



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2026 – 04:34 am BST

PDB ID : 2C3O / pdb_00002c3o
Title : CRYSTAL STRUCTURE OF THE FREE RADICAL INTERMEDIATE
OF PYRUVATE:FERREDOXIN OXIDOREDUCTASE FROM *Desulfovibrio*
africanus
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Fontecilla-Camps, J.C.
Deposited on : 2005-10-11
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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

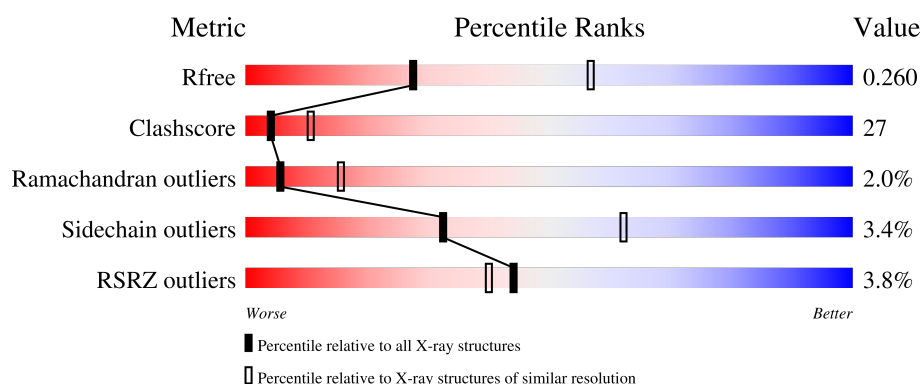
1 Overall quality at a glance

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	1231	5% 54% 42% .
1	B	1231	3% 55% 41% .

2 Entry composition [i](#)

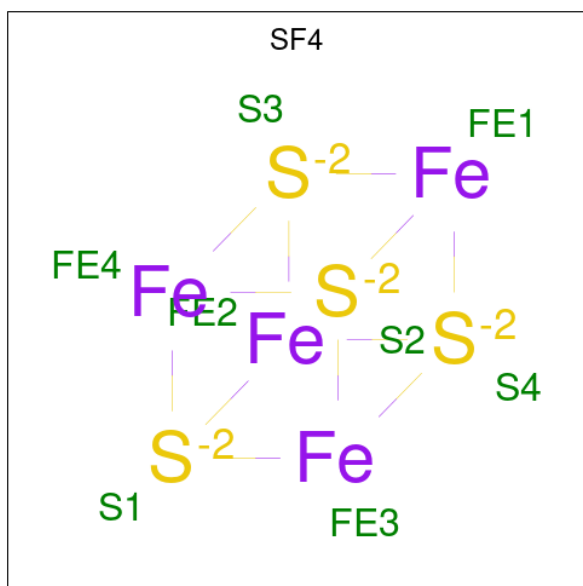
There are 7 unique types of molecules in this entry. The entry contains 19451 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PYRUVATE-FERREDOXIN OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1231	Total	C	N	O	S	0	0	0
			9383	5941	1599	1784	59			
1	B	1231	Total	C	N	O	S	0	0	0
			9383	5941	1599	1784	59			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



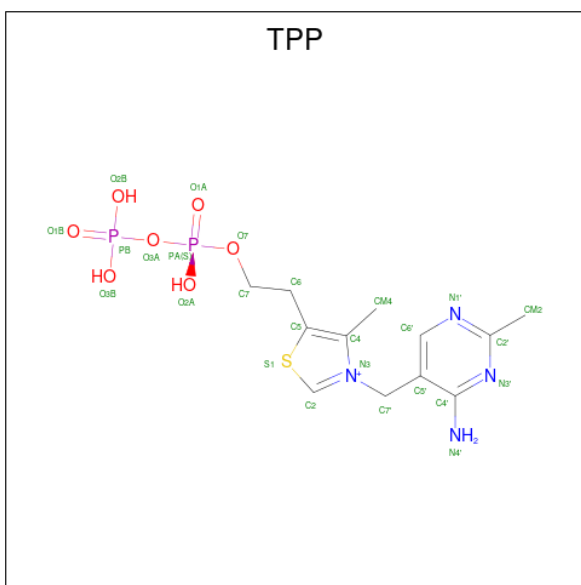
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $\text{C}_{12}\text{H}_{19}\text{N}_4\text{O}_7\text{P}_2\text{S}$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

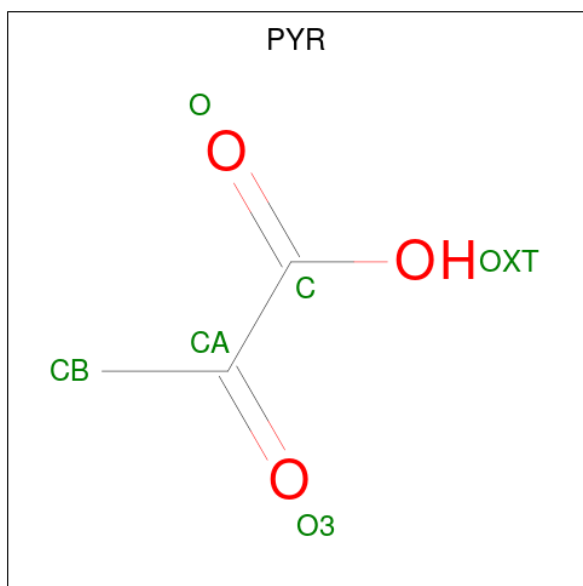
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

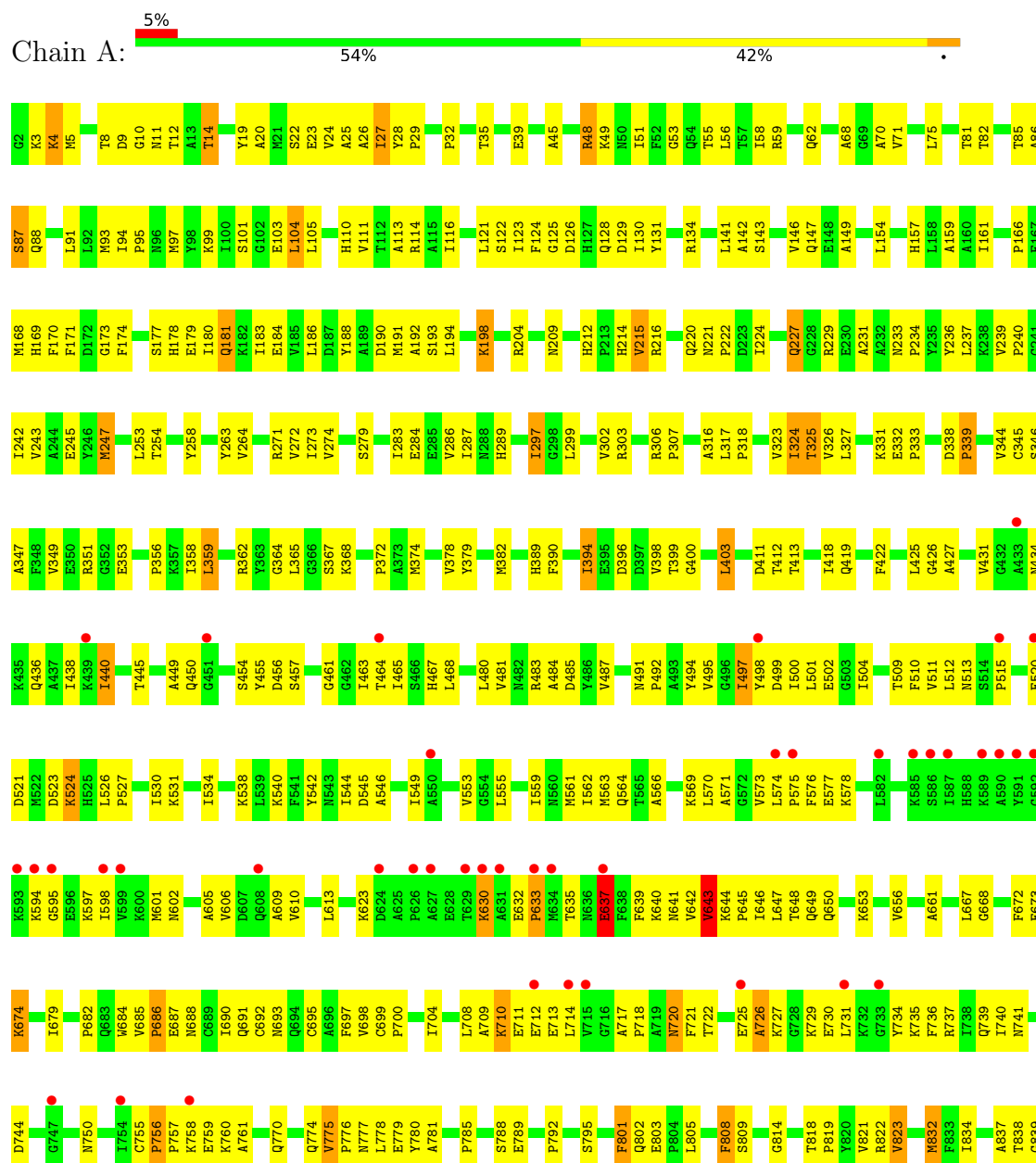
- Molecule 7 is water.

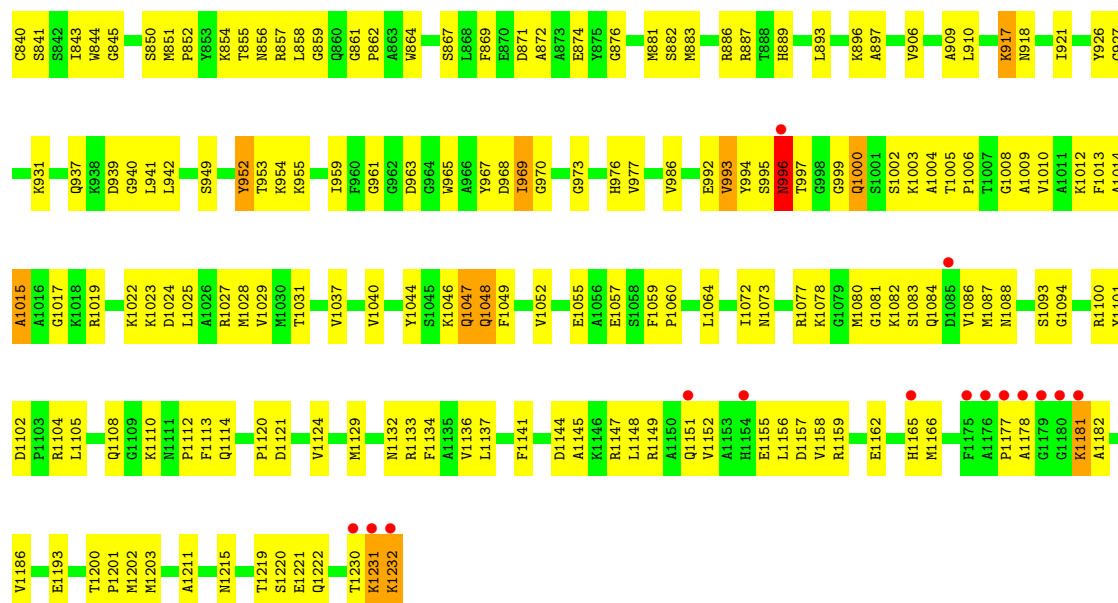
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	262	Total	O	0	0
			262	262		
7	B	307	Total	O	0	0
			307	307		

3 Residue-property plots

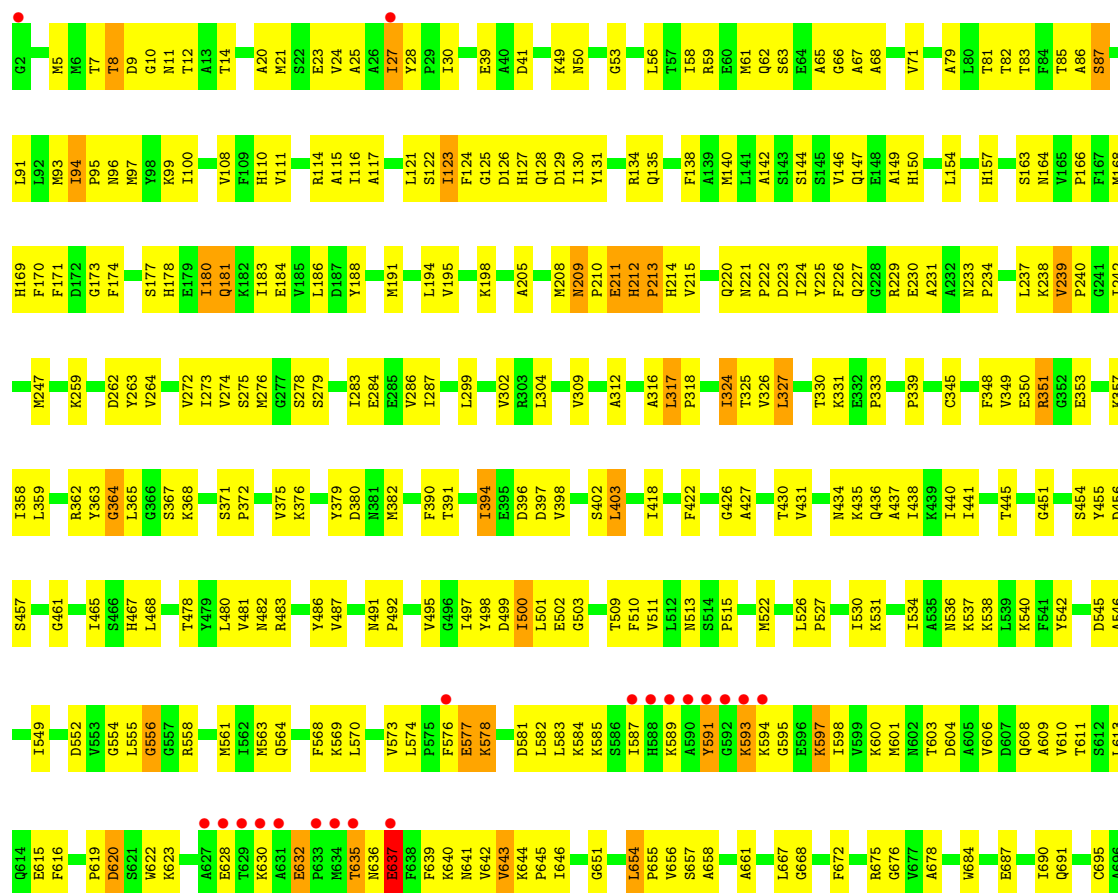
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

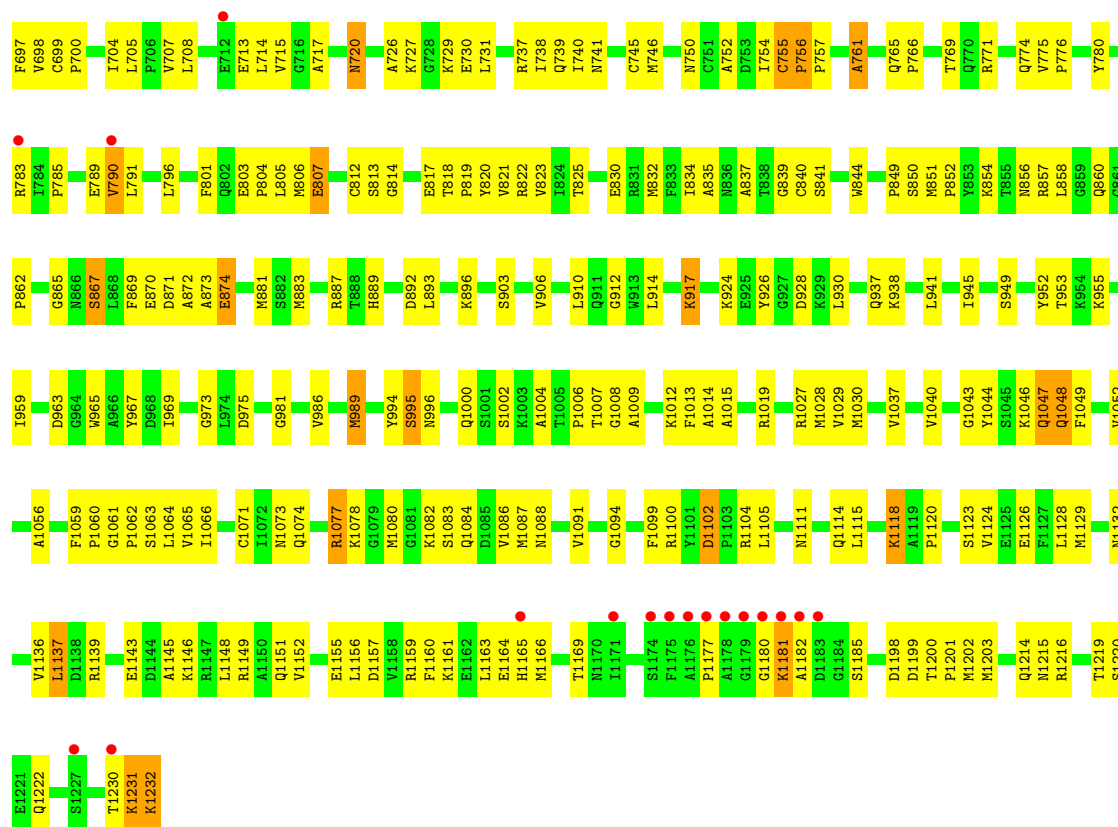
• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE





• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.65Å 145.24Å 204.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.11 – 2.70 38.11 – 2.71	Depositor EDS
% Data completeness (in resolution range)	94.4 (38.11-2.70) 94.5 (38.11-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.268 0.197 , 0.260	Depositor DCC
R_{free} test set	3476 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19451	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SF4, PYR, TPP, MG

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	0.33	0/9585	0.86	15/12954 (0.1%)
1	B	0.34	0/9585	0.88	27/12954 (0.2%)
All	All	0.34	0/19170	0.87	42/25908 (0.2%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	756	PRO	N-CA-C	8.72	121.34	110.70
1	B	125	GLY	N-CA-C	8.67	124.51	112.37
1	A	125	GLY	N-CA-C	8.43	124.87	111.64
1	A	755	CYS	CA-C-N	7.68	128.29	120.38
1	A	755	CYS	C-N-CA	7.68	128.29	120.38
1	A	1014	ALA	N-CA-C	-7.42	102.30	112.03
1	B	247	MET	N-CA-C	-7.21	103.43	111.28
1	B	756	PRO	N-CA-C	6.86	119.06	110.70
1	A	643	VAL	N-CA-C	6.72	117.47	110.62
1	B	1077	ARG	N-CA-C	6.60	119.03	111.11
1	B	500	ILE	N-CA-C	6.55	116.71	110.42
1	B	771	ARG	N-CA-C	6.40	117.92	111.07
1	B	94	ILE	CB-CA-C	-6.34	107.68	113.70
1	B	212	HIS	CA-C-N	6.26	126.23	120.03
1	B	212	HIS	C-N-CA	6.26	126.23	120.03
1	B	351	ARG	N-CA-C	-6.15	105.26	112.89
1	B	213	PRO	N-CA-C	6.01	120.42	111.41
1	B	755	CYS	CA-C-N	5.76	126.32	120.38
1	B	755	CYS	C-N-CA	5.76	126.32	120.38
1	A	247	MET	N-CA-C	-5.62	105.30	111.82
1	B	65	ALA	N-CA-C	-5.53	105.41	111.82
1	B	637	GLU	N-CA-C	-5.49	105.45	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	641	ASN	N-CA-C	5.46	119.94	113.28
1	A	698	VAL	N-CA-C	5.45	116.94	111.00
1	A	832	MET	N-CA-C	5.41	118.05	109.50
1	B	790	VAL	N-CA-C	5.38	115.82	110.23
1	A	485	ASP	N-CA-C	-5.35	106.92	113.50
1	B	591	TYR	CB-CA-C	-5.28	110.05	117.23
1	B	1102	ASP	CA-C-N	5.28	124.91	119.05
1	B	1102	ASP	C-N-CA	5.28	124.91	119.05
1	B	889	HIS	N-CA-C	-5.28	105.42	111.07
1	A	1141	PHE	CA-C-N	5.26	125.07	119.28
1	A	1141	PHE	C-N-CA	5.26	125.07	119.28
1	B	807	GLU	N-CA-C	5.24	117.16	109.24
1	B	801	PHE	N-CA-C	-5.20	106.25	112.59
1	A	637	GLU	N-CA-C	-5.15	106.84	113.02
1	B	761	ALA	N-CA-C	-5.15	106.68	113.17
1	B	1014	ALA	N-CA-C	-5.10	104.39	110.41
1	A	775	VAL	CB-CA-C	-5.09	108.86	113.70
1	B	620	ASP	N-CA-C	-5.07	106.60	112.89
1	A	801	PHE	N-CA-C	-5.02	106.75	112.92
1	B	205	ALA	N-CA-C	5.01	116.44	110.97

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	9383	0	9263	563	0
1	B	9383	0	9262	538	0
2	A	24	0	0	0	0
2	B	24	0	0	1	0
3	A	26	0	16	1	0
3	B	26	0	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	6	0	0	0	0
6	B	6	0	0	0	0
7	A	262	0	0	13	0
7	B	307	0	0	13	0
All	All	19451	0	18557	1026	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 27.

