



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:30 AM UTC

PDB ID : 2C3Y / pdb_00002c3y
Title : CRYSTAL STRUCTURE OF THE RADICAL FORM OF PYRUVATE:FERREDOXIN OXIDOREDUCTASE FROM *Desulfovibrio africanus*
Authors : Cavazza, C.; Contreras-Martel, C.; Pieulle, L.; Chabriere, E.; Hatchikian, E.C.; Fontecilla-Camps, J.C.
Deposited on : 2005-10-13
Resolution : 1.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

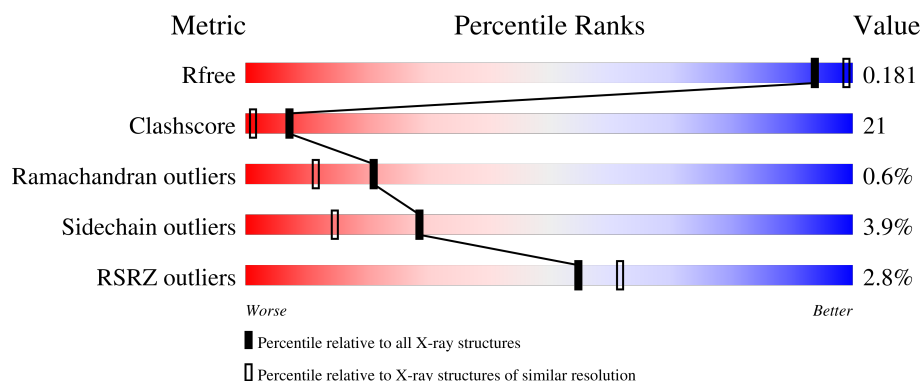
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	3% 64% 33% .
1	B	1231	3% 66% 31% .

2 Entry composition [i](#)

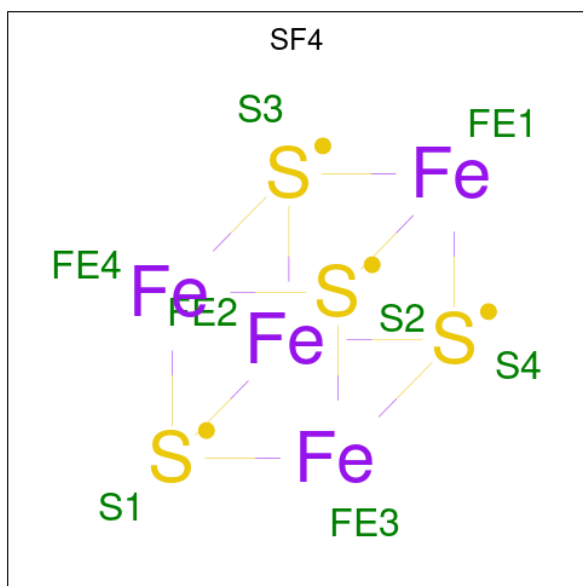
There are 7 unique types of molecules in this entry. The entry contains 20782 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			9347	5920	1591	1778	58			
1	B	1230	Total	C	N	O	S	0	0	0
			9341	5914	1595	1773	59			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



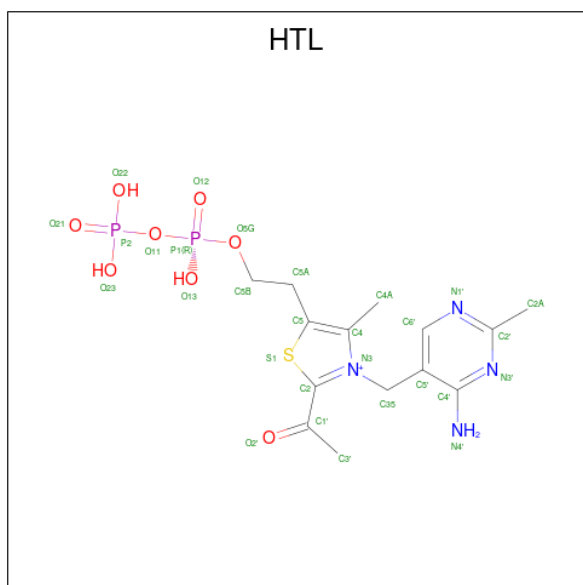
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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

- Molecule 3 is 2-ACETYL-THIAMINE DIPHOSPHATE (CCD ID: HTL) (formula: $C_{14}H_{21}N_4O_8P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 29	C 14	N 4	O 8	P 2	S 1	0	0
3	B	1	Total 29	C 14	N 4	O 8	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	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

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

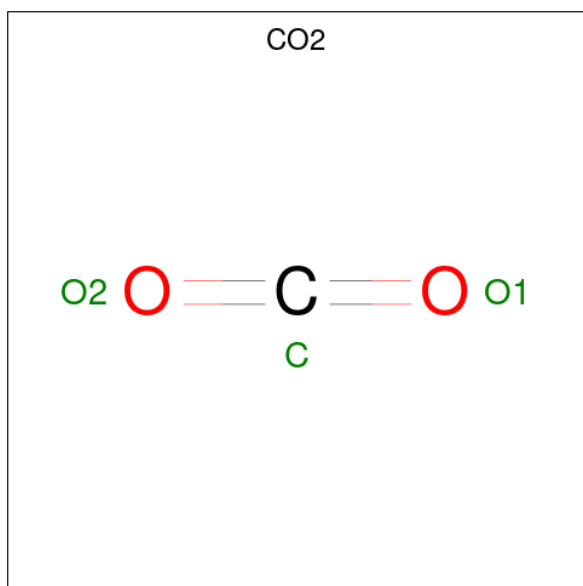
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

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

- Molecule 6 is CARBON DIOXIDE (CCD ID: CO2) (formula: CO₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		

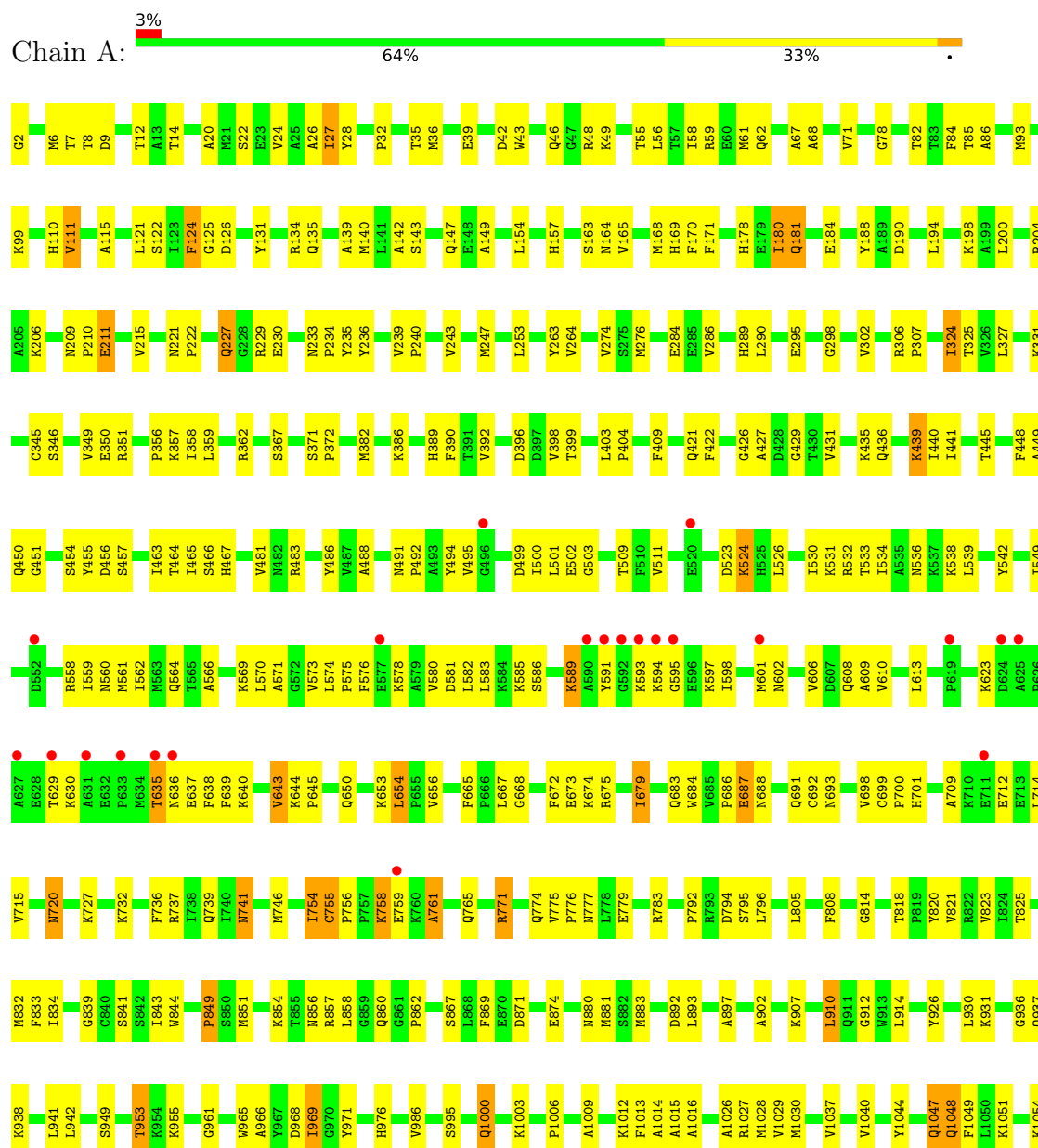
- Molecule 7 is water.

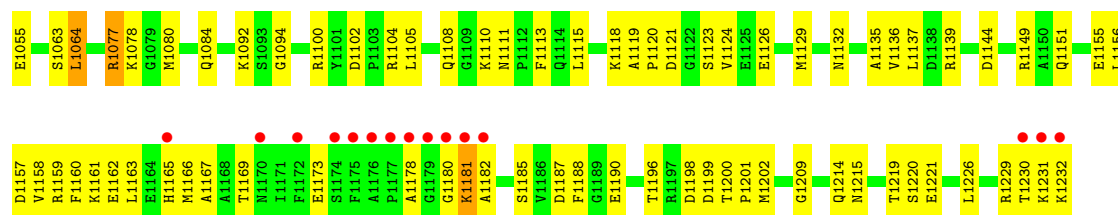
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	881	Total	O	0	0
			881	881		
7	B	1097	Total	O	0	0
			1097	1097		

3 Residue-property plots [i](#)

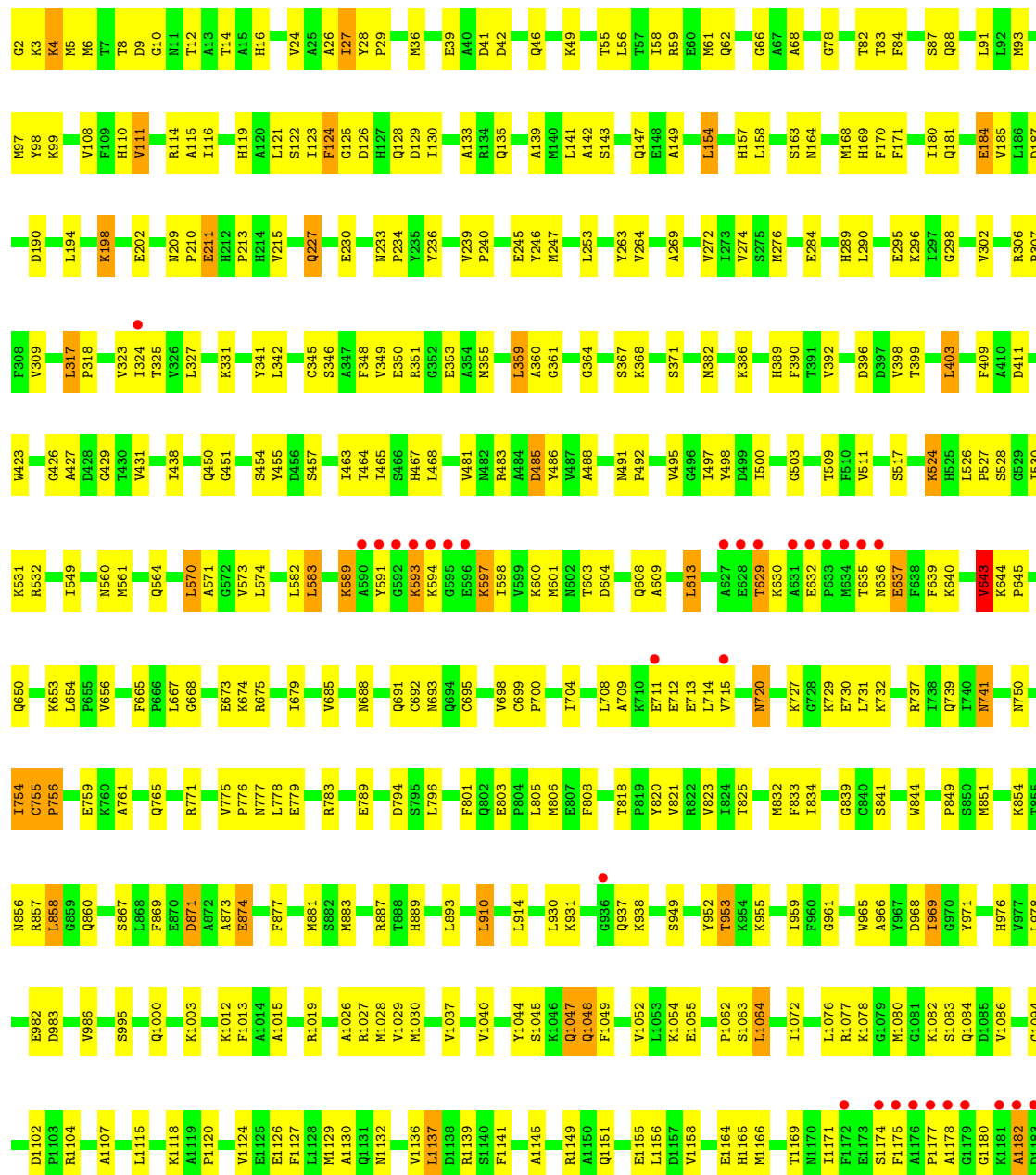
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	86.08Å 145.64Å 211.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.93 8.00 – 1.93	Depositor EDS
% Data completeness (in resolution range)	88.4 (8.00-1.93) 87.1 (8.00-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.93Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.186 , 0.228 0.186 , 0.181	Depositor DCC
R_{free} test set	17404 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 72.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20782	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: SF4, CA, HTL, CO2, 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	0.36	0/9543	0.89	27/12898 (0.2%)
1	B	0.37	0/9534	0.91	37/12884 (0.3%)
All	All	0.36	0/19077	0.90	64/25782 (0.2%)

