Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2026 – 05:57 am BST

PDB ID	:	2C3M / pdb_00002c3m
Title	:	Crystal Structure 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	:	2005-10-11
Resolution	:	1.84 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 (i) 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 (i)) were used in the production of this report:

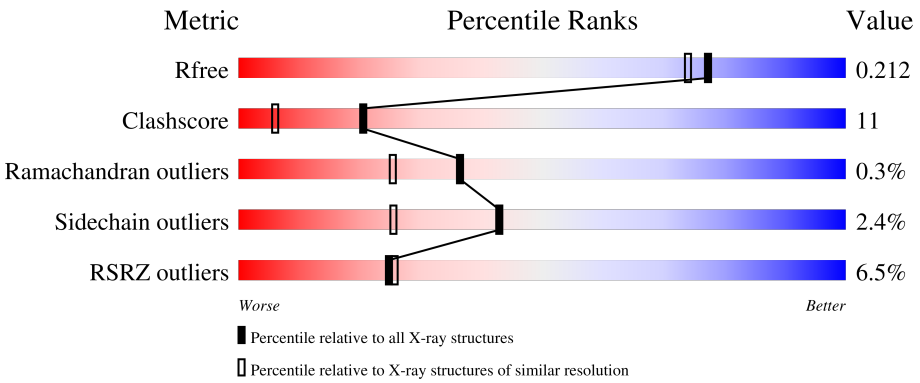
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	9% 76% 22% •
1	B	1231	4% 79% 19% •

2 Entry composition (i)

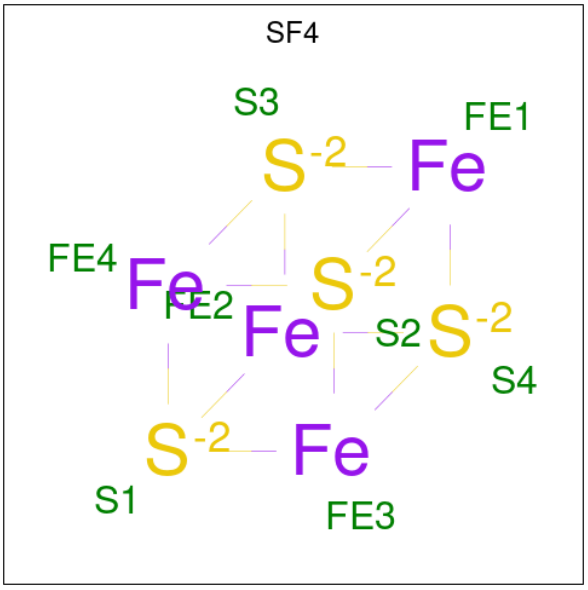
There are 7 unique types of molecules in this entry. The entry contains 20189 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	1231	9383	5941	1599	1784	59	0	0	0
1	B	1231	9383	5941	1599	1784	59	0	0	0

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



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

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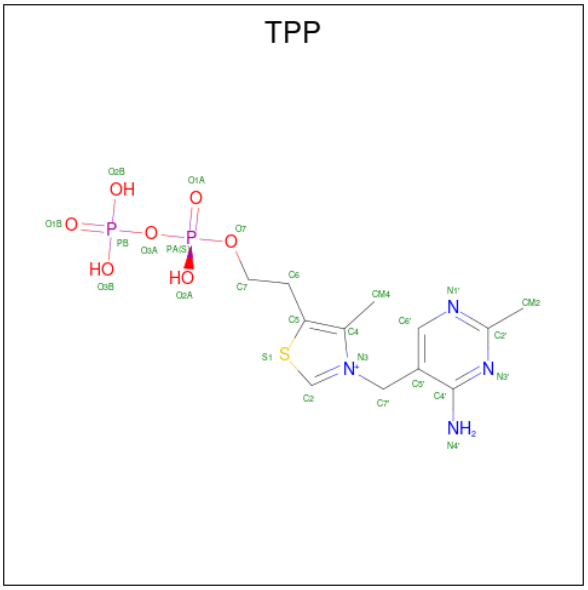
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	B	1	8	4	4	0	0
			Total	Fe	S		
2	B	1	8	4	4	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 7 is water.

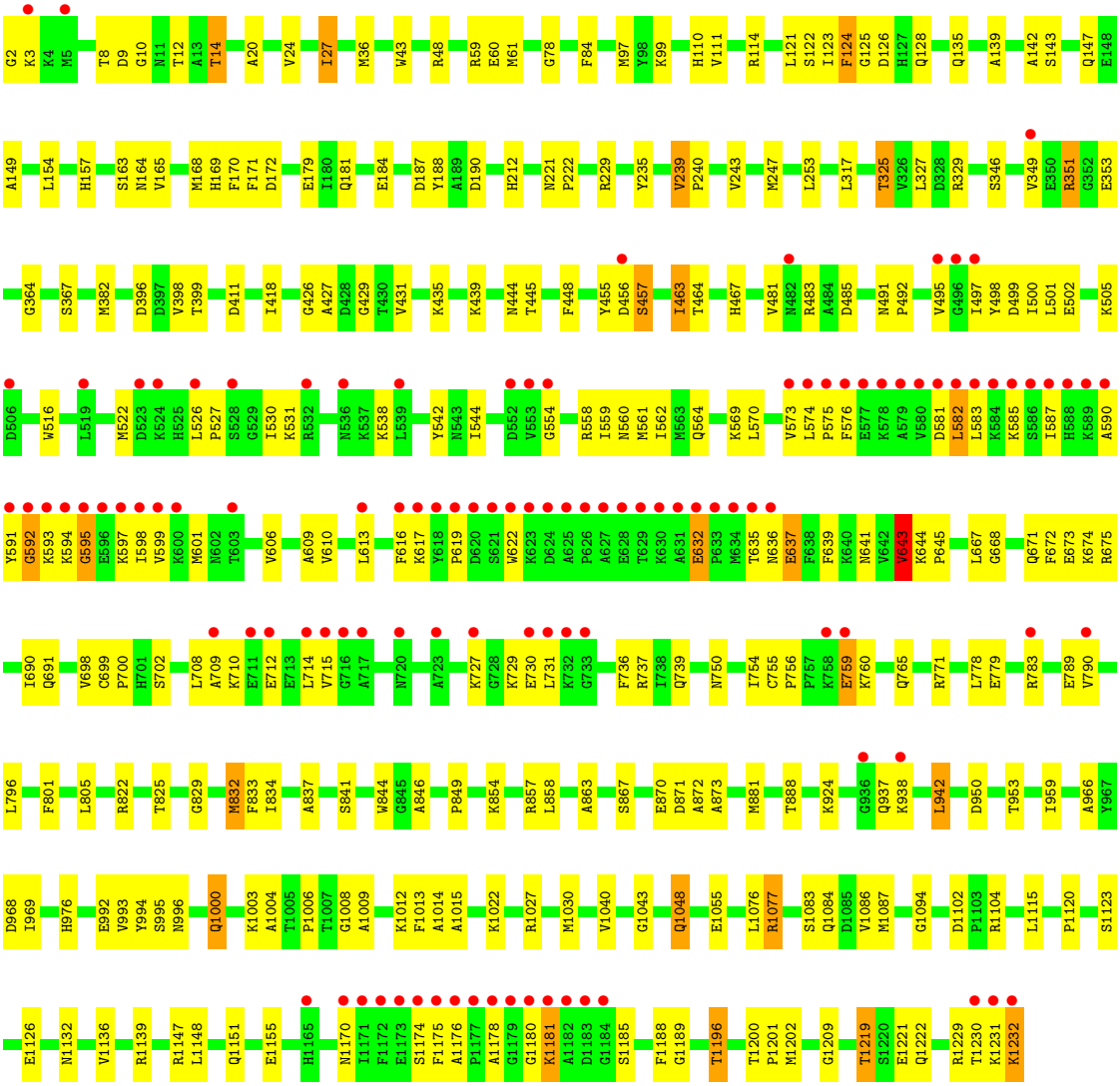
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	610	Total O 610 610	0	0
7	B	707	Total O 707 707	0	0

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.

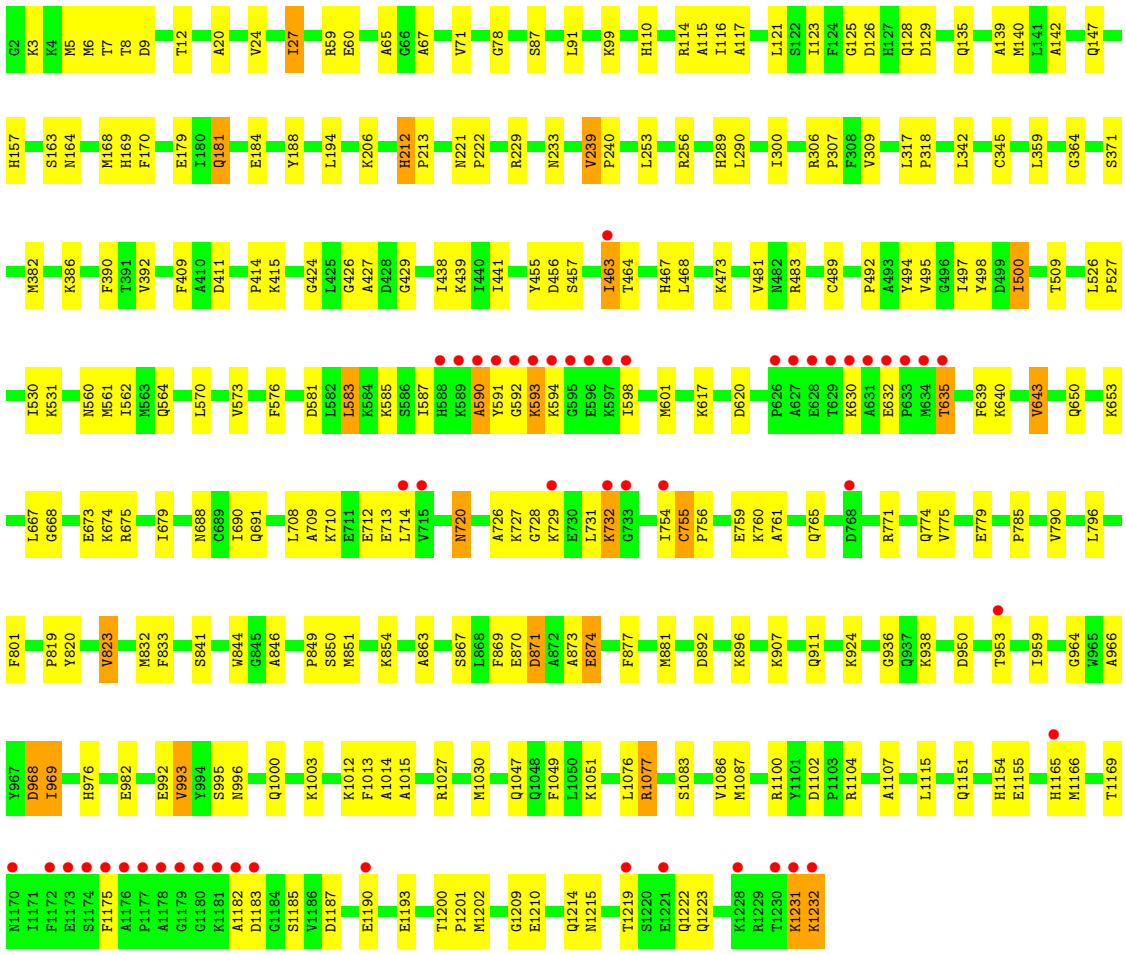
• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

