Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 04:29 pm GMT

PDB ID	:	2C3Y
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:

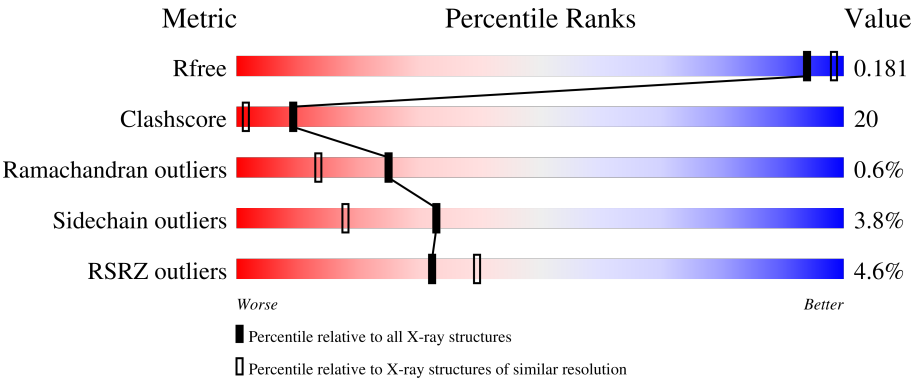
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 <=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	6% 66% 32% ·
1	B	1231	3% 69% 29% ·

2 Entry composition (i)

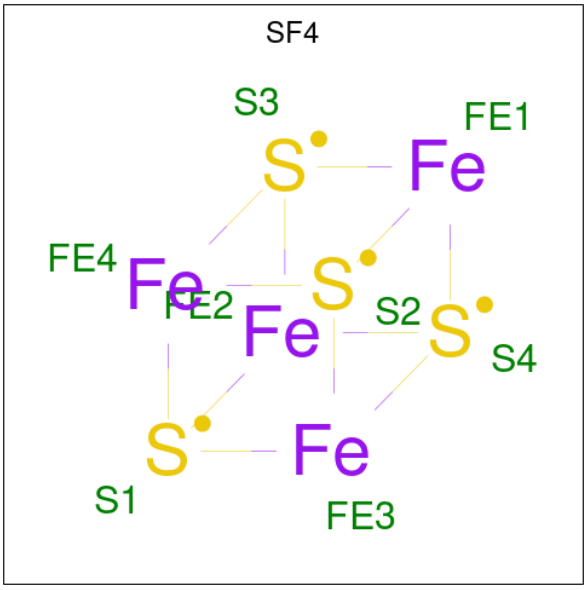
There are 7 unique types of molecules in this entry. The entry contains 20782 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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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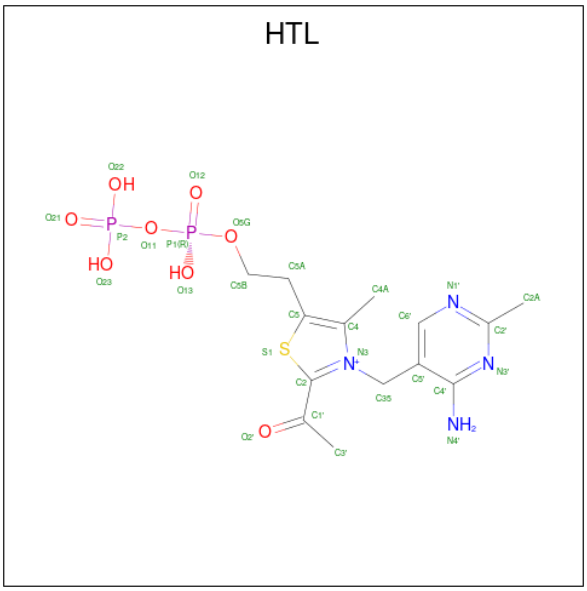
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0

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



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

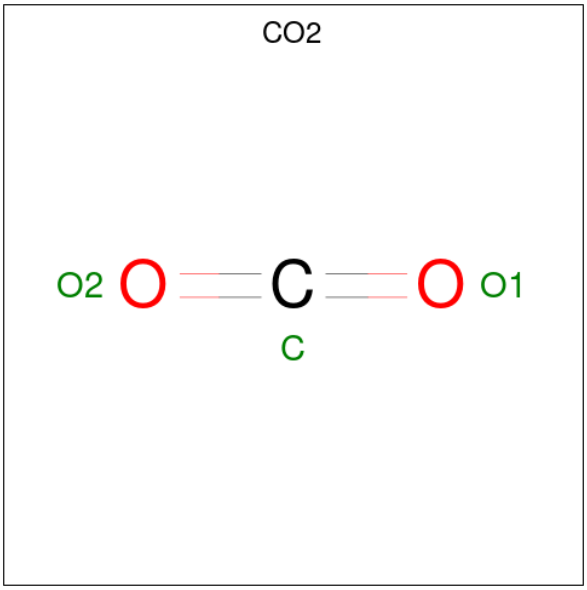
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO_2).



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

- Molecule 7 is water.