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	GLY	N-CA-C	10.02	127.37	111.64
1	B	125	GLY	N-CA-C	9.44	127.76	111.15
1	B	756	PRO	N-CA-C	9.15	121.86	110.70
1	A	756	PRO	N-CA-C	7.81	120.23	110.70
1	B	771	ARG	N-CA-C	7.47	119.42	111.28
1	A	969	ILE	N-CA-C	7.39	118.16	110.62
1	A	771	ARG	N-CA-C	7.20	118.78	111.07
1	A	27	ILE	N-CA-C	7.10	120.07	108.99
1	A	139	ALA	N-CA-C	-7.06	100.03	110.48
1	B	969	ILE	N-CA-C	6.97	117.73	110.62
1	B	27	ILE	N-CA-C	6.89	119.74	108.99
1	B	1141	PHE	CA-C-N	6.86	126.38	119.24
1	B	1141	PHE	C-N-CA	6.86	126.38	119.24
1	B	755	CYS	CA-C-N	6.78	127.36	120.38
1	B	755	CYS	C-N-CA	6.78	127.36	120.38
1	A	124	PHE	N-CA-C	6.59	119.04	110.53
1	A	755	CYS	CA-C-N	6.55	127.13	120.38
1	A	755	CYS	C-N-CA	6.55	127.13	120.38
1	B	679	ILE	N-CA-C	-6.54	105.36	111.45
1	B	801	PHE	N-CA-C	-6.39	104.79	112.59
1	B	139	ALA	N-CA-C	-6.38	101.05	110.48
1	B	871	ASP	N-CA-C	6.15	120.41	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1077	ARG	N-CA-C	6.08	118.70	111.71
1	B	966	ALA	N-CA-C	6.05	117.96	111.36
1	A	1231	LYS	CB-CA-C	-6.01	109.63	116.54
1	A	500	ILE	N-CA-C	5.89	117.34	110.62
1	A	995	SER	N-CA-C	5.88	117.56	111.03
1	B	833	PHE	N-CA-C	-5.87	100.62	109.95
1	B	637	GLU	N-CA-C	-5.86	104.98	111.36
1	B	668	GLY	N-CA-C	5.82	123.87	114.90
1	B	570	LEU	N-CA-C	5.73	121.30	113.97
1	A	761	ALA	N-CA-C	-5.67	106.36	113.28
1	A	968	ASP	N-CA-C	5.66	117.11	108.12
1	A	871	ASP	N-CA-C	5.64	119.74	112.41
1	A	1014	ALA	N-CA-C	-5.57	103.84	110.41
1	B	995	SER	N-CA-C	5.53	117.17	111.03
1	B	485	ASP	N-CA-C	-5.46	105.74	112.90
1	B	517	SER	N-CA-C	5.46	117.32	111.36
1	B	247	MET	N-CA-C	-5.45	105.42	111.36
1	A	966	ALA	N-CA-C	5.44	116.89	111.07
1	B	500	ILE	N-CA-C	5.43	116.16	110.62
1	B	213	PRO	N-CA-C	5.43	118.82	111.22
1	A	833	PHE	N-CA-C	-5.40	100.90	109.59
1	A	457	SER	N-CA-C	-5.38	106.22	112.89
1	A	668	GLY	N-CA-C	5.34	123.13	114.90
1	B	364	GLY	N-CA-C	5.33	125.82	113.18
1	A	78	GLY	N-CA-C	5.29	123.23	115.08
1	B	643	VAL	N-CA-C	5.27	116.04	110.72
1	A	1016	ALA	N-CA-C	-5.25	105.59	112.41
1	A	679	ILE	N-CA-C	-5.24	105.74	110.82
1	B	1164	GLU	N-CA-C	-5.23	105.75	111.82
1	B	371	SER	N-CA-C	5.21	116.12	110.13
1	B	968	ASP	N-CA-C	5.18	116.38	108.30
1	B	119	HIS	N-CA-C	-5.17	106.23	112.54
1	B	124	PHE	N-CA-C	5.16	117.18	110.53
1	B	457	SER	N-CA-C	-5.16	106.84	113.23
1	B	560	ASN	N-CA-C	5.15	117.29	111.11
1	A	448	PHE	N-CA-C	-5.14	102.14	110.32
1	B	685	VAL	CA-C-N	5.09	125.12	119.32
1	B	685	VAL	C-N-CA	5.09	125.12	119.32
1	A	580	VAL	N-CA-C	5.08	115.23	110.30
1	B	78	GLY	N-CA-C	5.08	123.39	114.76
1	A	559	ILE	N-CA-C	5.03	119.96	113.07
1	B	29	PRO	N-CA-C	5.01	118.72	110.55

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	9347	0	9203	440	0
1	B	9341	0	9207	393	0
2	A	24	0	0	0	0
2	B	24	0	0	0	0
3	A	29	0	18	1	0
3	B	29	0	18	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	881	0	0	25	0
7	B	1097	0	0	22	0
All	All	20782	0	18446	771	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 21.