Chain A: 9% 76% 22%



• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

Chain B: 4% 79% 19%


G2 K3 K4 M5 M6 T7 T8 D9 T12 A20 V24 I27 R59 E60 A65 G66 A67 V71 G78 S87 L91 K99 H110 R114 A115 I116 A117 L121 S122 I123 F124 G125 D126 H127 Q128 D129 Q135 A139 M140 L141 A142 Q147
H157 S163 N164 M168 H169 F170 E179 I180 Q181 E184 Y188 L194 K206 H212 P213 N221 P222 R229 N233 V239 P240 L253 R256 H289 L290 I300 R306 P307 F308 V309 L317 P318 L342 C345 L359 G364 S371
M382 K386 F390 T391 V392 F409 A410 D411 P414 K415 G424 L425 G426 A427 D428 G429 I438 K439 I440 I441 Y455 D456 S457 I463 T464 H467 L468 K473 V481 N482 R483 C489 P492 A493 Y494 V495 G496 I497 Y498 D499 I500 T509 L526 P527
I530 K531 N560 M561 I562 M563 Q564 L570 V573 F576 D581 L582 L583 K584 K585 S586 I587 H588 K589 A590 Y591 G592 K593 K594 G595 E596 K597 I598 M601 K617 D620 P626 A627 E628 T629 K630 A631 E632 P633 M634 T635 F639 K640 V643 Q650 K653
L667 G668 E673 K674 R675 I679 N688 G689 I690 Q691 L708 A709 K710 E711 E712 E713 L714 V715 N720 A726 K727 G728 K729 E730 L731 K732 G733 I754 C755 P756 E759 K760 A761 Q765 D768 R771 Q774 V775 E779 P785 V790 L796
F801 P819 Y820 V823 M832 F833 S841 W844 G845 A846 P849 S850 M851 K854 A863 S867 L868 F869 E870 D871 A872 A873 E874 F877 M881 D892 K896 K907 Q911 K924 G936 Q937 K938 D950 T953 I959 G964 W965 A966
Y967 D968 I969 H976 E982 E992 V993 Y994 S995 N996 Q1000 K1003 K1012 F1013 A1014 A1015 R1027 M1030 Q1047 Q1048 F1049 L1050 K1051 L1076 R1077 S1083 V1086 M1087 R1100 Y1101 D1102 P1103 R1104 A1107 L1115 Q1151 H1154 E1155 H1165 M1166 T1169
N1170 I1171 F1172 E1173 S1174 F1175 A1176 P1177 A1178 G1179 G1180 K1181 A1182 D1183 G1184 S1185 V1186 D1187 E1190 E1193 T1200 P1201 M1202 G1209 E1210 Q1214 N1215 T1219 S1220 E1221 Q1222 Q1223 K1228 R1229 T1230 K1231 K1232

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.02Å 146.16Å 211.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.12 – 1.84 51.12 – 1.84	Depositor EDS
% Data completeness (in resolution range)	93.4 (51.12-1.84) 93.5 (51.12-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.95 (at 1.84Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.222 0.182 , 0.212	Depositor DCC
R_{free} test set	10902 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	17.1	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20189	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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 (i)

5.1 Standard geometry (i)

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

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	0/9585	0.90	37/12954 (0.3%)
1	B	0.37	0/9585	0.92	42/12954 (0.3%)
All	All	0.36	0/19170	0.91	79/25908 (0.3%)

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	125	GLY	N-CA-C	9.27	126.19	111.64
1	A	125	GLY	N-CA-C	8.83	126.70	111.15
1	A	756	PRO	N-CA-C	8.71	121.32	110.70
1	B	756	PRO	N-CA-C	8.65	121.25	110.70
1	A	969	ILE	N-CA-C	7.91	118.69	110.62
1	A	27	ILE	N-CA-C	7.54	119.82	108.80
1	B	969	ILE	N-CA-C	7.39	118.16	110.62
1	B	139	ALA	N-CA-C	-7.34	99.61	110.48
1	A	139	ALA	N-CA-C	-7.33	100.16	110.50
1	B	993	VAL	CB-CA-C	-7.00	105.16	111.74
1	B	771	ARG	N-CA-C	6.98	118.89	111.28
1	A	755	CYS	CA-C-N	6.88	127.47	120.38
1	A	755	CYS	C-N-CA	6.88	127.47	120.38
1	B	27	ILE	N-CA-C	6.86	118.81	108.80
1	B	1014	ALA	N-CA-C	-6.74	102.45	110.41
1	A	771	ARG	N-CA-C	6.59	118.13	111.07
1	B	755	CYS	CA-C-N	6.48	127.06	120.38
1	B	755	CYS	C-N-CA	6.48	127.06	120.38
1	A	668	GLY	N-CA-C	6.41	124.53	115.30
1	B	590	ALA	N-CA-C	-6.36	102.30	110.19
1	B	679	ILE	N-CA-C	-6.30	105.59	111.45
1	B	643	VAL	N-CA-C	6.29	116.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	846	ALA	N-CA-C	6.26	117.80	110.41
1	A	995	SER	N-CA-C	6.22	117.94	111.03
1	B	576	PHE	N-CA-C	6.17	118.52	111.11
1	A	124	PHE	N-CA-C	6.16	119.53	110.59
1	B	593	LYS	N-CA-C	-6.10	105.76	112.72
1	B	212	HIS	CA-C-N	6.04	126.01	120.03
1	B	212	HIS	C-N-CA	6.04	126.01	120.03
1	B	968	ASP	N-CA-C	6.00	117.65	108.12
1	A	1014	ALA	N-CA-C	-5.93	103.41	110.41
1	A	500	ILE	N-CA-C	5.91	118.44	111.05
1	A	637	GLU	N-CA-C	-5.88	104.95	111.36
1	A	111	VAL	N-CA-C	5.87	116.33	108.11
1	B	560	ASN	N-CA-C	5.87	118.15	111.11
1	A	448	PHE	N-CA-C	-5.76	101.96	110.48
1	A	966	ALA	N-CA-C	5.74	117.61	111.36
1	B	668	GLY	N-CA-C	5.72	123.71	114.90
1	B	78	GLY	N-CA-C	5.64	123.77	115.08
1	B	371	SER	N-CA-C	5.63	116.61	110.13
1	B	1077	ARG	N-CA-C	5.59	119.36	112.54
1	B	774	GLN	N-CA-C	5.57	119.25	112.23
1	A	833	PHE	N-CA-C	-5.57	100.62	109.59
1	B	364	GLY	N-CA-C	5.56	126.35	113.18
1	A	78	GLY	N-CA-C	5.52	123.58	115.08
1	A	801	PHE	N-CA-C	-5.46	105.93	112.59
1	A	846	ALA	N-CA-C	5.46	118.29	109.83
1	B	65	ALA	N-CA-C	-5.42	105.46	111.36
1	B	570	LEU	N-CA-C	5.41	120.89	113.97
1	A	675	ARG	N-CA-C	5.40	117.17	111.28
1	B	966	ALA	N-CA-C	5.39	117.23	111.36
1	B	863	ALA	N-CA-C	-5.39	99.74	108.41
1	B	870	GLU	N-CA-C	5.38	119.69	113.18
1	A	863	ALA	N-CA-C	-5.37	99.76	108.41
1	B	213	PRO	N-CA-C	5.36	119.44	111.41
1	B	801	PHE	N-CA-C	-5.35	106.07	112.59
1	A	643	VAL	N-CA-C	5.35	116.12	110.72
1	A	364	GLY	N-CA-C	5.34	125.83	113.18
1	B	871	ASP	N-CA-C	5.33	119.34	112.41
1	B	832	MET	N-CA-C	5.33	118.42	109.95
1	A	1077	ARG	N-CA-C	5.32	117.77	111.33
1	A	871	ASP	N-CA-C	5.31	120.42	112.94
1	A	968	ASP	N-CA-C	5.30	116.55	108.12
1	B	833	PHE	N-CA-C	-5.30	101.05	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	239	VAL	CB-CA-C	-5.29	108.75	114.35
1	B	239	VAL	CB-CA-C	-5.28	108.69	113.70
1	A	559	ILE	N-CA-C	5.24	120.25	113.07
1	B	675	ARG	N-CA-C	5.23	116.98	111.28
1	A	888	THR	N-CA-C	-5.21	105.78	111.82
1	B	500	ILE	N-CA-C	5.20	117.55	111.05
1	A	485	ASP	N-CA-C	-5.19	106.10	112.90
1	A	457	SER	N-CA-C	-5.17	106.48	112.89
1	B	995	SER	N-CA-C	5.14	117.88	111.24
1	B	760	LYS	N-CA-C	5.13	117.54	110.35
1	A	172	ASP	N-CA-C	5.13	117.75	110.10
1	A	832	MET	N-CA-C	5.07	118.01	109.95
1	A	870	GLU	N-CA-C	5.05	119.44	113.28
1	B	457	SER	N-CA-C	-5.05	106.63	112.89
1	A	1170	ASN	N-CA-C	-5.04	106.38	112.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9383	0	9262	251	0
1	B	9383	0	9262	202	0
2	A	24	0	0	1	0
2	B	24	0	0	1	0
3	A	26	0	16	1	0
3	B	26	0	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	610	0	0	7	0
7	B	707	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20189	0	18556	420	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 11.

