/5/5/5
3	EST	B	354	-	-	-	0/4/4/4
4	NAP	D	362	-	-	8/35/67/67	0/5/5/5
3	EST	D	352	-	-	-	0/4/4/4
4	NAP	B	364	-	-	5/35/67/67	0/5/5/5
3	EST	C	353	-	-	-	0/4/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	361	NAP	P2B-O2B	-10.19	1.41	1.59
4	C	363	NAP	P2B-O2B	-9.71	1.42	1.59
4	D	362	NAP	P2B-O2B	-8.28	1.45	1.59
4	B	364	NAP	P2B-O2B	-8.01	1.45	1.59
4	C	363	NAP	C2N-N1N	6.10	1.41	1.35
4	A	361	NAP	C2N-N1N	5.74	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	362	NAP	PA-O3	4.70	1.64	1.59
4	B	364	NAP	C2N-N1N	4.60	1.40	1.35
4	D	362	NAP	C2N-N1N	4.51	1.39	1.35
4	D	362	NAP	C5A-N7A	-4.07	1.31	1.39
4	A	361	NAP	C5A-N7A	-3.84	1.32	1.39
4	B	364	NAP	PA-O3	3.72	1.63	1.59
4	D	362	NAP	PN-O3	3.63	1.63	1.59
4	D	362	NAP	P2B-O3X	-3.43	1.42	1.54
4	B	364	NAP	P2B-O3X	-3.39	1.42	1.54
4	C	363	NAP	P2B-O3X	-3.31	1.42	1.54
4	C	363	NAP	P2B-O1X	-3.30	1.40	1.50
4	C	363	NAP	C2B-C1B	3.25	1.61	1.53
4	C	363	NAP	C4A-N9A	-3.23	1.31	1.37
4	D	362	NAP	P2B-O1X	-3.14	1.40	1.50
4	B	364	NAP	PN-O3	3.10	1.62	1.59
4	C	363	NAP	P2B-O2X	-2.95	1.43	1.54
4	B	364	NAP	C5A-N7A	-2.92	1.33	1.39
4	A	361	NAP	P2B-O3X	-2.90	1.44	1.54
4	D	362	NAP	P2B-O2X	-2.78	1.44	1.54
4	B	364	NAP	P2B-O2X	-2.73	1.44	1.54
4	A	361	NAP	C6N-N1N	2.63	1.41	1.35
4	C	363	NAP	C5A-N7A	-2.56	1.34	1.39
4	A	361	NAP	P2B-O2X	-2.55	1.45	1.54
4	A	361	NAP	PA-O2A	-2.52	1.43	1.55
4	C	363	NAP	PA-O2A	-2.46	1.43	1.55
3	D	352	EST	C4-C3	2.44	1.42	1.39
4	C	363	NAP	O4D-C1D	2.42	1.44	1.40
4	B	364	NAP	P2B-O1X	-2.38	1.43	1.50
4	C	363	NAP	C6N-N1N	2.37	1.40	1.35
4	A	361	NAP	P2B-O1X	-2.21	1.43	1.50
4	B	364	NAP	C3N-C7N	2.20	1.53	1.50
3	A	351	EST	C12-C11	2.17	1.57	1.53
4	D	362	NAP	C8A-N9A	-2.16	1.33	1.37
4	D	362	NAP	C4A-N9A	-2.15	1.33	1.37
4	C	363	NAP	PN-O3	2.10	1.61	1.59
3	B	354	EST	C12-C13	-2.03	1.50	1.54
3	B	354	EST	C9-C8	2.02	1.56	1.54
4	B	364	NAP	C4A-N9A	-2.01	1.33	1.37