All (771) 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)
3:A:2236:HTL:C2	3:A:2236:HTL:C1'	1.89	1.51
3:B:2236:HTL:C1'	3:B:2236:HTL:C2	1.86	1.50
1:B:274:VAL:HG23	1:B:324:ILE:HD11	1.32	1.08
1:A:1200:THR:HG22	1:A:1202:MET:H	1.14	1.06
1:B:823:VAL:HG21	1:B:1049:PHE:HE2	1.22	1.04
1:B:1129:MET:HE3	1:B:1149:ARG:HD3	1.39	1.03
1:B:1200:THR:HG22	1:B:1202:MET:H	1.23	1.02
1:A:8:THR:HB	1:A:12:THR:HG21	1.44	1.00
1:A:198:LYS:H	1:A:198:LYS:HD2	1.23	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:VAL:HG11	1:A:1156:LEU:HD21	1.45	0.98
1:A:639:PHE:HA	1:A:643:VAL:CG1	1.96	0.94
1:A:823:VAL:HG21	1:A:1049:PHE:HE2	1.35	0.92
1:B:1124:VAL:HG11	1:B:1156:LEU:HD21	1.51	0.92
1:B:12:THR:HG22	1:B:39:GLU:OE1	1.69	0.92
1:B:227:GLN:H	1:B:227:GLN:HE21	1.17	0.92
1:B:454:SER:HB3	1:B:465:ILE:HG23	1.53	0.91
1:B:1137:LEU:HD12	1:B:1145:ALA:HB2	1.51	0.90
1:A:398:VAL:HG22	1:A:656:VAL:HG21	1.53	0.90
1:B:639:PHE:HA	1:B:643:VAL:HG13	1.53	0.90
1:A:1200:THR:HG21	1:A:1202:MET:HE3	1.56	0.88
1:B:823:VAL:HG21	1:B:1049:PHE:CE2	2.08	0.88
1:A:1129:MET:HE2	1:A:1129:MET:HA	1.56	0.88
1:A:558:ARG:HG2	1:A:560:ASN:ND2	1.90	0.86
1:A:8:THR:HB	1:A:12:THR:CG2	2.05	0.86
1:A:691:GLN:HE22	1:A:727:LYS:H	1.24	0.85
1:A:1077:ARG:HH11	1:A:1077:ARG:HB2	1.39	0.85
1:B:147:GLN:HE22	1:B:184:GLU:H	1.21	0.84
1:A:1027:ARG:HA	1:A:1030:MET:HE3	1.60	0.83
1:B:639:PHE:HA	1:B:643:VAL:CG1	2.08	0.83
1:B:5:MET:HE1	1:B:184:GLU:HB2	1.59	0.83
1:A:1080:MET:H	1:B:1215:ASN:ND2	1.77	0.83
1:A:601:MET:CA	1:A:602:ASN:N	2.43	0.82
1:B:711:GLU:CA	1:B:712:GLU:N	2.42	0.82
1:B:1126:GLU:CA	1:B:1127:PHE:N	2.43	0.82
1:B:712:GLU:CA	1:B:713:GLU:N	2.43	0.82
1:A:532:ARG:CA	1:A:533:THR:N	2.43	0.81
1:A:637:GLU:CA	1:A:638:PHE:N	2.43	0.81
1:B:245:GLU:CA	1:B:246:TYR:N	2.43	0.81
1:A:445:THR:HG21	1:A:574:LEU:HD21	1.61	0.81
1:A:9:ASP:OD2	1:A:12:THR:HG22	1.80	0.81
1:B:4:LYS:HB3	1:B:4:LYS:HZ3	1.46	0.81
1:A:35:THR:O	1:A:39:GLU:HG2	1.81	0.80
1:B:454:SER:HB3	1:B:465:ILE:CG2	2.12	0.80
1:B:398:VAL:HG22	1:B:656:VAL:HG21	1.62	0.79
1:B:56:LEU:HD23	1:B:58:ILE:HD11	1.64	0.79
1:A:644:LYS:HB3	1:A:645:PRO:HD3	1.65	0.79
1:A:931:LYS:HE2	1:A:949:SER:HB2	1.65	0.78
1:B:239:VAL:HG13	1:B:240:PRO:HD3	1.66	0.78
1:A:910:LEU:HD13	1:A:930:LEU:HD11	1.66	0.77
1:A:937:GLN:HG2	1:A:942:LEU:HB3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:ASN:HD21	1:A:1139:ARG:HH12	1.30	0.77
1:B:1200:THR:HG21	1:B:1202:MET:HE3	1.64	0.77
1:B:986:VAL:HG13	1:B:1064:LEU:HA	1.64	0.77
1:B:264:VAL:HG11	1:B:284:GLU:HG3	1.66	0.77
1:A:140:MET:HE3	1:A:168:MET:HE3	1.68	0.77
1:A:147:GLN:HE22	1:A:184:GLU:H	1.31	0.76
1:A:1111:ASN:HD21	1:A:1169:THR:HG22	1.50	0.76
1:B:49:LYS:NZ	1:B:55:THR:HG23	2.01	0.76
1:B:1077:ARG:HD2	1:B:1130:ALA:HA	1.66	0.76
1:B:1132:ASN:HD21	1:B:1139:ARG:HH12	1.33	0.76
1:A:569:LYS:HD3	1:A:613:LEU:HD23	1.66	0.76
1:A:639:PHE:HA	1:A:643:VAL:HG12	1.67	0.76
1:A:575:PRO:HG2	1:A:578:LYS:HB3	1.69	0.75
7:A:2174:HOH:O	1:B:953:THR:HG21	1.85	0.75
1:A:455:TYR:HB2	1:B:1201:PRO:HG3	1.66	0.75
1:A:1200:THR:HG22	1:A:1202:MET:N	1.98	0.75
1:A:1200:THR:HG23	1:A:1201:PRO:HD2	1.68	0.75
1:A:1151:GLN:O	1:A:1155:GLU:HG3	1.87	0.74
1:B:62:GLN:HA	7:B:2929:HOH:O	1.87	0.74
1:A:635:THR:HG23	1:A:639:PHE:HB3	1.68	0.74
1:B:986:VAL:HG12	1:B:1063:SER:O	1.87	0.74
1:A:110:HIS:HD2	1:A:169:HIS:HD2	1.36	0.74
1:B:549:ILE:HG23	1:B:608:GLN:HG2	1.68	0.74
1:A:1132:ASN:O	1:A:1136:VAL:HG23	1.87	0.74
1:B:1102:ASP:OD1	1:B:1104:ARG:HG2	1.88	0.74
1:A:691:GLN:NE2	1:A:727:LYS:H	1.86	0.73
1:A:227:GLN:H	1:A:227:GLN:HE21	1.37	0.73
1:B:856:ASN:HD21	1:B:860:GLN:HE21	1.34	0.73
1:B:1047:GLN:NE2	1:B:1047:GLN:H	1.86	0.73
1:A:1077:ARG:HB2	1:A:1077:ARG:NH1	2.04	0.73
1:A:805:LEU:HD23	1:A:862:PRO:HD3	1.69	0.72
1:A:883:MET:HE2	1:A:955:LYS:HG3	1.71	0.72
1:A:1102:ASP:OD1	1:A:1104:ARG:HG2	1.89	0.72
1:A:454:SER:HB2	1:A:465:ILE:CG2	2.19	0.72
1:A:635:THR:CG2	1:A:639:PHE:HB3	2.19	0.72
1:A:523:ASP:HA	1:A:531:LYS:NZ	2.04	0.72
1:A:82:THR:HG21	1:A:157:HIS:HE1	1.54	0.72
1:A:1230:THR:O	1:A:1232:LYS:HD3	1.90	0.72
1:A:264:VAL:HG11	1:A:284:GLU:HG3	1.70	0.72
1:A:1167:ALA:HA	7:A:2774:HOH:O	1.89	0.72
1:A:823:VAL:HG21	1:A:1049:PHE:CE2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:TYR:O	1:B:239:VAL:HG12	1.89	0.72
1:B:290:LEU:HD11	1:B:409:PHE:HZ	1.55	0.71
1:A:1080:MET:H	1:B:1215:ASN:HD21	1.37	0.71
1:B:593:LYS:HD2	1:B:594:LYS:N	2.04	0.71
1:B:245:GLU:O	1:B:246:TYR:N	2.24	0.71
1:B:245:GLU:CA	1:B:245:GLU:O	2.39	0.71
1:B:1126:GLU:O	1:B:1127:PHE:N	2.24	0.71
1:B:1126:GLU:CA	1:B:1126:GLU:O	2.39	0.71
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.37	0.71
1:A:759:GLU:CD	1:A:759:GLU:H	1.99	0.70
1:B:272:VAL:O	1:B:324:ILE:HD12	1.91	0.70
1:A:1078:LYS:O	1:B:1219:THR:HG23	1.90	0.70
1:B:691:GLN:HE22	1:B:727:LYS:H	1.37	0.70
1:A:986:VAL:CG2	1:A:1064:LEU:HA	2.22	0.70
1:A:601:MET:O	1:A:602:ASN:N	2.25	0.70
1:B:711:GLU:CA	1:B:711:GLU:O	2.39	0.70
1:B:711:GLU:O	1:B:712:GLU:N	2.24	0.70
1:A:637:GLU:O	1:A:638:PHE:N	2.24	0.70
1:A:601:MET:CA	1:A:601:MET:O	2.40	0.69
1:A:1181:LYS:H	1:B:1019:ARG:HH12	1.39	0.69
1:B:712:GLU:CA	1:B:712:GLU:O	2.40	0.69
1:A:325:THR:HG22	1:A:359:LEU:HB2	1.73	0.69
1:B:775:VAL:O	1:B:779:GLU:HG2	1.92	0.69
1:B:1200:THR:HG22	1:B:1202:MET:N	2.03	0.69
1:A:532:ARG:CA	1:A:532:ARG:O	2.40	0.69
1:A:532:ARG:O	1:A:533:THR:N	2.25	0.69
1:B:135:GLN:CD	1:B:135:GLN:H	2.00	0.69
1:B:712:GLU:O	1:B:713:GLU:N	2.25	0.69
1:A:1215:ASN:ND2	1:B:1080:MET:H	1.91	0.69
1:A:1029:VAL:HG23	1:A:1037:VAL:HG21	1.74	0.69
1:B:598:ILE:HA	1:B:601:MET:HE3	1.74	0.69
1:A:637:GLU:CA	1:A:637:GLU:O	2.40	0.69
1:B:883:MET:HE3	1:B:887:ARG:HD2	1.75	0.69
1:A:1108:GLN:HE21	1:A:1110:LYS:HD2	1.58	0.69
1:B:398:VAL:HG13	1:B:656:VAL:HG23	1.74	0.68
1:A:1129:MET:HE3	1:A:1149:ARG:HD3	1.75	0.68
1:A:198:LYS:HD2	1:A:198:LYS:N	2.05	0.68
1:A:1047:GLN:H	1:A:1047:GLN:NE2	1.90	0.68
1:A:739:GLN:NE2	1:A:777:ASN:HB3	2.08	0.68
1:A:111:VAL:HG13	1:A:170:PHE:HB3	1.73	0.68
1:A:558:ARG:HG2	1:A:560:ASN:HD21	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:PHE:O	1:B:355:MET:HE1	1.94	0.68
1:A:56:LEU:HD23	1:A:58:ILE:HD11	1.75	0.67
1:A:325:THR:HG21	7:A:2340:HOH:O	1.92	0.67
1:A:986:VAL:HG23	1:A:1064:LEU:HD23	1.76	0.67
1:A:398:VAL:HG13	1:A:656:VAL:HG23	1.75	0.67
1:A:523:ASP:HA	1:A:531:LYS:HZ1	1.58	0.67
1:B:325:THR:HG23	1:B:382:MET:SD	2.34	0.67
1:A:856:ASN:HD21	1:A:860:GLN:HE21	1.42	0.67
1:B:818:THR:HA	1:B:821:VAL:HG12	1.77	0.67
1:A:331:LYS:HE3	1:B:230:GLU:OE2	1.95	0.67
1:B:325:THR:HG22	1:B:359:LEU:HB2	1.77	0.67
1:A:953:THR:HG21	7:B:2219:HOH:O	1.94	0.66
1:A:499:ASP:OD2	1:A:502:GLU:HB2	1.95	0.66
1:B:1129:MET:HE3	1:B:1149:ARG:CD	2.22	0.66
1:A:986:VAL:HG22	1:A:1063:SER:O	1.95	0.66
1:B:1047:GLN:H	1:B:1047:GLN:CD	2.02	0.66
1:A:49:LYS:HE3	7:A:2036:HOH:O	1.96	0.66
1:B:239:VAL:CG1	1:B:240:PRO:HD3	2.26	0.66
1:A:239:VAL:CG2	1:A:240:PRO:HD3	2.26	0.65
1:A:635:THR:HG22	1:A:640:LYS:HG3	1.76	0.65
1:B:986:VAL:CG1	1:B:1064:LEU:HA	2.25	0.65
1:B:1137:LEU:HD12	1:B:1145:ALA:CB	2.24	0.65
1:A:198:LYS:H	1:A:198:LYS:CD	2.03	0.65
1:B:775:VAL:HB	1:B:776:PRO:HD3	1.78	0.65
1:A:324:ILE:C	1:A:324:ILE:HD13	2.21	0.65
1:A:215:VAL:HG11	1:B:851:MET:SD	2.37	0.65
1:A:754:ILE:HD11	1:A:1084:GLN:HB2	1.77	0.65
1:A:431:VAL:HG12	1:A:435:LYS:HE3	1.78	0.64
1:A:1219:THR:HG23	1:B:1078:LYS:O	1.96	0.64
1:B:10:GLY:O	1:B:14:THR:HG23	1.96	0.64
1:B:709:ALA:HB3	1:B:714:LEU:HD11	1.79	0.64
1:B:877:PHE:HE1	1:B:982:GLU:HG3	1.63	0.64
1:B:931:LYS:HE2	1:B:949:SER:HB2	1.80	0.64
1:A:1200:THR:CG2	1:A:1202:MET:HE3	2.28	0.64
1:A:398:VAL:HG22	1:A:656:VAL:CG2	2.28	0.64
1:A:233:ASN:HB2	7:A:2197:HOH:O	1.98	0.64
1:A:345:CYS:SG	1:B:349:VAL:HG21	2.38	0.64
1:A:593:LYS:HG3	1:A:594:LYS:H	1.63	0.63
1:A:82:THR:CG2	1:A:157:HIS:HE1	2.11	0.63
1:A:549:ILE:HG23	1:A:608:GLN:NE2	2.13	0.63
1:A:578:LYS:O	1:A:582:LEU:HD13	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ARG:HD3	1:B:353:GLU:HB2	1.81	0.63
1:A:163:SER:HB2	1:A:239:VAL:HG12	1.81	0.63
1:A:6:MET:HG2	1:A:8:THR:HG23	1.79	0.63
1:B:1029:VAL:HG23	1:B:1037:VAL:HG21	1.79	0.63
1:A:274:VAL:HG23	1:A:324:ILE:HD11	1.81	0.63
1:A:1113:PHE:HB3	7:A:2774:HOH:O	1.99	0.63
1:A:561:MET:CE	1:A:583:LEU:HD21	2.28	0.62
1:A:892:ASP:HB3	7:A:2649:HOH:O	1.99	0.62
1:B:1189:GLY:HA3	1:B:1196:THR:HG21	1.81	0.62
1:A:586:SER:HA	1:A:589:LYS:HZ3	1.65	0.62
1:B:1137:LEU:CD1	1:B:1145:ALA:HB2	2.28	0.62
1:A:851:MET:SD	1:B:215:VAL:HG11	2.39	0.62
1:B:1029:VAL:HG21	1:B:1064:LEU:HD12	1.81	0.62
1:B:1231:LYS:HB2	1:B:1231:LYS:NZ	2.15	0.61
1:A:164:ASN:HD22	1:A:206:LYS:NZ	1.97	0.61
1:B:6:MET:HE2	1:B:185:VAL:HG11	1.81	0.61
1:B:598:ILE:HD13	1:B:601:MET:CE	2.31	0.61
1:B:729:LYS:C	1:B:729:LYS:HD3	2.25	0.61