All (420) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1200:THR:HG22	1:B:1202:MET:H	1.17	1.09
1:A:691:GLN:HE22	1:A:727:LYS:H	1.02	1.02
1:A:639:PHE:HA	1:A:643:VAL:HG13	1.40	1.02
1:A:1200:THR:HG22	1:A:1202:MET:H	1.33	0.94
1:A:1200:THR:HG21	1:A:1202:MET:HE3	1.53	0.90
1:A:691:GLN:NE2	1:A:727:LYS:H	1.73	0.85
1:A:635:THR:HG22	1:A:636:ASN:H	1.43	0.83
1:B:635:THR:HG23	1:B:639:PHE:HB3	1.63	0.81
1:A:558:ARG:HG2	1:A:560:ASN:ND2	1.95	0.81
1:A:10:GLY:O	1:A:14:THR:HG23	1.82	0.78
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.29	0.78
1:B:591:TYR:C	1:B:593:LYS:H	1.92	0.78
1:A:1102:ASP:OD1	1:A:1104:ARG:HG2	1.84	0.77
1:B:1231:LYS:HG3	1:B:1232:LYS:H	1.49	0.76
1:B:823:VAL:HG11	1:B:1049:PHE:HE2	1.51	0.76
1:A:147:GLN:HE22	1:A:184:GLU:H	1.33	0.75
1:A:128:GLN:HE22	1:B:229:ARG:HE	1.34	0.75
1:A:594:LYS:HB3	1:A:598:ILE:HD12	1.70	0.74
1:B:635:THR:CG2	1:B:639:PHE:HB3	2.18	0.74
1:A:731:LEU:HD23	1:A:790:VAL:HG11	1.69	0.74
1:B:1200:THR:HG21	1:B:1202:MET:HE3	1.68	0.73
1:B:6:MET:HE3	1:B:8:THR:HG21	1.70	0.73
1:A:635:THR:HG22	1:A:636:ASN:N	2.02	0.73
1:A:691:GLN:HE22	1:A:727:LYS:N	1.84	0.72
1:A:1015:ALA:CB	1:B:1185:SER:HB2	2.19	0.72
1:A:325:THR:HG23	1:A:382:MET:SD	2.29	0.72
1:A:737:ARG:HE	1:A:739:GLN:NE2	1.88	0.72
1:A:351:ARG:HD3	1:A:353:GLU:HB2	1.72	0.71
1:B:924:LYS:HA	1:B:953:THR:HG22	1.72	0.71
1:B:1027:ARG:HA	1:B:1030:MET:HE3	1.73	0.71
1:B:1076:LEU:HD13	1:B:1086:VAL:HG21	1.72	0.71
1:A:1185:SER:HB2	1:B:1015:ALA:HB1	1.72	0.71
1:A:110:HIS:HD2	1:A:169:HIS:HD2	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:ILE:HD13	1:B:494:TYR:CE1	2.25	0.70
1:B:1219:THR:HG23	1:B:1222:GLN:H	1.55	0.70
1:B:1102:ASP:OD1	1:B:1104:ARG:HG2	1.92	0.70
1:B:5:MET:HE2	1:B:184:GLU:HB3	1.74	0.69
1:B:731:LEU:HD23	1:B:790:VAL:HG11	1.72	0.69
1:A:759:GLU:CD	1:A:759:GLU:H	1.98	0.69
1:A:1015:ALA:HB1	1:B:1185:SER:HB2	1.73	0.69
1:A:1174:SER:H	1:B:1154:HIS:HE1	1.40	0.69
1:A:591:TYR:C	1:A:593:LYS:H	2.00	0.69
1:B:8:THR:HB	1:B:12:THR:OG1	1.92	0.69
1:B:147:GLN:HE22	1:B:184:GLU:H	1.40	0.69
1:A:635:THR:HG21	1:A:639:PHE:CD2	2.28	0.69
1:B:691:GLN:HE22	1:B:727:LYS:H	1.40	0.68
1:A:857:ARG:HG3	1:A:858:LEU:HD22	1.75	0.68
1:B:617:LYS:HE2	1:B:617:LYS:HA	1.75	0.68
1:A:937:GLN:HG2	1:A:942:LEU:HB3	1.74	0.68
7:A:2376:HOH:O	1:B:1219:THR:HG21	1.94	0.68
1:B:110:HIS:HD2	1:B:169:HIS:CD2	2.11	0.67
1:A:3:LYS:HD3	1:A:184:GLU:OE2	1.94	0.67
1:A:135:GLN:H	1:A:135:GLN:NE2	1.93	0.67
1:A:1201:PRO:HG3	1:B:455:TYR:HB2	1.76	0.67
1:A:644:LYS:HB3	1:A:645:PRO:HD3	1.76	0.66
1:A:239:VAL:HG22	1:A:240:PRO:HD3	1.76	0.66
1:A:1123:SER:O	1:A:1126:GLU:HG2	1.96	0.66
1:B:1151:GLN:O	1:B:1155:GLU:HG3	1.95	0.65
1:A:593:LYS:HG3	1:A:594:LYS:N	2.11	0.65
1:A:593:LYS:HG3	1:A:594:LYS:H	1.61	0.65
1:B:561:MET:HE1	1:B:583:LEU:HD21	1.79	0.65
1:B:992:GLU:O	1:B:993:VAL:HG13	1.97	0.65
1:A:3:LYS:HD3	1:A:184:GLU:CD	2.22	0.64
1:A:709:ALA:HB3	1:A:714:LEU:HD11	1.80	0.64
1:A:1151:GLN:O	1:A:1155:GLU:HG3	1.98	0.64
1:B:877:PHE:HE1	1:B:982:GLU:HG3	1.62	0.64
1:B:691:GLN:NE2	1:B:727:LYS:H	1.95	0.64
1:B:5:MET:CE	1:B:184:GLU:HB3	2.28	0.63
1:A:1200:THR:HG23	1:A:1201:PRO:HD2	1.80	0.63
1:A:349:VAL:HG21	1:B:345:CYS:SG	2.39	0.63
1:B:6:MET:HE3	1:B:8:THR:CG2	2.29	0.63
1:A:1132:ASN:O	1:A:1136:VAL:HG22	1.99	0.63
1:B:710:LYS:HB2	1:B:712:GLU:HG2	1.80	0.63
1:B:1166:MET:O	1:B:1169:THR:HG22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:MET:HE2	1:A:834:ILE:HD11	1.79	0.63
1:A:1188:PHE:HE1	1:A:1196:THR:HG23	1.63	0.63
1:B:819:PRO:O	1:B:823:VAL:HG12	1.99	0.63
1:A:8:THR:HB	1:A:12:THR:OG1	2.00	0.62
1:B:1219:THR:HG22	1:B:1222:GLN:CG	2.30	0.62
1:A:544:ILE:HD12	1:A:613:LEU:HD22	1.81	0.61
1:B:527:PRO:HD2	1:B:530:ILE:HD12	1.82	0.61
1:A:1231:LYS:HG3	1:A:1232:LYS:H	1.66	0.61
1:A:445:THR:HG21	1:A:574:LEU:HD21	1.83	0.61
1:A:881:MET:HE2	1:B:24:VAL:HG13	1.82	0.61
1:B:140:MET:HE3	1:B:168:MET:CE	2.31	0.61
1:A:24:VAL:HG13	1:B:881:MET:HE2	1.82	0.61
1:A:561:MET:HE1	1:A:583:LEU:HD11	1.83	0.61
1:A:1181:LYS:HB2	1:A:1181:LYS:NZ	2.15	0.61
1:B:907:LYS:O	1:B:911:GLN:HG3	2.01	0.60
1:A:635:THR:HG23	1:A:672:PHE:CD2	2.36	0.60
1:B:164:ASN:HD22	1:B:206:LYS:NZ	1.99	0.60
1:B:775:VAL:O	1:B:779:GLU:HG2	2.01	0.60
7:A:2117:HOH:O	1:B:953:THR:HG21	2.00	0.60
1:A:881:MET:HE3	1:B:59:ARG:CG	2.32	0.60
1:A:976:HIS:HD2	1:B:1003:LYS:NZ	1.99	0.60
1:B:650:GLN:HE21	1:B:653:LYS:HD2	1.67	0.60
1:A:1147:ARG:HH11	1:A:1147:ARG:HB3	1.67	0.59
1:A:1188:PHE:CE1	1:A:1196:THR:HG23	2.37	0.59
1:B:1232:LYS:NZ	1:B:1232:LYS:HB3	2.17	0.59
1:A:14:THR:HG21	1:A:171:PHE:CE2	2.37	0.59
1:A:499:ASP:OD2	1:A:502:GLU:HB2	2.01	0.59
1:A:491:ASN:HD22	1:A:492:PRO:HD2	1.68	0.59
1:A:554:GLY:HA3	1:A:601:MET:HE2	1.83	0.59
1:A:635:THR:HG23	1:A:672:PHE:CG	2.38	0.59
1:A:1006:PRO:HG2	1:A:1009:ALA:HB2	1.84	0.59
1:A:737:ARG:HE	1:A:739:GLN:HE21	1.49	0.59
1:A:1147:ARG:HB3	1:A:1147:ARG:NH1	2.18	0.58
1:B:1107:ALA:HB2	1:B:1175:PHE:HB3	1.85	0.58
1:B:591:TYR:C	1:B:593:LYS:N	2.61	0.58
1:B:594:LYS:NZ	1:B:594:LYS:HB3	2.19	0.58
1:B:1200:THR:HG23	1:B:1201:PRO:HD2	1.86	0.58
1:A:976:HIS:HD2	1:B:1003:LYS:HZ3	1.49	0.58
1:B:164:ASN:HD22	1:B:206:LYS:HZ1	1.49	0.58
1:B:239:VAL:HB	1:B:240:PRO:HD3	1.86	0.58
1:A:99:LYS:HE3	1:B:867:SER:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ALA:HB2	1:A:170:PHE:CZ	2.39	0.58
1:A:97:MET:HE1	1:A:168:MET:HE3	1.85	0.58
1:A:110:HIS:HD2	1:A:169:HIS:CD2	2.21	0.58
1:A:639:PHE:HA	1:A:643:VAL:CG1	2.26	0.58
1:A:1185:SER:HB2	1:B:1015:ALA:CB	2.34	0.57
1:A:583:LEU:O	1:A:587:ILE:HG13	2.04	0.57
1:A:737:ARG:HH11	1:A:739:GLN:HE22	1.53	0.57
1:A:1232:LYS:NZ	1:A:1232:LYS:HB3	2.20	0.57
1:B:110:HIS:CD2	1:B:169:HIS:HD2	2.17	0.57
1:A:14:THR:HG22	1:A:149:ALA:HB1	1.86	0.57
1:A:581:ASP:OD2	1:A:585:LYS:HE3	2.05	0.57
1:A:143:SER:OG	1:A:171:PHE:HB3	2.05	0.57
1:A:43:TRP:HB3	1:A:48:ARG:HD3	1.87	0.57
1:A:992:GLU:O	1:A:993:VAL:HG13	2.05	0.57
1:A:731:LEU:CD2	1:A:790:VAL:HG11	2.35	0.56
1:A:710:LYS:HB2	1:A:710:LYS:NZ	2.20	0.56
1:B:635:THR:HG21	1:B:639:PHE:HD2	1.69	0.56
1:B:1231:LYS:O	1:B:1232:LYS:HB2	2.03	0.56
1:A:467:HIS:HD2	1:A:481:VAL:H	1.53	0.56
1:A:1174:SER:H	1:B:1154:HIS:CE1	2.23	0.56
1:A:873:ALA:HA	1:A:959:ILE:HD13	1.87	0.56
1:A:1219:THR:HG21	7:B:2455:HOH:O	2.05	0.56
1:A:444:ASN:HB2	1:A:582:LEU:HD21	1.86	0.56
1:A:609:ALA:O	1:A:613:LEU:HD23	2.07	0.55
1:B:233:ASN:HB2	7:B:2138:HOH:O	2.07	0.55