All (110) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	361	NAP	O4B-C1B-N9A	10.35	127.96	108.09
4	D	362	NAP	O4B-C1B-N9A	9.18	125.72	108.09
3	B	354	EST	C7-C8-C14	8.55	126.28	112.08
4	C	363	NAP	C2B-C1B-N9A	-6.14	103.64	113.75
3	B	354	EST	C11-C12-C13	5.82	122.57	112.74
4	B	364	NAP	N3A-C2A-N1A	-5.73	119.91	128.58
3	D	352	EST	C15-C14-C8	5.60	128.03	119.10
4	D	362	NAP	O7N-C7N-C3N	5.57	126.41	119.60
3	B	354	EST	C15-C14-C8	5.52	127.90	119.10
4	C	363	NAP	N3A-C2A-N1A	-5.50	120.26	128.58
4	A	361	NAP	N3A-C2A-N1A	-5.35	120.48	128.58
4	D	362	NAP	N3A-C2A-N1A	-5.35	120.49	128.58
3	A	351	EST	C16-C17-C13	5.21	108.63	104.52
4	B	364	NAP	C6N-N1N-C2N	-5.17	117.48	121.88
4	A	361	NAP	C5A-C4A-N3A	-5.12	119.67	126.72
3	B	354	EST	C12-C11-C9	5.01	118.83	112.34
3	D	352	EST	C6-C7-C8	4.78	118.60	110.61
4	B	364	NAP	O4B-C1B-N9A	4.71	117.14	108.09
4	C	363	NAP	C5A-C4A-N3A	-4.71	120.24	126.72
4	C	363	NAP	O4B-C1B-C2B	-4.69	98.51	106.59
3	C	353	EST	C7-C8-C14	4.65	119.81	112.08
4	C	363	NAP	O4B-C1B-N9A	4.58	116.88	108.09
3	D	352	EST	C7-C8-C14	4.55	119.64	112.08
3	A	351	EST	C6-C7-C8	4.52	118.16	110.61
4	A	361	NAP	C4D-O4D-C1D	4.35	113.91	109.92
4	D	362	NAP	C5A-C4A-N3A	-4.35	120.73	126.72
3	A	351	EST	C7-C8-C9	4.34	113.43	109.27
4	A	361	NAP	C2A-N3A-C4A	4.22	122.13	111.83
4	D	362	NAP	C6N-N1N-C2N	-4.20	118.30	121.88
4	B	364	NAP	C5A-C4A-N3A	-4.18	120.97	126.72
4	A	361	NAP	C6N-N1N-C2N	-4.07	118.41	121.88
3	A	351	EST	C18-C13-C17	-4.06	103.38	109.58
3	D	352	EST	C18-C13-C17	-4.02	103.44	109.58
3	D	352	EST	C10-C9-C8	3.95	116.35	111.59
4	C	363	NAP	N3A-C4A-N9A	3.91	133.82	127.17
4	D	362	NAP	C3N-C7N-N7N	-3.90	112.94	117.74
3	A	351	EST	C18-C13-C14	3.88	118.70	111.68
4	C	363	NAP	C3B-C2B-C1B	-3.86	95.41	102.81
3	C	353	EST	C9-C8-C14	3.86	114.05	108.68
4	B	364	NAP	C2A-N3A-C4A	3.78	121.06	111.83
4	B	364	NAP	C2D-C3D-C4D	-3.73	95.41	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	363	NAP	C2A-N3A-C4A	3.72	120.92	111.83
4	C	363	NAP	O7N-C7N-N7N	-3.70	117.28	122.62
3	C	353	EST	C18-C13-C17	-3.60	104.08	109.58
3	A	351	EST	C18-C13-C12	-3.58	105.33	110.61
4	D	362	NAP	C2A-N3A-C4A	3.55	120.50	111.83
4	B	364	NAP	N3A-C4A-N9A	3.51	133.15	127.17
3	A	351	EST	C14-C13-C17	3.47	102.79	99.25
4	D	362	NAP	O3D-C3D-C4D	-3.41	101.28	111.08
3	A	351	EST	C12-C13-C17	3.37	120.36	115.23
3	C	353	EST	C11-C9-C8	3.36	115.85	111.45
3	A	351	EST	C7-C8-C14	3.35	117.64	112.08
4	A	361	NAP	N3A-C4A-N9A	3.24	132.68	127.17
3	D	352	EST	C16-C17-C13	-3.24	101.97	104.52
4	A	361	NAP	O7N-C7N-N7N	-3.22	117.96	122.62
4	C	363	NAP	N9A-C8A-N7A	-3.21	109.39	113.94
3	C	353	EST	C14-C13-C17	3.17	102.49	99.25
3	D	352	EST	C9-C8-C14	3.16	113.08	108.68
3	D	352	EST	C7-C6-C5	3.16	118.86	112.87
4	D	362	NAP	O2A-PA-O1A	3.15	127.08	112.44
4	C	363	NAP	C4A-N9A-C8A	3.13	109.03	105.74
3	A	351	EST	C15-C14-C13	3.10	107.48	103.84
4	B	364	NAP	O3D-C3D-C4D	-3.07	102.26	111.08
4	A	361	NAP	O2N-PN-O1N	3.05	126.62	112.44
4	D	362	NAP	N3A-C4A-N9A	3.03	132.32	127.17
3	C	353	EST	C15-C14-C8	3.02	123.92	119.10
3	B	354	EST	C10-C9-C8	3.00	115.21	111.59
4	A	361	NAP	C2B-C1B-N9A	-2.94	108.91	113.75
3	A	351	EST	C1-C10-C5	-2.91	115.18	118.78
3	B	354	EST	C13-C14-C8	-2.87	110.34	114.41
4	A	361	NAP	N9A-C8A-N7A	-2.81	109.95	113.94
3	B	354	EST	C16-C17-C13	-2.81	102.31	104.52
3	D	352	EST	C18-C13-C14	2.80	116.76	111.68
4	A	361	NAP	C5A-N7A-C8A	2.80	107.84	103.45
4	A	361	NAP	C3N-C7N-N7N	2.76	121.14	117.74
4	C	363	NAP	O7N-C7N-C3N	2.76	122.97	119.60
4	D	362	NAP	P2B-O2B-C2B	-2.76	116.06	123.43
3	B	354	EST	O17-C17-C13	2.72	120.49	114.80
3	B	354	EST	C6-C7-C8	2.70	115.13	110.61
3	C	353	EST	C10-C9-C8	2.70	114.85	111.59
4	C	363	NAP	O2A-PA-O3	2.70	114.56	107.27
3	A	351	EST	C9-C8-C14	2.62	112.32	108.68
4	B	364	NAP	C5D-C4D-C3D	-2.53	106.12	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	351	EST	C7-C6-C5	2.52	117.65	112.87
3	B	354	EST	C18-C13-C17	-2.50	105.76	109.58
3	A	351	EST	C11-C12-C13	-2.48	108.55	112.74
4	B	364	NAP	O4D-C4D-C3D	-2.47	100.24	105.15
4	B	364	NAP	O2A-PA-O1A	2.46	123.89	112.44
3	B	354	EST	C3-C4-C5	-2.45	118.01	120.77
4	B	364	NAP	O3X-P2B-O2B	2.44	115.36	105.85
4	B	364	NAP	O7N-C7N-N7N	-2.41	119.13	122.62
4	C	363	NAP	C5N-C6N-N1N	-2.37	117.14	120.38
4	C	363	NAP	C5N-C4N-C3N	2.33	122.66	120.36
4	B	364	NAP	P2B-O2B-C2B	-2.31	117.25	123.43
4	A	361	NAP	O4B-C1B-C2B	-2.31	102.61	106.59
4	A	361	NAP	C4A-C5A-N7A	-2.27	107.98	110.58
3	D	352	EST	C12-C13-C14	2.25	110.61	107.25
3	D	352	EST	C12-C13-C17	-2.21	111.87	115.23
4	C	363	NAP	C1B-N9A-C8A	-2.21	122.19	127.09
3	D	352	EST	C18-C13-C12	2.21	113.86	110.61
4	D	362	NAP	C2B-C1B-N9A	2.18	117.34	113.75
3	C	353	EST	C11-C12-C13	-2.11	109.18	112.74
3	D	352	EST	O17-C17-C16	2.08	117.12	111.69
4	A	361	NAP	C5N-C4N-C3N	2.08	122.41	120.36
4	D	362	NAP	O2A-PA-O3	-2.07	101.68	107.27
3	B	354	EST	C4-C5-C10	2.06	122.08	119.49
3	C	353	EST	C7-C6-C5	2.04	116.73	112.87
4	B	364	NAP	N9A-C8A-N7A	-2.03	111.05	113.94
3	A	351	EST	C15-C14-C8	2.03	122.34	119.10
3	A	351	EST	C6-C5-C10	-2.00	118.15	121.11

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	361	NAP	C5B-O5B-PA-O1A
4	A	361	NAP	C5B-O5B-PA-O2A
4	A	361	NAP	C5B-O5B-PA-O3
4	A	361	NAP	C5D-O5D-PN-O3
4	A	361	NAP	O4D-C1D-N1N-C2N
4	C	363	NAP	C5B-O5B-PA-O1A
4	C	363	NAP	C5B-O5B-PA-O3
4	C	363	NAP	C5D-O5D-PN-O3
4	D	362	NAP	C5D-O5D-PN-O3
4	D	362	NAP	O4D-C1D-N1N-C2N