All (1026) 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:A:1200:THR:HG22	1:A:1202:MET:H	1.19	1.06
1:B:817:GLU:HB3	1:B:989:MET:HE2	1.30	1.05
1:B:1077:ARG:HH11	1:B:1077:ARG:HB2	1.22	1.02
1:B:239:VAL:HG13	1:B:240:PRO:HD3	1.42	1.02
1:A:198:LYS:H	1:A:198:LYS:HD2	1.24	1.00
1:A:147:GLN:HE22	1:A:184:GLU:H	1.10	0.97
1:A:690:ILE:HD11	1:A:692:CYS:HB3	1.44	0.97
1:A:1019:ARG:HH12	1:B:1180:GLY:HA3	1.27	0.96
1:B:198:LYS:H	1:B:198:LYS:HD2	1.28	0.96
1:B:1077:ARG:HB2	1:B:1077:ARG:NH1	1.81	0.94
1:B:914:LEU:HA	1:B:917:LYS:HZ3	1.30	0.94
1:B:873:ALA:HA	1:B:959:ILE:HD13	1.50	0.94
1:B:12:THR:HG22	1:B:39:GLU:OE1	1.68	0.93
1:B:708:LEU:HD21	1:B:731:LEU:HD22	1.51	0.93
1:B:883:MET:HE2	1:B:955:LYS:HG3	1.51	0.93
1:B:1200:THR:HG22	1:B:1202:MET:H	1.35	0.91
1:B:1102:ASP:OD1	1:B:1104:ARG:HG2	1.72	0.90
1:A:1080:MET:H	1:B:1215:ASN:ND2	1.71	0.89
1:B:274:VAL:HG23	1:B:324:ILE:HD11	1.55	0.89
1:A:445:THR:HG21	1:A:574:LEU:HD21	1.57	0.87
1:A:1215:ASN:ND2	1:B:1080:MET:H	1.72	0.87
1:B:639:PHE:HA	1:B:643:VAL:HG13	1.54	0.87
1:A:737:ARG:HH11	1:A:739:GLN:HE22	1.23	0.86
1:B:643:VAL:HB	1:B:849:PRO:HB2	1.55	0.86
1:A:726:ALA:HB1	1:A:731:LEU:HB3	1.57	0.85
1:A:455:TYR:HB2	1:B:1201:PRO:HG3	1.60	0.84
1:B:914:LEU:HD13	1:B:917:LYS:HZ1	1.44	0.83
1:A:509:THR:HG22	1:A:540:LYS:HB2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1231:LYS:HG3	1:B:1232:LYS:H	1.45	0.81
1:B:454:SER:HB3	1:B:465:ILE:HG23	1.61	0.81
1:A:12:THR:HG22	1:A:39:GLU:OE2	1.81	0.81
1:A:186:LEU:HD21	1:A:254:THR:HG22	1.63	0.81
1:A:1129:MET:HE3	1:A:1149:ARG:HD3	1.62	0.81
1:B:1006:PRO:HG2	1:B:1009:ALA:HB2	1.62	0.81
1:A:1077:ARG:HH11	1:A:1077:ARG:HB2	1.44	0.80
1:A:128:GLN:HE22	1:B:229:ARG:HE	1.29	0.80
1:B:823:VAL:HG21	1:B:1049:PHE:HE2	1.47	0.80
1:B:9:ASP:OD2	1:B:12:THR:HG23	1.82	0.80
1:A:194:LEU:HD21	1:A:253:LEU:HD11	1.64	0.79
1:A:325:THR:HG22	1:A:382:MET:SD	2.23	0.79
1:A:273:ILE:HD13	1:A:325:THR:HG23	1.65	0.79
1:B:1132:ASN:HD21	1:B:1139:ARG:HH12	1.28	0.79
1:B:239:VAL:CG1	1:B:240:PRO:HD3	2.14	0.78
1:A:11:ASN:ND2	1:A:177:SER:HB2	1.98	0.78
1:A:398:VAL:HG13	1:A:656:VAL:HG13	1.65	0.77
1:A:1231:LYS:HG3	1:A:1232:LYS:H	1.50	0.77
1:A:491:ASN:HD22	1:A:492:PRO:HD2	1.48	0.77
1:B:691:GLN:HE22	1:B:727:LYS:H	1.30	0.77
1:A:1093:SER:HB2	1:A:1124:VAL:HG22	1.68	0.76
1:A:147:GLN:NE2	1:A:184:GLU:H	1.84	0.76
1:A:1219:THR:HG22	1:A:1221:GLU:H	1.51	0.76
1:B:1047:GLN:NE2	1:B:1047:GLN:H	1.82	0.76
1:A:1219:THR:HB	1:A:1222:GLN:HG3	1.67	0.76
1:A:8:THR:HB	1:A:12:THR:OG1	1.87	0.75
1:A:867:SER:O	1:B:99:LYS:HE3	1.87	0.75
1:A:438:ILE:HD11	1:A:468:LEU:HD22	1.68	0.75
1:B:1219:THR:HB	1:B:1222:GLN:HG3	1.66	0.75
1:A:1102:ASP:OD1	1:A:1104:ARG:HG2	1.87	0.75
1:B:994:TYR:CE1	1:B:1002:SER:HB3	2.22	0.74
1:B:837:ALA:HB2	1:B:872:ALA:HB2	1.70	0.74
1:A:1077:ARG:HB2	1:A:1077:ARG:NH1	2.02	0.74
1:A:287:ILE:HD11	1:A:379:TYR:OH	1.88	0.74
1:A:809:SER:HB2	1:A:844:TRP:O	1.88	0.74
1:A:1019:ARG:NH1	1:B:1181:LYS:H	1.85	0.74
1:A:1145:ALA:HB1	1:A:1149:ARG:HH12	1.53	0.74
1:B:573:VAL:HG23	1:B:574:LEU:HG	1.70	0.74
1:B:578:LYS:HB3	7:B:2151:HOH:O	1.88	0.74
1:B:1083:SER:O	1:B:1087:MET:HG3	1.88	0.74
1:B:644:LYS:HB3	1:B:645:PRO:HD3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:VAL:HG23	1:A:504:ILE:HD13	1.70	0.73
1:A:909:ALA:HA	1:A:926:TYR:HD2	1.53	0.73
1:A:1215:ASN:HD21	1:B:1080:MET:H	1.35	0.73
1:B:593:LYS:HD2	1:B:594:LYS:N	2.02	0.73
1:A:639:PHE:HA	1:A:643:VAL:HG22	1.69	0.73
1:B:893:LEU:HB3	1:B:945:ILE:HD11	1.70	0.73
1:B:1143:GLU:O	1:B:1146:LYS:HG2	1.88	0.73
1:B:438:ILE:HD11	1:B:468:LEU:HD22	1.71	0.72
1:A:1132:ASN:O	1:A:1136:VAL:HG22	1.89	0.72
1:A:566:ALA:HA	1:A:613:LEU:HD21	1.71	0.72
1:B:7:THR:HB	1:B:180:ILE:HD11	1.69	0.72
1:B:430:THR:HG22	1:B:434:ASN:HD21	1.54	0.72
1:B:1132:ASN:ND2	1:B:1139:ARG:HH12	1.86	0.72
1:B:56:LEU:HD23	1:B:58:ILE:HD11	1.71	0.72
1:B:1007:THR:HB	1:B:1152:VAL:HG22	1.70	0.72
1:B:445:THR:HG21	1:B:574:LEU:HD21	1.72	0.72
1:B:123:ILE:HD13	1:B:123:ILE:H	1.55	0.72
1:A:222:PRO:HD3	1:B:124:PHE:CE2	2.25	0.71
1:B:11:ASN:ND2	1:B:177:SER:HB2	2.05	0.71
1:B:121:LEU:HD23	1:B:122:SER:N	2.04	0.71
1:A:1080:MET:H	1:B:1215:ASN:HD21	1.37	0.71
1:A:750:ASN:HD22	1:A:1084:GLN:HG2	1.55	0.71
1:A:142:ALA:HB2	1:A:170:PHE:CZ	2.26	0.71
1:B:775:VAL:HB	1:B:776:PRO:HD3	1.73	0.70
1:A:82:THR:HG21	1:A:157:HIS:HE1	1.56	0.70
1:B:1132:ASN:HD21	1:B:1139:ARG:NH1	1.90	0.70
1:A:874:GLU:HG2	1:B:66:GLY:HA2	1.73	0.70
1:A:27:ILE:HG22	1:A:28:TYR:N	2.06	0.70
1:A:247:MET:HE2	1:A:258:TYR:HB2	1.72	0.70
1:A:297:ILE:HB	1:A:379:TYR:CE2	2.26	0.70
1:A:606:VAL:O	1:A:610:VAL:HG23	1.92	0.70
1:B:1129:MET:HE3	1:B:1149:ARG:HD3	1.72	0.70
1:A:710:LYS:H	1:A:710:LYS:HD2	1.57	0.70
1:A:467:HIS:CD2	1:A:481:VAL:H	2.10	0.69
1:A:94:ILE:HB	1:A:95:PRO:HD3	1.73	0.69
1:B:914:LEU:HA	1:B:917:LYS:NZ	2.05	0.69
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.41	0.69
1:A:526:LEU:O	1:A:531:LYS:HE3	1.91	0.68
1:B:180:ILE:HD13	1:B:180:ILE:C	2.18	0.68
1:B:1040:VAL:HG12	1:B:1048:GLN:HE22	1.58	0.68
1:A:1083:SER:O	1:A:1087:MET:HG3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:GLN:O	1:A:1155:GLU:HG3	1.93	0.68
1:B:174:PHE:HA	1:B:178:HIS:HB2	1.76	0.68
1:A:575:PRO:HG2	1:A:578:LYS:HB3	1.76	0.68
1:A:708:LEU:HD21	1:A:731:LEU:HD22	1.76	0.67
1:A:1108:GLN:HE21	1:A:1110:LYS:HD2	1.59	0.67
1:B:209:ASN:OD1	1:B:211:GLU:HB2	1.93	0.67
1:B:1043:GLY:HA2	1:B:1084:GLN:HE21	1.59	0.67
1:A:857:ARG:HG3	1:A:858:LEU:HD12	1.74	0.67
1:B:5:MET:CE	1:B:184:GLU:HB2	2.24	0.67
1:B:926:TYR:O	1:B:930:LEU:HD13	1.94	0.67
1:A:147:GLN:HE22	1:A:184:GLU:N	1.90	0.67
1:B:224:ILE:HA	1:B:227:GLN:OE1	1.95	0.67
1:A:143:SER:OG	1:A:171:PHE:HB3	1.93	0.67
1:B:398:VAL:HG13	1:B:656:VAL:HG23	1.76	0.67
1:A:27:ILE:HD12	1:A:27:ILE:N	2.09	0.67
1:B:691:GLN:NE2	1:B:727:LYS:H	1.92	0.67
1:A:110:HIS:HD2	1:A:169:HIS:HD2	1.41	0.66
1:A:497:ILE:HG13	1:A:498:TYR:HD1	1.60	0.66
1:A:759:GLU:CD	1:A:759:GLU:H	2.02	0.66
1:A:897:ALA:HB3	1:A:910:LEU:HD21	1.77	0.66
1:A:832:MET:HE2	1:A:834:ILE:HD11	1.77	0.66
1:A:889:HIS:O	1:A:893:LEU:HD13	1.95	0.66
1:A:1019:ARG:NH1	1:B:1180:GLY:HA3	2.06	0.66
1:B:279:SER:O	1:B:283:ILE:HG13	1.95	0.66
1:B:1230:THR:O	1:B:1232:LYS:HG2	1.96	0.66
1:A:51:ILE:HB	1:A:192:ALA:HB2	1.76	0.66
1:A:10:GLY:O	1:A:14:THR:HG23	1.96	0.66
1:A:770:GLN:O	1:A:774:GLN:HG2	1.96	0.66
1:B:1156:LEU:HD12	1:B:1157:ASP:N	2.10	0.66
1:A:27:ILE:HG22	1:A:28:TYR:H	1.59	0.66
1:B:578:LYS:O	1:B:582:LEU:HD13	1.95	0.66
1:B:594:LYS:NZ	1:B:594:LYS:HB3	2.11	0.66
1:B:345:CYS:O	1:B:349:VAL:HG13	1.96	0.66
1:B:110:HIS:HD2	1:B:169:HIS:CD2	2.14	0.65
1:A:227:GLN:HE22	1:B:368:LYS:NZ	1.95	0.65
1:B:437:ALA:O	1:B:441:ILE:HG12	1.95	0.65
1:A:128:GLN:NE2	1:B:229:ARG:HE	1.95	0.65
1:A:530:ILE:O	1:A:534:ILE:HG12	1.96	0.65
1:A:264:VAL:HG11	1:A:284:GLU:HG3	1.78	0.65
1:A:297:ILE:HD13	1:A:297:ILE:H	1.62	0.65
1:A:737:ARG:NH1	1:A:739:GLN:HE22	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:VAL:HG13	1:B:791:LEU:H	1.60	0.65
1:B:1129:MET:HA	1:B:1129:MET:HE2	1.79	0.64
1:A:840:CYS:SG	1:A:996:ASN:HB3	2.36	0.64
1:B:210:PRO:O	1:B:213:PRO:HD3	1.97	0.64
1:B:1029:VAL:HG23	1:B:1037:VAL:HG21	1.80	0.64
1:A:713:GLU:OE1	1:A:785:PRO:HD2	1.98	0.64
1:A:774:GLN:HE21	1:A:774:GLN:HA	1.63	0.64
1:B:1082:LYS:O	1:B:1086:VAL:HG23	1.97	0.64
1:B:259:LYS:HB2	1:B:262:ASP:OD2	1.98	0.64
1:A:639:PHE:CD1	1:A:643:VAL:HG21	2.32	0.64
1:A:24:VAL:HG13	1:B:881:MET:HE2	1.79	0.64
1:A:750:ASN:ND2	1:A:1084:GLN:HG2	2.13	0.63
1:A:594:LYS:HB2	1:A:598:ILE:HD12	1.80	0.63
1:B:823:VAL:HG21	1:B:1049:PHE:CE2	2.31	0.63
1:A:467:HIS:CE1	1:A:480:LEU:HD22	2.32	0.63
1:A:1006:PRO:HG2	1:A:1009:ALA:HB2	1.80	0.63
1:A:14:THR:HG22	1:A:149:ALA:HB1	1.81	0.63
1:A:390:PHE:HB2	1:A:403:LEU:HD13	1.81	0.63
1:A:969:ILE:HG23	1:A:970:GLY:N	2.14	0.63
1:A:1200:THR:HG23	1:A:1202:MET:HE3	1.81	0.63
1:B:1181:LYS:HG3	1:B:1182:ALA:H	1.62	0.63
1:B:147:GLN:HE22	1:B:184:GLU:H	1.46	0.63
1:A:1015:ALA:HB1	1:B:1185:SER:HB2	1.81	0.62
1:A:1200:THR:CG2	1:A:1202:MET:HE3	2.29	0.62
1:B:91:LEU:HD11	1:B:116:ILE:HD12	1.81	0.62
1:B:593:LYS:CD	1:B:594:LYS:HG3	2.29	0.62
1:A:346:SER:HA	1:A:349:VAL:CG1	2.28	0.62
1:A:1094:GLY:HA3	1:A:1120:PRO:HG3	1.81	0.62
1:B:456:ASP:OD2	1:B:457:SER:N	2.32	0.62
1:B:239:VAL:HG13	1:B:240:PRO:CD	2.23	0.62
1:B:731:LEU:CD2	1:B:790:VAL:HG21	2.29	0.62
1:A:487:VAL:CG2	1:A:504:ILE:HD13	2.29	0.62
1:A:1201:PRO:HG3	1:B:455:TYR:HB2	1.79	0.62
1:B:287:ILE:HD11	1:B:379:TYR:OH	1.98	0.62
1:B:835:ALA:HB3	1:B:959:ILE:HG12	1.81	0.62
1:A:467:HIS:HD2	1:A:481:VAL:H	1.47	0.62
1:B:430:THR:HG22	1:B:434:ASN:ND2	2.14	0.62
1:A:937:GLN:HE21	1:A:939:ASP:H	1.47	0.62
1:A:1019:ARG:HH12	1:B:1180:GLY:CA	2.07	0.62
1:B:8:THR:O	1:B:180:ILE:HA	2.00	0.62
1:B:276:MET:HB2	1:B:302:VAL:CG1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1132:ASN:ND2	1:B:1136:VAL:HG13	2.15	0.62
1:A:691:GLN:HE22	1:A:726:ALA:HA	1.64	0.62
1:B:5:MET:HE1	1:B:184:GLU:HB2	1.82	0.62
1:A:687:GLU:C	1:A:688:ASN:HD22	2.07	0.61
1:A:818:THR:HA	1:A:821:VAL:HG22	1.80	0.61
1:B:398:VAL:HG22	1:B:656:VAL:HG21	1.82	0.61
1:B:497:ILE:HG13	1:B:498:TYR:CD1	2.34	0.61
1:A:609:ALA:O	1:A:613:LEU:HD13	2.00	0.61
1:B:263:TYR:HB2	1:B:316:ALA:HB1	1.82	0.61
1:A:274:VAL:HG21	1:A:324:ILE:HD11	1.83	0.61
1:A:1232:LYS:NZ	1:A:1232:LYS:HB3	2.14	0.61
1:A:338:ASP:HB3	1:A:339:PRO:HD2	1.82	0.61
1:A:497:ILE:HG13	1:A:498:TYR:CD1	2.35	0.61
1:A:639:PHE:CE1	1:A:672:PHE:HB2	2.35	0.61
1:B:569:LYS:C	1:B:570:LEU:HD12	2.25	0.61
1:A:99:LYS:HE3	1:B:867:SER:O	2.01	0.60
1:A:368:LYS:NZ	1:B:227:GLN:HE22	1.98	0.60
1:A:1010:VAL:HG21	1:A:1136:VAL:HG23	1.82	0.60
1:B:221:ASN:HB2	1:B:223:ASP:OD1	2.02	0.60
1:B:806:MET:SD	1:B:852:PRO:HB2	2.41	0.60
1:A:356:PRO:O	1:A:358:ILE:HG13	2.02	0.60
1:B:325:THR:HG22	1:B:382:MET:SD	2.41	0.60
1:B:593:LYS:HD3	1:B:594:LYS:HG3	1.83	0.60
1:A:1019:ARG:HH12	1:B:1181:LYS:H	1.48	0.60
1:B:434:ASN:O	1:B:438:ILE:HG12	2.01	0.60
1:B:434:ASN:HB3	1:B:468:LEU:HD11	1.83	0.60
1:A:3:LYS:NZ	1:A:254:THR:HA	2.17	0.60
1:B:1043:GLY:HA3	1:B:1087:MET:HB2	1.83	0.60
1:A:931:LYS:HE2	1:A:949:SER:HB2	1.82	0.60
1:A:976:HIS:CE1	1:B:61:MET:HA	2.36	0.60
1:A:331:LYS:O	1:A:333:PRO:HD3	2.02	0.60
1:A:1017:GLY:HA3	1:A:1137:LEU:HD11	1.84	0.60
1:A:5:MET:HE1	1:A:184:GLU:HB2	1.83	0.60
1:A:279:SER:O	1:A:283:ILE:HG12	2.02	0.60
1:A:1148:LEU:O	1:A:1152:VAL:HG23	2.01	0.60
1:A:1129:MET:HG3	7:A:2242:HOH:O	2.01	0.60
1:A:1219:THR:HG22	1:A:1221:GLU:N	2.17	0.60
1:B:67:ALA:O	1:B:71:VAL:HG23	2.02	0.60
1:A:650:GLN:HB3	1:A:653:LYS:HZ1	1.65	0.59
1:B:27:ILE:HD13	1:B:28:TYR:N	2.17	0.59
1:B:917:LYS:NZ	1:B:917:LYS:HB3	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:VAL:HG11	1:A:1064:LEU:HD13	1.82	0.59
1:B:140:MET:HE3	1:B:168:MET:CE	2.32	0.59
1:B:509:THR:HG22	1:B:540:LYS:HD3	1.84	0.59
1:B:872:ALA:HB3	1:B:965:TRP:CE2	2.37	0.59
1:B:737:ARG:HH11	1:B:739:GLN:HE22	1.51	0.59
1:B:513:ASN:HB2	1:B:563:MET:HE2	1.85	0.59
1:A:965:TRP:HA	1:A:969:ILE:CG2	2.33	0.59
1:B:869:PHE:CE2	1:B:969:ILE:HG21	2.38	0.59
1:A:227:GLN:HE22	1:B:368:LYS:HZ1	1.50	0.59
1:A:1203:MET:HE1	1:B:1073:ASN:HD21	1.67	0.59
1:B:606:VAL:O	1:B:610:VAL:HG23	2.03	0.59
1:B:620:ASP:OD1	1:B:623:LYS:HE2	2.03	0.59
1:B:741:ASN:C	1:B:741:ASN:HD22	2.11	0.59
1:A:239:VAL:CG1	1:A:240:PRO:HD3	2.32	0.59
1:B:1148:LEU:O	1:B:1152:VAL:HG23	2.02	0.59
1:A:345:CYS:O	1:A:349:VAL:HG12	2.03	0.58
1:A:68:ALA:HB2	1:A:93:MET:HG2	1.83	0.58
1:B:1044:TYR:OH	1:B:1118:LYS:HE2	2.03	0.58
1:B:832:MET:HE2	1:B:834:ILE:HD11	1.85	0.58
1:A:515:PRO:HA	1:A:545:ASP:OD2	2.04	0.58