1:A:164:ASN:HD22	1:A:206:LYS:HZ1	1.47	0.61
1:A:758:LYS:HB2	1:A:758:LYS:NZ	2.16	0.61
1:B:227:GLN:H	1:B:227:GLN:NE2	1.95	0.61
1:B:276:MET:HB2	1:B:302:VAL:CG2	2.30	0.61
1:A:14:THR:HG21	1:A:171:PHE:CE2	2.35	0.61
1:B:561:MET:HE1	1:B:583:LEU:HD21	1.83	0.61
1:A:235:TYR:O	1:A:239:VAL:HG13	2.01	0.61
1:B:1124:VAL:HG13	7:B:2985:HOH:O	2.00	0.61
1:A:1047:GLN:H	1:A:1047:GLN:HE21	1.48	0.60
1:B:143:SER:OG	1:B:171:PHE:HB3	2.01	0.60
1:B:691:GLN:NE2	1:B:727:LYS:H	1.99	0.60
1:A:1003:LYS:NZ	1:B:976:HIS:HD2	2.00	0.60
1:A:99:LYS:HE3	1:B:867:SER:O	2.01	0.60
1:A:325:THR:HG23	1:A:382:MET:SD	2.41	0.60
1:A:454:SER:HB2	1:A:465:ILE:HG23	1.82	0.60
1:A:1196:THR:HG23	1:B:1072:ILE:O	2.00	0.60
1:B:26:ALA:C	1:B:27:ILE:HD12	2.26	0.60
1:A:1015:ALA:CB	1:B:1185:SER:HB2	2.32	0.60
1:B:737:ARG:HH11	1:B:739:GLN:HE22	1.49	0.60
1:A:349:VAL:HG21	1:B:345:CYS:SG	2.42	0.60
1:B:1045:SER:OG	1:B:1047:GLN:NE2	2.35	0.60
1:A:805:LEU:HB2	1:A:825:THR:HB	1.84	0.59
1:A:43:TRP:HB3	1:A:48:ARG:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:HIS:HD2	1:A:169:HIS:CD2	2.20	0.59
1:A:1188:PHE:HE1	1:A:1196:THR:HG22	1.67	0.59
1:B:49:LYS:HZ2	1:B:55:THR:HG23	1.67	0.59
1:B:1118:LYS:HE3	7:B:3005:HOH:O	2.02	0.59
1:B:16:HIS:HD2	7:B:2039:HOH:O	1.85	0.59
1:B:198:LYS:O	1:B:202:GLU:HG3	2.03	0.59
1:B:1151:GLN:O	1:B:1155:GLU:HG3	2.01	0.59
1:B:121:LEU:C	1:B:121:LEU:HD23	2.28	0.59
1:B:571:ALA:HB3	7:B:2600:HOH:O	2.02	0.59
1:A:209:ASN:OD1	1:A:211:GLU:HB2	2.02	0.58
1:B:8:THR:HB	1:B:12:THR:OG1	2.03	0.58
1:B:49:LYS:HZ3	1:B:55:THR:HG23	1.67	0.58
1:A:236:TYR:O	1:A:239:VAL:HG22	2.03	0.58
1:B:794:ASP:OD1	1:B:1054:LYS:HD2	2.04	0.58
1:A:215:VAL:HG12	1:B:665:PHE:O	2.02	0.58
1:A:867:SER:O	1:B:99:LYS:HE3	2.04	0.58
1:A:581:ASP:O	1:A:585:LYS:HG2	2.04	0.58
1:A:194:LEU:HD21	1:A:253:LEU:HD11	1.84	0.58
1:B:820:TYR:O	1:B:823:VAL:HG22	2.03	0.58
1:B:708:LEU:HD21	1:B:731:LEU:HD22	1.85	0.58
1:A:566:ALA:HA	1:A:613:LEU:HD21	1.85	0.58
1:A:1158:VAL:O	1:A:1162:GLU:HG3	2.04	0.58
1:A:526:LEU:O	1:A:531:LYS:HE2	2.04	0.57
1:A:971:TYR:OH	1:A:1028:MET:HE2	2.03	0.57
1:A:575:PRO:HG2	1:A:578:LYS:CB	2.34	0.57
1:A:1165:HIS:HD2	1:B:1171:ILE:HD12	1.69	0.57
1:B:1044:TYR:OH	1:B:1118:LYS:HE2	2.04	0.57
1:A:142:ALA:HB2	1:A:170:PHE:CZ	2.39	0.57
1:A:1077:ARG:HH11	1:A:1077:ARG:CB	2.14	0.57
1:B:526:LEU:O	1:B:531:LYS:HE3	2.04	0.57
1:B:675:ARG:HD3	7:B:2700:HOH:O	2.03	0.57
1:A:68:ALA:HB2	1:A:93:MET:HG2	1.87	0.57
1:A:739:GLN:HE22	1:A:777:ASN:HB3	1.67	0.57
1:B:9:ASP:OD2	1:B:12:THR:HG23	2.04	0.57
1:A:561:MET:HE1	1:A:583:LEU:HD21	1.86	0.57
1:A:1181:LYS:HB2	1:A:1181:LYS:NZ	2.20	0.57
1:B:42:ASP:O	1:B:46:GLN:HG3	2.04	0.57
1:B:573:VAL:HG22	7:B:2600:HOH:O	2.05	0.57
1:A:1015:ALA:HB1	1:B:1185:SER:HB2	1.86	0.57
1:B:1187:ASP:HB3	1:B:1190:GLU:HG3	1.87	0.57
1:A:24:VAL:HG13	1:B:881:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLU:OE1	1:B:389:HIS:HE1	1.88	0.56
1:A:396:ASP:OD2	1:A:398:VAL:HG22	2.05	0.56
1:B:1219:THR:HG22	1:B:1220:SER:N	2.20	0.56
1:B:986:VAL:HG13	1:B:1064:LEU:HD23	1.86	0.56
1:B:82:THR:HG23	1:B:108:VAL:O	2.05	0.56
1:A:356:PRO:O	1:A:358:ILE:HD12	2.06	0.56
1:A:463:ILE:HD13	1:A:494:TYR:CE1	2.41	0.56
1:A:986:VAL:HG22	1:A:1064:LEU:HA	1.87	0.56
1:A:606:VAL:O	1:A:610:VAL:HG23	2.05	0.56
1:B:36:MET:HE3	1:B:84:PHE:HB3	1.87	0.56
1:B:883:MET:HE2	1:B:955:LYS:HG3	1.88	0.56
1:B:26:ALA:O	1:B:27:ILE:HD12	2.06	0.55
1:B:737:ARG:HE	1:B:739:GLN:NE2	2.04	0.55
1:A:561:MET:HE3	1:A:564:GLN:HB3	1.88	0.55
1:A:712:GLU:O	1:A:715:VAL:HG23	2.06	0.55
1:B:3:LYS:HE2	1:B:253:LEU:O	2.05	0.55
1:B:346:SER:O	1:B:350:GLU:HG3	2.07	0.55
1:B:857:ARG:HG3	1:B:858:LEU:HD13	1.88	0.55
1:B:110:HIS:HD2	1:B:169:HIS:CD2	2.23	0.55
1:B:110:HIS:HE1	1:B:157:HIS:NE2	2.04	0.55
1:A:635:THR:HG21	1:A:639:PHE:HD2	1.71	0.55
1:A:1003:LYS:HZ3	1:B:976:HIS:HD2	1.54	0.55
1:B:111:VAL:HG22	1:B:170:PHE:HB3	1.87	0.55
1:A:331:LYS:HD3	1:A:362:ARG:CZ	2.37	0.55
1:B:1200:THR:HG23	1:B:1201:PRO:HD2	1.88	0.55
1:B:877:PHE:CE1	1:B:982:GLU:HG3	2.42	0.55
1:B:41:ASP:HA	1:B:58:ILE:HD12	1.90	0.54
1:A:1219:THR:HG22	1:A:1220:SER:N	2.22	0.54
1:B:629:THR:HB	7:B:2644:HOH:O	2.07	0.54
1:A:111:VAL:HG13	1:A:170:PHE:CB	2.36	0.54
1:A:121:LEU:HD23	1:A:121:LEU:C	2.32	0.54
1:B:1166:MET:O	1:B:1169:THR:HG22	2.07	0.54
1:A:593:LYS:HG3	1:A:594:LYS:N	2.22	0.54
1:A:1185:SER:HB2	1:B:1015:ALA:HB1	1.89	0.54
1:B:121:LEU:HD23	1:B:122:SER:N	2.23	0.54
1:B:325:THR:HG21	7:B:2420:HOH:O	2.07	0.54
1:B:227:GLN:HE21	1:B:227:GLN:N	1.98	0.54
1:A:82:THR:HG21	1:A:157:HIS:CE1	2.39	0.54
1:B:390:PHE:HB2	1:B:403:LEU:HD13	1.89	0.54
1:A:194:LEU:HD21	1:A:253:LEU:CD1	2.37	0.54
1:A:1196:THR:HG22	1:A:1196:THR:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ALA:HA	1:B:135:GLN:HE22	1.73	0.54
1:B:597:LYS:NZ	1:B:597:LYS:HB3	2.23	0.54
1:B:983:ASP:HB2	7:B:2972:HOH:O	2.07	0.54
1:A:26:ALA:C	1:A:27:ILE:HD12	2.33	0.54
1:A:211:GLU:OE1	1:B:955:LYS:HE3	2.08	0.54
1:A:883:MET:HE2	1:A:955:LYS:CG	2.38	0.54
1:A:976:HIS:HD2	1:B:1003:LYS:NZ	2.06	0.54
1:B:392:VAL:HG22	1:B:403:LEU:HB2	1.89	0.54
1:B:351:ARG:HD2	7:B:2386:HOH:O	2.08	0.54
1:B:1189:GLY:CA	1:B:1196:THR:HG21	2.38	0.54
1:A:1094:GLY:HA3	1:A:1120:PRO:HG3	1.90	0.53
1:B:398:VAL:HG22	1:B:656:VAL:CG2	2.36	0.53
1:A:869:PHE:CE2	1:A:969:ILE:HG21	2.43	0.53
1:A:486:TYR:OH	1:A:511:VAL:HG11	2.08	0.53
1:B:351:ARG:CD	1:B:353:GLU:HB2	2.38	0.53
1:B:14:THR:HG21	1:B:171:PHE:CE2	2.43	0.53
1:A:741:ASN:C	1:A:741:ASN:HD22	2.16	0.53
1:A:1209:GLY:O	1:B:429:GLY:HA2	2.08	0.53
1:B:27:ILE:HG13	7:B:2075:HOH:O	2.09	0.53
1:B:1132:ASN:O	1:B:1136:VAL:HG22	2.08	0.53
1:A:27:ILE:HG23	1:A:28:TYR:N	2.24	0.53
1:A:239:VAL:HG23	1:A:240:PRO:HD3	1.91	0.53
1:B:209:ASN:OD1	1:B:211:GLU:HB2	2.09	0.53
1:A:1132:ASN:ND2	1:A:1139:ARG:HH12	2.03	0.53
1:A:857:ARG:HG3	1:A:858:LEU:HD12	1.91	0.53
1:B:438:ILE:HD11	1:B:468:LEU:HD22	1.91	0.53
1:A:820:TYR:O	1:A:823:VAL:HG22	2.09	0.53
1:A:147:GLN:NE2	1:A:184:GLU:H	2.03	0.52
1:B:6:MET:HE3	1:B:8:THR:OG1	2.08	0.52
1:B:765:GLN:HE21	1:B:765:GLN:HA	1.75	0.52
1:A:665:PHE:O	1:B:215:VAL:HG12	2.08	0.52
1:A:1187:ASP:HB3	1:A:1190:GLU:HG3	1.91	0.52
1:A:1219:THR:HG21	1:B:1082:LYS:HD3	1.91	0.52
1:A:635:THR:HG21	1:A:639:PHE:CD2	2.45	0.52
1:B:495:VAL:HG11	1:B:526:LEU:HD12	1.90	0.52
1:B:467:HIS:CD2	1:B:481:VAL:H	2.28	0.52
1:A:290:LEU:HB3	1:A:295:GLU:HG3	1.91	0.52
1:A:324:ILE:HD13	1:A:325:THR:N	2.23	0.52
1:A:687:GLU:H	1:A:687:GLU:CD	2.17	0.52
1:B:524:LYS:NZ	1:B:524:LYS:HB2	2.25	0.52
1:B:1132:ASN:ND2	1:B:1139:ARG:HH12	2.03	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:VAL:HG23	1:A:1064:LEU:HA	1.91	0.52
1:A:1044:TYR:OH	1:A:1118:LYS:HE2	2.10	0.52
1:A:180:ILE:O	1:A:450:GLN:HA	2.09	0.52
1:A:841:SER:HA	1:A:844:TRP:CE2	2.45	0.52
1:B:910:LEU:HD13	1:B:930:LEU:HD11	1.91	0.52
1:A:135:GLN:H	1:A:135:GLN:NE2	2.07	0.52
1:A:324:ILE:CG2	1:A:358:ILE:HG13	2.40	0.52
1:B:889:HIS:O	1:B:893:LEU:HD13	2.10	0.52
1:A:720:ASN:N	1:A:720:ASN:HD22	2.08	0.52
1:A:1180:GLY:O	1:A:1181:LYS:HB2	2.09	0.52
1:A:857:ARG:CG	1:A:858:LEU:HD12	2.41	0.51
1:A:1219:THR:HG22	1:A:1221:GLU:HG2	1.92	0.51
1:B:491:ASN:HD22	1:B:492:PRO:HD2	1.75	0.51
1:B:1136:VAL:HG12	1:B:1139:ARG:NH1	2.25	0.51
1:A:549:ILE:HB	1:A:562:ILE:HD13	1.93	0.51
1:A:1181:LYS:H	1:B:1019:ARG:NH1	2.08	0.51
1:B:27:ILE:CG2	1:B:28:TYR:N	2.71	0.51
1:B:1048:GLN:O	1:B:1052:VAL:HG23	2.10	0.51
1:A:818:THR:HA	1:A:821:VAL:HG22	1.91	0.51
1:A:902:ALA:O	1:A:907:LYS:HE3	2.11	0.51
1:A:1105:LEU:O	1:A:1108:GLN:HG2	2.11	0.51
1:B:198:LYS:N	1:B:198:LYS:HE3	2.26	0.51
1:A:650:GLN:CD	1:A:653:LYS:HZ3	2.18	0.51
1:B:323:VAL:HG21	1:B:386:LYS:NZ	2.25	0.51
1:B:423:TRP:CE3	1:B:463:ILE:HD11	2.46	0.51
1:B:467:HIS:HD2	1:B:481:VAL:H	1.59	0.51
1:B:1129:MET:HA	1:B:1129:MET:HE2	1.91	0.51
1:A:190:ASP:O	1:A:194:LEU:CD2	2.58	0.51
1:A:684:TRP:CE3	1:A:686:PRO:HG3	2.46	0.51
1:B:841:SER:HA	1:B:844:TRP:CE2	2.45	0.51
1:B:871:ASP:O	1:B:874:GLU:HG2	2.11	0.51
1:A:755:CYS:SG	1:A:761:ALA:HB3	2.51	0.51
1:A:1026:ALA:O	1:A:1029:VAL:HG22	2.10	0.51
1:B:239:VAL:CG1	1:B:307:PRO:HG2	2.41	0.51
1:B:1200:THR:CG2	1:B:1202:MET:HE3	2.36	0.51
1:A:239:VAL:HG22	1:A:240:PRO:HD3	1.92	0.51
1:A:1144:ASP:OD1	1:B:1182:ALA:HB2	2.10	0.51
1:A:274:VAL:CG2	1:A:324:ILE:HD11	2.41	0.51
1:A:1124:VAL:HG13	7:A:2786:HOH:O	2.10	0.51
1:B:233:ASN:HB2	7:B:2250:HOH:O	2.11	0.51
1:B:290:LEU:HD11	1:B:409:PHE:CZ	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:GLY:O	1:B:427:ALA:HB3	2.10	0.51
1:B:737:ARG:HE	1:B:739:GLN:HE21	1.57	0.51
1:A:691:GLN:HE22	1:A:727:LYS:N	2.01	0.51
1:B:87:SER:OG	1:B:88:GLN:N	2.44	0.51
1:B:609:ALA:O	1:B:613:LEU:HD22	2.11	0.51
1:B:1040:VAL:HG12	1:B:1048:GLN:HE22	1.75	0.51
1:A:1000:GLN:H	1:A:1000:GLN:NE2	2.09	0.50
1:A:456:ASP:OD1	1:A:463:ILE:HG22	2.10	0.50