1:A:953:THR:HG21	7:B:2118:HOH:O	2.05	0.55
1:A:730:GLU:CD	1:A:730:GLU:H	2.15	0.55
1:B:91:LEU:HD11	1:B:116:ILE:HD12	1.89	0.55
1:B:110:HIS:HE1	1:B:157:HIS:NE2	2.04	0.55
1:A:1136:VAL:HG12	1:A:1139:ARG:NH1	2.22	0.55
1:B:591:TYR:O	1:B:593:LYS:N	2.39	0.55
1:A:635:THR:CG2	1:A:636:ASN:H	2.17	0.55
1:A:121:LEU:HD23	1:A:121:LEU:C	2.32	0.54
1:A:467:HIS:CD2	1:A:481:VAL:H	2.25	0.54
1:A:1027:ARG:HA	1:A:1030:MET:HE3	1.89	0.54
1:A:398:VAL:HG23	1:A:399:THR:N	2.22	0.54
1:B:414:PRO:HB3	1:B:473:LYS:HD2	1.89	0.54
1:B:463:ILE:HD12	1:B:464:THR:H	1.72	0.54
1:B:1210:GLU:HG3	7:B:2695:HOH:O	2.08	0.54
1:B:630:LYS:O	1:B:630:LYS:HG3	2.08	0.54
1:A:698:VAL:HG13	1:A:1084:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:VAL:CG2	1:A:464:THR:HG21	2.39	0.53
1:A:1189:GLY:HA3	1:A:1196:THR:HG21	1.90	0.53
1:B:598:ILE:HD13	1:B:601:MET:HE2	1.89	0.53
1:A:1231:LYS:HG3	1:A:1232:LYS:N	2.23	0.53
1:B:729:LYS:O	1:B:732:LYS:HG3	2.08	0.53
1:A:121:LEU:HD23	1:A:122:SER:N	2.24	0.53
1:A:1200:THR:HG22	1:A:1202:MET:N	2.14	0.53
1:A:558:ARG:HG2	1:A:560:ASN:HD22	1.70	0.53
1:A:597:LYS:O	1:A:601:MET:HG3	2.09	0.52
1:B:121:LEU:C	1:B:121:LEU:HD23	2.34	0.52
1:A:562:ILE:HD12	1:A:562:ILE:N	2.24	0.52
1:A:1008:GLY:HA2	1:A:1148:LEU:HD13	1.92	0.52
1:A:1015:ALA:HB3	1:B:1185:SER:HB2	1.90	0.52
1:A:708:LEU:HD21	1:A:731:LEU:HD22	1.91	0.52
1:A:591:TYR:C	1:A:593:LYS:N	2.68	0.52
1:A:710:LYS:HB2	1:A:710:LYS:HZ2	1.73	0.52
1:A:796:LEU:HD23	1:A:796:LEU:C	2.34	0.52
1:B:820:TYR:O	1:B:823:VAL:HG13	2.10	0.52
1:B:142:ALA:HB2	1:B:170:PHE:CZ	2.45	0.52
1:A:444:ASN:CB	1:A:582:LEU:HD21	2.41	0.52
1:A:805:LEU:HD12	1:A:829:GLY:HA3	1.91	0.52
1:B:708:LEU:HD21	1:B:731:LEU:HD22	1.92	0.52
1:A:1132:ASN:ND2	1:A:1136:VAL:CG1	2.72	0.51
1:B:1051:LYS:HE2	1:B:1100:ARG:NH1	2.25	0.51
1:B:463:ILE:HD12	1:B:464:THR:N	2.25	0.51
1:A:635:THR:CG2	1:A:636:ASN:N	2.73	0.51
1:A:1132:ASN:CG	1:A:1136:VAL:HG13	2.36	0.51
1:B:561:MET:HE3	1:B:564:GLN:HB3	1.92	0.51
1:A:924:LYS:HA	1:A:953:THR:HG22	1.92	0.51
1:A:1076:LEU:HD13	1:A:1086:VAL:HG21	1.93	0.51
1:A:163:SER:HB2	1:A:239:VAL:HG12	1.93	0.51
1:A:593:LYS:CG	1:A:594:LYS:H	2.24	0.51
1:A:2:GLY:N	1:A:187:ASP:OD2	2.45	0.50
1:A:235:TYR:O	1:A:239:VAL:HG13	2.11	0.50
1:B:497:ILE:HG13	1:B:498:TYR:CD1	2.46	0.50
1:A:128:GLN:NE2	1:B:229:ARG:HE	2.03	0.50
1:B:1187:ASP:HB3	1:B:1190:GLU:HG3	1.92	0.50
1:B:1219:THR:HG22	1:B:1222:GLN:HG3	1.91	0.50
1:A:411:ASP:HB2	1:A:483:ARG:HD2	1.92	0.50
1:B:9:ASP:OD2	1:B:12:THR:HG23	2.10	0.50
1:B:424:GLY:O	1:B:463:ILE:HD12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ARG:HD2	7:B:2137:HOH:O	2.12	0.50
1:B:823:VAL:CG1	1:B:1049:PHE:HE2	2.21	0.50
1:A:59:ARG:CG	1:B:881:MET:HE3	2.41	0.50
1:B:590:ALA:O	1:B:591:TYR:C	2.55	0.50
1:A:698:VAL:HG11	1:A:1084:GLN:HG3	1.93	0.50
1:A:805:LEU:HB2	1:A:825:THR:HB	1.92	0.50
1:A:3:LYS:HE2	1:A:253:LEU:O	2.12	0.49
1:A:1219:THR:HG22	1:A:1222:GLN:H	1.77	0.49
1:B:709:ALA:HB3	1:B:714:LEU:HD21	1.93	0.49
1:A:483:ARG:O	1:A:505:LYS:HE3	2.13	0.49
1:A:1055:GLU:O	1:A:1104:ARG:NH1	2.44	0.49
1:B:317:LEU:HD13	1:B:318:PRO:O	2.12	0.49
1:A:754:ILE:C	1:A:754:ILE:HD12	2.38	0.49
1:A:841:SER:HA	1:A:844:TRP:CE2	2.47	0.49
1:A:1003:LYS:HZ3	1:B:976:HIS:HD2	1.61	0.49
1:B:390:PHE:CE1	1:B:392:VAL:HG23	2.47	0.49
1:B:164:ASN:ND2	1:B:206:LYS:NZ	2.61	0.49
1:B:691:GLN:HE22	1:B:726:ALA:HA	1.75	0.49
1:A:606:VAL:O	1:A:610:VAL:HG23	2.12	0.49
1:A:702:SER:HB2	1:A:822:ARG:HD2	1.94	0.49
1:B:936:GLY:O	1:B:938:LYS:HG2	2.11	0.49
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.94	0.49
1:A:396:ASP:OD2	1:A:398:VAL:HG22	2.13	0.49
1:A:526:LEU:O	1:A:531:LYS:HE3	2.12	0.49
1:A:544:ILE:HD12	1:A:613:LEU:CD2	2.42	0.49
1:B:667:LEU:HB3	1:B:854:LYS:HA	1.94	0.49
1:A:325:THR:CG2	1:A:382:MET:SD	3.01	0.49
1:A:1175:PHE:CD2	1:B:1151:GLN:HG3	2.48	0.49
1:A:1180:GLY:O	1:A:1181:LYS:HB2	2.13	0.49
1:A:1219:THR:HG23	7:A:2605:HOH:O	2.13	0.49
1:B:221:ASN:HB3	1:B:222:PRO:CD	2.43	0.49
1:A:325:THR:HG21	7:A:3239:HOH:O	2.13	0.49
1:B:492:PRO:O	1:B:495:VAL:HG22	2.12	0.48
1:A:750:ASN:HD21	1:A:1083:SER:HB2	1.78	0.48
1:B:489:CYS:SG	1:B:500:ILE:HD13	2.53	0.48
1:A:1003:LYS:NZ	1:B:976:HIS:HD2	2.12	0.48
1:A:1040:VAL:HG12	1:A:1048:GLN:HE22	1.77	0.48
1:B:20:ALA:HB2	1:B:188:TYR:CZ	2.48	0.48
1:A:591:TYR:O	1:A:593:LYS:N	2.45	0.48
1:B:290:LEU:HD11	1:B:409:PHE:HZ	1.79	0.48
1:A:1209:GLY:O	1:B:429:GLY:HA2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:841:SER:HA	1:B:844:TRP:CE2	2.48	0.48
1:B:390:PHE:CD1	1:B:392:VAL:HG23	2.48	0.48
1:A:20:ALA:HB2	1:A:188:TYR:CZ	2.49	0.48
1:A:526:LEU:HD11	1:A:530:ILE:HG21	1.96	0.48
1:A:594:LYS:HG2	1:A:595:GLY:H	1.77	0.48
1:A:455:TYR:HB2	1:B:1201:PRO:HD3	1.96	0.47
1:A:497:ILE:HG13	1:A:498:TYR:CD1	2.50	0.47
1:B:306:ARG:HA	1:B:307:PRO:C	2.40	0.47
1:B:873:ALA:HA	1:B:959:ILE:HD13	1.96	0.47
1:A:110:HIS:HE1	1:A:157:HIS:NE2	2.12	0.47
1:A:778:LEU:HD13	1:A:778:LEU:C	2.40	0.47
1:B:526:LEU:O	1:B:531:LYS:HE3	2.15	0.47
1:A:346:SER:HA	1:A:349:VAL:HG22	1.97	0.47
1:A:937:GLN:C	1:A:938:LYS:HD2	2.40	0.47
1:A:1004:ALA:O	1:A:1022:LYS:HG3	2.15	0.47
1:A:643:VAL:HB	1:A:849:PRO:HB2	1.96	0.47
1:B:850:SER:O	1:B:851:MET:HE2	2.15	0.47
1:A:239:VAL:CG2	1:A:240:PRO:HD3	2.45	0.46
1:B:27:ILE:HD11	1:B:1013:PHE:CE2	2.50	0.46
1:A:9:ASP:HA	1:A:179:GLU:O	2.15	0.46
1:A:730:GLU:CD	1:A:730:GLU:N	2.73	0.46
1:A:1102:ASP:CG	1:A:1104:ARG:HE	2.23	0.46
1:B:635:THR:HG22	1:B:640:LYS:HG3	1.96	0.46
1:B:765:GLN:HE21	1:B:765:GLN:HA	1.80	0.46
1:A:426:GLY:O	1:A:427:ALA:HB3	2.16	0.46
1:A:881:MET:HE3	1:B:59:ARG:HG3	1.98	0.46
1:B:7:THR:O	1:B:8:THR:HG23	2.14	0.46
1:A:992:GLU:O	1:A:993:VAL:CG1	2.64	0.46
1:B:1193:GLU:N	1:B:1193:GLU:OE2	2.48	0.46
1:A:2:GLY:HA2	1:A:190:ASP:OD2	2.16	0.46
1:A:673:GLU:O	1:A:674:LYS:C	2.58	0.46
1:A:1083:SER:O	1:A:1087:MET:HG3	2.16	0.46
1:B:67:ALA:O	1:B:71:VAL:HG23	2.16	0.46
1:B:135:GLN:H	1:B:135:GLN:NE2	2.12	0.46
1:B:720:ASN:N	1:B:720:ASN:HD22	2.14	0.46
1:A:435:LYS:O	1:A:439:LYS:HD3	2.16	0.46
1:A:542:TYR:CD2	1:A:570:LEU:HD21	2.51	0.46
1:B:3:LYS:HE2	1:B:253:LEU:O	2.15	0.46
1:B:184:GLU:HG3	7:B:2096:HOH:O	2.15	0.46
1:B:5:MET:HE2	1:B:184:GLU:CB	2.43	0.46
1:B:1219:THR:CG2	1:B:1222:GLN:HG3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:VAL:HG21	1:A:239:VAL:HG11	1.97	0.45
1:A:671:GLN:NE2	1:A:854:LYS:HD2	2.31	0.45
1:B:1200:THR:HG22	1:B:1202:MET:N	2.03	0.45