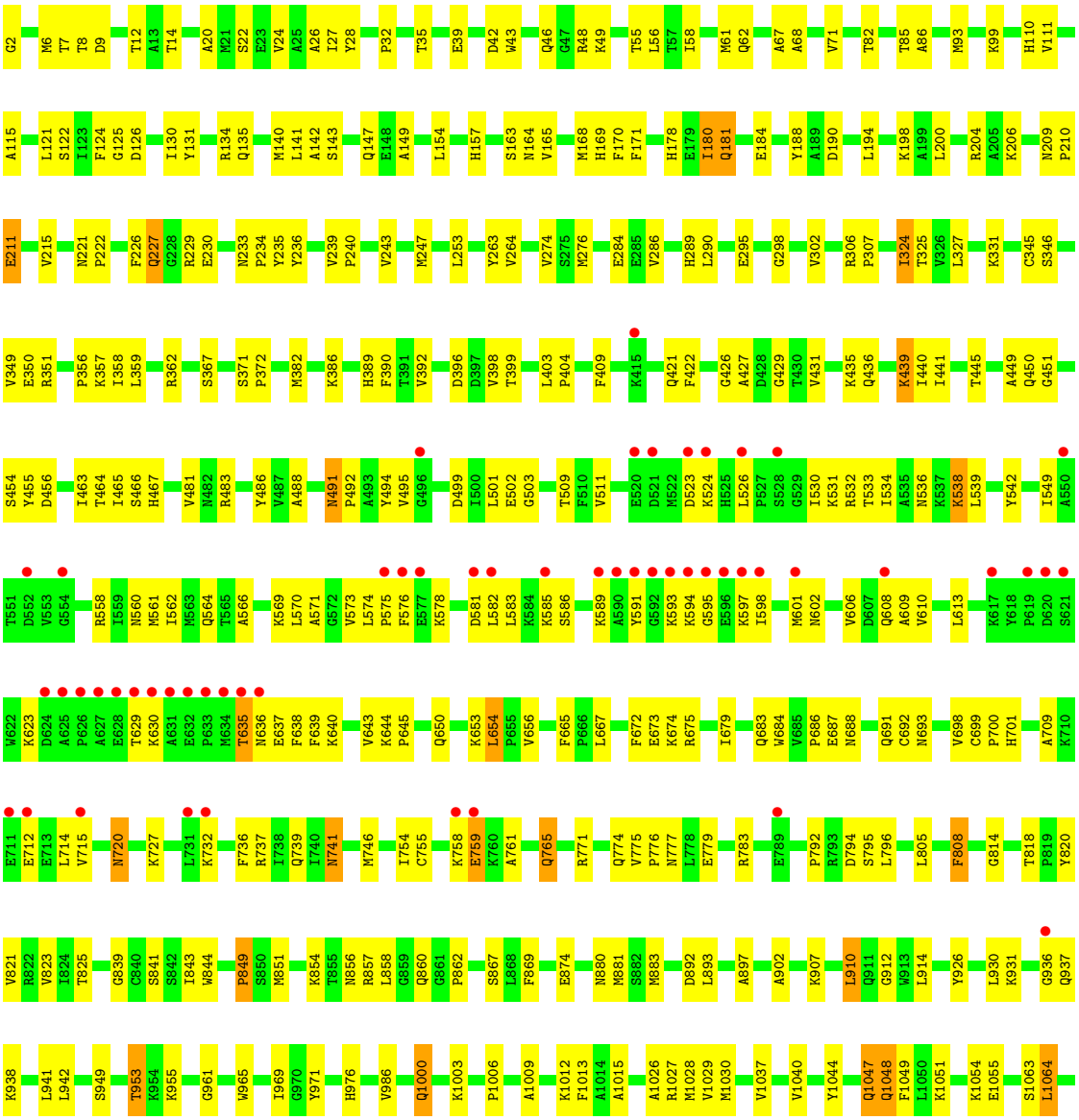
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	881	Total O 881 881	0	0
7	B	1097	Total O 1097 1097	0	0

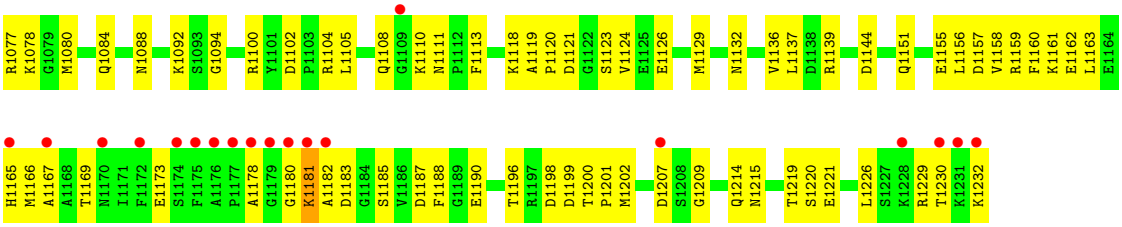
3 Residue-property plots (i)

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

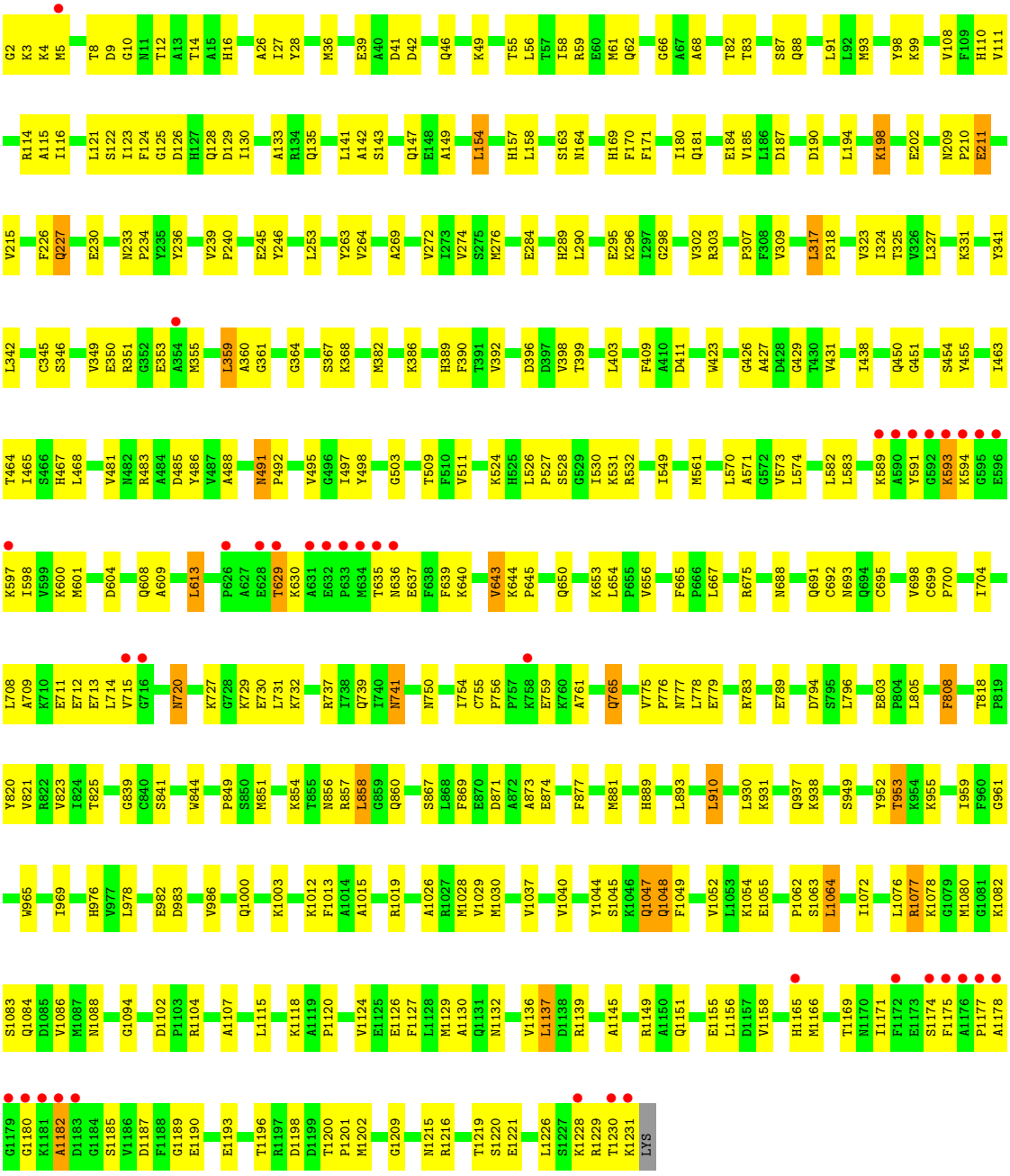
Chain A:





• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

Chain B:



4 Data and refinement statistics (i)

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 – 1.92	Depositor EDS
% Data completeness (in resolution range)	88.4 (8.00-1.93) 87.3 (8.00-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [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)	0.50 , 76.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CO2, HTL, MG, SF4

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	0.31	0/9543	0.58	1/12898 (0.0%)
1	B	0.32	0/9534	0.60	2/12884 (0.0%)
All	All	0.32	0/19077	0.59	3/25782 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	125	GLY	N-CA-C	5.87	127.76	113.10
1	A	125	GLY	N-CA-C	5.71	127.37	113.10
1	B	364	GLY	N-CA-C	5.09	125.82	113.10

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	428	0
1	B	9341	0	9207	369	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	23	0
All	All	20782	0	18446	738	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 20.

All (738) 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: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
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:B:823:VAL:HG21	1:B:1049:PHE:CE2	2.08	0.88
1:A:1003:LYS:HZ2	1:B:976:HIS:HD2	1.23	0.87
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:PHE:HA	1:B:643:VAL:CG1	2.08	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: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
1:A:1132:ASN:HD21	1:A:1139:ARG:HH12	1.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:B:5:MET:HE1	1:B:184:GLU:HB2	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:637:GLU:CA	1:A:637:GLU:O	2.40	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: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
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: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:A:759:GLU:CD	1:A:759:GLU:H	1.99	0.66
1:A:986:VAL:HG22	1:A:1063:SER:O	1.95	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: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:135:GLN:CD	1:B:135:GLN:H	2.00	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:351:ARG:HD3	1:B:353:GLU:HB2	1.81	0.63
1:B:598:ILE:HD13	1:B:601:MET:HE3	1.80	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:586:SER:HA	1:A:589:LYS:HZ3	1.64	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:B:1047:GLN:H	1:B:1047:GLN:CD	2.02	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:598:ILE:HD13	1:B:601:MET:CE	2.31	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:A:140:MET:HG2	1:A:168:MET:HE3	1.82	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:99:LYS:HE3	1:B:867:SER:O	2.01	0.60
1:A:324:ILE:C	1:A:324:ILE:HD13	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:THR:HG23	1:B:1072:ILE:O	2.00	0.60
1:B:1129:MET:CE	1:B:1149:ARG:HD3	2.31	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:A:1129:MET:HE2	1:A:1129:MET:HA	1.82	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
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: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:A:561:MET:HE1	1:A:583:LEU:HD21	1.84	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:A:1027:ARG:HA	1:A:1030:MET:HE3	1.86	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:4:LYS:HB3	1:B:4:LYS:HZ3	1.69	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:883:MET:HE1	1:A:955:LYS:HG3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:164:ASN:HD22	1:A:206:LYS:HZ1	1.51	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:B:729:LYS:C	1:B:729:LYS:HD3	2.25	0.56
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:A:561:MET:HE3	1:A:564:GLN:HB3	1.87	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:523:ASP:HA	1:A:531:LYS:HZ3	1.70	0.56
1:A:606:VAL:O	1:A:610:VAL:HG23	2.05	0.56
1:A:1129:MET:HA	1:A:1129:MET:CE	2.36	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: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:26:ALA:C	1:B:27:ILE:HD12	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1003:LYS:NZ	1:B:976:HIS:HD2	2.00	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:121:LEU:HD23	1:B:121:LEU:C	2.28	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
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:211:GLU:OE1	1:B:955:LYS:HE3	2.08	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:B:349:VAL:HA	1:B:355:MET:HE1	1.91	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: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:523:ASP:HA	1:A:531:LYS:HZ1	1.72	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:A:1003:LYS:HZ2	1:B:976:HIS:CD2	2.15	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:5:MET:CE	1:B:184:GLU:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1028:MET:HE2	1:B:1028:MET:HE2	1.90	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ILE:CG2	1:A:28:TYR:N	2.74	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: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
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: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:1129:MET:HE3	1:B:1149:ARG:HD3	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:B:82:THR:HG22	1:B:83:THR:N	2.26	0.50
1:A:227:GLN:HE22	1:B:368:LYS:HZ3	1.60	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:A:221:ASN:HB3	1:A:222:PRO:CD	2.41	0.50
1:A:121:LEU:HD23	1:A:121:LEU:C	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:26:ALA:C	1:A:27:ILE:HD12	2.33	0.49
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.95	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: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:A:741:ASN:C	1:A:741:ASN:HD22	2.16	0.48