1:A:734:TYR:C	1:A:735:LYS:HD2	2.28	0.58
1:B:351:ARG:HD2	7:B:2094:HOH:O	2.03	0.58
1:A:286:VAL:HG22	1:A:372:PRO:HB3	1.85	0.58
1:B:1064:LEU:HD21	1:B:1066:ILE:HG13	1.84	0.58
1:B:583:LEU:O	1:B:587:ILE:HG13	2.04	0.58
1:B:1043:GLY:HA2	1:B:1084:GLN:NE2	2.18	0.58
1:A:523:ASP:HA	1:A:531:LYS:HE2	1.86	0.58
1:A:850:SER:O	1:A:851:MET:HE2	2.04	0.58
1:B:1048:GLN:O	1:B:1052:VAL:HG23	2.04	0.58
1:B:1012:LYS:O	1:B:1013:PHE:HB2	2.04	0.57
1:A:124:PHE:CE2	1:B:222:PRO:HD3	2.39	0.57
1:A:883:MET:O	1:A:887:ARG:HG3	2.05	0.57
1:A:1024:ASP:O	1:A:1028:MET:HG3	2.04	0.57
1:B:49:LYS:HD2	1:B:53:GLY:O	2.04	0.57
1:B:82:THR:HG22	1:B:83:THR:N	2.19	0.57
1:A:1200:THR:HG22	1:A:1202:MET:N	2.04	0.57
1:B:746:MET:HB3	1:B:813:SER:OG	2.04	0.57
1:B:892:ASP:OD1	1:B:896:LYS:HE3	2.04	0.57
1:B:1064:LEU:C	1:B:1064:LEU:HD23	2.29	0.57
1:A:511:VAL:HA	1:A:542:TYR:O	2.04	0.57
1:B:1232:LYS:NZ	1:B:1232:LYS:HB3	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:THR:O	1:A:39:GLU:HG2	2.04	0.57
1:A:422:PHE:O	1:A:465:ILE:HA	2.03	0.57
1:A:1133:ARG:HG3	1:A:1134:PHE:CD1	2.39	0.57
1:B:283:ILE:O	1:B:287:ILE:HD13	2.04	0.57
1:B:690:ILE:HG12	2:B:2233:SF4:S2	2.45	0.57
1:B:1151:GLN:O	1:B:1155:GLU:HG3	2.04	0.57
1:A:97:MET:HE1	1:A:168:MET:HE3	1.86	0.57
1:A:247:MET:HE2	1:A:258:TYR:CB	2.34	0.57
1:A:690:ILE:CD1	1:A:692:CYS:HB3	2.26	0.57
1:A:845:GLY:HA2	1:A:852:PRO:HG3	1.86	0.57
1:A:426:GLY:O	1:A:427:ALA:HB3	2.05	0.57
1:B:94:ILE:HB	1:B:95:PRO:HD3	1.86	0.57
1:A:838:THR:HB	1:A:869:PHE:HB2	1.86	0.57
1:B:554:GLY:C	1:B:556:GLY:H	2.13	0.57
1:B:857:ARG:HG3	1:B:858:LEU:HD13	1.87	0.57
1:B:130:ILE:HG13	1:B:131:TYR:N	2.20	0.57
1:B:765:GLN:HE21	1:B:765:GLN:HA	1.69	0.57
1:B:110:HIS:HE1	1:B:157:HIS:NE2	2.03	0.56
1:B:114:ARG:NE	1:B:123:ILE:HA	2.20	0.56
1:B:275:SER:O	1:B:302:VAL:HG12	2.05	0.56
1:B:351:ARG:HD3	1:B:353:GLU:HB2	1.87	0.56
1:B:1047:GLN:H	1:B:1047:GLN:HE21	1.51	0.56
1:A:49:LYS:HD2	1:A:53:GLY:O	2.06	0.56
1:A:273:ILE:HG23	1:A:327:LEU:HD13	1.87	0.56
1:A:520:GLU:HG3	1:A:521:ASP:N	2.20	0.56
1:B:86:ALA:HA	1:B:111:VAL:HG23	1.86	0.56
1:B:394:ILE:HD13	1:B:394:ILE:H	1.70	0.56
1:B:581:ASP:O	1:B:585:LYS:HG2	2.06	0.56
1:B:1007:THR:HG21	1:B:1151:GLN:NE2	2.20	0.56
1:A:263:TYR:HB2	1:A:316:ALA:HB1	1.88	0.56
1:A:1181:LYS:HB2	1:A:1181:LYS:NZ	2.20	0.56
1:B:111:VAL:HG13	1:B:170:PHE:HB3	1.88	0.56
1:B:561:MET:HE2	1:B:583:LEU:HD21	1.87	0.56
1:B:180:ILE:HD12	1:B:438:ILE:HG21	1.88	0.56
1:B:526:LEU:O	1:B:531:LYS:HE3	2.05	0.56
1:B:837:ALA:HB2	1:B:872:ALA:CB	2.34	0.56
1:A:454:SER:HB2	1:A:465:ILE:HG23	1.88	0.56
1:A:523:ASP:HA	1:A:531:LYS:CE	2.35	0.56
1:A:561:MET:HE3	1:A:564:GLN:HB3	1.88	0.56
1:B:467:HIS:HD2	1:B:481:VAL:H	1.54	0.56
1:B:906:VAL:O	1:B:910:LEU:HD13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:VAL:CG2	1:A:324:ILE:HD11	2.36	0.56
1:A:374:MET:O	1:A:378:VAL:HG23	2.05	0.56
1:B:912:GLY:HA3	1:B:926:TYR:CD2	2.41	0.56
1:A:700:PRO:HG2	1:A:814:GLY:HA2	1.87	0.56
1:B:364:GLY:HA2	1:B:368:LYS:HB3	1.88	0.56
1:B:856:ASN:HD21	1:B:860:GLN:HB2	1.70	0.56
1:B:790:VAL:HG13	1:B:791:LEU:N	2.21	0.55
1:A:965:TRP:HA	1:A:969:ILE:HG22	1.89	0.55
1:A:26:ALA:C	1:A:27:ILE:HD12	2.32	0.55
1:A:1000:GLN:HA	1:A:1012:LYS:HB2	1.88	0.55
1:B:522:MET:HG2	1:B:616:PHE:CZ	2.41	0.55
1:B:1064:LEU:CD2	1:B:1066:ILE:HG13	2.35	0.55
1:A:27:ILE:HD13	1:A:58:ILE:HG23	1.87	0.55
1:A:642:VAL:O	1:A:646:ILE:HG13	2.06	0.55
1:A:58:ILE:HD12	1:A:58:ILE:N	2.22	0.55
1:A:81:THR:HG22	1:A:82:THR:N	2.21	0.55
1:A:331:LYS:HD3	1:A:362:ARG:NE	2.21	0.55
1:A:396:ASP:O	1:A:400:GLY:HA2	2.07	0.55
1:A:1029:VAL:HG13	1:A:1037:VAL:HG21	1.88	0.55
1:B:436:GLN:O	1:B:440:ILE:HG12	2.07	0.55
1:B:841:SER:HA	1:B:844:TRP:CE2	2.42	0.55
1:A:630:LYS:HD2	1:A:630:LYS:C	2.31	0.55
1:A:869:PHE:CZ	1:A:969:ILE:HG21	2.41	0.55
1:A:881:MET:HE2	1:B:24:VAL:HG13	1.89	0.55
1:B:731:LEU:HD23	1:B:790:VAL:HG21	1.89	0.55
1:B:820:TYR:O	1:B:823:VAL:HG22	2.06	0.55
1:A:906:VAL:O	1:A:910:LEU:HB2	2.06	0.55
1:B:238:LYS:O	1:B:242:ILE:HG12	2.06	0.55
1:A:25:ALA:HB1	1:A:27:ILE:HD11	1.89	0.55
1:A:708:LEU:HD22	1:A:801:PHE:CE1	2.42	0.55
1:A:1100:ARG:HH12	1:A:1114:GLN:NE2	2.03	0.55
1:B:7:THR:HA	1:B:181:GLN:O	2.08	0.55
1:B:208:MET:O	1:B:209:ASN:HB2	2.07	0.55
1:A:188:TYR:HA	1:A:191:MET:HE3	1.89	0.54
1:A:239:VAL:HG13	1:A:240:PRO:HD3	1.88	0.54
1:A:969:ILE:HG23	1:A:970:GLY:H	1.72	0.54
1:A:331:LYS:HD3	1:A:362:ARG:CZ	2.37	0.54
1:A:1158:VAL:HG12	1:A:1162:GLU:OE2	2.07	0.54
1:B:124:PHE:HB3	1:B:367:SER:OG	2.07	0.54
1:B:1059:PHE:HA	1:B:1104:ARG:NH2	2.21	0.54
1:A:434:ASN:O	1:A:438:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LEU:HD12	1:A:513:ASN:H	1.73	0.54
1:A:59:ARG:HG2	1:B:881:MET:HE3	1.89	0.54
1:A:883:MET:HE2	1:A:955:LYS:HG3	1.89	0.54
1:A:1129:MET:HE3	1:A:1149:ARG:CD	2.35	0.54
1:B:635:THR:HG23	1:B:640:LYS:HG3	1.90	0.54
1:A:157:HIS:O	1:A:161:ILE:HD13	2.07	0.54
1:B:135:GLN:CD	1:B:135:GLN:H	2.15	0.54
1:B:274:VAL:HG23	1:B:324:ILE:CD1	2.34	0.54
1:A:994:TYR:CE1	1:A:1002:SER:HB3	2.43	0.54
1:B:697:PHE:CD2	1:B:1046:LYS:HD3	2.43	0.54
1:B:803:GLU:O	1:B:805:LEU:HD13	2.08	0.54
1:B:1027:ARG:HA	1:B:1030:MET:HE3	1.89	0.54
1:A:123:ILE:HD13	1:B:1202:MET:HE2	1.89	0.54
1:B:87:SER:HA	1:B:129:ASP:HB3	1.89	0.54
1:A:287:ILE:HD11	1:A:379:TYR:CZ	2.43	0.53
1:A:573:VAL:HG22	7:A:2138:HOH:O	2.08	0.53
1:A:992:GLU:O	1:A:993:VAL:HB	2.08	0.53
1:B:552:ASP:HB2	1:B:608:GLN:HE22	1.73	0.53
1:A:215:VAL:HG11	1:B:851:MET:SD	2.49	0.53
1:A:227:GLN:H	1:A:227:GLN:NE2	2.06	0.53
1:A:487:VAL:O	1:A:510:PHE:HD1	1.92	0.53
1:A:1093:SER:HA	1:A:1121:ASP:OD1	2.08	0.53
1:B:7:THR:O	1:B:8:THR:HG23	2.08	0.53
1:A:365:LEU:HD22	1:B:226:PHE:CE2	2.44	0.53
1:B:994:TYR:HE1	1:B:1002:SER:HB3	1.72	0.53
1:A:1009:ALA:O	1:A:1017:GLY:HA2	2.08	0.53
1:B:499:ASP:OD2	1:B:502:GLU:HB2	2.08	0.53
1:A:542:TYR:CD2	1:A:570:LEU:HD21	2.43	0.53
1:B:186:LEU:O	1:B:191:MET:HE2	2.08	0.53
1:B:527:PRO:HB2	1:B:530:ILE:HD13	1.91	0.53
1:B:549:ILE:HD12	1:B:549:ILE:N	2.23	0.53
1:B:593:LYS:HD2	1:B:594:LYS:H	1.72	0.53
1:B:805:LEU:HB2	1:B:825:THR:HB	1.91	0.53
1:A:967:TYR:CG	1:A:1004:ALA:HB2	2.43	0.53
1:B:93:MET:O	1:B:97:MET:HG3	2.09	0.53
1:A:959:ILE:HG13	1:A:986:VAL:HG12	1.91	0.53
1:A:1158:VAL:O	1:A:1162:GLU:HG3	2.09	0.53
1:A:1219:THR:CG2	1:A:1220:SER:N	2.72	0.53
1:B:81:THR:HG22	1:B:82:THR:N	2.23	0.53
1:B:465:ILE:HD13	7:B:2126:HOH:O	2.09	0.53
1:A:737:ARG:HE	1:A:739:GLN:NE2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:LEU:HD11	1:B:530:ILE:HG21	1.90	0.53
1:A:695:CYS:HB2	1:A:704:ILE:HD13	1.91	0.53
1:A:837:ALA:HB2	1:A:872:ALA:HB2	1.90	0.53
1:A:1044:TYR:HD1	1:A:1088:ASN:HD22	1.57	0.53
1:B:583:LEU:O	1:B:583:LEU:HD23	2.09	0.53
1:B:912:GLY:HA3	1:B:926:TYR:CE2	2.43	0.53
1:A:194:LEU:HD21	1:A:253:LEU:CD1	2.35	0.52
1:A:425:LEU:HD11	1:A:461:GLY:HA2	1.90	0.52
1:A:512:LEU:O	1:A:544:ILE:HG22	2.08	0.52
1:A:571:ALA:HB3	7:A:2138:HOH:O	2.09	0.52
1:A:792:PRO:HB2	1:A:795:SER:HB3	1.90	0.52
1:A:808:PHE:N	1:A:808:PHE:CD2	2.77	0.52
1:A:1008:GLY:HA2	1:A:1148:LEU:HD13	1.91	0.52
1:B:1123:SER:O	1:B:1126:GLU:HG2	2.09	0.52
1:A:805:LEU:HD23	1:A:862:PRO:HD3	1.91	0.52
1:B:41:ASP:HA	1:B:58:ILE:HD12	1.91	0.52
1:B:591:TYR:C	1:B:593:LYS:H	2.15	0.52
1:A:690:ILE:HD12	1:A:690:ILE:O	2.09	0.52
1:B:1099:PHE:HB3	1:B:1115:LEU:HD23	1.92	0.52
1:B:286:VAL:HG21	1:B:375:VAL:HB	1.91	0.52
1:B:684:TRP:CH2	1:B:737:ARG:HA	2.45	0.52
1:A:173:GLY:O	1:A:174:PHE:HB2	2.09	0.52
1:B:127:HIS:HB3	1:B:130:ILE:HD11	1.91	0.52
1:B:144:SER:O	1:B:278:SER:HA	2.10	0.52
1:B:324:ILE:HD12	1:B:325:THR:N	2.25	0.52
1:B:390:PHE:HB2	1:B:403:LEU:HD13	1.91	0.52
1:B:698:VAL:HG13	1:B:1084:GLN:OE1	2.09	0.52
1:A:714:LEU:HD12	1:A:714:LEU:N	2.25	0.52
1:A:774:GLN:HA	1:A:774:GLN:NE2	2.24	0.52
1:B:163:SER:O	1:B:164:ASN:HB2	2.10	0.52
1:B:893:LEU:HB3	1:B:945:ILE:CD1	2.37	0.52
1:B:595:GLY:C	1:B:597:LYS:H	2.17	0.52
1:B:642:VAL:C	1:B:645:PRO:HD2	2.35	0.52
1:B:870:GLU:OE2	1:B:870:GLU:N	2.41	0.52
1:B:1198:ASP:OD1	1:B:1203:MET:HE3	2.09	0.52
1:B:1029:VAL:HG21	1:B:1064:LEU:HD13	1.92	0.52
1:B:1064:LEU:HD23	1:B:1065:VAL:N	2.25	0.52
1:A:9:ASP:HA	1:A:179:GLU:O	2.10	0.52
1:A:396:ASP:HA	1:A:656:VAL:CG1	2.40	0.52
1:B:140:MET:HE3	1:B:168:MET:HE1	1.92	0.52
1:A:526:LEU:HD11	1:A:530:ILE:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:ASN:N	1:A:720:ASN:HD22	2.08	0.51
1:B:180:ILE:HD13	1:B:181:GLN:N	2.25	0.51
1:A:27:ILE:CG2	1:A:28:TYR:H	2.23	0.51
1:A:717:ALA:HB2	1:A:780:TYR:CZ	2.45	0.51
1:B:584:LYS:HE2	1:B:603:THR:HG23	1.93	0.51
1:A:691:GLN:HE22	1:A:727:LYS:N	2.09	0.51
1:A:788:SER:HB2	1:A:802:GLN:HE22	1.75	0.51
1:A:124:PHE:HB3	1:A:367:SER:OG	2.10	0.51
1:A:236:TYR:O	1:A:239:VAL:HG12	2.11	0.51
1:B:887:ARG:NH2	1:B:952:TYR:O	2.42	0.51
1:A:87:SER:HB2	1:A:114:ARG:CG	2.41	0.51
1:A:729:LYS:HD2	1:A:730:GLU:OE2	2.10	0.51
1:B:131:TYR:CD1	1:B:330:THR:HG21	2.45	0.51
1:B:264:VAL:HG11	1:B:284:GLU:HG3	1.92	0.51
1:A:394:ILE:CG2	1:B:227:GLN:HE21	2.24	0.51
1:A:697:PHE:CD2	1:A:1046:LYS:HD3	2.45	0.51
1:A:1019:ARG:CZ	1:B:1181:LYS:H	2.23	0.51
1:A:1077:ARG:HH11	1:A:1077:ARG:CB	2.18	0.51
1:B:422:PHE:O	1:B:465:ILE:HA	2.11	0.51
1:B:1137:LEU:HD12	1:B:1145:ALA:HA	1.92	0.51
1:A:3:LYS:O	1:A:4:LYS:HB2	2.10	0.51
1:A:121:LEU:HD23	1:A:121:LEU:C	2.35	0.51
1:A:146:VAL:HG12	1:A:183:ILE:HD13	1.93	0.51
1:A:273:ILE:CD1	1:A:325:THR:HG23	2.39	0.51
1:A:436:GLN:O	1:A:440:ILE:HG12	2.11	0.51
1:A:917:LYS:NZ	1:A:917:LYS:HB3	2.26	0.51
1:B:82:THR:HG23	1:B:108:VAL:O	2.11	0.51
1:B:221:ASN:HB3	1:B:222:PRO:CD	2.41	0.51
1:B:750:ASN:ND2	1:B:1084:GLN:HG2	2.26	0.51
1:B:981:GLY:C	1:B:1062:PRO:HD3	2.36	0.51
1:A:45:ALA:CB	1:B:1185:SER:HB3	2.40	0.51
1:A:75:LEU:HB2	1:A:105:LEU:HD13	1.93	0.51
1:A:398:VAL:HG23	1:A:399:THR:N	2.26	0.51
1:A:709:ALA:HB3	1:A:714:LEU:HD11	1.93	0.51
1:A:1200:THR:HG23	1:A:1201:PRO:HD2	1.92	0.51
1:B:327:LEU:HB3	1:B:363:TYR:CE1	2.46	0.51
1:A:48:ARG:O	1:A:55:THR:HG22	2.11	0.51
1:A:413:THR:HG21	1:A:419:GLN:NE2	2.25	0.51
1:A:555:LEU:HD11	1:A:605:ALA:HB2	1.93	0.51
1:A:597:LYS:O	1:A:601:MET:HG3	2.10	0.51
1:A:726:ALA:HB1	1:A:731:LEU:CB	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:VAL:HG12	1:A:1052:VAL:HG21	1.92	0.51
1:B:142:ALA:HB2	1:B:170:PHE:CZ	2.46	0.51
1:B:530:ILE:HD12	1:B:530:ILE:N	2.26	0.51
1:B:591:TYR:C	1:B:593:LYS:N	2.68	0.51
1:A:14:THR:CG2	1:A:149:ALA:HB1	2.41	0.50
1:A:242:ILE:O	1:A:245:GLU:HB3	2.11	0.50
1:A:839:GLY:O	1:A:843:ILE:HG12	2.12	0.50
1:A:1144:ASP:HA	1:A:1147:ARG:HH12	1.75	0.50
1:A:1047:GLN:CD	1:A:1047:GLN:H	2.18	0.50
1:B:121:LEU:HD12	7:B:2226:HOH:O	2.12	0.50
1:B:486:TYR:OH	1:B:511:VAL:HG11	2.10	0.50
1:B:554:GLY:HA3	1:B:601:MET:HE2	1.93	0.50
1:B:814:GLY:O	1:B:1080:MET:HE3	2.10	0.50
1:B:937:GLN:O	1:B:938:LYS:HD2	2.10	0.50
1:A:198:LYS:HD2	1:A:198:LYS:N	2.08	0.50
1:B:115:ALA:HA	1:B:126:ASP:OD2	2.11	0.50
1:B:941:LEU:O	1:B:945:ILE:HG12	2.12	0.50
1:A:1186:VAL:HG12	1:B:1015:ALA:O	2.11	0.50
1:B:1077:ARG:HH11	1:B:1077:ARG:CB	2.08	0.50
1:A:331:LYS:HE3	1:B:230:GLU:OE2	2.11	0.50
1:A:775:VAL:N	1:A:776:PRO:HD2	2.26	0.50
1:B:558:ARG:HA	7:B:2148:HOH:O	2.10	0.50
1:A:27:ILE:CG2	1:A:28:TYR:N	2.73	0.50
1:B:24:VAL:HG12	1:B:25:ALA:N	2.26	0.50
1:B:138:PHE:CE2	1:B:166:PRO:HB2	2.45	0.50
1:B:796:LEU:C	1:B:796:LEU:HD23	2.36	0.50
1:A:82:THR:CG2	1:A:157:HIS:HE1	2.22	0.50
1:A:857:ARG:HG3	1:A:858:LEU:CD1	2.42	0.50
1:A:684:TRP:CH2	1:A:686:PRO:HB3	2.46	0.50
1:A:882:SER:OG	1:B:79:ALA:HB2	2.12	0.50
1:A:883:MET:HE2	1:A:955:LYS:CG	2.42	0.50
1:A:1025:LEU:O	1:A:1029:VAL:HG12	2.11	0.50