1:A:796:LEU:HD23	1:A:796:LEU:C	2.36	0.50
1:A:534:ILE:HA	1:A:539:LEU:HD12	1.92	0.50
1:B:650:GLN:HE22	1:B:653:LYS:NZ	2.09	0.50
1:B:1027:ARG:HA	1:B:1030:MET:HE3	1.92	0.50
1:A:194:LEU:N	1:A:194:LEU:HD22	2.26	0.50
1:A:483:ARG:HA	1:A:503:GLY:O	2.11	0.50
1:A:774:GLN:HA	1:A:774:GLN:NE2	2.26	0.50
1:A:1051:LYS:HE3	1:A:1100:ARG:NH1	2.26	0.50
1:A:1129:MET:HA	1:A:1129:MET:CE	2.36	0.50
1:B:82:THR:HG22	1:B:83:THR:N	2.26	0.50
1:A:359:LEU:N	1:A:359:LEU:HD12	2.26	0.50
1:B:486:TYR:HA	1:B:509:THR:HG23	1.93	0.50
1:B:778:LEU:C	1:B:778:LEU:HD13	2.36	0.50
1:A:881:MET:HE3	1:B:59:ARG:HG2	1.94	0.50
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.41	0.50
1:A:538:LYS:HD2	1:A:538:LYS:N	2.27	0.50
1:B:114:ARG:NE	1:B:123:ILE:HA	2.26	0.50
1:B:1132:ASN:CG	1:B:1136:VAL:HG13	2.36	0.49
1:A:435:LYS:HE2	7:A:2407:HOH:O	2.12	0.49
1:A:821:VAL:HG11	7:A:2275:HOH:O	2.12	0.49
1:A:346:SER:HA	1:A:349:VAL:HG22	1.93	0.49
1:A:431:VAL:CG1	1:A:435:LYS:HE3	2.42	0.49
1:A:549:ILE:HG23	1:A:608:GLN:HE21	1.77	0.49
1:B:27:ILE:HG23	1:B:28:TYR:N	2.27	0.49
1:A:110:HIS:HE1	1:A:157:HIS:NE2	2.10	0.49
1:A:180:ILE:HG23	1:A:451:GLY:N	2.28	0.49
1:A:636:ASN:ND2	1:A:672:PHE:CE1	2.81	0.49
1:A:936:GLY:O	1:A:938:LYS:HD3	2.12	0.49
1:B:644:LYS:HB3	1:B:645:PRO:HD3	1.93	0.49
1:A:115:ALA:HB2	1:A:126:ASP:OD1	2.13	0.49
1:B:28:TYR:HE1	7:B:2929:HOH:O	1.95	0.49
1:A:639:PHE:HA	1:A:643:VAL:HG13	1.87	0.49
1:A:1219:THR:CG2	1:A:1221:GLU:HG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:VAL:CG2	1:B:464:THR:HG21	2.43	0.49
1:B:528:SER:O	1:B:532:ARG:HG3	2.13	0.49
1:B:1198:ASP:OD1	1:B:1203:MET:HE3	2.13	0.49
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.95	0.49
1:A:1156:LEU:HD12	1:A:1156:LEU:C	2.38	0.49
1:B:961:GLY:HA3	1:B:965:TRP:CE3	2.48	0.49
1:A:346:SER:O	1:A:349:VAL:HG22	2.12	0.49
1:A:1166:MET:O	1:A:1169:THR:HG22	2.12	0.49
1:A:27:ILE:CG2	1:A:28:TYR:N	2.74	0.49
1:A:227:GLN:HE22	1:B:368:LYS:HZ3	1.61	0.49
1:A:1199:ASP:CG	1:A:1214:GLN:HE22	2.20	0.49
1:A:42:ASP:O	1:A:46:GLN:HG3	2.12	0.48
1:A:1215:ASN:HD21	1:B:1080:MET:H	1.59	0.48
1:B:147:GLN:NE2	1:B:184:GLU:H	2.00	0.48
1:B:495:VAL:HG12	1:B:527:PRO:CD	2.44	0.48
1:A:180:ILE:HD12	1:A:181:GLN:N	2.28	0.48
1:B:361:GLY:HA3	1:B:390:PHE:CZ	2.48	0.48
1:A:55:THR:HG22	7:A:2032:HOH:O	2.13	0.48
1:A:698:VAL:HG11	1:A:1084:GLN:HG3	1.94	0.48
1:B:68:ALA:HB2	1:B:93:MET:HG2	1.94	0.48
1:A:131:TYR:O	1:A:134:ARG:HG2	2.13	0.48
1:A:227:GLN:H	1:A:227:GLN:NE2	2.06	0.48
1:A:698:VAL:HG13	7:A:2538:HOH:O	2.13	0.48
1:B:739:GLN:NE2	1:B:777:ASN:HB3	2.27	0.48
1:B:593:LYS:HD2	1:B:593:LYS:C	2.38	0.48
1:A:536:ASN:ND2	1:A:623:LYS:HG2	2.28	0.48
1:B:589:LYS:NZ	1:B:589:LYS:HB3	2.28	0.48
1:A:230:GLU:OE2	1:B:331:LYS:HE2	2.13	0.48
1:A:390:PHE:HB2	1:A:403:LEU:HD13	1.96	0.48
1:A:881:MET:HE3	1:B:59:ARG:CG	2.44	0.48
1:A:1188:PHE:CE1	1:A:1196:THR:HG22	2.47	0.48
1:B:411:ASP:HB2	1:B:483:ARG:HD2	1.95	0.48
1:A:421:GLN:HA	1:A:466:SER:O	2.14	0.48
1:A:14:THR:CG2	1:A:149:ALA:HB1	2.44	0.48
1:A:351:ARG:HD3	7:A:2318:HOH:O	2.13	0.48
1:A:404:PRO:HG2	7:A:2372:HOH:O	2.13	0.48
1:B:805:LEU:HB2	1:B:825:THR:HB	1.96	0.48
1:B:873:ALA:HA	1:B:959:ILE:HD13	1.96	0.47
1:A:163:SER:O	1:A:164:ASN:HB2	2.15	0.47
1:A:463:ILE:HD13	1:A:494:TYR:CZ	2.50	0.47
1:A:858:LEU:HD12	1:A:858:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ASN:HD22	1:B:491:ASN:C	2.21	0.47
1:A:709:ALA:HB3	1:A:714:LEU:HD11	1.95	0.47
1:A:1173:GLU:HG2	1:B:1158:VAL:HG11	1.96	0.47
1:B:495:VAL:HG12	1:B:527:PRO:HD3	1.97	0.47
1:A:398:VAL:HG23	1:A:399:THR:N	2.28	0.47
1:B:348:PHE:C	1:B:355:MET:HE1	2.38	0.47
1:A:635:THR:CG2	1:A:636:ASN:N	2.77	0.47
1:A:673:GLU:O	1:A:674:LYS:C	2.57	0.47
1:A:12:THR:HG21	7:A:2004:HOH:O	2.15	0.47
1:A:121:LEU:HD23	1:A:122:SER:N	2.30	0.47
1:A:276:MET:HB2	1:A:302:VAL:CG2	2.44	0.47
1:A:491:ASN:HD22	1:A:492:PRO:HD2	1.79	0.47
1:A:561:MET:HE3	1:A:561:MET:O	2.15	0.47
1:A:1226:LEU:O	1:A:1230:THR:HG23	2.14	0.47
1:B:937:GLN:O	1:B:938:LYS:HD2	2.15	0.47
1:B:1026:ALA:O	1:B:1030:MET:HG3	2.14	0.47
1:B:1077:ARG:HB3	1:B:1077:ARG:NH1	2.29	0.47
1:B:1107:ALA:HB2	1:B:1175:PHE:HB3	1.97	0.47
1:A:289:HIS:ND1	1:A:290:LEU:HD12	2.30	0.47
1:B:346:SER:HA	1:B:349:VAL:HG22	1.97	0.47
1:B:396:ASP:OD2	1:B:398:VAL:HG22	2.14	0.47
1:B:573:VAL:HG23	1:B:574:LEU:HG	1.95	0.47
1:A:239:VAL:CG2	1:A:307:PRO:HG2	2.45	0.47
1:A:243:VAL:O	1:A:247:MET:HG3	2.15	0.47
1:A:679:ILE:HD11	1:B:1216:ARG:HH22	1.80	0.47
1:A:912:GLY:HA3	1:A:926:TYR:CD2	2.50	0.47
1:A:1092:LYS:HB3	1:A:1121:ASP:OD2	2.14	0.47
1:B:4:LYS:HZ3	1:B:4:LYS:CB	2.23	0.47
1:B:491:ASN:HD22	1:B:492:PRO:CD	2.27	0.47
1:B:692:CYS:O	1:B:693:ASN:HB2	2.15	0.47
1:B:883:MET:HE2	1:B:955:LYS:CG	2.45	0.47
1:B:1055:GLU:O	1:B:1104:ARG:NH1	2.39	0.47
1:A:1132:ASN:CG	1:A:1136:VAL:CG2	2.88	0.47
1:A:1165:HIS:CE1	1:B:1165:HIS:CE1	3.03	0.47
1:B:389:HIS:HD2	7:B:2123:HOH:O	1.98	0.47
1:A:754:ILE:CD1	1:A:1084:GLN:HB2	2.45	0.46
1:B:483:ARG:HA	1:B:503:GLY:O	2.15	0.46
1:B:598:ILE:HD13	1:B:601:MET:HE1	1.96	0.46
1:A:429:GLY:HA2	1:B:1209:GLY:O	2.14	0.46
1:A:595:GLY:C	1:A:597:LYS:H	2.23	0.46
1:A:1201:PRO:HD3	1:B:455:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ALA:HB2	1:B:126:ASP:OD1	2.15	0.46
1:B:276:MET:HB2	1:B:302:VAL:HG21	1.98	0.46
1:B:485:ASP:O	1:B:509:THR:HG22	2.15	0.46
1:B:806:MET:HE2	1:B:821:VAL:HG11	1.98	0.46
1:B:2:GLY:N	1:B:187:ASP:OD2	2.48	0.46
1:B:390:PHE:CD1	1:B:392:VAL:HG23	2.51	0.46
1:B:1026:ALA:O	1:B:1029:VAL:HG22	2.15	0.46
1:A:27:ILE:HG13	7:A:2068:HOH:O	2.16	0.46
1:A:575:PRO:HD2	1:A:578:LYS:HD3	1.97	0.46
1:A:591:TYR:HD1	1:A:593:LYS:NZ	2.13	0.46
1:A:1077:ARG:HG3	1:B:1193:GLU:CD	2.40	0.46
1:A:357:LYS:HD3	1:A:386:LYS:HD3	1.97	0.46
1:A:1165:HIS:CD2	1:B:1171:ILE:HD12	2.50	0.46
1:B:698:VAL:HG11	1:B:1084:GLN:HG3	1.98	0.46
1:A:643:VAL:HG23	1:A:849:PRO:HG2	1.98	0.46
1:B:163:SER:O	1:B:164:ASN:HB2	2.15	0.46
1:A:22:SER:OG	1:A:82:THR:CG2	2.63	0.46
1:A:358:ILE:C	1:A:359:LEU:HD12	2.41	0.46
1:A:441:ILE:HD13	1:A:573:VAL:HG21	1.98	0.46
1:A:1132:ASN:OD1	1:A:1136:VAL:CG2	2.64	0.46
1:A:1200:THR:HG23	1:A:1201:PRO:CD	2.41	0.46
1:B:600:LYS:HE3	1:B:604:ASP:OD2	2.16	0.46
1:B:741:ASN:C	1:B:741:ASN:HD22	2.23	0.46
1:A:229:ARG:HE	1:B:128:GLN:NE2	2.14	0.46
1:A:431:VAL:CG2	1:A:464:THR:HG21	2.46	0.46
1:B:398:VAL:HG23	1:B:399:THR:N	2.31	0.46
1:A:1006:PRO:HG2	1:A:1009:ALA:HB2	1.98	0.46
1:B:720:ASN:N	1:B:720:ASN:HD22	2.14	0.46
1:A:467:HIS:CD2	1:A:481:VAL:H	2.34	0.46
1:A:210:PRO:HG3	1:B:955:LYS:HD2	1.98	0.45
1:B:5:MET:CE	1:B:184:GLU:HB2	2.39	0.45
1:B:240:PRO:HB3	1:B:309:VAL:HG21	1.96	0.45
1:A:635:THR:HG23	1:A:636:ASN:N	2.31	0.45
1:A:667:LEU:HB3	1:A:854:LYS:HA	1.97	0.45
1:A:389:HIS:HE1	1:B:350:GLU:OE2	1.99	0.45
1:B:346:SER:O	1:B:349:VAL:HG22	2.17	0.45
1:A:229:ARG:HE	1:B:128:GLN:HE22	1.63	0.45
1:B:796:LEU:C	1:B:796:LEU:HD23	2.41	0.45
1:A:1055:GLU:O	1:A:1104:ARG:NH1	2.47	0.45
1:B:124:PHE:HB3	1:B:367:SER:HB2	1.98	0.45
1:B:269:ALA:HA	1:B:296:LYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1219:THR:HG22	1:B:1221:GLU:OE1	2.16	0.45
1:A:180:ILE:HG23	1:A:451:GLY:CA	2.46	0.45
1:B:720:ASN:H	1:B:720:ASN:ND2	2.15	0.45
1:B:361:GLY:HA3	1:B:390:PHE:CE1	2.51	0.45
1:B:714:LEU:N	1:B:714:LEU:HD12	2.32	0.45
1:A:190:ASP:O	1:A:194:LEU:HD23	2.17	0.45
1:A:227:GLN:HE21	1:A:227:GLN:N	2.11	0.45
1:B:295:GLU:HG2	7:B:2333:HOH:O	2.17	0.45
1:B:1077:ARG:HB3	1:B:1077:ARG:HH11	1.81	0.45
1:B:1193:GLU:N	1:B:1193:GLU:OE2	2.50	0.45
1:B:1226:LEU:O	1:B:1230:THR:HG23	2.17	0.45
1:A:306:ARG:HA	1:A:307:PRO:C	2.40	0.45
1:A:779:GLU:O	1:A:783:ARG:HD3	2.16	0.45
1:B:632:GLU:O	1:B:632:GLU:CD	2.60	0.45
1:A:227:GLN:HE22	1:B:368:LYS:NZ	2.14	0.45
1:A:422:PHE:O	1:A:465:ILE:HD12	2.17	0.45
1:A:759:GLU:O	1:A:759:GLU:HG2	2.17	0.45
1:A:1080:MET:N	1:B:1215:ASN:ND2	2.58	0.45
1:A:1221:GLU:HG3	7:B:2753:HOH:O	2.17	0.45
1:B:635:THR:HG23	1:B:640:LYS:HG3	1.98	0.45
1:A:26:ALA:HB3	1:A:71:VAL:HG23	1.98	0.44
1:A:56:LEU:HD23	1:A:58:ILE:CD1	2.44	0.44
1:A:426:GLY:O	1:A:427:ALA:HB3	2.17	0.44
1:A:1012:LYS:O	1:A:1013:PHE:HB2	2.18	0.44
1:B:495:VAL:HG13	1:B:530:ILE:HD12	2.00	0.44
1:A:558:ARG:CG	1:A:560:ASN:ND2	2.74	0.44
1:A:737:ARG:HE	1:A:739:GLN:NE2	2.15	0.44
1:A:771:ARG:O	1:A:775:VAL:HG23	2.17	0.44
1:A:961:GLY:HA3	1:A:965:TRP:CE3	2.51	0.44
1:A:1040:VAL:HG12	1:A:1048:GLN:HE22	1.81	0.44
1:A:1219:THR:CG2	1:A:1220:SER:N	2.80	0.44
1:B:142:ALA:HB2	1:B:170:PHE:CZ	2.53	0.44
1:B:233:ASN:HB2	1:B:234:PRO:HD3	1.99	0.44
1:B:561:MET:HE3	1:B:564:GLN:HB3	1.99	0.44
1:A:290:LEU:HD11	1:A:409:PHE:HZ	1.82	0.44
1:A:465:ILE:HG21	7:A:2419:HOH:O	2.17	0.44
1:A:720:ASN:ND2	1:A:720:ASN:H	2.15	0.44
1:A:20:ALA:HB2	1:A:188:TYR:CZ	2.52	0.44
1:A:501:LEU:N	1:A:501:LEU:HD12	2.33	0.44