1:A:1027:ARG:HA	1:A:1030:MET:CE	2.43	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: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: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:B:1129:MET:HE2	1:B:1149:ARG:HD3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:687:GLU:H	1:A:687:GLU:CD	2.17	0.47
1:A:635:THR:CG2	1:A:636:ASN:N	2.77	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:1226:LEU:O	1:A:1230:THR:HG23	2.14	0.47
1:B:4:LYS:HB3	1:B:4:LYS:NZ	2.29	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:A:971:TYR:OH	1:A:1028:MET:HE2	2.14	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: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:1055:GLU:O	1:B:1104:ARG:NH1	2.39	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:A:429:GLY:HA2	1:B:1209:GLY:O	2.14	0.46
1:A:1201:PRO:HD3	1:B:455:TYR:HB2	1.97	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ASP:O	1:B:509:THR:HG22	2.15	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: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:A:758:LYS:HB2	1:A:758:LYS:HZ2	1.79	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:441:ILE:HD13	1:A:573:VAL:HG21	1.98	0.46
1:A:561:MET:HE3	1:A:561:MET:O	2.16	0.46
1:A:883:MET:CE	1:A:955:LYS:HG3	2.45	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:A:1200:THR:HG21	1:A:1202:MET:CE	2.46	0.46
1:B:600:LYS:HE3	1:B:604:ASP:OD2	2.16	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:B:778:LEU:C	1:B:778:LEU:HD13	2.36	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:1200:THR:HG21	1:A:1202:MET:HE3	1.98	0.46
1:A:210:PRO:HG3	1:B:955:LYS:HD2	1.98	0.45
1:A:796:LEU:HD23	1:A:796:LEU:C	2.36	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: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
1:B:1219:THR:HG22	1:B:1221:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1132:ASN:CG	1:B:1136:VAL:HG13	2.36	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:779:GLU:O	1:A:783:ARG:HD3	2.16	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:A:1199:ASP:CG	1:A:1214:GLN:HE22	2.20	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:1200:THR:HG21	1:B:1202:MET:HE3	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
1:A:683:GLN:HE21	1:A:765:GLN:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1156:LEU:HD12	1:A:1156:LEU:C	2.38	0.44
1:A:1165:HIS:CE1	1:B:1165:HIS:HE1	2.34	0.44
1:B:263:TYR:OH	1:B:298:GLY:HA3	2.18	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: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: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:593:LYS:HD2	1:B:593:LYS:C	2.38	0.43
1:B:1219:THR:CG2	1:B:1220:SER:N	2.81	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:B:190:ASP:O	1:B:194:LEU:HD13	2.19	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1198:ASP:OD2	1:A:1200:THR:HB	2.18	0.43
1:B:491:ASN:HD22	1:B:491:ASN:C	2.21	0.43
1:B:720:ASN:HD22	1:B:720:ASN:H	1.67	0.43
1:B:803:GLU:O	1:B:805:LEU:HD13	2.19	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:198:LYS:H	1:B:198:LYS:HZ2	1.67	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: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:A:573:VAL:HG12	7:A:2465:HOH:O	2.17	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:1200:THR:HG23	1:B:1201:PRO:CD	2.49	0.42
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:A:673:GLU:O	1:A:674:LYS:C	2.57	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:650:GLN:HE22	1:A:653:LYS:HZ1	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:881:MET:HE3	1:B:59:ARG:HB2	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:B:355:MET:HE2	7:B:2386:HOH:O	2.18	0.42
1:A:636:ASN:ND2	1:A:672:PHE:HE1	2.16	0.42
1:A:692:CYS:O	1:A:693:ASN:HB2	2.20	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:A:1132:ASN:CG	1:A:1136:VAL:CG2	2.88	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:B:561:MET:HE3	1:B:561:MET:O	2.20	0.42
1:A:636:ASN:O	1:A:640:LYS:HG3	2.20	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:595:GLY:C	1:A:597:LYS:H	2.23	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:650:GLN:HE22	1:B:653:LYS:HZ3	1.68	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
1:B:949:SER:HA	1:B:952:TYR:CE2	2.55	0.41
1:A:1077:ARG:HG3	1:B:1193:GLU:CD	2.40	0.41
1:B:4:LYS:HZ3	1:B:185:VAL:HG23	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HG23	1:A:240:PRO:CD	2.51	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:741:ASN:C	1:B:741:ASN:HD22	2.23	0.41
1:B:953:THR:HG22	7:B:2882:HOH:O	2.20	0.41
1:A:24:VAL:HG13	1:B:881:MET:HE1	2.01	0.41
1:A:358:ILE:C	1:A:359:LEU:HD12	2.41	0.41
1:A:396:ASP:OD2	1:A:398:VAL:CG2	2.68	0.41
1:A:130:ILE:O	1:A:140:MET:HE3	2.20	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:HG23	1:B:302:VAL:O	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: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:B:796:LEU:C	1:B:796:LEU:HD23	2.41	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:306:ARG:HA	1:A:307:PRO:C	2.40	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:1180:GLY:O	1:B:1182:ALA:N	2.49	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%)	25	13
1	B	1221/1231 (99%)	1179 (97%)	34 (3%)	8 (1%)	22	11
All	All	2444/2462 (99%)	2345 (96%)	84 (3%)	15 (1%)	25	13

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	732	LYS
1	A	576	PHE

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Mol	Chain	Res	Type
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 (i)

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%)	936 (96%)	34 (4%)	36	21
1	B	971/978 (99%)	931 (96%)	40 (4%)	30	15
All	All	1941/1956 (99%)	1867 (96%)	74 (4%)	33	18

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	LEU
1	A	154	LEU
1	A	180	ILE
1	A	181	GLN
1	A	211	GLU
1	A	226	PHE
1	A	227	GLN
1	A	324	ILE
1	A	327	LEU
1	A	439	LYS