1:B:642:VAL:O	1:B:645:PRO:HD2	2.12	0.50
1:B:713:GLU:OE1	1:B:785:PRO:HD2	2.11	0.50
1:A:62:GLN:NE2	1:B:973:GLY:HA2	2.26	0.50
1:A:524:LYS:HB2	1:A:524:LYS:NZ	2.26	0.50
1:A:661:ALA:HA	1:B:231:ALA:CB	2.42	0.50
1:A:803:GLU:OE1	1:A:856:ASN:HB2	2.10	0.50
1:B:651:GLY:O	1:B:654:LEU:HB2	2.12	0.50
1:B:812:CYS:HB3	7:B:2210:HOH:O	2.11	0.50
1:A:841:SER:HA	1:A:844:TRP:CZ2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:TYR:HA	1:A:1112:PRO:O	2.11	0.49
1:A:1203:MET:HE3	1:B:995:SER:O	2.12	0.49
1:A:131:TYR:O	1:A:134:ARG:HG2	2.12	0.49
1:B:1064:LEU:HD21	1:B:1066:ILE:CG1	2.42	0.49
1:A:11:ASN:HD21	1:A:177:SER:HB2	1.75	0.49
1:A:216:ARG:O	1:B:865:GLY:HA2	2.12	0.49
7:A:2252:HOH:O	1:B:1132:ASN:HB3	2.13	0.49
1:B:491:ASN:HD22	1:B:492:PRO:HD2	1.77	0.49
1:B:646:ILE:HG21	1:B:849:PRO:HD3	1.93	0.49
1:A:23:GLU:C	1:A:56:LEU:HD12	2.38	0.49
1:A:394:ILE:HD13	1:A:394:ILE:H	1.78	0.49
1:B:538:LYS:HE3	7:B:2158:HOH:O	2.12	0.49
1:B:542:TYR:CD2	1:B:570:LEU:HD21	2.47	0.49
1:B:700:PRO:HG2	1:B:814:GLY:HA2	1.94	0.49
1:A:325:THR:HB	1:A:359:LEU:HB2	1.93	0.49
1:A:1003:LYS:HE2	1:A:1023:LYS:HD2	1.93	0.49
1:A:1019:ARG:HH12	1:B:1181:LYS:N	2.08	0.49
1:A:1113:PHE:CD1	1:A:1166:MET:HE2	2.48	0.49
1:A:1113:PHE:CG	1:A:1166:MET:HE2	2.47	0.49
1:A:220:GLN:HG2	1:A:224:ILE:HD11	1.95	0.49
1:A:630:LYS:HD2	1:A:630:LYS:O	2.12	0.49
1:B:821:VAL:HG13	1:B:989:MET:HE3	1.95	0.49
1:A:124:PHE:HB3	1:A:367:SER:CB	2.43	0.49
1:A:351:ARG:O	1:A:353:GLU:HG3	2.12	0.49
1:B:513:ASN:ND2	1:B:546:ALA:HB3	2.27	0.49
1:A:271:ARG:HA	1:A:323:VAL:O	2.13	0.49
1:A:602:ASN:O	1:A:606:VAL:HG23	2.13	0.49
1:A:845:GLY:HA2	1:A:852:PRO:CG	2.43	0.49
1:B:63:SER:HB3	1:B:969:ILE:HG13	1.94	0.49
1:A:494:TYR:HB3	1:A:500:ILE:HD11	1.95	0.49
1:A:559:ILE:HD12	1:A:559:ILE:C	2.38	0.49
1:A:639:PHE:CA	1:A:643:VAL:HG22	2.41	0.49
1:A:1048:GLN:O	1:A:1052:VAL:HG23	2.13	0.49
1:B:173:GLY:O	1:B:174:PHE:HB2	2.13	0.49
1:B:561:MET:HE3	1:B:564:GLN:HB3	1.95	0.49
1:B:676:GLY:HA2	7:B:2193:HOH:O	2.12	0.49
1:B:986:VAL:O	1:B:986:VAL:HG23	2.13	0.49
1:B:1059:PHE:C	1:B:1061:GLY:H	2.21	0.49
1:A:881:MET:HE3	1:B:59:ARG:HG2	1.94	0.48
1:A:1005:THR:HG23	7:A:2214:HOH:O	2.13	0.48
1:B:331:LYS:HB2	1:B:362:ARG:HD3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:844:TRP:O	1:B:852:PRO:HG3	2.13	0.48
1:B:924:LYS:HG2	1:B:928:ASP:OD2	2.13	0.48
1:B:986:VAL:HG22	1:B:1063:SER:O	2.12	0.48
1:A:82:THR:HG21	1:A:157:HIS:CE1	2.43	0.48
1:A:823:VAL:HG11	1:A:1049:PHE:HE2	1.78	0.48
1:B:619:PRO:HG2	1:B:622:TRP:CD1	2.47	0.48
1:B:910:LEU:O	1:B:914:LEU:HD23	2.13	0.48
1:B:1219:THR:HG22	1:B:1220:SER:N	2.27	0.48
1:B:5:MET:HE2	1:B:184:GLU:HB2	1.94	0.48
1:B:220:GLN:HE21	1:B:225:TYR:HA	1.77	0.48
1:B:573:VAL:O	1:B:574:LEU:HD23	2.13	0.48
1:B:10:GLY:O	1:B:14:THR:HG23	2.13	0.48
1:B:730:GLU:N	1:B:730:GLU:OE1	2.46	0.48
1:A:29:PRO:HB3	1:A:1000:GLN:HG2	1.94	0.48
1:A:368:LYS:HZ1	1:B:227:GLN:HE22	1.61	0.48
1:A:394:ILE:HB	1:B:227:GLN:HG3	1.93	0.48
1:A:841:SER:HA	1:A:844:TRP:CE2	2.48	0.48
1:B:111:VAL:HG13	1:B:170:PHE:CB	2.43	0.48
1:B:1199:ASP:CG	1:B:1214:GLN:HE22	2.22	0.48
1:A:686:PRO:HG3	1:A:722:THR:HG21	1.96	0.48
1:A:1012:LYS:O	1:A:1013:PHE:HB2	2.12	0.48
1:B:914:LEU:HD13	1:B:917:LYS:NZ	2.22	0.48
1:A:637:GLU:O	1:A:641:ASN:HB2	2.14	0.48
1:A:1059:PHE:CD1	1:A:1060:PRO:HD2	2.48	0.48
1:B:396:ASP:H	1:B:402:SER:HB3	1.78	0.48
1:B:530:ILE:O	1:B:534:ILE:HG13	2.13	0.48
1:A:70:ALA:HA	1:B:874:GLU:O	2.14	0.48
1:A:1144:ASP:HA	1:A:1147:ARG:NH1	2.29	0.48
1:B:351:ARG:HD3	1:B:353:GLU:OE2	2.14	0.48
1:B:577:GLU:O	1:B:578:LYS:C	2.56	0.48
1:A:181:GLN:HA	1:A:449:ALA:O	2.13	0.48
1:A:463:ILE:HD11	1:A:649:GLN:NE2	2.29	0.48
1:A:523:ASP:HA	1:A:531:LYS:NZ	2.28	0.48
1:A:573:VAL:HG23	1:A:574:LEU:HG	1.96	0.48
1:A:691:GLN:HE22	1:A:727:LYS:H	1.61	0.48
1:A:720:ASN:HD22	1:A:720:ASN:H	1.60	0.48
1:B:766:PRO:HB2	1:B:769:THR:HG23	1.95	0.48
1:A:114:ARG:NE	1:A:123:ILE:HA	2.29	0.48
1:A:569:LYS:HD2	1:A:610:VAL:HG13	1.96	0.48
1:A:575:PRO:O	1:A:576:PHE:C	2.57	0.48
1:B:584:LYS:HA	1:B:587:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:GLU:O	1:A:674:LYS:C	2.56	0.47
1:A:1028:MET:HE3	1:B:1028:MET:O	2.14	0.47
1:A:1222:GLN:NE2	1:B:752:ALA:HB3	2.29	0.47
1:B:595:GLY:C	1:B:597:LYS:N	2.71	0.47
1:A:643:VAL:O	1:A:647:LEU:HG	2.14	0.47
1:B:14:THR:CG2	1:B:149:ALA:HB1	2.44	0.47
1:B:309:VAL:HG12	1:B:312:ALA:H	1.78	0.47
1:B:324:ILE:HG23	1:B:358:ILE:HD13	1.96	0.47
1:A:121:LEU:HD23	1:A:122:SER:N	2.28	0.47
1:A:688:ASN:HD22	1:A:688:ASN:N	2.10	0.47
1:A:927:GLY:O	1:A:931:LYS:HG3	2.15	0.47
1:A:1165:HIS:CD2	1:B:1165:HIS:NE2	2.82	0.47
1:B:467:HIS:CE1	1:B:480:LEU:HD22	2.50	0.47
1:B:491:ASN:HD22	1:B:491:ASN:C	2.23	0.47
1:B:656:VAL:C	1:B:658:ALA:H	2.22	0.47
1:B:949:SER:HA	1:B:952:TYR:CE1	2.50	0.47
1:A:720:ASN:H	1:A:720:ASN:ND2	2.12	0.47
1:A:968:ASP:OD2	1:A:1003:LYS:NZ	2.44	0.47
1:B:698:VAL:HG11	1:B:1084:GLN:HG3	1.95	0.47
1:B:839:GLY:O	1:B:840:CYS:C	2.58	0.47
1:B:1019:ARG:NE	1:B:1148:LEU:HD11	2.29	0.47
1:A:113:ALA:HB1	1:A:126:ASP:O	2.14	0.47
1:A:273:ILE:HD11	1:A:382:MET:HE2	1.95	0.47
1:A:645:PRO:O	1:A:650:GLN:HB2	2.14	0.47
1:A:1230:THR:O	1:A:1231:LYS:C	2.58	0.47
1:B:180:ILE:CD1	1:B:438:ILE:HG21	2.44	0.47
1:B:451:GLY:HA2	1:B:468:LEU:HD23	1.97	0.47
1:B:695:CYS:HB2	1:B:704:ILE:HD13	1.96	0.47
1:B:963:ASP:HB2	1:B:1004:ALA:CB	2.45	0.47
1:A:126:ASP:OD2	1:A:126:ASP:C	2.57	0.47
1:B:558:ARG:HG3	1:B:558:ARG:HH11	1.78	0.47
1:B:729:LYS:C	1:B:729:LYS:HD3	2.39	0.47
1:B:1056:ALA:HB1	1:B:1063:SER:HB3	1.95	0.47
1:A:22:SER:O	1:A:56:LEU:HD13	2.15	0.47
1:A:130:ILE:C	1:A:130:ILE:HD12	2.40	0.47
1:A:209:ASN:HB3	1:A:212:HIS:CE1	2.49	0.47
1:A:569:LYS:HD3	1:A:613:LEU:HD23	1.96	0.47
1:A:872:ALA:HB3	1:A:965:TRP:CE2	2.50	0.47
1:A:917:LYS:HB3	1:A:917:LYS:HZ3	1.78	0.47
1:B:278:SER:HB2	1:B:478:THR:HG21	1.96	0.47
1:B:850:SER:O	1:B:851:MET:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ALA:O	1:A:51:ILE:HG23	2.14	0.47
1:A:45:ALA:HB1	1:B:1185:SER:HB3	1.96	0.47
1:A:418:ILE:HD12	1:A:418:ILE:N	2.30	0.47
1:A:648:THR:O	1:A:650:GLN:HG2	2.15	0.47
1:A:650:GLN:CD	1:A:653:LYS:HZ1	2.23	0.47
1:B:397:ASP:OD1	1:B:655:PRO:HB2	2.15	0.47
1:B:491:ASN:HD22	1:B:492:PRO:CD	2.28	0.47
1:B:821:VAL:HG23	1:B:822:ARG:N	2.29	0.47
1:B:823:VAL:CG2	1:B:1049:PHE:HE2	2.23	0.47
1:A:691:GLN:NE2	1:A:727:LYS:H	2.13	0.47
1:B:272:VAL:O	1:B:324:ILE:HD12	2.14	0.47
1:B:487:VAL:O	1:B:510:PHE:HD1	1.97	0.47
1:B:668:GLY:HA2	7:B:2169:HOH:O	2.13	0.47
1:B:737:ARG:NH1	1:B:739:GLN:HE22	2.12	0.47
1:B:830:GLU:HB2	1:B:860:GLN:NE2	2.30	0.47
1:A:484:ALA:O	1:A:504:ILE:HD12	2.15	0.46
1:B:1156:LEU:HD12	1:B:1156:LEU:C	2.39	0.46
1:A:750:ASN:OD1	1:A:1081:GLY:HA2	2.15	0.46
1:A:839:GLY:HA2	3:A:2236:TPP:S1	2.55	0.46
1:B:720:ASN:N	1:B:720:ASN:HD22	2.13	0.46
1:B:1044:TYR:CD2	1:B:1091:VAL:HG11	2.50	0.46
1:A:286:VAL:CG2	1:A:372:PRO:HB3	2.45	0.46
1:A:967:TYR:CD2	1:A:1004:ALA:HB2	2.50	0.46
1:B:583:LEU:HD23	1:B:583:LEU:C	2.40	0.46
1:A:129:ASP:OD2	1:A:130:ILE:N	2.45	0.46
1:A:190:ASP:O	1:A:193:SER:OG	2.33	0.46
1:A:570:LEU:N	1:A:570:LEU:HD12	2.30	0.46
1:A:717:ALA:HB2	1:A:780:TYR:CE2	2.51	0.46
1:A:949:SER:HA	1:A:952:TYR:CZ	2.51	0.46
1:A:1044:TYR:HD1	1:A:1088:ASN:ND2	2.12	0.46
1:A:1102:ASP:OD1	1:A:1104:ARG:CG	2.60	0.46
1:A:1132:ASN:OD1	1:A:1136:VAL:HG13	2.14	0.46
1:A:1193:GLU:CD	1:B:1077:ARG:HG3	2.41	0.46
1:A:204:ARG:HG2	1:A:204:ARG:HH21	1.81	0.46
1:A:682:PRO:HG2	1:A:740:ILE:HD12	1.96	0.46
1:A:690:ILE:HD12	1:A:690:ILE:C	2.41	0.46
1:B:20:ALA:O	1:B:50:ASN:HB2	2.15	0.46
1:B:594:LYS:HB3	1:B:594:LYS:HZ3	1.79	0.46
1:A:499:ASP:OD2	1:A:502:GLU:HB2	2.16	0.46
1:A:456:ASP:OD2	1:A:457:SER:N	2.49	0.46
1:A:876:GLY:HA3	1:A:959:ILE:CD1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:LYS:O	1:A:1086:VAL:HG23	2.16	0.46
1:B:233:ASN:N	1:B:234:PRO:CD	2.79	0.46
1:B:418:ILE:N	1:B:418:ILE:HD12	2.30	0.46
1:B:937:GLN:C	1:B:938:LYS:HD2	2.41	0.46
1:A:527:PRO:O	1:A:531:LYS:HG3	2.15	0.46
1:A:921:ILE:N	1:A:921:ILE:HD12	2.30	0.46
1:B:272:VAL:HG12	1:B:273:ILE:N	2.30	0.46
1:B:461:GLY:O	1:B:675:ARG:NH2	2.49	0.46
1:A:9:ASP:OD2	1:A:12:THR:HG23	2.15	0.46
1:A:59:ARG:CG	1:B:881:MET:HE3	2.46	0.46
1:A:546:ALA:C	1:A:559:ILE:HG22	2.41	0.46
1:A:553:VAL:HG23	1:A:555:LEU:HG	1.97	0.46
1:B:500:ILE:HG22	1:B:501:LEU:HD12	1.97	0.46
1:B:914:LEU:CD1	1:B:917:LYS:HZ1	2.23	0.46
1:A:1105:LEU:O	1:A:1108:GLN:HG2	2.16	0.45
1:B:20:ALA:HB2	1:B:188:TYR:CE2	2.51	0.45
1:B:684:TRP:CD2	1:B:738:ILE:HB	2.51	0.45
1:B:755:CYS:SG	1:B:761:ALA:HB3	2.57	0.45
1:A:71:VAL:O	1:A:75:LEU:HG	2.16	0.45
1:A:289:HIS:CD2	1:A:412:THR:HG22	2.52	0.45
1:A:639:PHE:HA	1:A:643:VAL:CG2	2.40	0.45
1:B:14:THR:HG21	1:B:171:PHE:CE2	2.51	0.45
1:B:131:TYR:O	1:B:134:ARG:HG2	2.17	0.45
1:B:465:ILE:HG12	1:B:467:HIS:CE1	2.51	0.45
1:A:306:ARG:HA	1:A:307:PRO:C	2.40	0.45
1:A:644:LYS:HB3	1:A:645:PRO:HD3	1.99	0.45
1:A:838:THR:HB	1:A:869:PHE:CB	2.47	0.45
1:A:973:GLY:HA2	1:B:62:GLN:NE2	2.32	0.45
1:B:96:ASN:O	1:B:100:ILE:HG13	2.15	0.45
1:B:123:ILE:O	1:B:174:PHE:HE2	1.99	0.45
1:B:209:ASN:HB3	1:B:212:HIS:CE1	2.52	0.45
1:B:482:ASN:OD1	1:B:483:ARG:HG3	2.15	0.45
1:B:549:ILE:HD12	1:B:549:ILE:H	1.81	0.45
1:B:628:GLU:HG2	7:B:2140:HOH:O	2.15	0.45
1:A:538:LYS:HD2	1:A:538:LYS:N	2.31	0.45
1:A:1000:GLN:H	1:A:1000:GLN:NE2	2.14	0.45
1:A:1159:ARG:O	1:A:1162:GLU:HB2	2.17	0.45
1:B:611:THR:HG22	1:B:611:THR:O	2.17	0.45
1:B:871:ASP:O	1:B:874:GLU:HG2	2.16	0.45
1:A:520:GLU:HG3	1:A:521:ASP:H	1.80	0.45
1:A:1072:ILE:HD12	1:A:1073:ASN:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2124:HOH:O	1:B:1199:ASP:HB3	2.15	0.45
1:B:27:ILE:HD13	1:B:28:TYR:C	2.42	0.45
1:B:542:TYR:CZ	1:B:615:GLU:HG2	2.51	0.45
1:B:1200:THR:CG2	1:B:1202:MET:HE3	2.47	0.45
1:A:91:LEU:O	1:A:94:ILE:HG12	2.15	0.45
1:B:594:LYS:NZ	1:B:597:LYS:HD3	2.31	0.45
1:B:729:LYS:HB3	1:B:730:GLU:OE1	2.16	0.45
1:A:99:LYS:HE2	1:B:117:ALA:HB1	1.98	0.45
1:A:233:ASN:HB2	1:A:234:PRO:HD3	1.99	0.45
1:A:864:TRP:CE3	1:B:215:VAL:HG23	2.52	0.45
1:A:1047:GLN:OE1	1:A:1047:GLN:N	2.46	0.45
1:B:140:MET:O	1:B:304:LEU:HD12	2.16	0.45
1:B:691:GLN:HE22	1:B:726:ALA:HA	1.81	0.45
1:B:714:LEU:N	1:B:714:LEU:HD12	2.31	0.45
1:B:756:PRO:N	1:B:757:PRO:HD2	2.32	0.45
1:B:818:THR:OG1	1:B:819:PRO:HD3	2.16	0.45
1:A:718:PRO:HB2	1:A:720:ASN:ND2	2.32	0.45
1:A:937:GLN:HG2	1:A:942:LEU:HB3	1.99	0.45
1:B:317:LEU:HD11	1:B:348:PHE:CZ	2.52	0.45
1:A:398:VAL:HG22	1:A:656:VAL:HG11	1.99	0.45
1:A:741:ASN:C	1:A:741:ASN:HD22	2.24	0.45
1:A:1181:LYS:HB2	1:A:1181:LYS:HZ3	1.82	0.45
1:B:513:ASN:HB2	1:B:563:MET:CE	2.47	0.45
1:B:597:LYS:HZ2	1:B:598:ILE:HD13	1.81	0.45
1:B:632:GLU:O	1:B:632:GLU:CD	2.60	0.45
1:B:325:THR:HA	1:B:359:LEU:O	2.17	0.45
1:B:396:ASP:OD2	1:B:398:VAL:HG22	2.17	0.45
1:B:495:VAL:HG12	1:B:527:PRO:CD	2.47	0.45
1:B:635:THR:OG1	1:B:636:ASN:N	2.49	0.45
1:A:87:SER:HB2	1:A:114:ARG:HG2	1.99	0.44
1:A:101:SER:HA	1:A:166:PRO:HG3	1.98	0.44
1:A:237:LEU:O	1:A:240:PRO:HD2	2.16	0.44
1:A:344:VAL:O	1:A:347:ALA:HB3	2.16	0.44
1:A:411:ASP:HB2	1:A:483:ARG:HD3	1.98	0.44
1:A:559:ILE:O	1:A:563:MET:HG2	2.17	0.44
1:B:351:ARG:CD	1:B:353:GLU:HB2	2.47	0.44
1:B:1159:ARG:O	1:B:1163:LEU:HG	2.18	0.44
1:A:20:ALA:HB2	1:A:188:TYR:CZ	2.52	0.44
1:A:691:GLN:HG2	1:A:736:PHE:CD2	2.52	0.44
1:A:722:THR:O	1:A:737:ARG:NH2	2.50	0.44
1:A:1003:LYS:HE3	1:B:975:ASP:OD1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:ARG:O	1:A:1031:THR:HG23	2.17	0.44
1:B:537:LYS:O	1:B:538:LYS:C	2.60	0.44
1:A:338:ASP:HB3	1:A:339:PRO:CD	2.45	0.44
1:A:632:GLU:CD	1:A:632:GLU:O	2.60	0.44