1:A:575:PRO:O	1:A:576:PHE:C	2.59	0.45
1:B:673:GLU:O	1:B:674:LYS:C	2.58	0.45
1:B:710:LYS:HG3	1:B:713:GLU:OE2	2.16	0.45
1:B:731:LEU:CD2	1:B:790:VAL:HG11	2.41	0.45
1:A:667:LEU:HB3	1:A:854:LYS:HA	1.98	0.45
1:B:114:ARG:NE	1:B:123:ILE:HA	2.31	0.45
1:B:495:VAL:HA	1:B:500:ILE:HD12	1.99	0.45
1:B:720:ASN:H	1:B:720:ASN:ND2	2.15	0.45
1:A:99:LYS:HE2	1:B:117:ALA:HB1	1.98	0.45
1:B:562:ILE:HD12	1:B:562:ILE:N	2.30	0.45
1:A:709:ALA:CB	1:A:714:LEU:HD11	2.46	0.45
1:B:823:VAL:HG11	1:B:1049:PHE:CE2	2.41	0.45
1:A:243:VAL:O	1:A:247:MET:HG3	2.17	0.45
1:A:398:VAL:HG23	1:A:399:THR:H	1.82	0.45
1:A:867:SER:O	1:B:99:LYS:HE3	2.16	0.45
1:A:1189:GLY:CA	1:A:1196:THR:HG21	2.47	0.45
1:B:240:PRO:HB3	1:B:309:VAL:HG21	1.99	0.45
1:B:992:GLU:O	1:B:993:VAL:CG1	2.65	0.45
1:A:20:ALA:HB2	1:A:188:TYR:CE1	2.52	0.45
1:A:97:MET:HE1	1:A:168:MET:CE	2.47	0.45
1:A:163:SER:O	1:A:164:ASN:HB2	2.17	0.45
1:B:632:GLU:O	1:B:632:GLU:CD	2.60	0.45
1:B:635:THR:HG21	1:B:639:PHE:CD2	2.50	0.45
1:B:871:ASP:O	1:B:874:GLU:HG2	2.17	0.45
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.48	0.44
1:A:491:ASN:HD22	1:A:492:PRO:CD	2.29	0.44
1:A:950:ASP:OD2	1:B:212:HIS:HE1	2.00	0.44
1:B:426:GLY:O	1:B:427:ALA:HB3	2.17	0.44
3:B:2236:TPP:HN42	3:B:2236:TPP:H2	1.82	0.44
1:A:27:ILE:HB	7:A:2051:HOH:O	2.18	0.44
1:B:441:ILE:HD13	1:B:573:VAL:HG11	1.98	0.44
1:A:516:TRP:O	1:A:522:MET:HE2	2.17	0.44
1:A:690:ILE:HG12	2:A:2233:SF4:S2	2.58	0.44
1:A:699:CYS:HA	1:A:700:PRO:HD3	1.84	0.44
1:A:1181:LYS:HB2	1:A:1181:LYS:HZ2	1.79	0.44
1:B:87:SER:HA	1:B:129:ASP:HB3	1.98	0.44
1:B:1219:THR:HG22	1:B:1222:GLN:CD	2.42	0.44
1:A:1043:GLY:HA3	1:A:1087:MET:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:LYS:HG3	1:B:728:GLY:N	2.31	0.44
1:B:1219:THR:CG2	1:B:1222:GLN:H	2.26	0.44
1:A:1132:ASN:ND2	1:A:1136:VAL:HG13	2.32	0.44
1:A:590:ALA:O	1:A:591:TYR:C	2.61	0.44
1:A:698:VAL:O	1:A:698:VAL:HG12	2.18	0.44
1:B:411:ASP:HB2	1:B:483:ARG:HD2	2.00	0.44
1:B:1214:GLN:O	1:B:1215:ASN:HB2	2.17	0.44
1:A:418:ILE:HD12	1:A:573:VAL:HA	1.98	0.44
3:A:2236:TPP:HN42	3:A:2236:TPP:H2	1.83	0.43
1:B:690:ILE:HG12	2:B:2233:SF4:S2	2.58	0.43
1:B:713:GLU:OE1	1:B:785:PRO:HD2	2.18	0.43
1:B:1219:THR:O	1:B:1223:GLN:HG3	2.18	0.43
1:A:60:GLU:O	1:B:976:HIS:HE1	2.00	0.43
1:A:495:VAL:HG12	1:A:527:PRO:CD	2.49	0.43
1:A:569:LYS:HG3	1:A:576:PHE:CD2	2.54	0.43
1:A:858:LEU:HD22	1:A:858:LEU:N	2.33	0.43
1:A:765:GLN:HE21	1:A:765:GLN:HA	1.82	0.43
1:A:1000:GLN:H	1:A:1000:GLN:NE2	2.17	0.43
1:A:1230:THR:O	1:A:1231:LYS:C	2.61	0.43
1:A:1229:ARG:HH12	1:B:765:GLN:HE22	1.66	0.43
1:A:779:GLU:O	1:A:783:ARG:HD3	2.19	0.43
1:A:632:GLU:CD	1:A:632:GLU:O	2.62	0.43
1:A:456:ASP:OD2	1:A:457:SER:N	2.52	0.43
1:A:592:GLY:HA2	1:A:599:VAL:CG2	2.49	0.43
1:A:837:ALA:HB2	1:A:872:ALA:HB2	2.00	0.43
1:A:1200:THR:HG23	1:A:1201:PRO:CD	2.45	0.43
1:B:1083:SER:O	1:B:1087:MET:HG3	2.19	0.43
1:A:635:THR:HG22	1:A:639:PHE:HB3	2.01	0.42
1:A:976:HIS:HE1	1:B:60:GLU:O	2.02	0.42
1:A:1000:GLN:HA	1:A:1012:LYS:HB2	2.00	0.42
1:B:317:LEU:HD13	1:B:317:LEU:C	2.44	0.42
1:A:229:ARG:HD2	7:B:2065:HOH:O	2.19	0.42
1:A:483:ARG:HG2	1:A:483:ARG:HH11	1.84	0.42
1:B:456:ASP:OD1	1:B:463:ILE:HG22	2.18	0.42
1:A:126:ASP:HB2	1:A:329:ARG:HG2	2.01	0.42
1:A:636:ASN:HD22	1:A:672:PHE:HE1	1.63	0.42
1:B:755:CYS:SG	1:B:761:ALA:HB3	2.60	0.42
1:A:561:MET:HE3	1:A:564:GLN:HB3	2.01	0.42
1:A:691:GLN:HG2	1:A:736:PHE:CD2	2.54	0.42
1:A:796:LEU:C	1:A:796:LEU:CD2	2.93	0.42
1:A:463:ILE:C	1:A:463:ILE:HD12	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:GLU:CD	1:A:759:GLU:N	2.72	0.42
1:A:1012:LYS:O	1:A:1013:PHE:HB2	2.20	0.42
1:A:501:LEU:HD11	1:A:530:ILE:HG23	2.02	0.42
1:A:616:PHE:HB2	7:A:2313:HOH:O	2.20	0.42
1:A:712:GLU:O	1:A:715:VAL:HG23	2.20	0.42
1:B:1232:LYS:HB3	1:B:1232:LYS:HZ3	1.85	0.42
1:A:538:LYS:HD2	1:A:538:LYS:N	2.35	0.41
1:A:1132:ASN:HD21	1:A:1136:VAL:CG1	2.33	0.41
1:B:9:ASP:HA	1:B:179:GLU:O	2.20	0.41
1:A:221:ASN:HB3	1:A:222:PRO:HD2	2.02	0.41
1:A:346:SER:O	1:A:349:VAL:HG22	2.20	0.41
1:A:1232:LYS:HB3	1:A:1232:LYS:HZ2	1.86	0.41
7:A:2581:HOH:O	1:B:1077:ARG:HG2	2.19	0.41
1:B:300:ILE:HD11	1:B:317:LEU:HD23	2.00	0.41
1:B:317:LEU:HA	1:B:318:PRO:HD3	1.95	0.41
1:B:892:ASP:OD2	1:B:896:LYS:NZ	2.52	0.41
1:A:24:VAL:CG1	1:B:881:MET:HE2	2.48	0.41
1:A:576:PHE:C	1:A:576:PHE:CD1	2.98	0.41
1:A:1175:PHE:CD2	1:A:1176:ALA:N	2.88	0.41
1:B:438:ILE:HD11	1:B:468:LEU:HD22	2.02	0.41
1:B:581:ASP:O	1:B:585:LYS:HG2	2.20	0.41
1:B:594:LYS:HB3	1:B:594:LYS:HZ2	1.85	0.41
1:A:114:ARG:NE	1:A:123:ILE:HA	2.35	0.41
1:A:429:GLY:HA2	1:B:1209:GLY:O	2.21	0.41
1:A:1094:GLY:HA3	1:A:1120:PRO:HG3	2.03	0.41
1:A:617:LYS:HD3	1:A:617:LYS:HA	1.92	0.41
1:A:729:LYS:HB3	1:A:730:GLU:OE2	2.21	0.41
1:B:720:ASN:HD22	1:B:720:ASN:H	1.69	0.41
1:A:593:LYS:CG	1:A:594:LYS:N	2.76	0.41
1:A:994:TYR:HB2	1:A:1000:GLN:HE21	1.85	0.41
1:B:650:GLN:HE22	1:B:653:LYS:NZ	2.18	0.41
1:B:964:GLY:O	1:B:968:ASP:HB2	2.21	0.41
1:B:289:HIS:ND1	1:B:290:LEU:HD12	2.36	0.41
1:B:593:LYS:O	1:B:593:LYS:HG2	2.20	0.41
1:A:36:MET:HE3	1:A:84:PHE:HB3	2.03	0.41
1:A:61:MET:HA	1:B:976:HIS:CE1	2.56	0.41
1:A:229:ARG:HE	1:B:128:GLN:HE22	1.68	0.41
1:B:20:ALA:HB2	1:B:188:TYR:CE1	2.56	0.41
1:B:163:SER:O	1:B:164:ASN:HB2	2.20	0.41
1:B:181:GLN:HE21	1:B:181:GLN:HB3	1.63	0.41
1:B:184:GLU:CD	1:B:256:ARG:HH12	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:TYR:HB3	1:B:500:ILE:HD11	2.03	0.41
1:B:639:PHE:HA	1:B:643:VAL:HB	2.03	0.41
1:B:714:LEU:N	1:B:714:LEU:HD22	2.35	0.41
1:A:1219:THR:HG22	1:A:1221:GLU:N	2.34	0.41
1:B:7:THR:HG21	1:B:439:LYS:HA	2.03	0.40
1:B:467:HIS:CD2	1:B:481:VAL:H	2.40	0.40
1:A:212:HIS:HE1	1:B:950:ASP:OD2	2.03	0.40
1:B:869:PHE:CE2	1:B:969:ILE:HG21	2.55	0.40
1:B:1012:LYS:O	1:B:1013:PHE:HB2	2.21	0.40
1:A:619:PRO:HG2	1:A:622:TRP:CD1	2.57	0.40
1:B:7:THR:O	1:B:7:THR:HG23	2.22	0.40
1:B:115:ALA:HB2	1:B:126:ASP:OD1	2.21	0.40
1:B:221:ASN:HB3	1:B:222:PRO:HD2	2.02	0.40
1:B:382:MET:O	1:B:386:LYS:NZ	2.54	0.40
1:A:637:GLU:HG3	1:A:641:ASN:HD22	1.86	0.40
1:B:587:ILE:O	1:B:590:ALA:O	2.40	0.40
1:B:688:ASN:HB3	1:B:759:GLU:O	2.20	0.40
1:B:850:SER:C	1:B:851:MET:HE2	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1229/1231 (100%)	1181 (96%)	44 (4%)	4 (0%)	36	25
1	B	1229/1231 (100%)	1184 (96%)	41 (3%)	4 (0%)	36	25
All	All	2458/2462 (100%)	2365 (96%)	85 (4%)	8 (0%)	36	25