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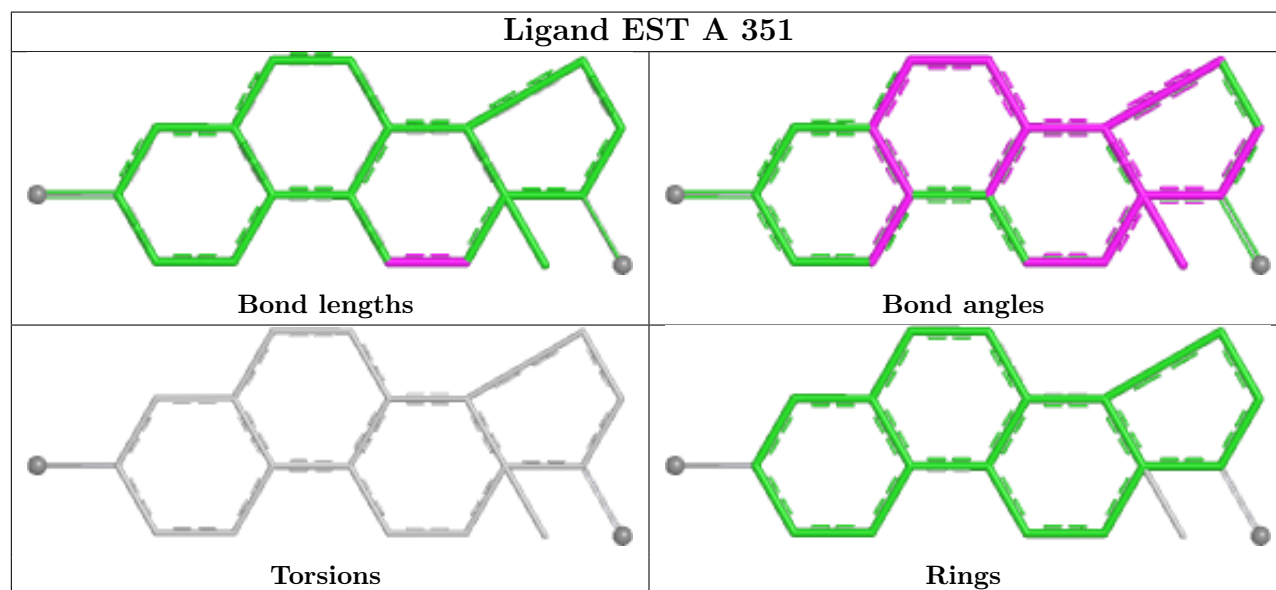
Mol	Chain	Res	Type	Atoms
4	A	361	NAP	O4B-C4B-C5B-O5B
4	A	361	NAP	C3B-C4B-C5B-O5B
4	C	363	NAP	O4B-C4B-C5B-O5B
4	C	363	NAP	C3B-C4B-C5B-O5B
4	A	361	NAP	C1B-C2B-O2B-P2B
4	A	361	NAP	PN-O3-PA-O1A
4	D	362	NAP	PA-O3-PN-O1N
4	A	361	NAP	PN-O3-PA-O5B
4	D	362	NAP	PN-O3-PA-O5B
4	B	364	NAP	PA-O3-PN-O2N
4	A	361	NAP	C5D-O5D-PN-O1N
4	B	364	NAP	C5D-O5D-PN-O1N
4	C	363	NAP	C5B-O5B-PA-O2A
4	C	363	NAP	C5D-O5D-PN-O1N
4	D	362	NAP	C5D-O5D-PN-O1N
4	D	362	NAP	PA-O3-PN-O2N
4	C	363	NAP	C2B-O2B-P2B-O2X
4	A	361	NAP	O4D-C1D-N1N-C6N
4	B	364	NAP	O4B-C4B-C5B-O5B
4	B	364	NAP	O4D-C1D-N1N-C6N
4	D	362	NAP	O4D-C1D-N1N-C6N
4	C	363	NAP	PN-O3-PA-O1A
4	C	363	NAP	PN-O3-PA-O5B
4	A	361	NAP	C3B-C2B-O2B-P2B
4	B	364	NAP	PA-O3-PN-O1N
4	C	363	NAP	C2B-C1B-N9A-C8A
4	D	362	NAP	O4B-C1B-N9A-C8A

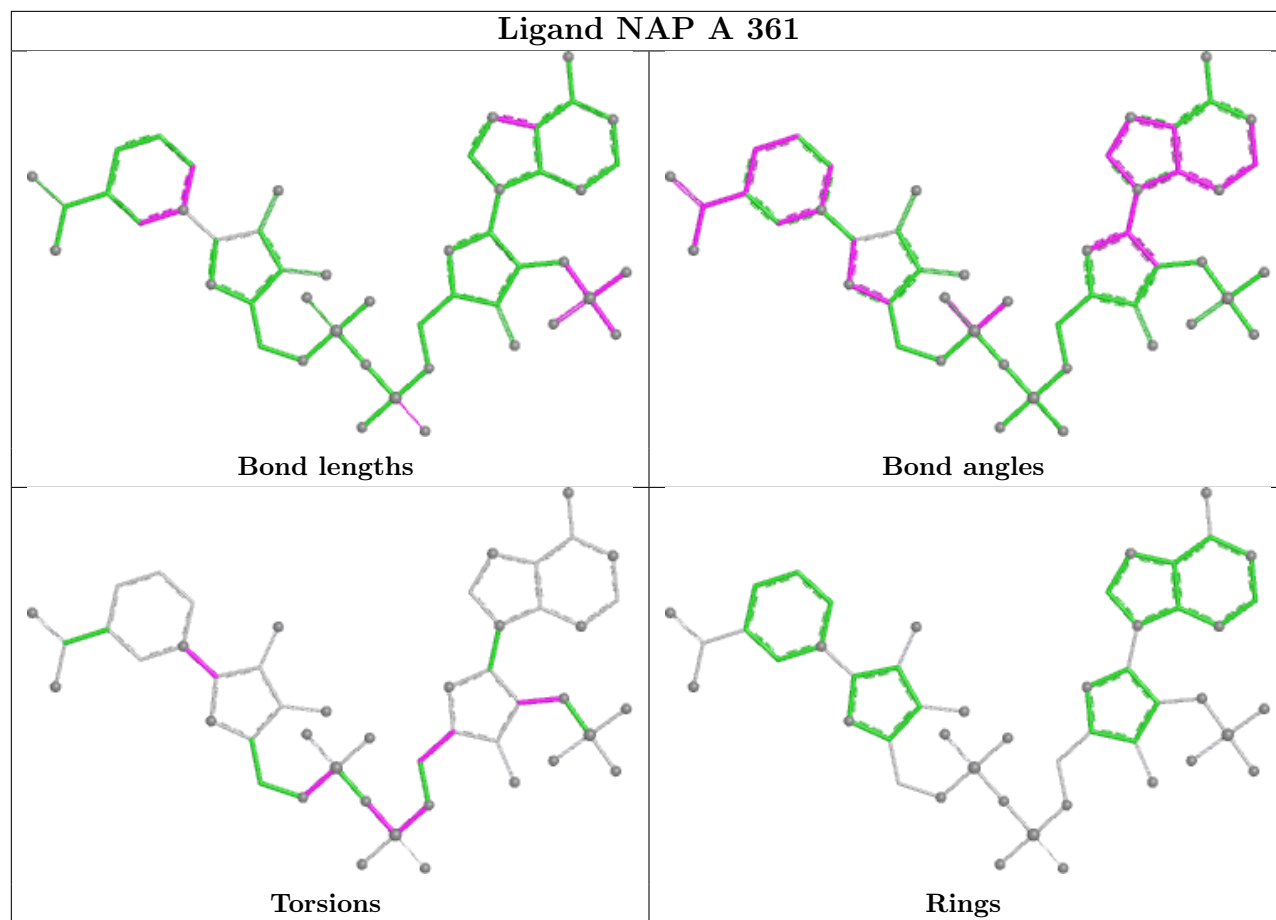
There are no ring outliers.