1:A:691:GLN:CD	1:A:727:LYS:HG3	2.42	0.44
1:A:818:THR:OG1	1:A:819:PRO:HD3	2.18	0.44
1:A:996:ASN:HD22	1:A:997:THR:N	2.14	0.44
1:A:1055:GLU:O	1:A:1104:ARG:NH1	2.51	0.44
1:B:20:ALA:HB2	1:B:188:TYR:CZ	2.52	0.44
1:B:750:ASN:HD22	1:B:1084:GLN:HG2	1.82	0.44
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.99	0.44
1:A:243:VAL:O	1:A:247:MET:HG3	2.18	0.44
1:A:886:ARG:O	1:A:889:HIS:HB3	2.16	0.44
1:A:918:ASN:HA	1:A:954:LYS:HD2	2.00	0.44
1:B:600:LYS:O	1:B:604:ASP:N	2.48	0.44
1:B:804:PRO:HG2	1:B:807:GLU:OE2	2.17	0.44
1:A:32:PRO:HB2	1:A:178:HIS:CE1	2.52	0.44
1:A:396:ASP:HA	1:A:656:VAL:HG12	2.00	0.44
1:A:858:LEU:HD12	1:A:858:LEU:N	2.32	0.44
1:A:869:PHE:CE2	1:A:969:ILE:HG21	2.52	0.44
1:A:1193:GLU:OE2	1:B:1077:ARG:HG3	2.17	0.44
1:B:591:TYR:O	1:B:593:LYS:N	2.50	0.44
1:A:190:ASP:O	1:A:194:LEU:HD23	2.17	0.44
1:B:326:VAL:N	1:B:359:LEU:O	2.51	0.44
1:B:667:LEU:HB3	1:B:854:LYS:HA	1.99	0.44
1:A:327:LEU:N	1:A:327:LEU:HD12	2.31	0.44
1:A:411:ASP:HB2	1:A:483:ARG:CD	2.48	0.44
1:A:778:LEU:HD13	1:A:778:LEU:C	2.42	0.44
1:B:85:THR:O	1:B:111:VAL:HG23	2.17	0.44
1:B:561:MET:CE	1:B:583:LEU:HD21	2.48	0.44
1:B:949:SER:HA	1:B:952:TYR:CZ	2.53	0.44
1:A:501:LEU:N	1:A:501:LEU:HD12	2.33	0.44
1:B:549:ILE:HG23	1:B:608:GLN:NE2	2.32	0.44
1:B:569:LYS:HE3	1:B:576:PHE:CE2	2.53	0.44
1:A:569:LYS:C	1:A:570:LEU:HD12	2.43	0.44
1:A:729:LYS:HD3	1:A:729:LYS:C	2.42	0.44
1:A:1145:ALA:HB1	1:A:1149:ARG:NH1	2.29	0.44
1:B:49:LYS:HB3	1:B:53:GLY:HA2	1.99	0.44
1:B:830:GLU:HB2	1:B:860:GLN:HE21	1.83	0.44
1:B:953:THR:HG23	1:B:955:LYS:NZ	2.33	0.44
1:B:1166:MET:O	1:B:1169:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:PHE:HB3	1:B:367:SER:CB	2.48	0.43
1:B:198:LYS:HD2	1:B:198:LYS:N	2.12	0.43
1:B:214:HIS:HB3	7:B:2048:HOH:O	2.17	0.43
1:B:495:VAL:HG11	1:B:526:LEU:HD12	1.99	0.43
1:B:555:LEU:O	1:B:556:GLY:C	2.60	0.43
1:B:1124:VAL:O	1:B:1128:LEU:HG	2.18	0.43
1:A:222:PRO:HD3	1:B:124:PHE:CD2	2.52	0.43
1:A:963:ASP:HB2	1:A:1004:ALA:CB	2.47	0.43
1:B:738:ILE:HG22	1:B:740:ILE:CD1	2.48	0.43
1:B:1132:ASN:HB2	7:B:2276:HOH:O	2.17	0.43
1:B:1157:ASP:OD2	1:B:1161:LYS:NZ	2.51	0.43
1:A:103:GLU:O	1:A:104:LEU:C	2.62	0.43
1:B:23:GLU:O	1:B:56:LEU:HD12	2.18	0.43
1:B:391:THR:HB	1:B:394:ILE:HD11	2.00	0.43
1:B:591:TYR:HA	1:B:593:LYS:HE2	2.00	0.43
1:B:699:CYS:HA	1:B:700:PRO:HD3	1.84	0.43
1:B:1078:LYS:HB2	1:B:1082:LYS:HG3	2.00	0.43
1:A:159:ALA:HA	1:A:242:ILE:CG2	2.48	0.43
1:A:283:ILE:O	1:A:287:ILE:HG12	2.17	0.43
1:A:545:ASP:O	1:A:549:ILE:HG12	2.18	0.43
1:A:699:CYS:HA	1:A:700:PRO:HD3	1.81	0.43
1:A:710:LYS:HD2	1:A:710:LYS:N	2.29	0.43
1:B:140:MET:HE3	1:B:168:MET:HE2	2.01	0.43
1:B:363:TYR:O	1:B:365:LEU:HD12	2.18	0.43
1:B:376:LYS:HZ2	1:B:380:ASP:CG	2.26	0.43
1:B:1219:THR:HB	1:B:1222:GLN:CG	2.42	0.43
1:A:272:VAL:O	1:A:324:ILE:HA	2.18	0.43
1:B:501:LEU:HD11	1:B:510:PHE:CE2	2.53	0.43
1:B:656:VAL:HG23	1:B:657:SER:N	2.33	0.43
1:A:667:LEU:N	1:A:667:LEU:HD12	2.33	0.43
1:A:688:ASN:N	1:A:688:ASN:ND2	2.64	0.43
1:A:710:LYS:C	1:A:712:GLU:N	2.77	0.43
1:A:969:ILE:CG2	1:A:970:GLY:N	2.82	0.43
1:B:774:GLN:HA	1:B:774:GLN:NE2	2.33	0.43
1:B:967:TYR:CG	1:B:1004:ALA:HB2	2.54	0.43
1:B:1008:GLY:HA2	1:B:1148:LEU:HD13	1.99	0.43
1:A:346:SER:HA	1:A:349:VAL:HG12	2.00	0.43
1:A:686:PRO:HG2	1:A:687:GLU:OE2	2.19	0.43
1:A:1231:LYS:HG3	1:A:1232:LYS:N	2.25	0.43
1:B:1012:LYS:O	1:B:1013:PHE:CB	2.66	0.43
1:B:1052:VAL:HG22	1:B:1100:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:O	1:A:81:THR:HA	2.19	0.43
1:A:68:ALA:HB2	1:A:93:MET:CG	2.48	0.43
1:A:231:ALA:HB1	1:B:661:ALA:HA	2.00	0.43
1:A:855:THR:HB	1:A:859:GLY:C	2.43	0.43
1:A:909:ALA:HA	1:A:926:TYR:CD2	2.43	0.43
1:A:994:TYR:O	1:A:999:GLY:HA2	2.19	0.43
1:A:1022:LYS:HD2	7:A:2215:HOH:O	2.18	0.43
1:A:1028:MET:HE2	1:B:1028:MET:HB3	2.01	0.43
1:A:721:PHE:CZ	1:A:781:ALA:HB2	2.54	0.43
1:A:973:GLY:O	1:A:977:VAL:HG23	2.19	0.43
1:A:1072:ILE:HA	7:A:2226:HOH:O	2.19	0.43
1:B:68:ALA:HB2	1:B:93:MET:HG2	2.00	0.43
1:B:111:VAL:O	1:B:170:PHE:HA	2.19	0.43
1:B:188:TYR:HA	1:B:191:MET:HE3	2.00	0.43
1:B:431:VAL:CG1	1:B:435:LYS:HE3	2.49	0.43
1:B:1232:LYS:HB3	1:B:1232:LYS:HZ2	1.83	0.43
1:A:87:SER:OG	1:A:88:GLN:N	2.52	0.43
1:A:214:HIS:HB3	7:A:2045:HOH:O	2.18	0.43
1:A:668:GLY:HA2	7:A:2186:HOH:O	2.19	0.43
1:A:779:GLU:HA	1:A:779:GLU:OE1	2.18	0.43
1:A:949:SER:HA	1:A:952:TYR:CE2	2.54	0.43
1:A:961:GLY:HA3	1:A:965:TRP:CE3	2.54	0.43
1:A:1156:LEU:HD12	1:A:1157:ASP:N	2.34	0.43
1:B:11:ASN:HD21	1:B:177:SER:HB2	1.80	0.43
1:A:297:ILE:HD13	1:A:297:ILE:N	2.28	0.42
1:A:679:ILE:HB	1:B:1216:ARG:O	2.19	0.42
1:A:679:ILE:N	1:A:679:ILE:HD12	2.33	0.42
1:B:620:ASP:C	1:B:622:TRP:H	2.25	0.42
1:B:740:ILE:N	1:B:740:ILE:HD12	2.34	0.42
1:B:1094:GLY:HA3	1:B:1120:PRO:HG3	2.00	0.42
1:A:710:LYS:HG2	1:A:712:GLU:HB2	2.01	0.42
1:A:821:VAL:HG23	1:A:822:ARG:N	2.34	0.42
1:A:1219:THR:HG22	1:A:1220:SER:N	2.34	0.42
1:B:491:ASN:C	1:B:491:ASN:ND2	2.77	0.42
1:B:536:ASN:C	1:B:538:LYS:H	2.28	0.42
1:A:264:VAL:HG11	1:A:284:GLU:CG	2.47	0.42
1:A:861:GLY:O	1:B:210:PRO:HA	2.19	0.42
1:A:1010:VAL:HG21	1:A:1136:VAL:CG2	2.47	0.42
1:A:1156:LEU:HD12	1:A:1156:LEU:C	2.44	0.42
1:A:1211:ALA:HA	1:B:427:ALA:O	2.19	0.42
1:B:21:MET:HE1	1:B:195:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1200:THR:HG23	1:A:1201:PRO:CD	2.50	0.42
1:B:656:VAL:C	1:B:658:ALA:N	2.77	0.42
1:A:229:ARG:HH21	1:B:128:GLN:NE2	2.17	0.42
1:A:283:ILE:HB	1:A:299:LEU:HD22	2.02	0.42
1:A:871:ASP:HA	1:A:874:GLU:OE2	2.19	0.42
1:B:129:ASP:OD2	1:B:130:ILE:N	2.48	0.42
1:B:226:PHE:C	1:B:226:PHE:CD2	2.98	0.42
1:B:1105:LEU:HD11	1:B:1114:GLN:NE2	2.35	0.42
1:A:110:HIS:HE1	1:A:157:HIS:NE2	2.17	0.42
1:A:674:LYS:HD3	1:A:744:ASP:OD2	2.20	0.42
1:B:368:LYS:HD3	7:B:2099:HOH:O	2.17	0.42
1:B:515:PRO:HA	1:B:545:ASP:OD2	2.20	0.42
1:A:326:VAL:C	1:A:327:LEU:HD12	2.44	0.42
1:A:368:LYS:NZ	1:B:227:GLN:NE2	2.66	0.42
1:A:661:ALA:HA	1:B:231:ALA:HB1	2.02	0.42
1:A:805:LEU:HD23	1:A:861:GLY:HA2	1.99	0.42
1:A:986:VAL:HG22	1:A:1064:LEU:HA	2.02	0.42
1:B:316:ALA:O	1:B:318:PRO:HD3	2.20	0.42
1:B:783:ARG:O	1:B:785:PRO:HD3	2.19	0.42
1:B:1044:TYR:HA	1:B:1088:ASN:ND2	2.35	0.42
1:A:271:ARG:HB3	1:A:382:MET:HE3	2.01	0.42
1:A:287:ILE:HD12	1:A:297:ILE:HG12	2.00	0.42
1:A:774:GLN:HE21	1:A:774:GLN:CA	2.28	0.42
1:B:1129:MET:HE3	1:B:1149:ARG:CD	2.44	0.42
1:A:27:ILE:HD13	1:A:58:ILE:CG2	2.50	0.42
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.49	0.42
1:A:893:LEU:O	1:A:896:LYS:HB2	2.19	0.42
1:A:1078:LYS:HB2	1:A:1082:LYS:HG3	2.01	0.42
1:B:283:ILE:O	1:B:287:ILE:CD1	2.68	0.42
1:B:630:LYS:HE2	1:B:632:GLU:OE2	2.20	0.42
1:B:636:ASN:ND2	1:B:672:PHE:CE1	2.88	0.42
1:B:687:GLU:CD	1:B:687:GLU:H	2.28	0.42
1:B:1071:CYS:O	1:B:1074:GLN:HB2	2.20	0.42
1:A:823:VAL:CG1	1:A:1049:PHE:HE2	2.33	0.42
1:B:283:ILE:CG2	1:B:299:LEU:HD22	2.50	0.42
1:B:426:GLY:O	1:B:427:ALA:HB3	2.20	0.42
1:B:483:ARG:HG2	1:B:483:ARG:HH11	1.85	0.42
1:A:431:VAL:CG2	1:A:464:THR:HG21	2.50	0.41
1:A:635:THR:HG23	1:A:640:LYS:HE3	2.02	0.41
1:A:685:VAL:HB	1:A:761:ALA:HA	2.02	0.41
1:B:49:LYS:HD2	1:B:53:GLY:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:H	1:B:123:ILE:CD1	2.28	0.41
1:B:869:PHE:CZ	3:B:2236:TPP:H71	2.54	0.41
1:A:3:LYS:NZ	1:A:253:LEU:O	2.48	0.41
1:A:667:LEU:HB3	1:A:854:LYS:HA	2.03	0.41
1:A:896:LYS:HB3	1:A:941:LEU:HD13	2.02	0.41
1:A:1108:GLN:NE2	1:A:1110:LYS:HD2	2.32	0.41
1:A:1219:THR:HB	1:A:1222:GLN:CG	2.43	0.41
1:B:276:MET:HB2	1:B:302:VAL:HG13	2.00	0.41
1:B:467:HIS:CD2	1:B:481:VAL:H	2.34	0.41
1:B:678:ALA:HB2	1:B:745:CYS:O	2.20	0.41
1:B:695:CYS:O	1:B:704:ILE:HD12	2.20	0.41
1:A:303:ARG:HH21	1:A:303:ARG:HG3	1.85	0.41
1:A:1132:ASN:C	1:A:1134:PHE:H	2.28	0.41
1:B:264:VAL:HG11	1:B:284:GLU:CD	2.45	0.41
1:A:181:GLN:HE21	1:A:181:GLN:HB3	1.54	0.41
1:A:394:ILE:HG21	1:B:227:GLN:HE21	1.84	0.41
1:A:874:GLU:HG2	1:B:66:GLY:CA	2.45	0.41
1:B:609:ALA:O	1:B:613:LEU:HD23	2.20	0.41
1:A:332:GLU:OE2	1:B:135:GLN:HB3	2.21	0.41
1:A:389:HIS:HE1	1:B:350:GLU:OE1	2.03	0.41
1:A:650:GLN:CB	1:A:653:LYS:HZ1	2.32	0.41
1:A:837:ALA:HB2	1:A:872:ALA:CB	2.48	0.41
1:A:1080:MET:H	1:B:1215:ASN:HD22	1.63	0.41
1:A:1215:ASN:ND2	1:B:1080:MET:N	2.54	0.41
1:B:30:ILE:O	1:B:30:ILE:HG23	2.20	0.41
1:B:720:ASN:H	1:B:720:ASN:ND2	2.18	0.41
1:B:994:TYR:HE1	1:B:1002:SER:CB	2.32	0.41
1:B:1132:ASN:CG	1:B:1136:VAL:HG13	2.46	0.41
1:A:23:GLU:O	1:A:56:LEU:HD12	2.20	0.41
1:A:349:VAL:HG11	1:B:345:CYS:HB3	2.03	0.41
1:A:562:ILE:N	1:A:562:ILE:HD12	2.36	0.41
1:A:632:GLU:HA	1:A:633:PRO:HD3	1.95	0.41
1:A:756:PRO:HB2	1:A:757:PRO:CD	2.51	0.41
1:B:568:PHE:CD2	1:B:583:LEU:HD12	2.56	0.41
1:B:917:LYS:HZ3	1:B:917:LYS:HB3	1.85	0.41
1:A:3:LYS:HB2	7:A:2001:HOH:O	2.20	0.41
1:A:19:TYR:CZ	1:A:48:ARG:HB3	2.56	0.41
1:A:49:LYS:HD2	1:A:53:GLY:C	2.46	0.41
1:A:116:ILE:HG12	1:A:128:GLN:HB3	2.00	0.41
1:A:124:PHE:CD2	1:B:222:PRO:HD3	2.55	0.41
1:A:483:ARG:HG2	1:A:483:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:PRO:HG2	1:A:777:ASN:ND2	2.36	0.41
1:A:788:SER:HB2	1:A:802:GLN:NE2	2.36	0.41
1:A:996:ASN:C	1:A:996:ASN:ND2	2.79	0.41
1:B:741:ASN:C	1:B:741:ASN:ND2	2.77	0.41
1:B:1111:ASN:HD21	1:B:1169:THR:HG22	1.86	0.41
1:A:317:LEU:HA	1:A:318:PRO:HD3	1.87	0.41
1:A:520:GLU:HG3	1:A:521:ASP:OD1	2.21	0.41
1:B:126:ASP:OD2	1:B:126:ASP:C	2.63	0.41
1:B:240:PRO:HB3	1:B:309:VAL:HG21	2.02	0.41
1:B:331:LYS:O	1:B:333:PRO:HD3	2.19	0.41
1:B:391:THR:CB	1:B:394:ILE:HD11	2.50	0.41
1:B:803:GLU:OE1	1:B:856:ASN:HB2	2.20	0.41
1:A:86:ALA:O	1:A:87:SER:C	2.63	0.41
1:A:99:LYS:O	1:A:103:GLU:HG3	2.20	0.41
1:A:116:ILE:HD11	1:A:129:ASP:HB3	2.03	0.41
1:A:146:VAL:O	1:A:149:ALA:HB3	2.20	0.41
1:A:231:ALA:CB	1:B:661:ALA:HA	2.51	0.41
1:A:317:LEU:HD13	1:A:317:LEU:C	2.46	0.41
1:A:569:LYS:HG2	1:A:570:LEU:HD12	2.03	0.41
1:A:650:GLN:CD	1:A:653:LYS:NZ	2.79	0.41
1:A:710:LYS:C	1:A:712:GLU:H	2.29	0.41
1:A:720:ASN:N	1:A:720:ASN:ND2	2.69	0.41
1:A:725:GLU:O	1:A:726:ALA:C	2.63	0.41
1:B:8:THR:C	1:B:180:ILE:HG12	2.46	0.41
1:B:82:THR:CG2	1:B:83:THR:N	2.84	0.41
1:B:705:LEU:O	1:B:707:VAL:HG23	2.20	0.41
1:A:426:GLY:O	1:A:427:ALA:CB	2.69	0.41
1:A:692:CYS:O	1:A:693:ASN:HB2	2.20	0.41
7:A:2187:HOH:O	1:B:208:MET:HG2	2.20	0.41
1:B:146:VAL:HG12	1:B:183:ILE:HD13	2.03	0.41
1:B:584:LYS:CE	1:B:603:THR:HG23	2.50	0.41
1:A:887:ARG:HD3	7:A:2196:HOH:O	2.20	0.40
1:B:233:ASN:O	1:B:237:LEU:HG	2.20	0.40
1:B:371:SER:HB2	1:B:372:PRO:HD2	2.03	0.40
1:B:870:GLU:HB3	1:B:969:ILE:HG12	2.02	0.40
1:A:85:THR:OG1	1:A:86:ALA:N	2.55	0.40
1:A:396:ASP:OD2	1:A:398:VAL:HG22	2.21	0.40
1:A:1057:GLU:C	1:A:1057:GLU:CD	2.89	0.40
1:A:1129:MET:HE2	1:A:1129:MET:HA	2.03	0.40
1:B:637:GLU:OE1	1:B:637:GLU:N	2.55	0.40
1:B:717:ALA:HA	1:B:780:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:GLU:HB3	1:A:735:LYS:NZ	2.36	0.40
1:B:150:HIS:ND1	1:B:150:HIS:C	2.80	0.40
1:B:805:LEU:HD23	1:B:862:PRO:HD3	2.03	0.40
1:B:1160:PHE:O	1:B:1164:GLU:N	2.50	0.40
1:A:56:LEU:HB3	1:A:58:ILE:HD11	2.02	0.40
1:A:87:SER:HB2	1:A:114:ARG:HB3	2.03	0.40
1:A:455:TYR:HB3	1:B:1199:ASP:O	2.22	0.40
1:B:7:THR:HG21	1:B:438:ILE:HG22	2.03	0.40
1:B:210:PRO:C	1:B:213:PRO:HD3	2.46	0.40
1:B:903:SER:OG	1:B:906:VAL:HG23	2.22	0.40
1:A:51:ILE:CB	1:A:192:ALA:HB2	2.50	0.40
1:A:180:ILE:O	1:A:450:GLN:HA	2.21	0.40
1:A:918:ASN:CA	1:A:954:LYS:HD2	2.51	0.40
1:A:1132:ASN:C	1:A:1134:PHE:N	2.78	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	1229/1231 (100%)	1105 (90%)	96 (8%)	28 (2%)	5	13
1	B	1229/1231 (100%)	1120 (91%)	89 (7%)	20 (2%)	7	20
All	All	2458/2462 (100%)	2225 (90%)	185 (8%)	48 (2%)	6	16