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1178	ALA
1	A	595	GLY
1	B	732	LYS
1	B	1231	LYS
1	B	1182	ALA
1	A	760	LYS
1	B	592	GLY
1	A	592	GLY

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	978/978 (100%)	955 (98%)	23 (2%)	43	25
1	B	978/978 (100%)	955 (98%)	23 (2%)	43	25
All	All	1956/1956 (100%)	1910 (98%)	46 (2%)	43	25

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	154	LEU
1	A	181	GLN
1	A	317	LEU
1	A	325	THR
1	A	327	LEU
1	A	351	ARG
1	A	463	ILE
1	A	582	LEU
1	A	632	GLU
1	A	643	VAL
1	A	759	GLU
1	A	789	GLU
1	A	942	LEU
1	A	996	ASN
1	A	1000	GLN

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Mol	Chain	Res	Type
1	A	1048	GLN
1	A	1077	ARG
1	A	1115	LEU
1	A	1181	LYS
1	A	1196	THR
1	A	1219	THR
1	A	1232	LYS
1	B	181	GLN
1	B	194	LEU
1	B	342	LEU
1	B	359	LEU
1	B	415	LYS
1	B	463	ILE
1	B	509	THR
1	B	583	LEU
1	B	620	ASP
1	B	635	THR
1	B	720	ASN
1	B	754	ILE
1	B	796	LEU
1	B	823	VAL
1	B	849	PRO
1	B	874	GLU
1	B	996	ASN
1	B	1000	GLN
1	B	1047	GLN
1	B	1115	LEU
1	B	1165	HIS
1	B	1183	ASP
1	B	1232	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	46	GLN
1	A	96	ASN
1	A	110	HIS
1	A	128	GLN
1	A	135	GLN
1	A	147	GLN
1	A	164	ASN

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Mol	Chain	Res	Type
1	A	169	HIS
1	A	181	GLN
1	A	212	HIS
1	A	220	GLN
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	560	ASN
1	A	608	GLN
1	A	641	ASN
1	A	671	GLN
1	A	683	GLN
1	A	688	ASN
1	A	691	GLN
1	A	720	ASN
1	A	739	GLN
1	A	750	ASN
1	A	765	GLN
1	A	777	ASN
1	A	836	ASN
1	A	866	ASN
1	A	918	ASN
1	A	937	GLN
1	A	976	HIS
1	A	996	ASN
1	A	1000	GLN
1	A	1048	GLN
1	A	1073	ASN
1	A	1084	GLN
1	A	1088	ASN
1	A	1108	GLN
1	A	1170	ASN
1	B	11	ASN
1	B	16	HIS
1	B	46	GLN
1	B	96	ASN
1	B	110	HIS