1:A:683:GLN:NE2	1:A:765:GLN:HG3	2.32	0.44
1:A:775:VAL:N	1:A:776:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:GLN:HE21	1:A:765:GLN:HG3	1.83	0.44
1:B:194:LEU:HD11	1:B:253:LEU:HD11	2.00	0.44
1:A:22:SER:OG	1:A:82:THR:HG23	2.17	0.44
1:A:439:LYS:HE3	1:A:439:LYS:N	2.33	0.44
1:A:684:TRP:CZ3	1:A:686:PRO:HG3	2.52	0.44
1:A:794:ASP:OD1	1:A:1054:LYS:HD2	2.17	0.44
1:A:1123:SER:O	1:A:1126:GLU:HG2	2.18	0.44
1:A:1165:HIS:CE1	1:B:1165:HIS:HE1	2.34	0.44
1:B:97:MET:HE1	1:B:168:MET:HE2	1.99	0.44
1:B:263:TYR:OH	1:B:298:GLY:HA3	2.18	0.44
1:B:323:VAL:HG21	1:B:386:LYS:HZ2	1.83	0.44
1:B:465:ILE:HG13	1:B:467:HIS:CE1	2.52	0.44
1:B:486:TYR:OH	1:B:511:VAL:HG11	2.18	0.44
1:B:673:GLU:O	1:B:674:LYS:C	2.60	0.44
1:B:699:CYS:HA	1:B:700:PRO:HD3	1.79	0.44
1:A:32:PRO:HB2	1:A:178:HIS:CE1	2.53	0.44
1:A:883:MET:CE	1:A:955:LYS:HG3	2.45	0.44
1:A:1181:LYS:HB2	1:A:1181:LYS:HZ2	1.83	0.44
1:B:14:THR:OG1	1:B:36:MET:SD	2.74	0.44
1:B:87:SER:HA	1:B:129:ASP:HB3	2.00	0.44
1:B:154:LEU:HD22	1:B:158:LEU:CD1	2.48	0.44
1:B:667:LEU:HB3	1:B:854:LYS:HA	2.00	0.44
1:A:233:ASN:HD21	1:B:331:LYS:NZ	2.15	0.43
1:A:1219:THR:HG22	1:A:1221:GLU:H	1.82	0.43
1:A:8:THR:HB	1:A:12:THR:HG23	1.95	0.43
1:A:650:GLN:NE2	1:A:653:LYS:NZ	2.66	0.43
1:A:2:GLY:N	1:A:190:ASP:OD1	2.51	0.43
1:A:26:ALA:O	1:A:27:ILE:HD12	2.18	0.43
1:A:165:VAL:HG21	1:A:239:VAL:HG11	1.99	0.43
1:A:467:HIS:HD2	1:A:481:VAL:H	1.66	0.43
1:A:1159:ARG:O	1:A:1163:LEU:HG	2.18	0.43
1:B:1219:THR:CG2	1:B:1220:SER:N	2.81	0.43
1:A:59:ARG:CG	1:B:881:MET:HE3	2.48	0.43
1:A:143:SER:OG	1:A:171:PHE:HB3	2.18	0.43
1:A:495:VAL:HG11	1:A:526:LEU:HD12	2.00	0.43
1:A:583:LEU:O	1:A:583:LEU:HD23	2.17	0.43
1:A:1015:ALA:HB3	1:B:1185:SER:HB2	2.00	0.43
1:A:1129:MET:HE1	1:A:1135:ALA:HA	2.01	0.43
1:B:190:ASP:O	1:B:194:LEU:HD13	2.19	0.43
1:A:754:ILE:O	1:A:755:CYS:C	2.61	0.43
1:A:758:LYS:HB2	1:A:758:LYS:HZ2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ALA:HB2	1:A:941:LEU:CD2	2.49	0.43
1:A:955:LYS:HD2	1:B:210:PRO:HG3	2.00	0.43
1:A:1157:ASP:O	1:A:1161:LYS:HG3	2.19	0.43
1:B:695:CYS:HB2	1:B:704:ILE:HD13	2.01	0.43
1:B:978:LEU:O	1:B:1062:PRO:HG2	2.19	0.43
1:B:1012:LYS:O	1:B:1013:PHE:HB2	2.19	0.43
1:A:62:GLN:HB3	1:B:976:HIS:CG	2.53	0.43
1:A:436:GLN:O	1:A:440:ILE:HG13	2.19	0.43
1:B:91:LEU:HD11	1:B:116:ILE:HD12	2.00	0.43
1:B:691:GLN:HE22	1:B:727:LYS:N	2.12	0.43
1:B:1076:LEU:HD13	1:B:1086:VAL:HG21	1.99	0.43
1:B:1226:LEU:HD13	1:B:1229:ARG:HH22	1.83	0.43
1:A:536:ASN:HD22	1:A:623:LYS:HG2	1.84	0.43
1:A:583:LEU:HD23	1:A:583:LEU:C	2.44	0.43
1:A:637:GLU:N	1:A:638:PHE:N	2.66	0.43
1:A:675:ARG:HD3	7:A:2519:HOH:O	2.17	0.43
1:A:688:ASN:HB3	1:A:759:GLU:O	2.19	0.43
1:A:699:CYS:HA	1:A:700:PRO:HD3	1.83	0.43
1:A:832:MET:HE2	1:A:834:ILE:HD11	2.00	0.43
1:A:1198:ASP:OD2	1:A:1200:THR:HB	2.18	0.43
1:B:720:ASN:HD22	1:B:720:ASN:H	1.67	0.43
1:B:754:ILE:O	1:B:755:CYS:C	2.61	0.43
1:B:803:GLU:O	1:B:805:LEU:HD13	2.19	0.43
1:B:971:TYR:OH	1:B:1028:MET:HE2	2.18	0.43
1:A:701:HIS:CE1	1:A:746:MET:HG3	2.54	0.43
1:A:1000:GLN:HA	1:A:1012:LYS:HB2	2.00	0.43
1:B:779:GLU:HB3	1:B:783:ARG:HH21	1.83	0.43
1:A:371:SER:HB2	1:A:372:PRO:HD2	2.01	0.43
1:A:398:VAL:CG2	7:B:2250:HOH:O	2.67	0.43
1:A:976:HIS:HD2	1:B:1003:LYS:HZ2	1.66	0.43
1:B:1137:LEU:HD12	1:B:1145:ALA:CA	2.49	0.43
1:A:36:MET:HE3	1:A:84:PHE:HB3	2.01	0.43
1:A:431:VAL:O	1:A:435:LYS:HG3	2.19	0.43
1:B:750:ASN:HD21	1:B:1083:SER:HB2	1.84	0.43
1:B:832:MET:HE2	1:B:834:ILE:HD11	2.01	0.43
1:A:573:VAL:HG12	7:A:2465:HOH:O	2.17	0.42
1:A:881:MET:HE2	1:B:24:VAL:HG13	1.99	0.42
1:B:14:THR:CG2	1:B:149:ALA:HB1	2.48	0.42
1:B:239:VAL:HG13	1:B:240:PRO:CD	2.41	0.42
1:B:650:GLN:NE2	1:B:653:LYS:HZ2	2.17	0.42
1:B:1200:THR:HG23	1:B:1201:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:GLY:O	1:A:843:ILE:HG12	2.19	0.42
1:B:839:GLY:HA2	3:B:2236:HTL:S1	2.59	0.42
1:B:1045:SER:HA	1:B:1047:GLN:HE22	1.84	0.42
1:B:180:ILE:HG22	1:B:451:GLY:O	2.18	0.42
1:B:650:GLN:NE2	1:B:653:LYS:NZ	2.67	0.42
1:B:1132:ASN:OD1	1:B:1136:VAL:CG1	2.67	0.42
1:A:495:VAL:HG13	1:A:530:ILE:CD1	2.49	0.42
1:A:542:TYR:CD2	1:A:570:LEU:HD21	2.54	0.42
1:A:609:ALA:O	1:A:613:LEU:HB2	2.19	0.42
1:A:720:ASN:HD22	1:A:720:ASN:H	1.67	0.42
1:A:164:ASN:ND2	1:A:206:LYS:NZ	2.66	0.42
1:B:698:VAL:HG13	7:B:2721:HOH:O	2.18	0.42
1:B:1228:LYS:O	1:B:1231:LYS:HG3	2.19	0.42
1:A:85:THR:O	1:A:86:ALA:HB2	2.19	0.42
1:A:792:PRO:HB2	1:A:795:SER:HB3	2.02	0.42
1:A:1229:ARG:HH12	1:B:765:GLN:HE22	1.66	0.42
1:B:98:TYR:OH	1:B:135:GLN:HG2	2.18	0.42
7:A:2322:HOH:O	1:B:350:GLU:HG2	2.19	0.42
1:B:111:VAL:HG21	1:B:130:ILE:HG22	2.00	0.42
1:B:180:ILE:HG23	1:B:451:GLY:N	2.35	0.42
1:A:636:ASN:ND2	1:A:672:PHE:HE1	2.16	0.42
1:A:808:PHE:CD2	1:A:808:PHE:N	2.88	0.42
1:A:897:ALA:HB2	1:A:941:LEU:HD22	2.02	0.42
1:A:1118:LYS:HE3	7:A:2780:HOH:O	2.19	0.42
1:B:198:LYS:H	1:B:198:LYS:CE	2.33	0.42
1:B:317:LEU:HD23	1:B:318:PRO:HD2	2.01	0.42
1:A:636:ASN:O	1:A:640:LYS:HG3	2.20	0.42
1:B:491:ASN:C	1:B:491:ASN:ND2	2.78	0.42
1:B:779:GLU:HB3	1:B:783:ARG:NH2	2.35	0.42
1:B:808:PHE:CD2	1:B:808:PHE:N	2.86	0.42
1:A:210:PRO:CG	1:B:955:LYS:HD2	2.50	0.42
1:A:286:VAL:O	1:A:290:LEU:HD13	2.20	0.42
1:A:727:LYS:NZ	1:A:727:LYS:HB3	2.35	0.42
1:A:976:HIS:CE1	1:B:61:MET:HA	2.54	0.42
1:A:1080:MET:N	1:B:1215:ASN:HD21	2.10	0.42
1:B:803:GLU:OE1	1:B:856:ASN:HB2	2.20	0.42
1:A:181:GLN:HA	1:A:449:ALA:O	2.20	0.41
1:A:302:VAL:O	1:A:302:VAL:HG23	2.19	0.41
1:A:371:SER:HB2	1:A:372:PRO:CD	2.50	0.41
1:B:143:SER:HB3	1:B:169:HIS:HE1	1.84	0.41
1:B:488:ALA:HA	1:B:511:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:949:SER:HA	1:B:952:TYR:CE2	2.55	0.41
1:A:523:ASP:HA	1:A:531:LYS:HZ3	1.85	0.41
1:B:56:LEU:HG	1:B:58:ILE:CG1	2.50	0.41
1:B:755:CYS:SG	1:B:761:ALA:HB3	2.60	0.41
1:B:1198:ASP:OD2	1:B:1200:THR:HB	2.20	0.41
1:A:239:VAL:HG23	1:A:240:PRO:CD	2.51	0.41
1:A:1028:MET:HE2	1:B:1028:MET:HE2	2.02	0.41
1:B:135:GLN:H	1:B:135:GLN:NE2	2.17	0.41
1:B:198:LYS:H	1:B:198:LYS:NZ	2.17	0.41
1:B:306:ARG:HA	1:B:307:PRO:C	2.45	0.41
1:B:953:THR:HG22	7:B:2882:HOH:O	2.20	0.41
1:A:396:ASP:OD2	1:A:398:VAL:CG2	2.68	0.41
1:A:595:GLY:C	1:A:597:LYS:N	2.79	0.41
1:A:349:VAL:HG23	1:A:350:GLU:N	2.35	0.41
1:A:392:VAL:CG2	1:A:403:LEU:HD22	2.50	0.41
1:A:720:ASN:N	1:A:720:ASN:ND2	2.68	0.41
1:A:1136:VAL:HG22	1:A:1139:ARG:NH1	2.36	0.41
1:A:398:VAL:HG21	7:B:2250:HOH:O	2.20	0.41
1:A:986:VAL:HG23	1:A:986:VAL:O	2.20	0.41
1:B:789:GLU:N	1:B:789:GLU:OE2	2.54	0.41
1:A:454:SER:HB2	1:A:465:ILE:HG22	2.00	0.41
1:B:302:VAL:O	1:B:302:VAL:HG23	2.21	0.41
1:B:396:ASP:OD2	1:B:656:VAL:HG21	2.21	0.41
1:A:200:LEU:O	1:A:204:ARG:HG2	2.21	0.41
1:A:524:LYS:HB2	1:A:524:LYS:NZ	2.36	0.41
1:A:571:ALA:HB3	7:A:2465:HOH:O	2.20	0.41
1:A:594:LYS:HB2	1:A:598:ILE:HD12	2.02	0.41
1:B:198:LYS:HE3	1:B:198:LYS:H	1.86	0.41
1:B:264:VAL:HG11	1:B:284:GLU:CG	2.44	0.41
1:B:276:MET:CB	1:B:302:VAL:CG2	2.97	0.41
1:B:289:HIS:ND1	1:B:290:LEU:HD12	2.36	0.41
1:B:341:TYR:CD1	1:B:360:ALA:HB2	2.55	0.41
1:B:737:ARG:HH11	1:B:739:GLN:NE2	2.17	0.41
1:B:823:VAL:CG2	1:B:1049:PHE:CE2	2.93	0.41
1:B:1102:ASP:CG	1:B:1104:ARG:HE	2.29	0.41
1:A:324:ILE:C	1:A:324:ILE:CD1	2.91	0.41
1:A:691:GLN:HG2	1:A:736:PHE:CD2	2.56	0.41
7:A:2197:HOH:O	1:B:398:VAL:HG21	2.21	0.41
1:B:180:ILE:O	1:B:450:GLN:HA	2.21	0.41
1:A:1159:ARG:HD3	7:A:2816:HOH:O	2.20	0.40
1:A:566:ALA:HA	1:A:613:LEU:CD2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:LEU:HD12	1:A:654:LEU:HA	1.91	0.40
1:A:700:PRO:HG2	1:A:814:GLY:HA2	2.03	0.40
1:A:874:GLU:HG2	1:B:66:GLY:HA2	2.03	0.40
1:B:111:VAL:HG22	1:B:170:PHE:CB	2.51	0.40
1:B:497:ILE:HG13	1:B:498:TYR:CD1	2.55	0.40
1:B:712:GLU:O	1:B:715:VAL:HG23	2.21	0.40
1:A:233:ASN:HB2	1:A:234:PRO:HD3	2.02	0.40
1:A:263:TYR:OH	1:A:298:GLY:HA3	2.21	0.40
1:A:692:CYS:O	1:A:693:ASN:HB2	2.20	0.40
1:A:941:LEU:HD23	1:A:941:LEU:C	2.46	0.40
1:B:688:ASN:HB3	1:B:759:GLU:O	2.20	0.40
1:B:755:CYS:HA	1:B:756:PRO:HD3	1.87	0.40
1:B:869:PHE:CE2	1:B:969:ILE:HG21	2.56	0.40
1:B:1094:GLY:HA3	1:B:1120:PRO:HG3	2.04	0.40
1:B:1137:LEU:HD13	1:B:1137:LEU:O	2.21	0.40
1:A:7:THR:HB	1:A:180:ILE:HD11	2.03	0.40
1:A:61:MET:HG3	1:A:67:ALA:HA	2.02	0.40
1:A:234:PRO:HD3	7:A:2197:HOH:O	2.20	0.40
1:A:488:ALA:CB	1:A:511:VAL:HG13	2.52	0.40
1:B:382:MET:O	1:B:386:LYS:NZ	2.43	0.40
1:B:1047:GLN:CD	1:B:1047:GLN:N	2.76	0.40
1:B:1180:GLY:O	1:B:1182:ALA:N	2.49	0.40
1:A:59:ARG:HG2	1:B:881:MET:HE3	2.03	0.40
1:A:1119:ALA:HA	1:A:1160:PHE:CE2	2.57	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	1223/1231 (99%)	1166 (95%)	50 (4%)	7 (1%)	21 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	1221/1231 (99%)	1179 (97%)	34 (3%)	8 (1%)	18 9
All	All	2444/2462 (99%)	2345 (96%)	84 (3%)	15 (1%)	21 11