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1231	LYS
1	B	556	GLY
1	B	577	GLU
1	B	597	LYS

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Mol	Chain	Res	Type
1	A	4	LYS
1	A	87	SER
1	A	339	PRO
1	A	364	GLY
1	A	623	LYS
1	A	726	ALA
1	B	357	LYS
1	B	578	LYS
1	B	1231	LYS
1	A	993	VAL
1	A	995	SER
1	A	996	ASN
1	A	1015	ALA
1	A	1177	PRO
1	A	1178	ALA
1	A	1182	ALA
1	B	996	ASN
1	B	1177	PRO
1	B	1181	LYS
1	A	104	LEU
1	A	577	GLU
1	A	633	PRO
1	A	674	LYS
1	A	952	TYR
1	B	87	SER
1	B	995	SER
1	A	595	GLY
1	A	711	GLU
1	A	760	LYS
1	A	940	GLY
1	B	339	PRO
1	B	589	LYS
1	B	635	THR
1	B	867	SER
1	B	1060	PRO
1	A	969	ILE
1	B	503	GLY
1	A	440	ILE
1	A	495	VAL
1	B	209	ASN
1	B	364	GLY
1	A	497	ILE

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Mol	Chain	Res	Type
1	A	686	PRO
1	B	715	VAL

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	978/978 (100%)	943 (96%)	35 (4%)	31	60
1	B	978/978 (100%)	947 (97%)	31 (3%)	34	64
All	All	1956/1956 (100%)	1890 (97%)	66 (3%)	32	62

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	27	ILE
1	A	48	ARG
1	A	111	VAL
1	A	141	LEU
1	A	154	LEU
1	A	181	GLN
1	A	198	LYS
1	A	215	VAL
1	A	227	GLN
1	A	297	ILE
1	A	302	VAL
1	A	324	ILE
1	A	325	THR
1	A	359	LEU
1	A	394	ILE
1	A	403	LEU
1	A	524	LYS
1	A	630	LYS
1	A	637	GLU
1	A	643	VAL

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Mol	Chain	Res	Type
1	A	710	LYS
1	A	720	ASN
1	A	758	LYS
1	A	789	GLU
1	A	808	PHE
1	A	823	VAL
1	A	917	LYS
1	A	953	THR
1	A	996	ASN
1	A	1000	GLN
1	A	1047	GLN
1	A	1048	GLN
1	A	1181	LYS
1	A	1232	LYS
1	B	8	THR
1	B	27	ILE
1	B	123	ILE
1	B	154	LEU
1	B	180	ILE
1	B	181	GLN
1	B	194	LEU
1	B	211	GLU
1	B	239	VAL
1	B	317	LEU
1	B	324	ILE
1	B	327	LEU
1	B	394	ILE
1	B	403	LEU
1	B	593	LYS
1	B	632	GLU
1	B	637	GLU
1	B	643	VAL
1	B	654	LEU
1	B	720	ASN
1	B	754	ILE
1	B	789	GLU
1	B	874	GLU
1	B	917	LYS
1	B	989	MET
1	B	1000	GLN
1	B	1047	GLN
1	B	1048	GLN

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Mol	Chain	Res	Type
1	B	1118	LYS
1	B	1137	LEU
1	B	1232	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	16	HIS
1	A	46	GLN
1	A	96	ASN
1	A	110	HIS
1	A	128	GLN
1	A	147	GLN
1	A	164	ASN
1	A	169	HIS
1	A	220	GLN
1	A	221	ASN
1	A	227	GLN
1	A	233	ASN
1	A	288	ASN
1	A	289	HIS
1	A	389	HIS
1	A	434	ASN
1	A	444	ASN
1	A	467	HIS
1	A	491	ASN
1	A	513	ASN
1	A	588	HIS
1	A	614	GLN
1	A	649	GLN
1	A	671	GLN
1	A	688	ASN
1	A	691	GLN
1	A	693	ASN
1	A	720	ASN
1	A	739	GLN
1	A	741	ASN
1	A	750	ASN
1	A	770	GLN
1	A	774	GLN
1	A	777	ASN

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Mol	Chain	Res	Type
1	A	802	GLN
1	A	860	GLN
1	A	866	ASN
1	A	911	GLN
1	A	918	ASN
1	A	937	GLN
1	A	976	HIS
1	A	1000	GLN
1	A	1048	GLN
1	A	1073	ASN
1	A	1084	GLN
1	A	1088	ASN
1	A	1108	GLN
1	A	1151	GLN
1	A	1215	ASN
1	B	11	ASN
1	B	16	HIS
1	B	46	GLN
1	B	96	ASN
1	B	110	HIS
1	B	128	GLN
1	B	135	GLN
1	B	147	GLN
1	B	164	ASN
1	B	169	HIS
1	B	181	GLN
1	B	212	HIS
1	B	220	GLN
1	B	221	ASN
1	B	227	GLN
1	B	233	ASN
1	B	248	GLN
1	B	288	ASN
1	B	389	HIS
1	B	419	GLN
1	B	434	ASN
1	B	467	HIS
1	B	491	ASN
1	B	513	ASN
1	B	536	ASN
1	B	608	GLN
1	B	614	GLN

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Mol	Chain	Res	Type
1	B	636	ASN
1	B	641	ASN
1	B	680	ASN
1	B	688	ASN
1	B	691	GLN
1	B	693	ASN
1	B	720	ASN
1	B	739	GLN
1	B	741	ASN
1	B	750	ASN
1	B	765	GLN
1	B	774	GLN
1	B	777	ASN
1	B	802	GLN
1	B	860	GLN
1	B	866	ASN
1	B	918	ASN
1	B	937	GLN
1	B	976	HIS
1	B	1000	GLN
1	B	1047	GLN
1	B	1048	GLN
1	B	1073	ASN
1	B	1088	ASN
1	B	1108	GLN
1	B	1114	GLN
1	B	1132	ASN
1	B	1215	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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	TPP	B	2236	4	25,27,27	2.86	8 (32%)	37,40,40	1.63	8 (21%)
2	SF4	A	2234	1	0,12,12	-	-	-	-	-
6	PYR	B	2239	-	5,5,5	0.98	0	3,6,6	2.12	1 (33%)
2	SF4	B	2233	1	0,12,12	-	-	-	-	-
2	SF4	A	2235	1	0,12,12	-	-	-	-	-
6	PYR	A	2239	-	5,5,5	1.10	0	3,6,6	2.03	1 (33%)
2	SF4	B	2235	1	0,12,12	-	-	-	-	-
2	SF4	B	2234	1	0,12,12	-	-	-	-	-
2	SF4	A	2233	1	0,12,12	-	-	-	-	-
3	TPP	A	2236	4	25,27,27	3.08	9 (36%)	37,40,40	1.74	8 (21%)