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Mol	Chain	Res	Type
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	421	GLN
1	B	434	ASN
1	B	467	HIS
1	B	476	GLN
1	B	525	HIS
1	B	608	GLN
1	B	650	GLN
1	B	688	ASN
1	B	691	GLN
1	B	720	ASN
1	B	750	ASN
1	B	765	GLN
1	B	777	ASN
1	B	880	ASN
1	B	976	HIS
1	B	996	ASN
1	B	1000	GLN
1	B	1073	ASN
1	B	1084	GLN
1	B	1088	ASN
1	B	1108	GLN
1	B	1154	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	-	-	-		
3	TPP	A	2236	5	25,27,27	2.47	10 (40%)	37,40,40	1.57	8 (21%)
2	SF4	B	2233	1	0,12,12	-	-	-		
2	SF4	B	2235	1	0,12,12	-	-	-		
3	TPP	B	2236	5	25,27,27	2.47	9 (36%)	37,40,40	1.58	9 (24%)
2	SF4	B	2234	1	0,12,12	-	-	-		
2	SF4	A	2234	1	0,12,12	-	-	-		
2	SF4	A	2233	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	A	2236	5	-	3/17/17/17	0/2/2/2
2	SF4	A	2235	1	-	-	0/6/5/5
2	SF4	B	2233	1	-	-	0/6/5/5
2	SF4	B	2235	1	-	-	0/6/5/5
2	SF4	A	2234	1	-	-	0/6/5/5
2	SF4	B	2234	1	-	-	0/6/5/5
3	TPP	B	2236	5	-	5/17/17/17	0/2/2/2
2	SF4	A	2233	1	-	-	0/6/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2236	TPP	C5'-C4'	6.38	1.53	1.42
3	B	2236	TPP	C2'-N1'	5.84	1.43	1.34
3	B	2236	TPP	C5'-C4'	5.67	1.52	1.42
3	A	2236	TPP	C6'-N1'	4.61	1.44	1.34
3	B	2236	TPP	C4'-N3'	4.23	1.41	1.35
3	A	2236	TPP	CM4-C4	4.22	1.58	1.49
3	B	2236	TPP	C6-C5	3.98	1.58	1.50
3	A	2236	TPP	C2'-N1'	3.31	1.39	1.34
3	B	2236	TPP	C6'-N1'	3.07	1.40	1.34
3	A	2236	TPP	C2-N3	3.01	1.40	1.32
3	B	2236	TPP	C4-N3	3.01	1.46	1.39
3	B	2236	TPP	C2-N3	2.91	1.39	1.32
3	A	2236	TPP	C2'-N3'	2.86	1.39	1.34
3	A	2236	TPP	C4'-N3'	2.75	1.39	1.35
3	A	2236	TPP	C4-N3	2.74	1.45	1.39
3	B	2236	TPP	C2'-N3'	2.59	1.38	1.34
3	A	2236	TPP	C6'-C5'	2.51	1.43	1.37
3	A	2236	TPP	C6-C5	2.18	1.54	1.50
3	B	2236	TPP	C6'-C5'	2.16	1.42	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2236	TPP	C6'-N1'-C2'	4.44	123.51	115.96
3	A	2236	TPP	C6'-N1'-C2'	3.71	122.27	115.96
3	A	2236	TPP	C4-C5-S1	3.36	116.05	110.56
3	B	2236	TPP	N1'-C2'-N3'	-3.10	120.20	125.54
3	B	2236	TPP	C4-C5-S1	2.90	115.29	110.56
3	A	2236	TPP	C5-C4-N3	-2.58	106.81	111.69
3	A	2236	TPP	N1'-C2'-N3'	-2.54	121.17	125.54
3	B	2236	TPP	CM2-C2'-N1'	2.50	119.89	117.14
3	B	2236	TPP	C5'-C4'-N3'	2.48	125.15	121.24
3	B	2236	TPP	C5-C4-N3	-2.36	107.22	111.69
3	A	2236	TPP	CM4-C4-N3	2.21	125.80	120.52
3	A	2236	TPP	CM2-C2'-N3'	2.20	120.59	117.15
3	A	2236	TPP	C2-S1-C5	-2.16	89.72	91.21
3	B	2236	TPP	N4'-C4'-N3'	-2.13	114.02	117.03
3	A	2236	TPP	N4'-C4'-N3'	-2.11	114.06	117.03
3	B	2236	TPP	CM4-C4-N3	2.10	125.53	120.52
3	B	2236	TPP	C5'-C6'-N1'	-2.07	120.37	123.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2236	TPP	C5'-C7'-N3-C2
3	B	2236	TPP	C5'-C7'-N3-C2
3	B	2236	TPP	C5'-C7'-N3-C4
3	A	2236	TPP	C5'-C7'-N3-C4
3	A	2236	TPP	PA-O3A-PB-O2B
3	B	2236	TPP	PA-O3A-PB-O2B
3	B	2236	TPP	C5-C6-C7-O7
3	B	2236	TPP	S1-C5-C6-C7

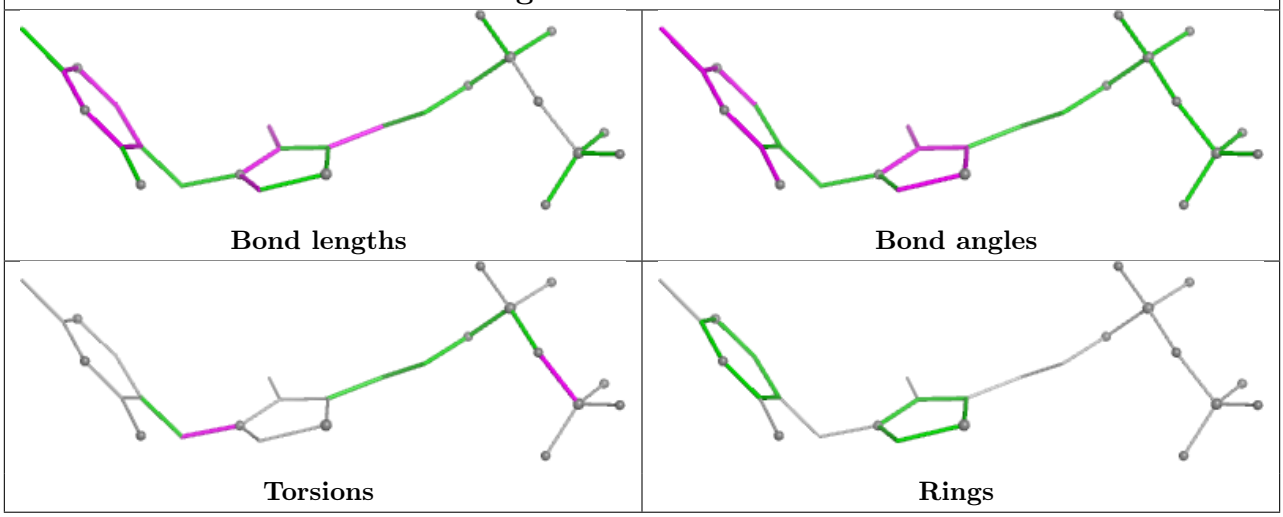
There are no ring outliers.

4 monomers are involved in 4 short contacts:

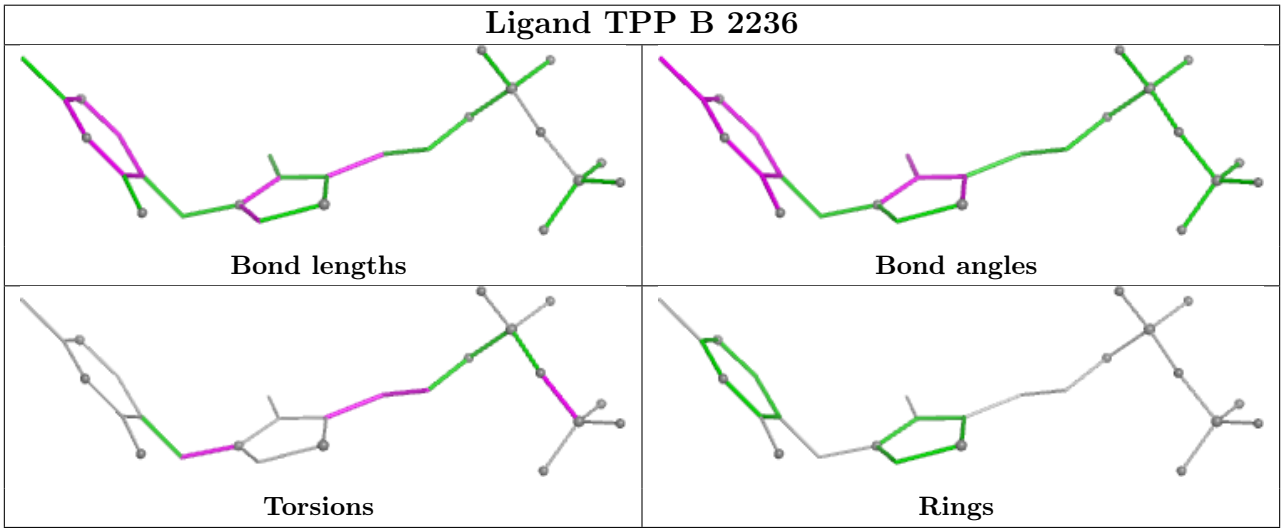
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2236	TPP	1	0
2	B	2233	SF4	1	0
3	B	2236	TPP	1	0
2	A	2233	SF4	1	0

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 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 TPP A 2236