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Mol	Chain	Res	Type
1	A	491	ASN
1	A	509	THR
1	A	538	LYS
1	A	635	THR
1	A	654	LEU
1	A	720	ASN
1	A	741	ASN
1	A	759	GLU
1	A	765	GLN
1	A	808	PHE
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	1088	ASN
1	A	1137	LEU
1	A	1183	ASP
1	A	1207	ASP
1	B	141	LEU
1	B	154	LEU
1	B	181	GLN
1	B	198	LYS
1	B	211	GLU
1	B	226	PHE
1	B	227	GLN
1	B	303	ARG
1	B	317	LEU
1	B	327	LEU
1	B	342	LEU
1	B	359	LEU
1	B	491	ASN
1	B	570	LEU
1	B	582	LEU
1	B	583	LEU
1	B	593	LYS
1	B	613	LEU

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Mol	Chain	Res	Type
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	765	GLN
1	B	808	PHE
1	B	849	PRO
1	B	858	LEU
1	B	910	LEU
1	B	953	THR
1	B	1000	GLN
1	B	1047	GLN
1	B	1048	GLN
1	B	1064	LEU
1	B	1077	ARG
1	B	1088	ASN
1	B	1115	LEU
1	B	1137	LEU

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	110	HIS
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

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Mol	Chain	Res	Type
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	560	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	836	ASN
1	A	860	GLN
1	A	866	ASN
1	A	880	ASN
1	A	918	ASN
1	A	976	HIS
1	A	1000	GLN
1	A	1047	GLN
1	A	1048	GLN
1	A	1084	GLN
1	A	1088	ASN
1	A	1108	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

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Mol	Chain	Res	Type
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	288	ASN
1	B	389	HIS
1	B	421	GLN
1	B	434	ASN
1	B	467	HIS
1	B	491	ASN
1	B	513	ASN
1	B	536	ASN
1	B	636	ASN
1	B	650	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
1	B	750	ASN
1	B	765	GLN
1	B	774	GLN
1	B	777	ASN
1	B	836	ASN
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

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Mol	Chain	Res	Type
1	B	1048	GLN
1	B	1084	GLN
1	B	1088	ASN
1	B	1108	GLN
1	B	1132	ASN
1	B	1151	GLN
1	B	1165	HIS
1	B	1215	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	A	2235	1	0,12,12	-	-	-		
2	SF4	B	2235	1	0,12,12	-	-	-		
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	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CO2	B	2239	-	2,2,2	1.29	0	1,1,1	0.54	0
6	CO2	A	2239	-	2,2,2	1.49	0	1,1,1	0.55	0
3	HTL	A	2236	4	23,30,30	5.36	10 (43%)	31,45,45	3.05	9 (29%)
3	HTL	B	2236	4	23,30,30	5.36	10 (43%)	31,45,45	3.33	7 (22%)

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	A	2235	1	-	-	0/6/5/5
2	SF4	B	2235	1	-	-	0/6/5/5
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	-	1/16/21/21	0/2/2/2
3	HTL	B	2236	4	-	1/16/21/21	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2236	HTL	C5A-C5	21.71	1.60	1.50
3	B	2236	HTL	C5A-C5	20.64	1.60	1.50
3	B	2236	HTL	C2'-N1'	9.03	1.48	1.34
3	B	2236	HTL	C4'-N3'	7.99	1.46	1.35
3	A	2236	HTL	C2'-N1'	6.88	1.45	1.34
3	A	2236	HTL	C4'-N3'	5.97	1.43	1.35
3	A	2236	HTL	C6'-N1'	5.79	1.46	1.34
3	A	2236	HTL	C5'-C4'	4.37	1.50	1.42
3	B	2236	HTL	C6'-N1'	3.97	1.42	1.34
3	B	2236	HTL	C5'-C4'	3.78	1.49	1.42
3	A	2236	HTL	C5-S1	3.64	1.80	1.74
3	B	2236	HTL	O2'-C1'	3.60	1.33	1.22
3	A	2236	HTL	O2'-C1'	3.41	1.33	1.22
3	B	2236	HTL	C3'-C1'	3.24	1.59	1.49
3	A	2236	HTL	C6'-C5'	3.02	1.44	1.37
3	B	2236	HTL	P2-O22	-2.71	1.44	1.54
3	B	2236	HTL	C2'-N3'	2.70	1.38	1.34
3	B	2236	HTL	C5-S1	2.45	1.78	1.74
3	A	2236	HTL	C2'-N3'	2.39	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2236	HTL	C3'-C1'	2.33	1.56	1.49

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2236	HTL	C5A-C5-C4	-14.66	115.67	127.43
3	A	2236	HTL	C5A-C5-C4	-12.96	117.03	127.43
3	B	2236	HTL	C2A-C2'-N1'	6.70	124.52	117.14
3	A	2236	HTL	C2A-C2'-N1'	5.60	123.30	117.14
3	B	2236	HTL	N1'-C2'-N3'	-4.49	117.81	125.54
3	B	2236	HTL	C4A-C4-N3	3.97	127.69	122.69
3	A	2236	HTL	N1'-C2'-N3'	-3.74	119.11	125.54
3	A	2236	HTL	C4A-C4-N3	3.72	127.37	122.69
3	A	2236	HTL	C5'-C35-N3	-3.58	107.34	113.26
3	B	2236	HTL	C5'-C35-N3	-3.27	107.85	113.26
3	A	2236	HTL	C2'-N3'-C4'	2.99	122.74	118.08
3	B	2236	HTL	C6'-N1'-C2'	2.57	120.33	115.96
3	A	2236	HTL	O2'-C1'-C3'	-2.55	114.44	120.17
3	B	2236	HTL	C2'-N3'-C4'	2.17	121.47	118.08
3	A	2236	HTL	C4-N3-C2	2.16	109.84	108.64
3	A	2236	HTL	O22-P2-O21	2.09	118.87	110.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2236	HTL	P1-O11-P2-O21
3	A	2236	HTL	P1-O11-P2-O21

There are no ring outliers.