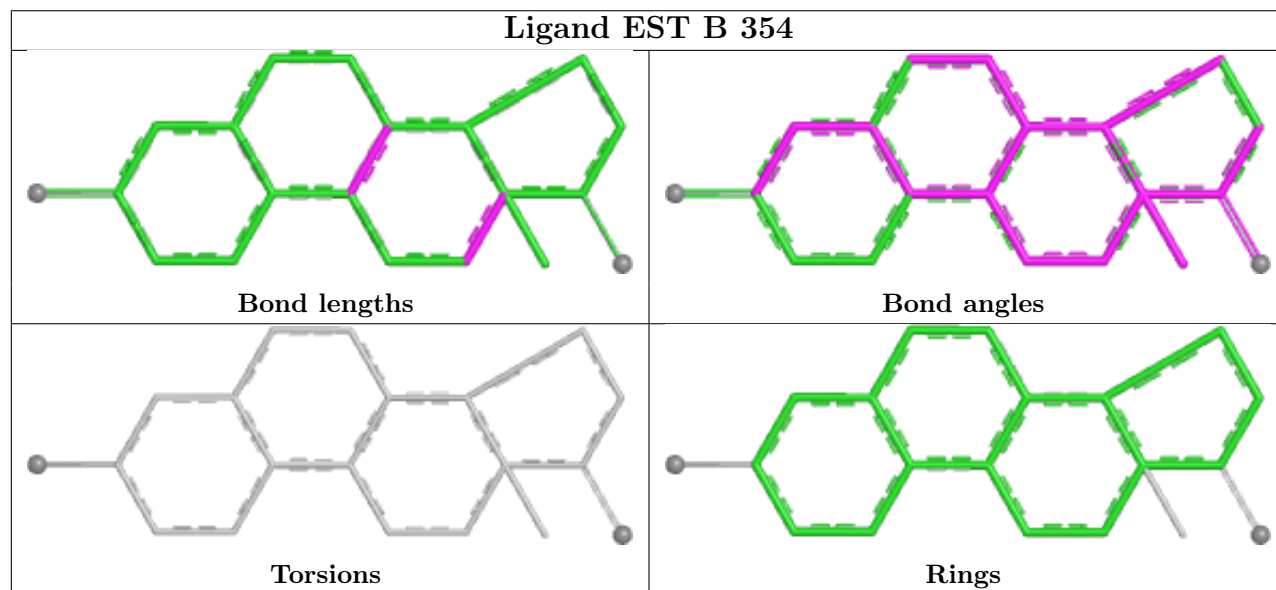
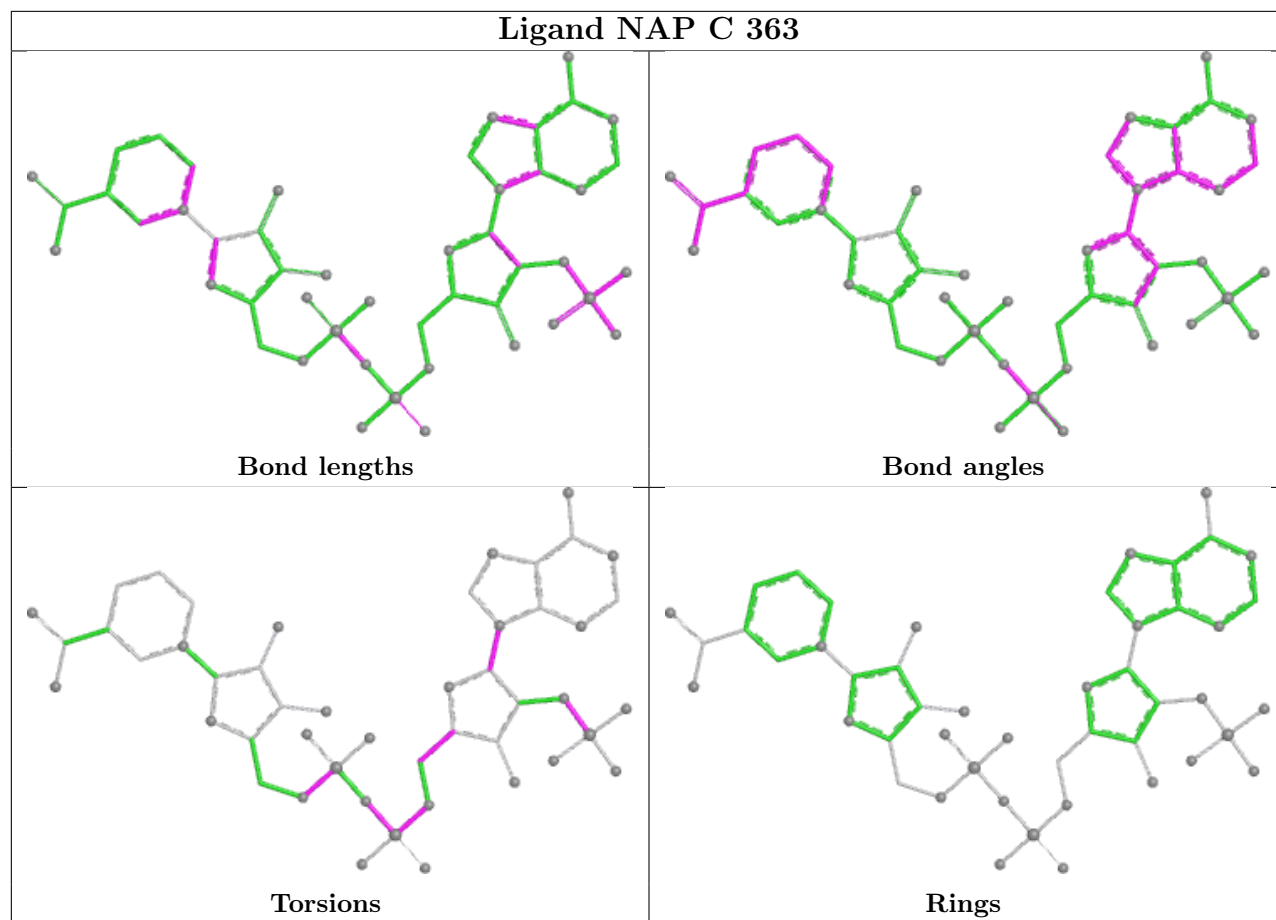
10 monomers are involved in 49 short contacts:

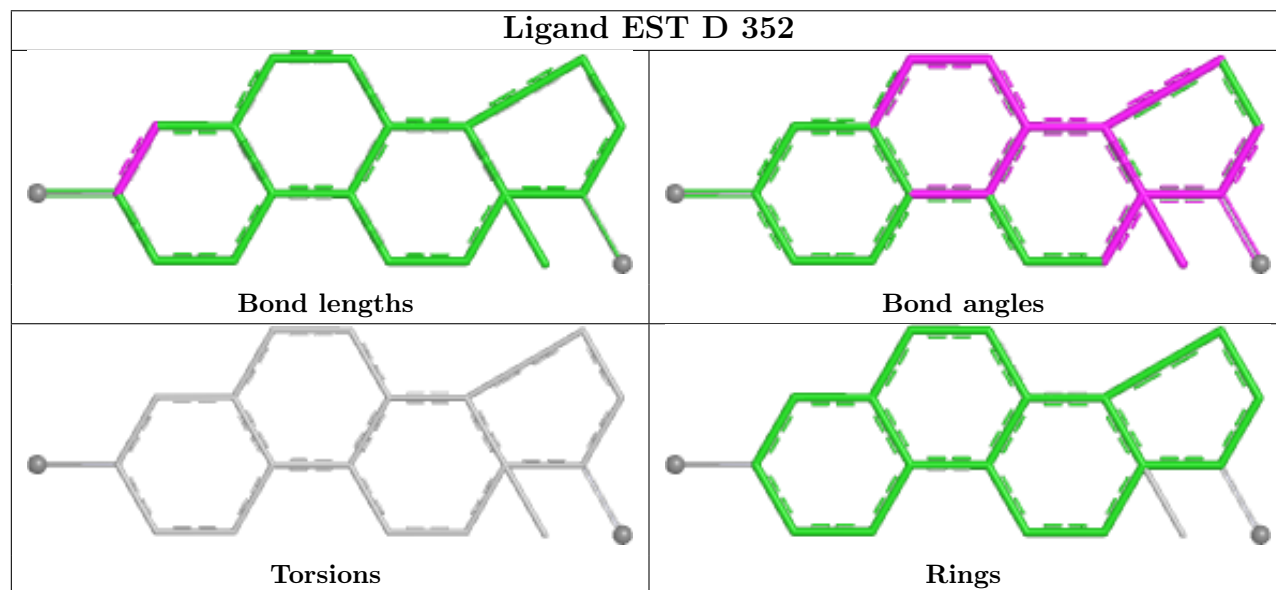
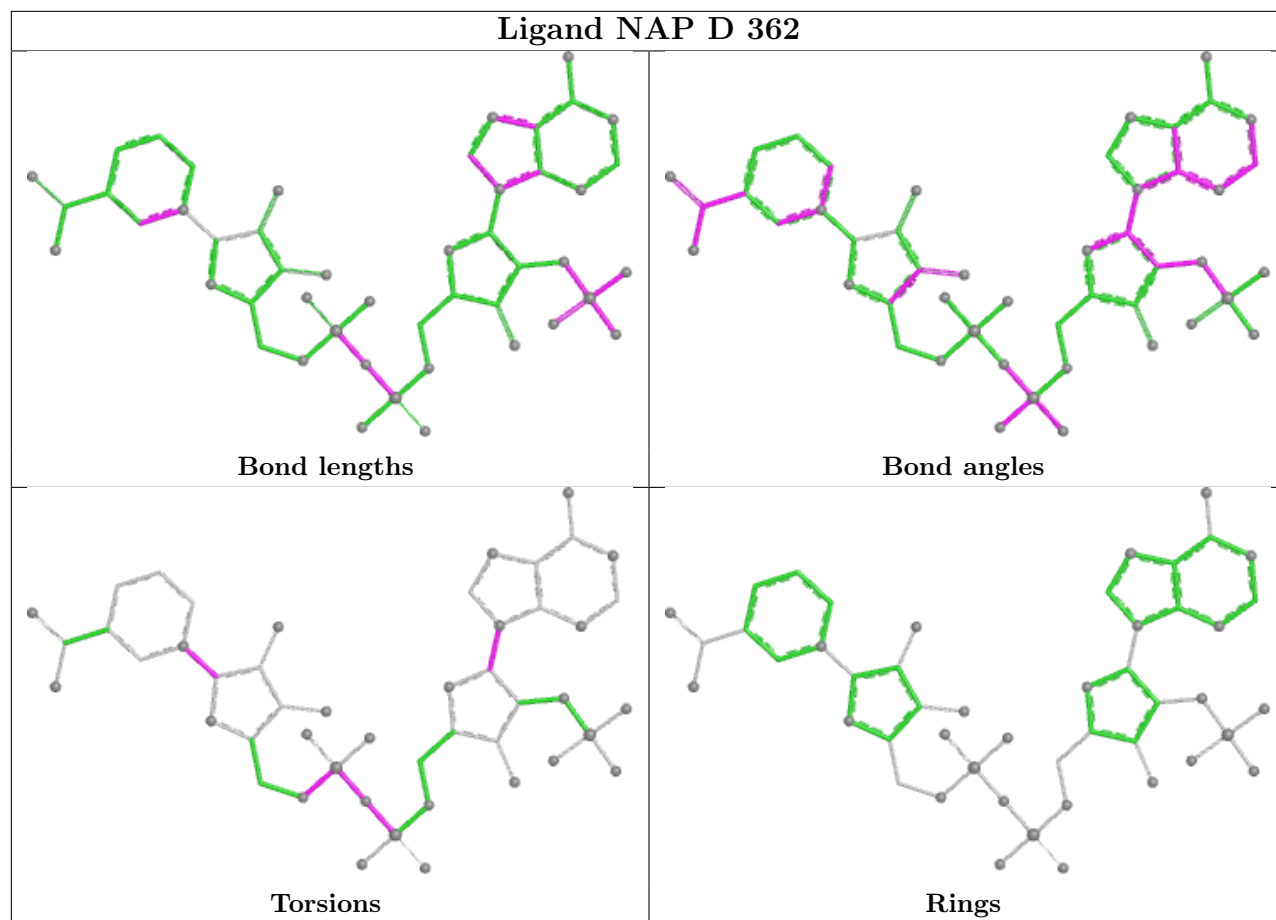
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	351	EST	10	0
4	A	361	NAP	6	0
4	C	363	NAP	5	0
3	B	354	EST	7	0
4	D	362	NAP	5	0
3	D	352	EST	6	0
2	D	402	SO4	2	0
4	B	364	NAP	6	0
3	C	353	EST	3	0
2	C	403	SO4	2	0