Ligand TPP B 2236



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1231/1231 (100%)	0.25	110 (8%)	15	16	10, 20, 60, 92	0
1	B	1231/1231 (100%)	-0.05	51 (4%)	41	44	8, 18, 41, 90	0
All	All	2462/2462 (100%)	0.10	161 (6%)	25	26	8, 19, 51, 92	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1175	PHE	9.5
1	B	1178	ALA	8.7
1	A	1175	PHE	6.7
1	B	1176	ALA	6.6
1	A	1182	ALA	6.3
1	B	631	ALA	6.2
1	B	1182	ALA	6.2
1	A	1176	ALA	5.9
1	B	1177	PRO	5.7
1	B	1174	SER	5.6
1	B	627	ALA	5.6
1	B	591	TYR	5.6
1	B	590	ALA	5.5
1	B	629	THR	5.4
1	A	587	ILE	5.4
1	A	1177	PRO	5.3
1	A	631	ALA	5.2
1	B	595	GLY	5.0
1	B	630	LYS	5.0
1	A	1178	ALA	4.9
1	A	1165	HIS	4.9
1	A	626	PRO	4.8
1	B	1181	LYS	4.7
1	B	593	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	592	GLY	4.7
1	B	589	LYS	4.6
1	A	599	VAL	4.5
1	A	629	THR	4.4
1	A	627	ALA	4.4
1	A	1172	PHE	4.3
1	A	1179	GLY	4.3
1	A	591	TYR	4.3
1	B	1230	THR	4.2
1	A	598	ILE	4.2
1	B	1180	GLY	4.2
1	A	589	LYS	4.2
1	A	1181	LYS	4.1
1	A	714	LEU	4.1
1	B	628	GLU	4.1
1	B	633	PRO	4.0
1	A	1230	THR	4.0
1	A	553	VAL	4.0
1	B	594	LYS	4.0
1	A	1174	SER	3.9
1	A	580	VAL	3.9
1	A	593	LYS	3.9
1	A	625	ALA	3.9
1	A	633	PRO	3.9
1	B	1179	GLY	3.9
1	A	576	PHE	3.8
1	A	636	ASN	3.8
1	B	1232	LYS	3.7
1	B	732	LYS	3.7
1	A	497	ILE	3.6
1	A	592	GLY	3.6
1	A	1231	LYS	3.6
1	A	597	LYS	3.6
1	A	594	LYS	3.5
1	A	1180	GLY	3.5
1	A	618	TYR	3.5
1	A	586	SER	3.5
1	A	588	HIS	3.5
1	A	759	GLU	3.4
1	B	634	MET	3.4
1	B	598	ILE	3.4
1	B	632	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	590	ALA	3.4
1	A	574	LEU	3.3
1	B	635	THR	3.3
1	B	1183	ASP	3.3
1	A	595	GLY	3.3
1	A	1184	GLY	3.3
1	A	630	LYS	3.2
1	B	1165	HIS	3.2
1	A	624	ASP	3.2
1	A	526	LEU	3.2
1	A	579	ALA	3.2
1	A	582	LEU	3.1
1	A	715	VAL	3.1
1	A	616	PHE	3.1
1	A	596	GLU	3.1
1	A	622	TRP	3.1
1	A	519	LEU	3.0
1	B	715	VAL	3.0
1	B	1231	LYS	3.0
1	A	635	THR	3.0
1	B	596	GLU	3.0
1	B	1221	GLU	3.0
1	B	1173	GLU	2.9
1	A	732	LYS	2.9
1	B	597	LYS	2.9
1	A	1171	ILE	2.9
1	A	717	ALA	2.9
1	B	754	ILE	2.9
1	A	790	VAL	2.8
1	B	1172	PHE	2.8
1	A	617	LYS	2.7
1	A	577	GLU	2.7
1	A	482	ASN	2.7
1	A	634	MET	2.7
1	B	714	LEU	2.7
1	A	1232	LYS	2.7
1	A	1183	ASP	2.6
1	A	495	VAL	2.6
1	B	768	ASP	2.6
1	A	628	GLU	2.6
1	A	730	GLU	2.6
1	A	552	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	463	ILE	2.6
1	A	1170	ASN	2.6
1	B	729	LYS	2.5
1	A	573	VAL	2.5
1	A	711	GLU	2.5
1	A	583	LEU	2.5
1	A	554	GLY	2.5
1	B	1228	LYS	2.5
1	A	613	LEU	2.5
1	A	603	THR	2.5
1	B	733	GLY	2.4
1	A	578	LYS	2.4
1	B	1219	THR	2.4
1	A	731	LEU	2.4
1	A	620	ASP	2.4
1	A	3	LYS	2.4
1	A	349	VAL	2.3
1	A	528	SER	2.3
1	A	720	ASN	2.3
1	A	5	MET	2.3
1	A	938	LYS	2.3
1	A	709	ALA	2.3
1	A	523	ASP	2.3
1	A	727	LYS	2.3
1	A	716	GLY	2.2
1	A	581	ASP	2.2
1	B	953	THR	2.2
1	A	536	ASN	2.2
1	B	588	HIS	2.2
1	A	585	LYS	2.2
1	A	758	LYS	2.2
1	A	532	ARG	2.2
1	A	712	GLU	2.2
1	A	539	LEU	2.2
1	A	619	PRO	2.2
1	B	626	PRO	2.2
1	A	575	PRO	2.1
1	A	600	LYS	2.1
1	A	783	ARG	2.1
1	A	632	GLU	2.1
1	A	723	ALA	2.1
1	A	733	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	584	LYS	2.1
1	A	1173	GLU	2.1
1	A	524	LYS	2.1
1	A	936	GLY	2.1
1	A	456	ASP	2.1
1	A	623	LYS	2.0
1	B	1170	ASN	2.0
1	A	506	ASP	2.0
1	B	1190	GLU	2.0
1	A	621	SER	2.0
1	A	496	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
2	SF4	A	2233	8/8	0.97	0.05	23,24,25,25	0
2	SF4	B	2233	8/8	0.98	0.04	17,18,19,20	0
3	TPP	A	2236	26/26	0.98	0.05	8,12,14,16	0
6	CA	A	2239	1/1	0.98	0.12	45,45,45,45	0
6	CA	B	2239	1/1	0.98	0.16	40,40,40,40	0
2	SF4	A	2235	8/8	0.99	0.02	15,15,16,17	0
3	TPP	B	2236	26/26	0.99	0.04	7,9,13,14	0
4	CL	B	2237	1/1	0.99	0.03	20,20,20,20	0
5	MG	A	2238	1/1	0.99	0.05	9,9,9,9	0
5	MG	B	2238	1/1	0.99	0.05	5,5,5,5	0
2	SF4	A	2234	8/8	0.99	0.03	18,20,21,22	0
2	SF4	B	2234	8/8	0.99	0.03	13,15,16,16	0

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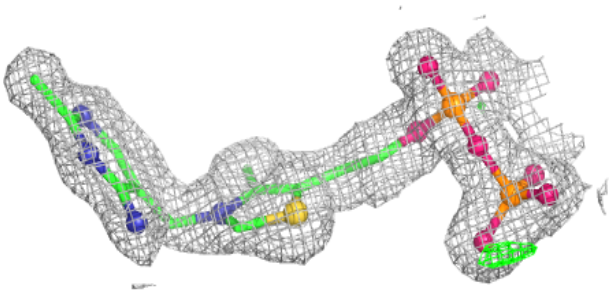
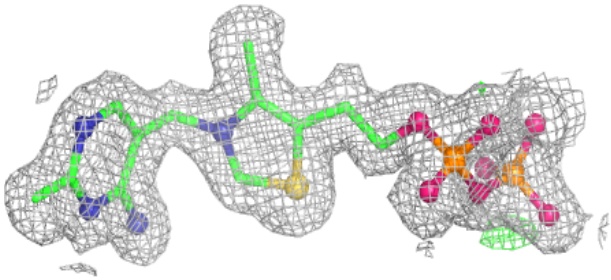
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	A	2237	1/1	1.00	0.04	21,21,21,21	0
2	SF4	B	2235	8/8	1.00	0.02	9,11,12,12	0

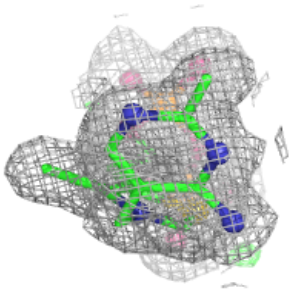
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 2236:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

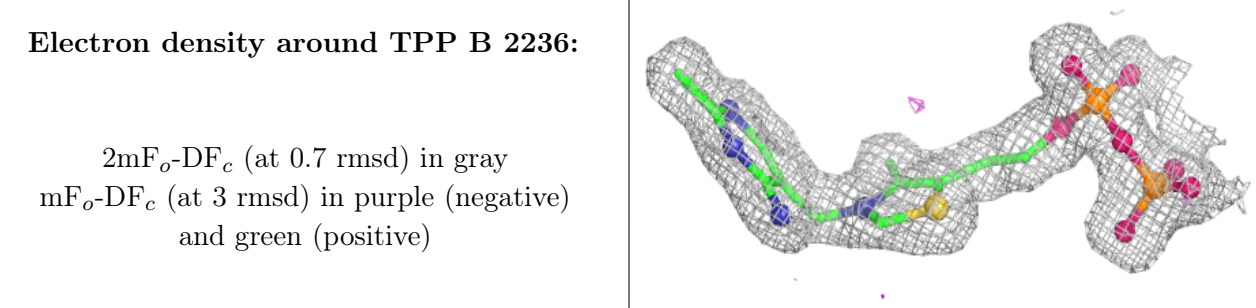


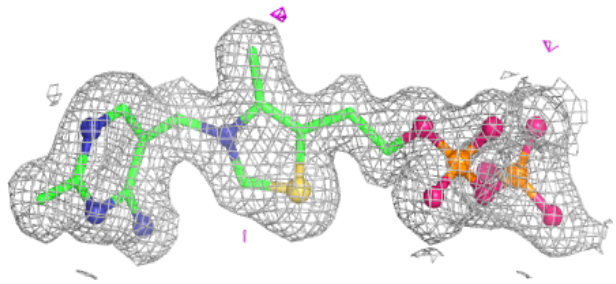


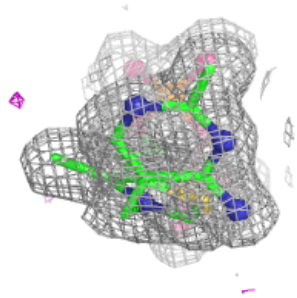


Electron density around TPP B 2236:

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







6.5 Other polymers (i)

There are no such residues in this entry.