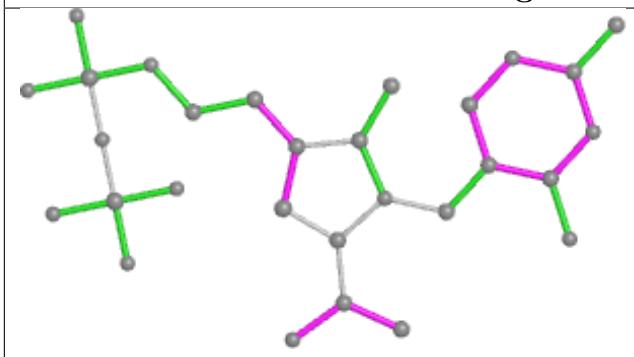
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2236	HTL	1	0
3	B	2236	HTL	2	0

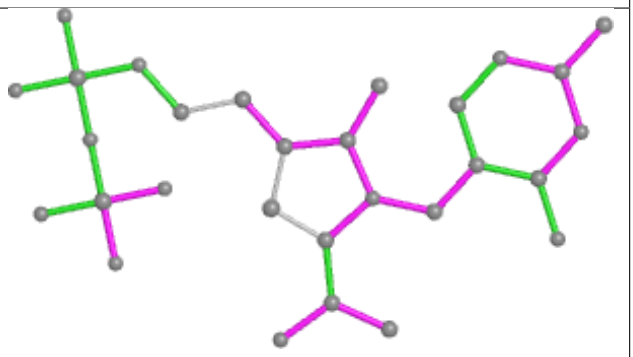
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