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	732	LYS
1	A	576	PHE
1	A	629	THR
1	B	629	THR
1	B	732	LYS
1	B	1177	PRO
1	B	1178	ALA
1	A	630	LYS
1	A	1181	LYS
1	B	591	TYR
1	B	630	LYS
1	B	1174	SER
1	A	1178	ALA
1	A	1182	ALA
1	B	1182	ALA

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	970/978 (99%)	938 (97%)	32 (3%)	33 20
1	B	971/978 (99%)	927 (96%)	44 (4%)	24 11
All	All	1941/1956 (99%)	1865 (96%)	76 (4%)	28 15

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	VAL

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Mol	Chain	Res	Type
1	A	154	LEU
1	A	180	ILE
1	A	181	GLN
1	A	211	GLU
1	A	227	GLN
1	A	324	ILE
1	A	327	LEU
1	A	439	LYS
1	A	509	THR
1	A	524	LYS
1	A	589	LYS
1	A	635	THR
1	A	643	VAL
1	A	654	LEU
1	A	687	GLU
1	A	720	ASN
1	A	741	ASN
1	A	754	ILE
1	A	758	LYS
1	A	849	PRO
1	A	880	ASN
1	A	893	LEU
1	A	910	LEU
1	A	914	LEU
1	A	953	THR
1	A	1000	GLN
1	A	1047	GLN
1	A	1048	GLN
1	A	1064	LEU
1	A	1115	LEU
1	A	1137	LEU
1	B	4	LYS
1	B	111	VAL
1	B	141	LEU
1	B	154	LEU
1	B	181	GLN
1	B	184	GLU
1	B	198	LYS
1	B	211	GLU
1	B	227	GLN
1	B	317	LEU
1	B	327	LEU

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Mol	Chain	Res	Type
1	B	342	LEU
1	B	359	LEU
1	B	403	LEU
1	B	524	LYS
1	B	570	LEU
1	B	582	LEU
1	B	583	LEU
1	B	589	LYS
1	B	593	LYS
1	B	597	LYS
1	B	603	THR
1	B	613	LEU
1	B	636	ASN
1	B	637	GLU
1	B	643	VAL
1	B	654	LEU
1	B	720	ASN
1	B	730	GLU
1	B	741	ASN
1	B	754	ILE
1	B	849	PRO
1	B	858	LEU
1	B	874	GLU
1	B	910	LEU
1	B	914	LEU
1	B	953	THR
1	B	1000	GLN
1	B	1047	GLN
1	B	1048	GLN
1	B	1064	LEU
1	B	1115	LEU
1	B	1137	LEU
1	B	1231	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) 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

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Mol	Chain	Res	Type
1	A	128	GLN
1	A	135	GLN
1	A	147	GLN
1	A	164	ASN
1	A	169	HIS
1	A	181	GLN
1	A	212	HIS
1	A	220	GLN
1	A	221	ASN
1	A	227	GLN
1	A	233	ASN
1	A	288	ASN
1	A	389	HIS
1	A	421	GLN
1	A	434	ASN
1	A	467	HIS
1	A	491	ASN
1	A	513	ASN
1	A	536	ASN
1	A	543	ASN
1	A	602	ASN
1	A	608	GLN
1	A	636	ASN
1	A	641	ASN
1	A	650	GLN
1	A	683	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	765	GLN
1	A	774	GLN
1	A	777	ASN
1	A	860	GLN
1	A	880	ASN
1	A	976	HIS
1	A	1000	GLN
1	A	1047	GLN
1	A	1048	GLN

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Mol	Chain	Res	Type
1	A	1073	ASN
1	A	1084	GLN
1	A	1108	GLN
1	A	1114	GLN
1	A	1132	ASN
1	A	1165	HIS
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	389	HIS
1	B	421	GLN
1	B	434	ASN
1	B	467	HIS
1	B	482	ASN
1	B	491	ASN
1	B	513	ASN
1	B	536	ASN
1	B	543	ASN
1	B	636	ASN
1	B	650	GLN
1	B	671	GLN
1	B	683	GLN
1	B	688	ASN
1	B	691	GLN
1	B	693	ASN
1	B	720	ASN
1	B	739	GLN
1	B	741	ASN

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Mol	Chain	Res	Type
1	B	750	ASN
1	B	765	GLN
1	B	774	GLN
1	B	777	ASN
1	B	860	GLN
1	B	880	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	1165	HIS
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	$\# Z > 2$
2	SF4	B	2235	1	0,12,12	-	-	-		
2	SF4	A	2235	1	0,12,12	-	-	-		
6	CO2	B	2239	-	2,2,2	1.35	0	1,1,1	0.49	0
6	CO2	A	2239	-	2,2,2	1.56	0	1,1,1	0.50	0
3	HTL	B	2236	4	29,30,30	7.04	15 (51%)	35,45,45	2.34	9 (25%)
2	SF4	B	2233	1	0,12,12	-	-	-		
2	SF4	B	2234	1	0,12,12	-	-	-		
2	SF4	A	2233	1	0,12,12	-	-	-		
2	SF4	A	2234	1	0,12,12	-	-	-		
3	HTL	A	2236	4	29,30,30	7.16	14 (48%)	35,45,45	2.17	12 (34%)

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
2	SF4	B	2235	1	-	-	0/6/5/5
2	SF4	A	2235	1	-	-	0/6/5/5
3	HTL	B	2236	4	-	3/19/21/21	0/2/2/2
2	SF4	B	2233	1	-	-	0/6/5/5
2	SF4	B	2234	1	-	-	0/6/5/5
2	SF4	A	2233	1	-	-	0/6/5/5
2	SF4	A	2234	1	-	-	0/6/5/5
3	HTL	A	2236	4	-	4/19/21/21	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2236	HTL	C1'-C2	33.16	1.89	1.48
3	B	2236	HTL	C1'-C2	30.68	1.86	1.48
3	B	2236	HTL	C2'-N1'	9.52	1.48	1.34
3	A	2236	HTL	C2-N3	9.42	1.58	1.34
3	B	2236	HTL	C2-N3	9.32	1.58	1.34
3	B	2236	HTL	C5-C4	9.11	1.54	1.35
3	B	2236	HTL	C4'-N3'	8.56	1.46	1.35
3	A	2236	HTL	C2'-N1'	7.26	1.45	1.34
3	A	2236	HTL	C5-C4	7.17	1.50	1.35
3	A	2236	HTL	C4'-N3'	6.39	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2236	HTL	C6'-N1'	5.99	1.46	1.34
3	B	2236	HTL	C35-N3	5.17	1.53	1.47
3	B	2236	HTL	O2'-C1'	4.71	1.33	1.23
3	B	2236	HTL	C3'-C1'	4.67	1.59	1.50
3	A	2236	HTL	C5'-C4'	4.57	1.50	1.42
3	A	2236	HTL	C5A-C5	4.56	1.60	1.50
3	A	2236	HTL	O2'-C1'	4.45	1.33	1.23
3	B	2236	HTL	C5A-C5	4.34	1.60	1.50
3	B	2236	HTL	C6'-N1'	4.11	1.42	1.34
3	B	2236	HTL	C5'-C4'	3.96	1.49	1.42
3	A	2236	HTL	C5-S1	3.34	1.80	1.74
3	A	2236	HTL	C3'-C1'	3.28	1.56	1.50
3	A	2236	HTL	C6'-C5'	3.19	1.44	1.37
3	A	2236	HTL	C35-N3	2.87	1.50	1.47
3	B	2236	HTL	P2-O22	-2.80	1.44	1.54
3	B	2236	HTL	C2'-N3'	2.78	1.38	1.34
3	A	2236	HTL	C2'-N3'	2.46	1.38	1.34
3	B	2236	HTL	C5-S1	2.25	1.78	1.74
3	B	2236	HTL	C6'-C5'	2.02	1.41	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2236	HTL	C2A-C2'-N1'	6.87	124.52	117.20
3	A	2236	HTL	C2A-C2'-N1'	5.73	123.30	117.20
3	B	2236	HTL	C5A-C5-S1	-5.10	108.35	119.29
3	B	2236	HTL	C5A-C5-C4	-4.98	115.67	128.17
3	B	2236	HTL	N1'-C2'-N3'	-4.64	117.81	125.53
3	A	2236	HTL	C5A-C5-C4	-4.44	117.03	128.17
3	B	2236	HTL	C4A-C4-N3	4.39	127.69	121.95
3	A	2236	HTL	C4A-C4-N3	4.15	127.37	121.95
3	A	2236	HTL	N1'-C2'-N3'	-3.86	119.11	125.53
3	A	2236	HTL	C5A-C5-S1	-3.41	111.98	119.29
3	A	2236	HTL	C2'-N3'-C4'	3.02	122.74	118.10
3	B	2236	HTL	O5G-C5B-C5A	2.91	120.31	108.63
3	A	2236	HTL	O5G-C5B-C5A	2.85	120.07	108.63
3	B	2236	HTL	C6'-N1'-C2'	2.60	120.33	116.07
3	B	2236	HTL	C35-N3-C4	-2.40	119.95	123.95
3	A	2236	HTL	O2'-C1'-C3'	-2.38	114.44	119.77
3	A	2236	HTL	C3'-C1'-C2	2.22	120.42	118.17
3	B	2236	HTL	C2'-N3'-C4'	2.19	121.47	118.10
3	A	2236	HTL	C35-N3-C4	-2.07	120.49	123.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2236	HTL	O22-P2-O21	2.06	118.87	110.83
3	A	2236	HTL	C35-C5'-C6'	2.01	124.47	120.69

There are no chirality outliers.