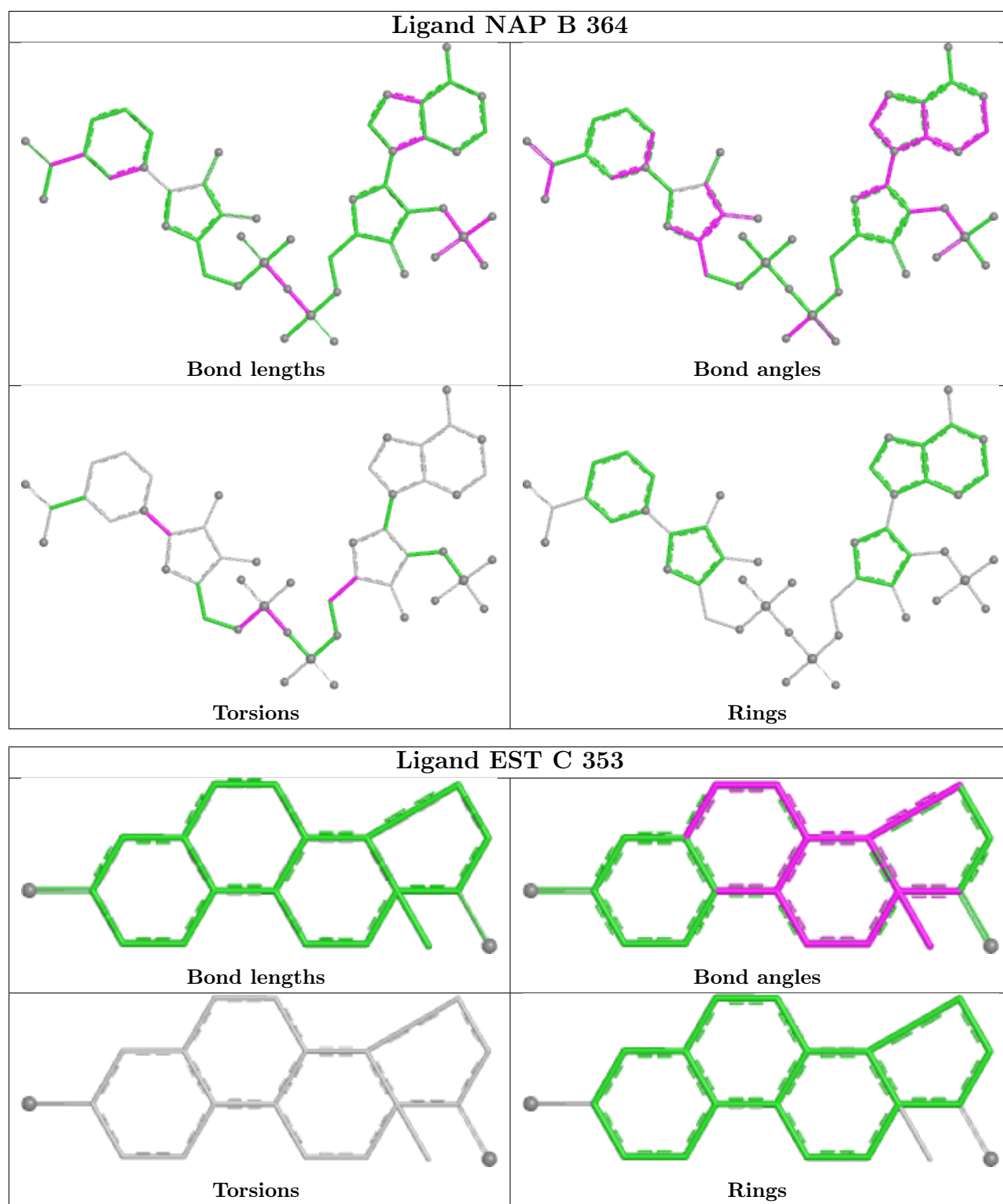
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	281/327 (85%)	-0.11	11 (3%) 43 39	8, 22, 47, 55	10 (3%)
1	B	280/327 (85%)	-0.18	9 (3%) 50 46	8, 22, 41, 52	13 (4%)
1	C	285/327 (87%)	0.03	13 (4%) 37 34	8, 23, 48, 56	11 (3%)
1	D	281/327 (85%)	-0.23	9 (3%) 50 46	10, 22, 42, 50	10 (3%)
All	All	1127/1308 (86%)	-0.12	42 (3%) 45 41	8, 22, 45, 56	44 (3%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	264	ARG	10.0
1	D	2	ARG	7.5
1	A	281	ARG	7.5
1	C	201	GLU	7.3
1	D	202	GLU	7.0
1	B	268	ASP	6.9
1	B	264	ARG	5.6
1	A	264	ARG	5.6
1	A	197	LEU	5.5
1	C	197	LEU	5.3
1	C	258	ARG	5.1
1	B	203	VAL	5.1
1	D	267	LEU	5.0
1	A	2	ARG	4.8
1	C	228	GLU	4.4
1	C	268	ASP	4.4
1	D	245	ARG	4.4
1	D	197	LEU	3.9
1	A	131	ARG	3.9
1	C	235	GLU	3.7
1	B	197	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	198	GLY	3.6
1	A	1	ALA	3.4
1	B	206	ARG	3.4
1	A	228	GLU	3.2
1	C	196	VAL	3.1
1	A	285	GLY	2.9
1	B	260	LEU	2.9
1	A	28	GLN	2.8
1	C	285	GLY	2.7
1	D	1	ALA	2.6
1	A	205	ASP	2.5
1	B	273	SER	2.3
1	C	199	SER	2.3
1	B	78	ARG	2.2
1	D	196	VAL	2.2
1	D	206	ARG	2.2
1	C	28	GLN	2.2
1	D	207	THR	2.2
1	C	198	GLY	2.1
1	B	281	ARG	2.0
1	C	266	ARG	2.0

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 [i](#)

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($\text{\AA}^2$)	Q<0.9
3	EST	B	354	20/20	0.65	0.16	56,58,59,59	0
3	EST	D	352	20/20	0.74	0.15	47,50,51,51	0