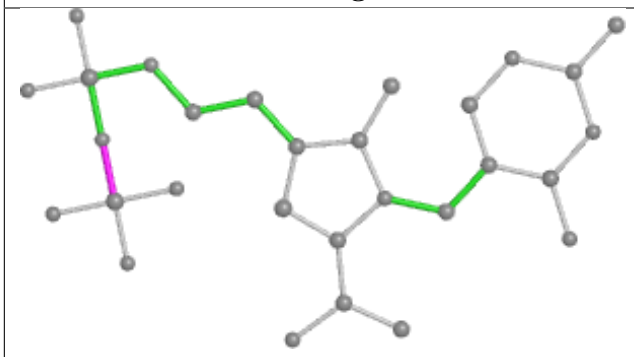
Ligand HTL A 2236



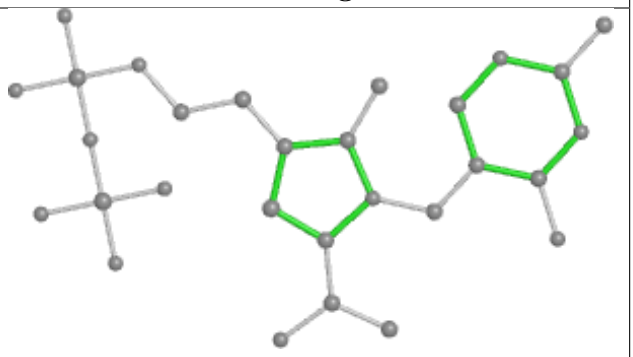
Bond lengths



Bond angles

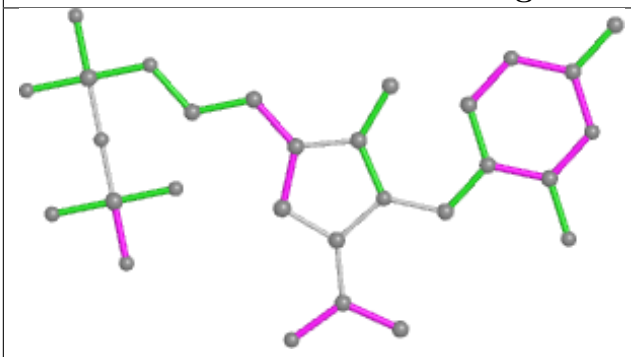


Torsions

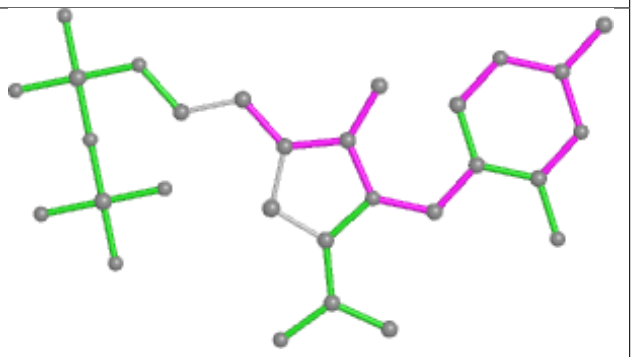


Rings

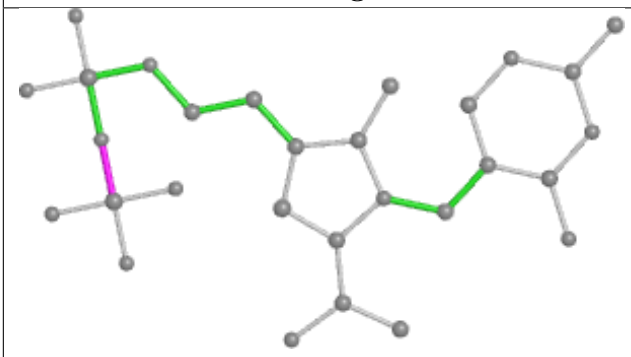
Ligand HTL B 2236



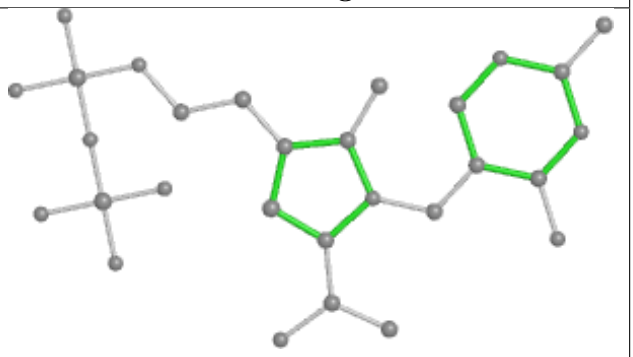
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.05	74 (6%)	21	28	8, 19, 49, 97	0
1	B	1230/1231 (99%)	-0.15	38 (3%)	49	56	8, 17, 39, 87	0
All	All	2461/2462 (99%)	-0.05	112 (4%)	32	39	8, 18, 46, 97	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1176	ALA	8.7
1	B	595	GLY	8.6
1	A	1178	ALA	8.3
1	A	1176	ALA	8.0
1	A	629	THR	7.2
1	A	1177	PRO	7.1
1	B	631	ALA	7.1
1	A	1179	GLY	6.6
1	B	1181	LYS	6.5
1	A	631	ALA	6.4
1	A	593	LYS	6.2
1	A	1232	LYS	6.2
1	A	633	PRO	6.2
1	B	1178	ALA	6.0
1	B	629	THR	6.0
1	B	593	LYS	6.0
1	B	1174	SER	5.9
1	B	1177	PRO	5.8
1	B	628	GLU	5.5
1	B	1175	PHE	5.5
1	A	595	GLY	5.4
1	B	715	VAL	5.3
1	B	594	LYS	5.3
1	A	632	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	594	LYS	5.1
1	A	627	ALA	5.0
1	B	1183	ASP	5.0
1	B	632	GLU	4.9
1	A	597	LYS	4.9
1	A	630	LYS	4.8
1	A	635	THR	4.8
1	B	1179	GLY	4.5
1	A	1231	LYS	4.5
1	A	634	MET	4.3
1	A	628	GLU	4.3
1	B	1172	PHE	4.2
1	A	1181	LYS	4.2
1	A	520	GLU	4.0
1	A	1175	PHE	3.9
1	A	601	MET	3.9
1	B	1231	LYS	3.9
1	A	577	GLU	3.8
1	A	758	LYS	3.6
1	B	354	ALA	3.5
1	A	1180	GLY	3.5
1	A	711	GLU	3.5
1	A	1230	THR	3.5
1	A	596	GLU	3.4
1	A	576	PHE	3.4
1	A	636	ASN	3.4
1	A	1172	PHE	3.4
1	A	715	VAL	3.3
1	A	590	ALA	3.3
1	A	1174	SER	3.3
1	B	1182	ALA	3.2
1	B	590	ALA	3.2
1	B	633	PRO	3.1
1	B	1180	GLY	3.1
1	B	716	GLY	3.1
1	A	589	LYS	3.1
1	A	624	ASP	3.1
1	A	619	PRO	3.0
1	A	712	GLU	3.0
1	B	589	LYS	3.0
1	A	554	GLY	2.9
1	A	759	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	617	LYS	2.8
1	A	581	ASP	2.8
1	B	634	MET	2.8
1	A	1170	ASN	2.8
1	B	1230	THR	2.7
1	A	1228	LYS	2.7
1	B	591	TYR	2.7
1	A	621	SER	2.7
1	B	596	GLU	2.7
1	A	789	GLU	2.7
1	A	731	LEU	2.7
1	A	496	GLY	2.6
1	A	626	PRO	2.6
1	B	635	THR	2.6
1	A	936	GLY	2.6
1	A	1109	GLY	2.6
1	A	620	ASP	2.5
1	B	636	ASN	2.5
1	A	598	ILE	2.5
1	B	592	GLY	2.5
1	A	608	GLN	2.5
1	A	1165	HIS	2.5
1	B	758	LYS	2.4
1	B	5	MET	2.4
1	A	732	LYS	2.4
1	B	597	LYS	2.4
1	A	591	TYR	2.4
1	A	1182	ALA	2.3
1	A	582	LEU	2.3
1	A	415	LYS	2.3
1	A	524	LYS	2.3
1	A	552	ASP	2.3
1	A	1167	ALA	2.3
1	A	526	LEU	2.3
1	A	592	GLY	2.2
1	B	1228	LYS	2.2
1	A	550	ALA	2.2
1	B	1165	HIS	2.2
1	B	626	PRO	2.1
1	A	523	ASP	2.1
1	A	585	LYS	2.1
1	A	528	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	521	ASP	2.1
1	A	1207	ASP	2.0
1	A	575	PRO	2.0
1	A	625	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