All (7) torsion outliers are listed below:

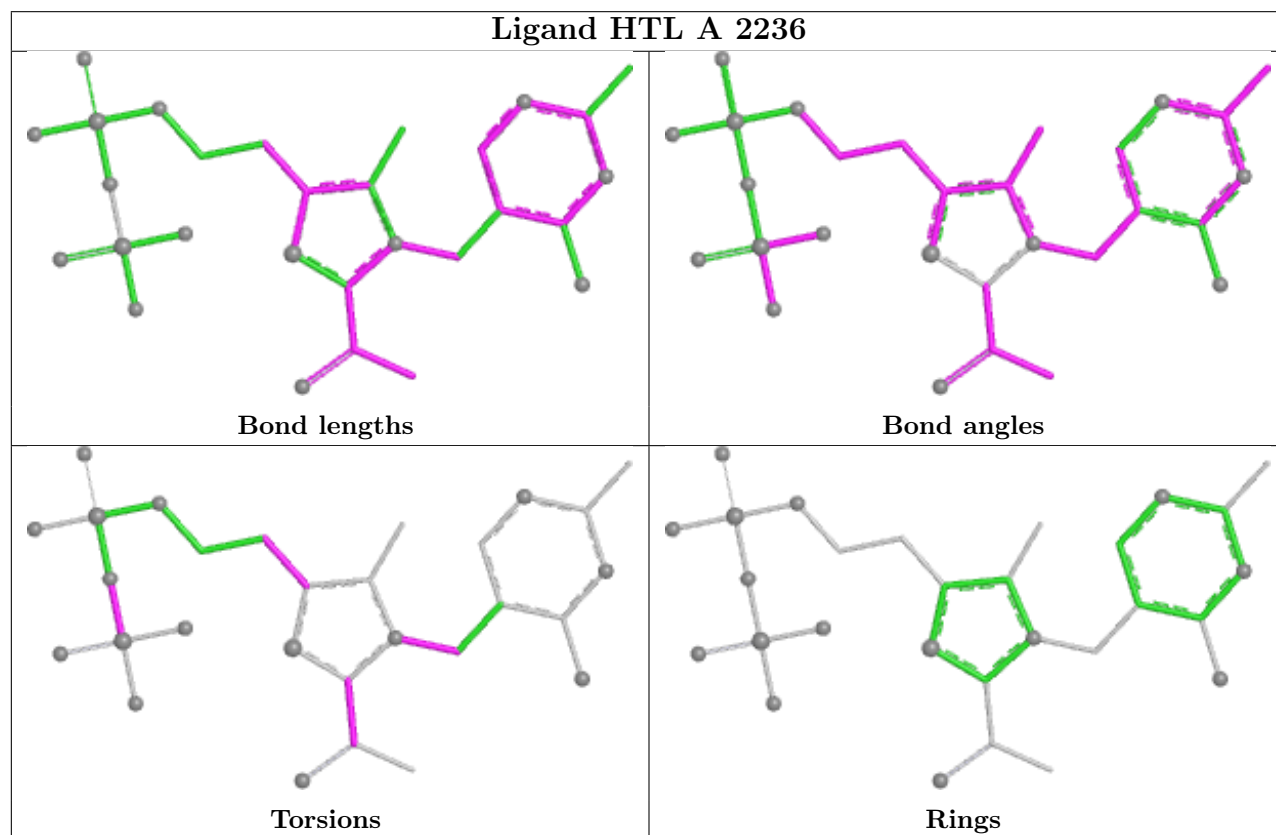
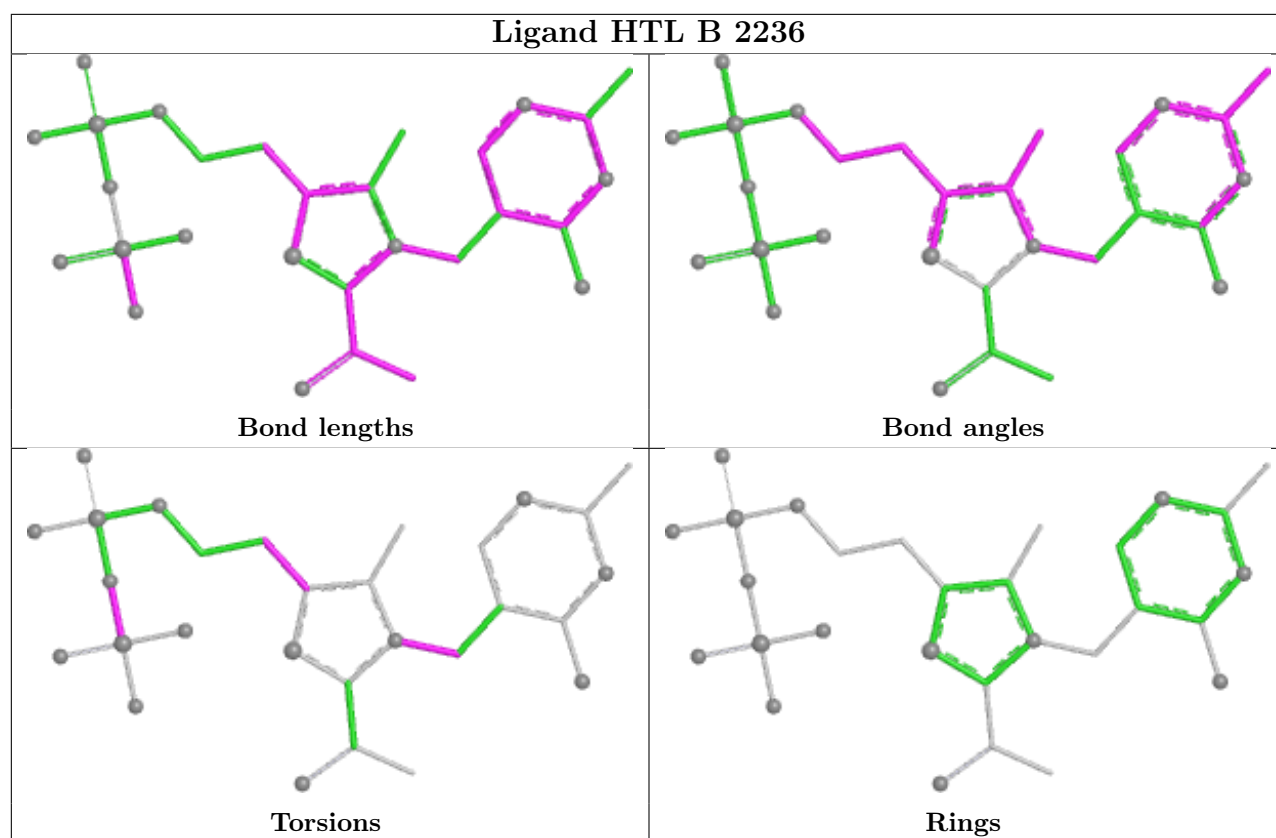
Mol	Chain	Res	Type	Atoms
3	A	2236	HTL	O2'-C1'-C2-S1
3	A	2236	HTL	S1-C5-C5A-C5B
3	B	2236	HTL	S1-C5-C5A-C5B
3	B	2236	HTL	P1-O11-P2-O21
3	A	2236	HTL	P1-O11-P2-O21
3	A	2236	HTL	C5'-C35-N3-C2
3	B	2236	HTL	C5'-C35-N3-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2236	HTL	2	0
3	A	2236	HTL	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

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	1231/1231 (100%)	-0.19	37 (3%)	52	58	8, 19, 49, 97	0
1	B	1230/1231 (99%)	-0.37	32 (2%)	57	64	8, 17, 39, 87	0
All	All	2461/2462 (99%)	-0.28	69 (2%)	55	62	8, 18, 46, 97	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	595	GLY	4.8
1	A	1178	ALA	4.6
1	B	631	ALA	4.5
1	B	1176	ALA	4.4
1	A	1179	GLY	4.3
1	A	629	THR	4.3
1	A	631	ALA	4.0
1	B	590	ALA	4.0
1	B	632	GLU	4.0
1	A	635	THR	3.9
1	B	1178	ALA	3.8
1	A	1176	ALA	3.7
1	B	1175	PHE	3.6
1	B	629	THR	3.4
1	B	593	LYS	3.4
1	A	1177	PRO	3.4
1	A	1230	THR	3.4
1	A	592	GLY	3.4
1	A	1175	PHE	3.3
1	A	627	ALA	3.2
1	B	1174	SER	3.2
1	A	595	GLY	3.1
1	B	1183	ASP	3.1
1	B	628	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1180	GLY	3.0
1	B	1177	PRO	3.0
1	A	619	PRO	2.9
1	A	633	PRO	2.9
1	B	627	ALA	2.9
1	A	601	MET	2.9
1	A	636	ASN	2.9
1	A	1181	LYS	2.9
1	B	594	LYS	2.9
1	B	1182	ALA	2.7
1	A	590	ALA	2.6
1	A	593	LYS	2.6
1	A	496	GLY	2.6
1	B	1181	LYS	2.6
1	A	520	GLU	2.6
1	B	635	THR	2.6
1	B	1231	LYS	2.5
1	B	1172	PHE	2.5
1	A	1174	SER	2.5
1	B	633	PRO	2.5
1	B	591	TYR	2.5
1	A	1172	PHE	2.5
1	B	711	GLU	2.5
1	A	594	LYS	2.5
1	B	636	ASN	2.4
1	A	759	GLU	2.4
1	A	1232	LYS	2.4
1	B	1179	GLY	2.4
1	B	634	MET	2.4
1	A	1165	HIS	2.4
1	B	715	VAL	2.4
1	B	592	GLY	2.3
1	A	711	GLU	2.2
1	B	324	ILE	2.2
1	A	1170	ASN	2.2
1	A	624	ASP	2.2
1	A	1182	ALA	2.2
1	A	591	TYR	2.1
1	A	577	GLU	2.1
1	B	596	GLU	2.1
1	A	625	ALA	2.0
1	A	552	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	1221	GLU	2.0
1	A	1231	LYS	2.0
1	B	936	GLY	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](#)

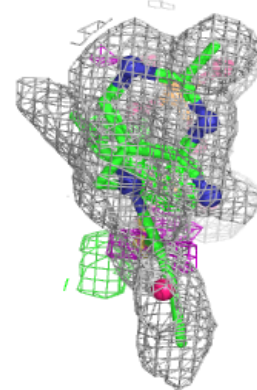
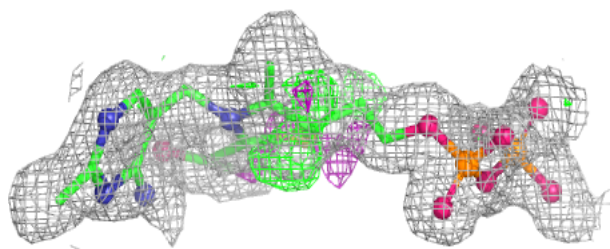
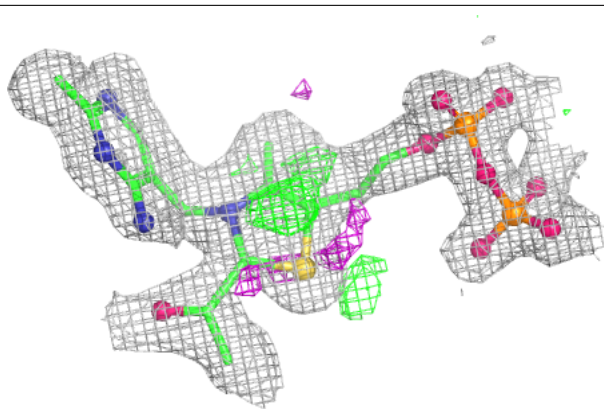
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CO2	B	2239	3/3	0.86	0.16	20,20,24,32	0
6	CO2	A	2239	3/3	0.90	0.10	22,22,29,33	0
3	HTL	A	2236	29/29	0.96	0.06	10,17,30,32	0
3	HTL	B	2236	29/29	0.96	0.06	10,16,25,28	0
4	MG	A	2237	1/1	0.97	0.08	15,15,15,15	0
2	SF4	A	2233	8/8	0.98	0.04	21,22,23,23	0
5	CA	B	2238	1/1	0.98	0.11	38,38,38,38	0
2	SF4	B	2234	8/8	0.99	0.02	10,12,13,14	0
4	MG	B	2237	1/1	0.99	0.03	10,10,10,10	0
5	CA	A	2238	1/1	0.99	0.13	39,39,39,39	0
2	SF4	B	2235	8/8	0.99	0.03	8,11,12,13	0
2	SF4	A	2234	8/8	0.99	0.03	17,18,18,18	0
2	SF4	B	2233	8/8	0.99	0.03	14,16,16,17	0
2	SF4	A	2235	8/8	1.00	0.02	12,14,15,15	0

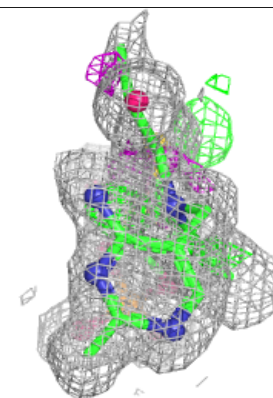
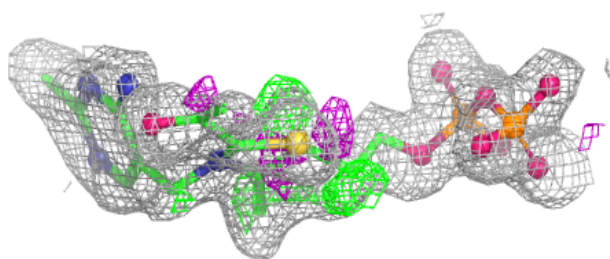
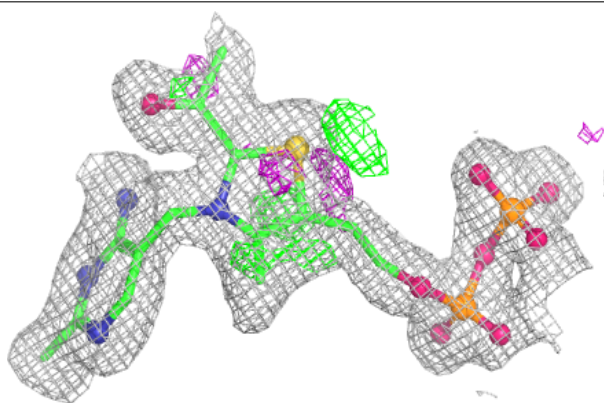
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTL 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 HTL 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.