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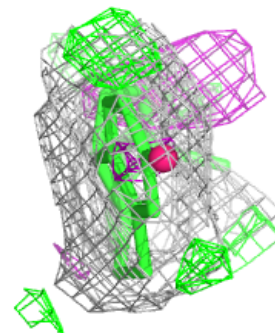
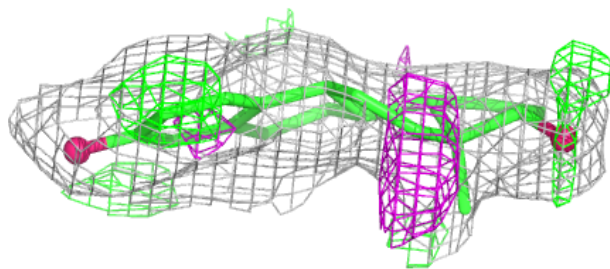
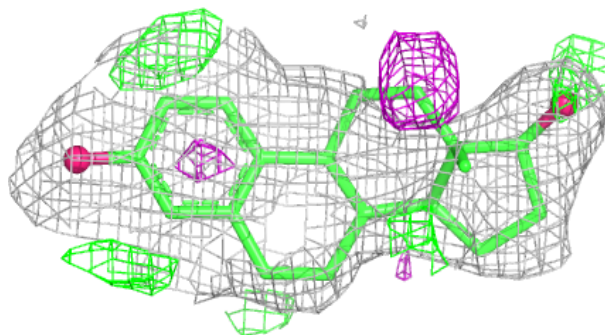
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EST	A	351	20/20	0.76	0.16	48,50,51,52	0
3	EST	C	353	20/20	0.82	0.13	61,63,64,64	1
2	SO4	A	401	5/5	0.92	0.09	42,43,43,43	0
2	SO4	C	403	5/5	0.92	0.10	43,43,44,44	0
2	SO4	D	402	5/5	0.95	0.09	42,43,43,43	0
2	SO4	B	400	5/5	0.96	0.07	46,47,47,47	0
4	NAP	A	361	48/48	0.97	0.07	13,16,19,21	0
4	NAP	C	363	48/48	0.97	0.06	13,17,21,23	0
4	NAP	B	364	48/48	0.98	0.06	10,17,21,23	0
4	NAP	D	362	48/48	0.98	0.06	12,17,21,22	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.

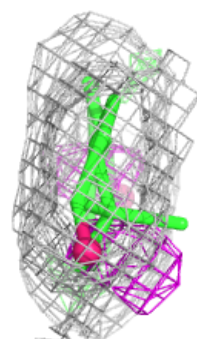
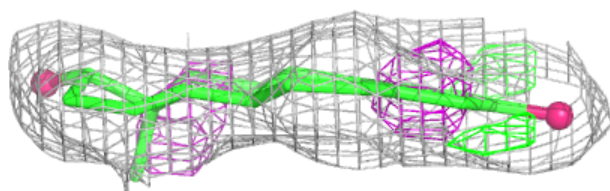
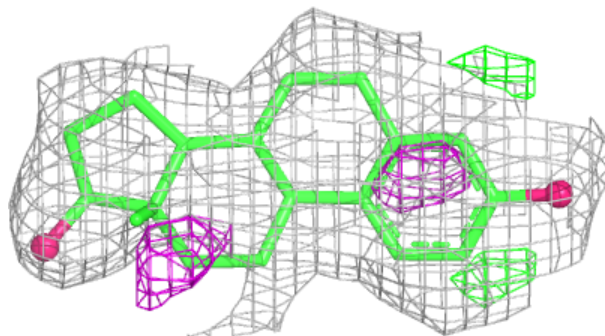
Electron density around EST B 354:

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

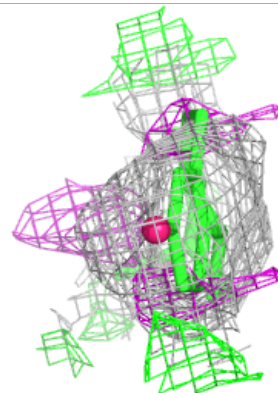
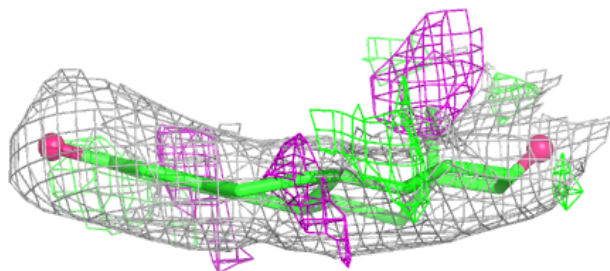
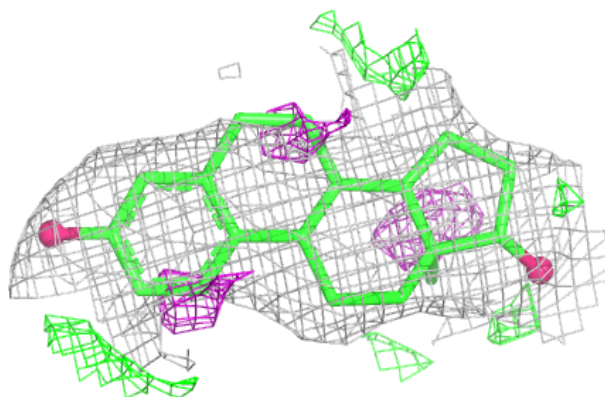


Electron density around EST D 352:

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

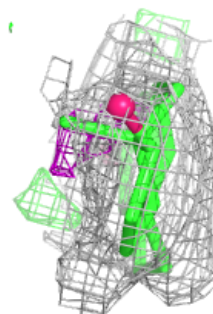
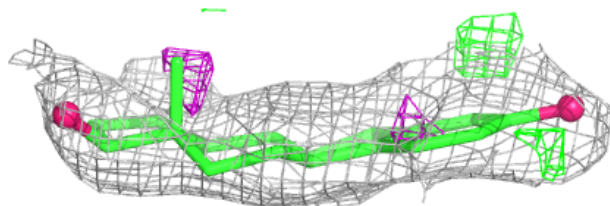
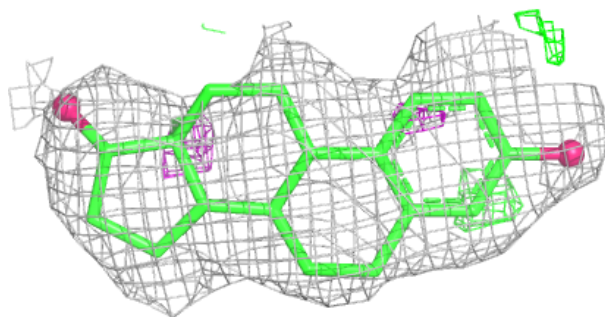
**Electron density around EST A 351:**

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

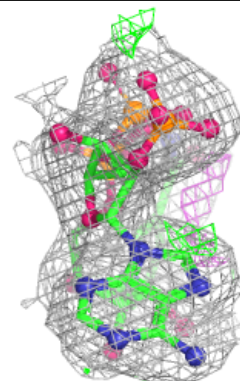
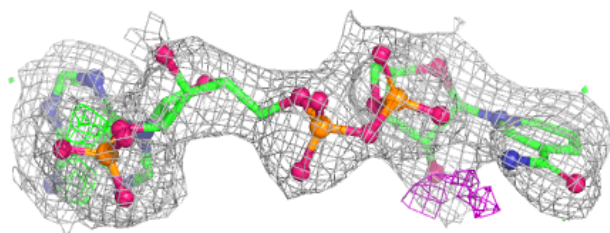
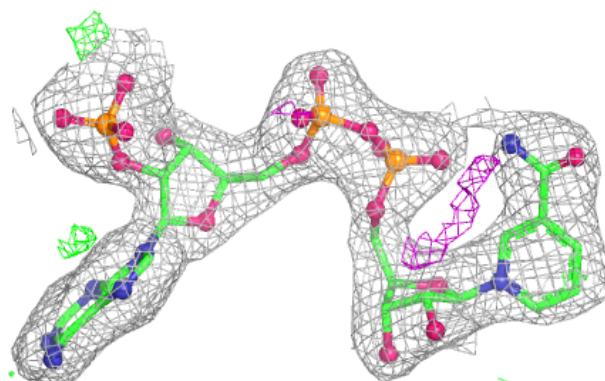