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	TPP	B	2236	4	-	3/17/17/17	0/2/2/2
2	SF4	A	2234	1	-	-	0/6/5/5
6	PYR	B	2239	-	-	0/4/4/4	-
2	SF4	B	2233	1	-	-	0/6/5/5
2	SF4	A	2235	1	-	-	0/6/5/5
6	PYR	A	2239	-	-	0/4/4/4	-
2	SF4	B	2235	1	-	-	0/6/5/5
2	SF4	B	2234	1	-	-	0/6/5/5
2	SF4	A	2233	1	-	-	0/6/5/5
3	TPP	A	2236	4	-	5/17/17/17	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2236	TPP	C4'-N3'	8.88	1.47	1.35
3	B	2236	TPP	C6'-C5'	6.59	1.51	1.37
3	B	2236	TPP	C2'-N3'	6.33	1.45	1.34
3	A	2236	TPP	C2'-N3'	5.00	1.42	1.34
3	A	2236	TPP	C2'-N1'	4.99	1.42	1.34
3	B	2236	TPP	C4'-N3'	4.90	1.42	1.35
3	B	2236	TPP	C6'-N1'	4.79	1.44	1.34
3	B	2236	TPP	C4-N3	4.75	1.50	1.39
3	A	2236	TPP	C5'-C4'	4.73	1.51	1.42
3	A	2236	TPP	C4-N3	4.61	1.49	1.39
3	A	2236	TPP	C6'-N1'	4.61	1.44	1.34
3	B	2236	TPP	C2'-N1'	3.98	1.40	1.34
3	A	2236	TPP	C6'-C5'	3.76	1.45	1.37
3	B	2236	TPP	C5'-C4'	3.62	1.49	1.42
3	A	2236	TPP	CM4-C4	2.70	1.55	1.49
3	B	2236	TPP	PA-O7	-2.20	1.50	1.59
3	A	2236	TPP	C5-C4	2.07	1.39	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2236	TPP	C5'-C7'-N3	4.30	122.59	112.97
3	B	2236	TPP	C5'-C7'-N3	3.96	121.83	112.97
3	B	2236	TPP	C6-C5-S1	-3.52	112.44	120.89
3	A	2236	TPP	C6'-N1'-C2'	3.51	121.94	115.96
3	A	2236	TPP	CM2-C2'-N3'	3.50	122.62	117.15
6	B	2239	PYR	OXT-C-CA	3.39	123.24	113.97
6	A	2239	PYR	OXT-C-CA	3.25	122.86	113.97
3	A	2236	TPP	N1'-C2'-N3'	-3.03	120.32	125.54
3	B	2236	TPP	N1'-C2'-N3'	-2.81	120.70	125.54
3	A	2236	TPP	C7-C6-C5	2.77	121.53	112.73
3	B	2236	TPP	C4-C5-S1	2.75	115.04	110.56
3	B	2236	TPP	C5-C4-N3	-2.44	107.06	111.69
3	A	2236	TPP	C6-C5-S1	-2.29	115.41	120.89
3	B	2236	TPP	C6'-N1'-C2'	2.23	119.77	115.96
3	A	2236	TPP	O3B-PB-O3A	2.23	112.10	104.64
3	B	2236	TPP	C6'-C5'-C4'	-2.18	112.75	115.72
3	B	2236	TPP	CM2-C2'-N3'	2.09	120.42	117.15
3	A	2236	TPP	C5-C4-N3	-2.09	107.73	111.69

There are no chirality outliers.

All (8) torsion outliers are listed below:

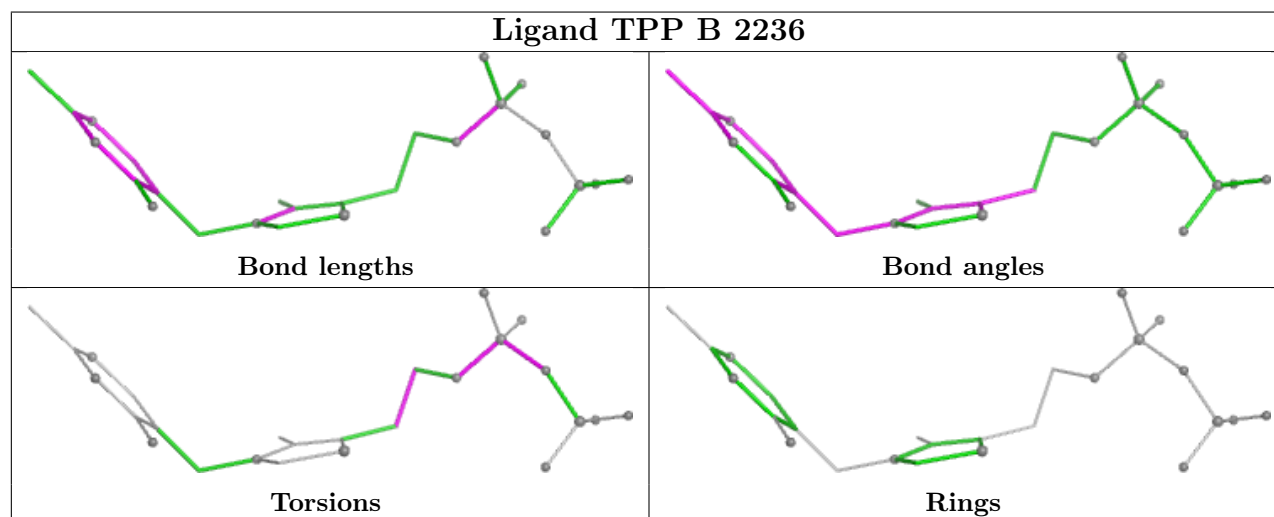
Mol	Chain	Res	Type	Atoms
3	A	2236	TPP	C5-C6-C7-O7
3	A	2236	TPP	C7-O7-PA-O3A
3	B	2236	TPP	C5-C6-C7-O7
3	B	2236	TPP	C7-O7-PA-O1A
3	A	2236	TPP	PB-O3A-PA-O7
3	B	2236	TPP	PB-O3A-PA-O7
3	A	2236	TPP	C7-O7-PA-O1A
3	A	2236	TPP	C7-O7-PA-O2A

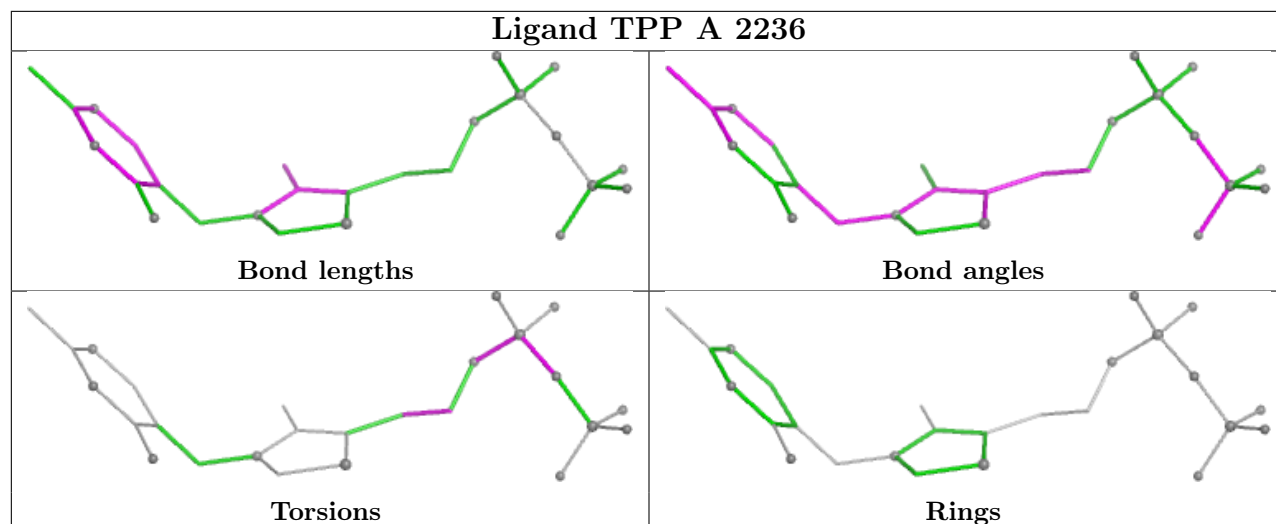
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2236	TPP	1	0
2	B	2233	SF4	1	0
3	A	2236	TPP	1	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

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	1231/1231 (100%)	0.19	57 (4%) 37 34	3, 26, 71, 114	0
1	B	1231/1231 (100%)	-0.07	37 (3%) 52 49	2, 18, 55, 117	0
All	All	2462/2462 (100%)	0.06	94 (3%) 44 40	2, 22, 64, 117	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	576	PHE	6.4
1	B	1180	GLY	5.4
1	B	1179	GLY	4.7
1	B	1178	ALA	4.3
1	A	1178	ALA	4.2
1	A	595	GLY	4.2
1	A	592	GLY	4.1
1	A	1180	GLY	4.0
1	B	592	GLY	4.0
1	B	593	LYS	3.9
1	B	1165	HIS	3.8
1	B	1175	PHE	3.7
1	B	1181	LYS	3.6
1	B	1174	SER	3.6
1	B	630	LYS	3.6
1	B	1182	ALA	3.6
1	A	1181	LYS	3.3
1	A	747	GLY	3.3
1	A	1179	GLY	3.3
1	B	634	MET	3.3
1	A	1230	THR	3.2
1	B	631	ALA	3.2
1	B	1176	ALA	3.2
1	A	593	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	590	ALA	3.1
1	A	587	ILE	3.1
1	A	731	LEU	3.1
1	B	589	LYS	3.0
1	A	754	ILE	3.0
1	A	1177	PRO	3.0
1	A	758	LYS	3.0
1	A	589	LYS	2.9
1	A	1176	ALA	2.9
1	A	591	TYR	2.9
1	B	594	LYS	2.8
1	A	1231	LYS	2.8
1	B	635	THR	2.8
1	A	550	ALA	2.8
1	B	628	GLU	2.8
1	A	575	PRO	2.7
1	A	1232	LYS	2.7
1	A	631	ALA	2.7
1	B	637	GLU	2.6
1	B	590	ALA	2.6
1	A	574	LEU	2.6
1	A	608	GLN	2.6
1	B	629	THR	2.5
1	A	451	GLY	2.5
1	B	1230	THR	2.5
1	A	585	LYS	2.5
1	A	586	SER	2.4
1	B	712	GLU	2.4
1	A	630	LYS	2.4
1	A	715	VAL	2.4
1	A	624	ASP	2.4
1	A	637	GLU	2.4
1	A	714	LEU	2.4
1	B	1227	SER	2.4
1	B	1183	ASP	2.4
1	A	633	PRO	2.4
1	B	1177	PRO	2.4
1	B	1171	ILE	2.3
1	A	712	GLU	2.3
1	A	1085	ASP	2.3
1	B	790	VAL	2.3
1	B	588	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	591	TYR	2.3
1	A	634	MET	2.3
1	A	996	ASN	2.3
1	A	626	PRO	2.3
1	A	627	ALA	2.3
1	A	1154	HIS	2.3
1	B	783	ARG	2.3
1	A	733	GLY	2.3
1	A	1175	PHE	2.3
1	B	627	ALA	2.2
1	A	1165	HIS	2.2
1	B	633	PRO	2.2
1	A	582	LEU	2.2
1	A	594	LYS	2.2
1	B	2	GLY	2.2
1	A	599	VAL	2.2
1	A	629	THR	2.1
1	A	464	THR	2.1
1	A	439	LYS	2.1
1	B	27	ILE	2.1
1	A	520	GLU	2.1
1	A	725	GLU	2.1
1	A	433	ALA	2.0
1	A	515	PRO	2.0
1	A	1151	GLN	2.0
1	B	587	ILE	2.0
1	A	598	ILE	2.0
1	A	498	TYR	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,

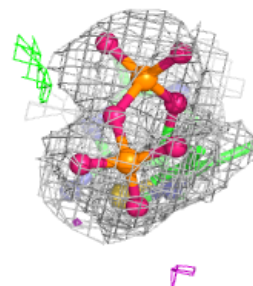
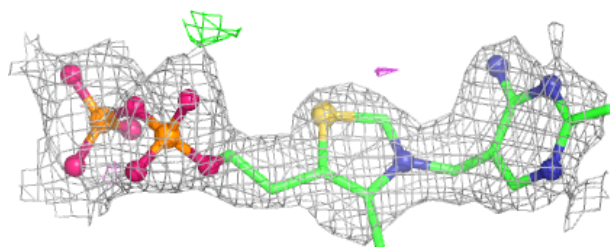
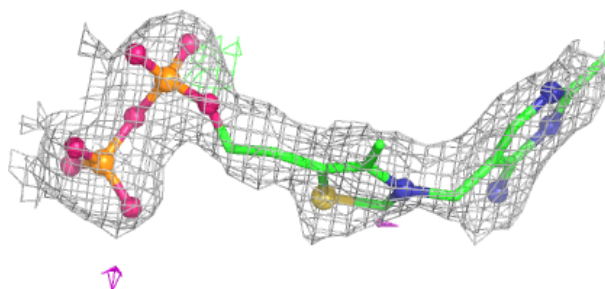
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PYR	A	2239	6/6	0.80	0.20	50,55,57,58	0
5	CA	A	2238	1/1	0.92	0.08	61,61,61,61	0
6	PYR	B	2239	6/6	0.93	0.10	17,23,25,26	0
3	TPP	A	2236	26/26	0.96	0.10	23,36,48,52	0
3	TPP	B	2236	26/26	0.97	0.07	3,14,23,31	0
2	SF4	A	2233	8/8	0.98	0.06	32,34,36,36	0
2	SF4	A	2234	8/8	0.98	0.04	28,29,32,33	0
4	MG	A	2237	1/1	0.98	0.04	16,16,16,16	0
2	SF4	A	2235	8/8	0.98	0.04	20,25,26,28	0
5	CA	B	2238	1/1	0.98	0.06	47,47,47,47	0
2	SF4	B	2233	8/8	0.98	0.03	20,22,24,24	0
2	SF4	B	2234	8/8	0.98	0.04	7,10,12,13	0
2	SF4	B	2235	8/8	0.99	0.03	6,11,12,12	0
4	MG	B	2237	1/1	1.00	0.03	3,3,3,3	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.

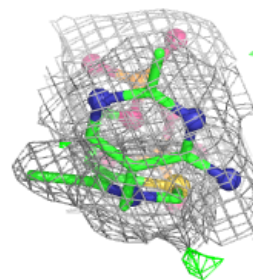
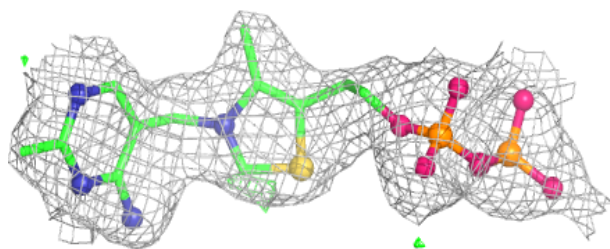
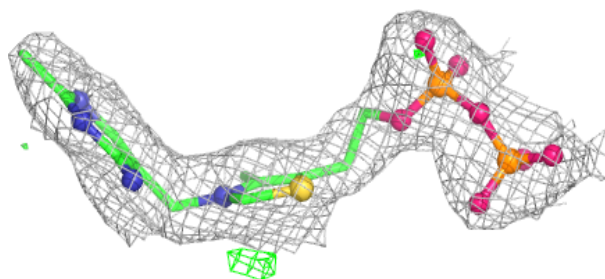
Electron density around TPP A 2236:

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 TPP B 2236:

$2mF_o-DF_c$ (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.