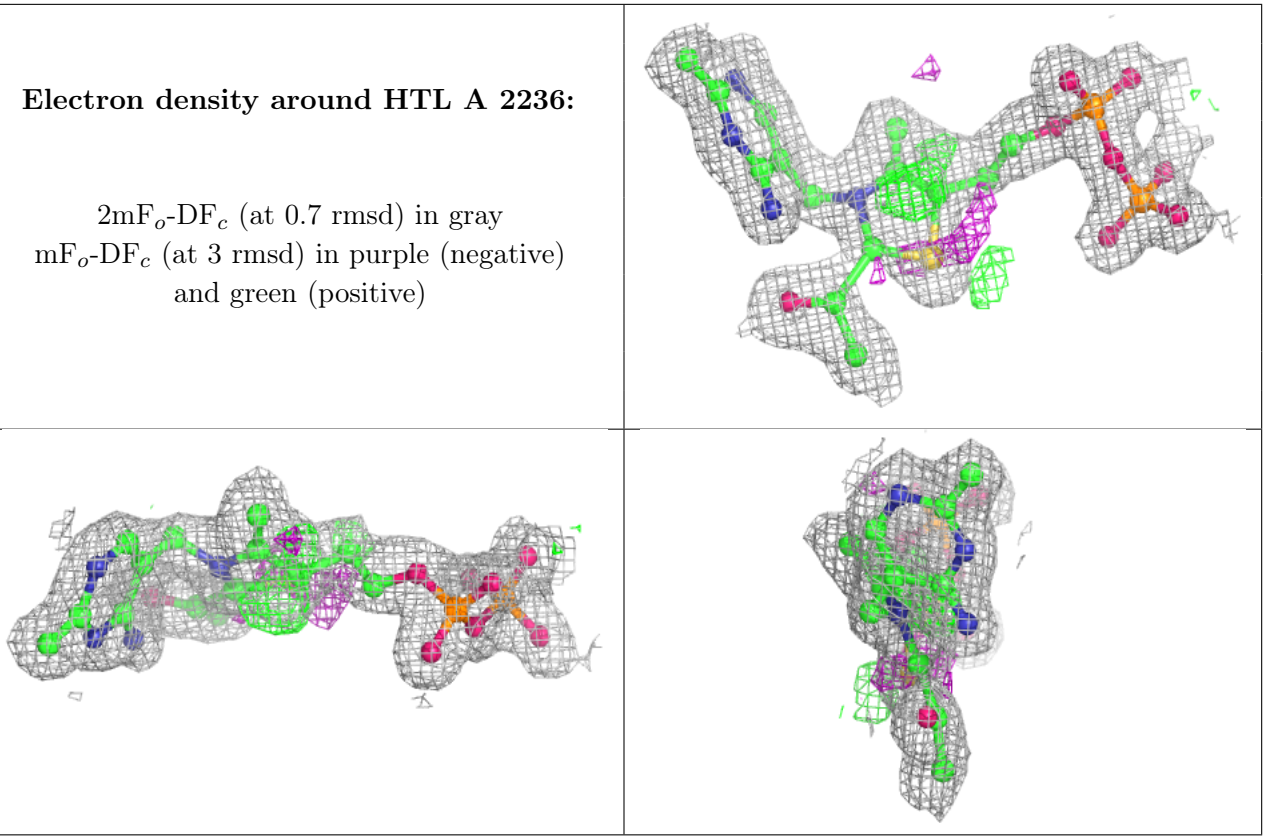
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.89	0.22	20,20,24,32	0
6	CO2	A	2239	3/3	0.95	0.14	22,22,29,33	0
3	HTL	A	2236	29/29	0.96	0.09	10,17,30,32	0
3	HTL	B	2236	29/29	0.97	0.10	10,16,25,28	0
4	MG	A	2237	1/1	0.98	0.12	15,15,15,15	0
2	SF4	B	2235	8/8	0.99	0.04	8,11,12,13	0
2	SF4	A	2233	8/8	0.99	0.05	21,22,23,23	0
2	SF4	A	2234	8/8	0.99	0.04	17,18,18,18	0
2	SF4	A	2235	8/8	0.99	0.04	12,14,15,15	0
4	MG	B	2237	1/1	0.99	0.07	10,10,10,10	0
5	CA	A	2238	1/1	0.99	0.14	39,39,39,39	0
5	CA	B	2238	1/1	0.99	0.09	38,38,38,38	0
2	SF4	B	2233	8/8	0.99	0.04	14,16,16,17	0
2	SF4	B	2234	8/8	0.99	0.03	10,12,13,14	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.

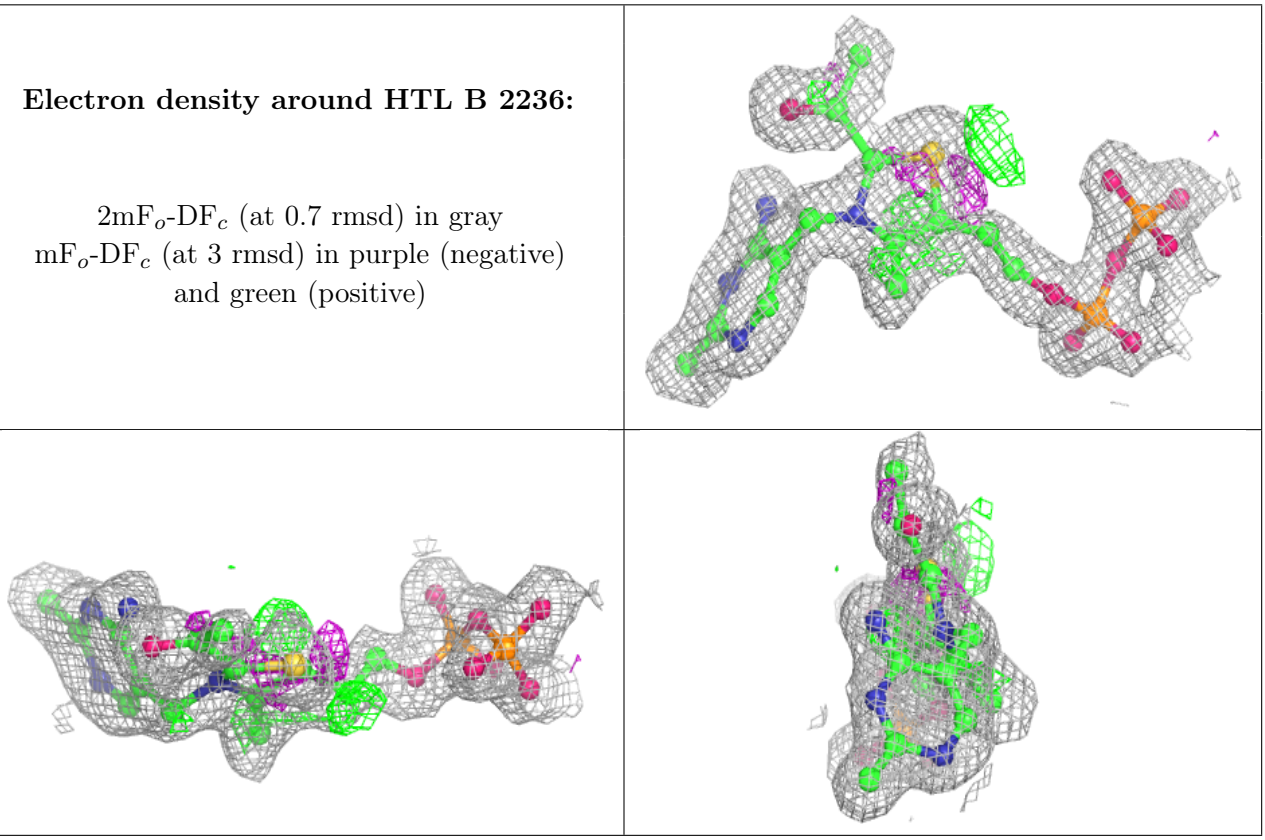
Electron density around HTL A 2236:

$2mF_o$-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.