Electron density around EST C 353:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

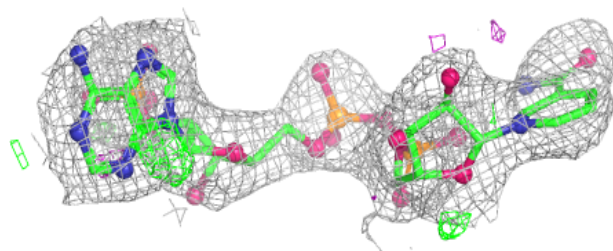
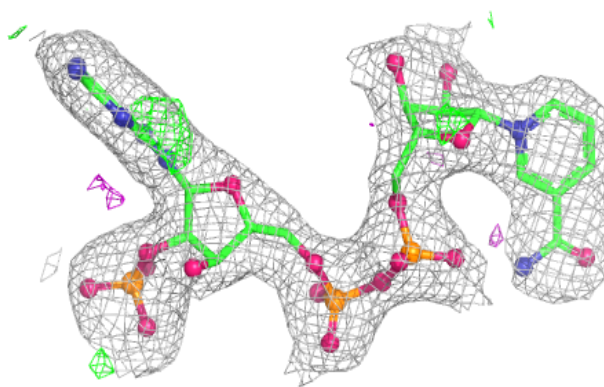
**Electron density around NAP A 361:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

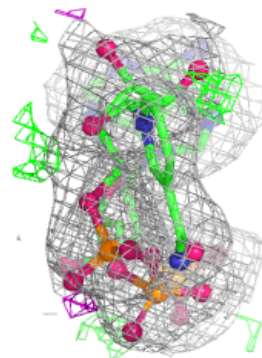
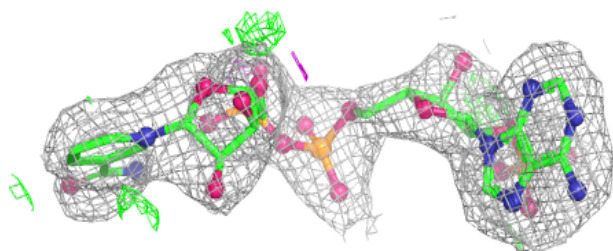
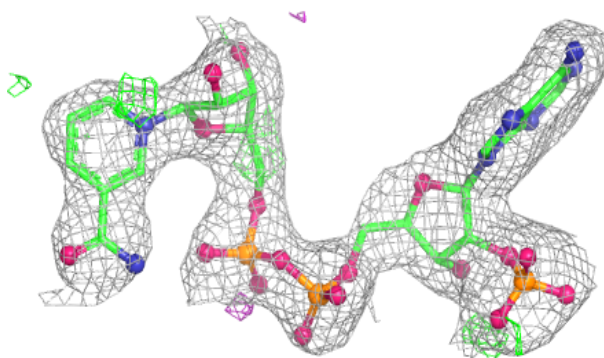


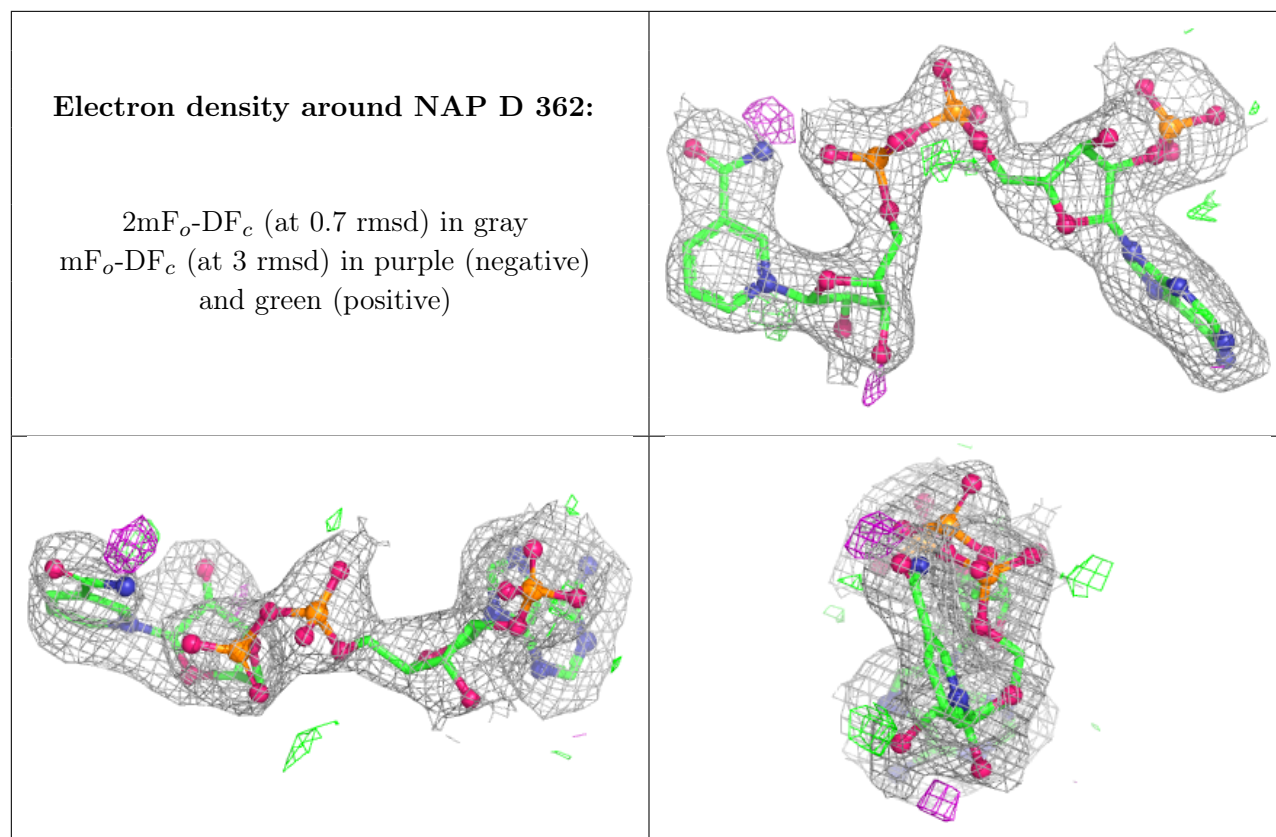
Electron density around NAP C 363:

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

**Electron density around NAP B 364:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.