Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2026 – 01:51 pm BST

PDB ID	:	2C42 / pdb_00002c42
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	:	2005-10-14
Resolution	:	1.78 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:

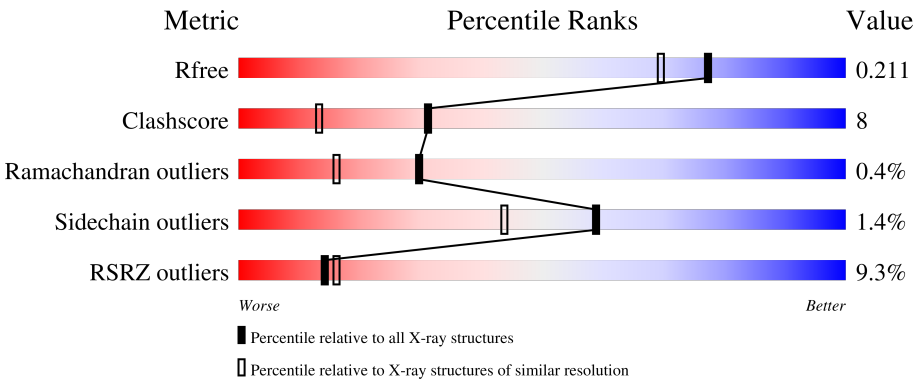
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	12% 80% 19% •
1	B	1231	6% 83% 15% •

2 Entry composition (i)

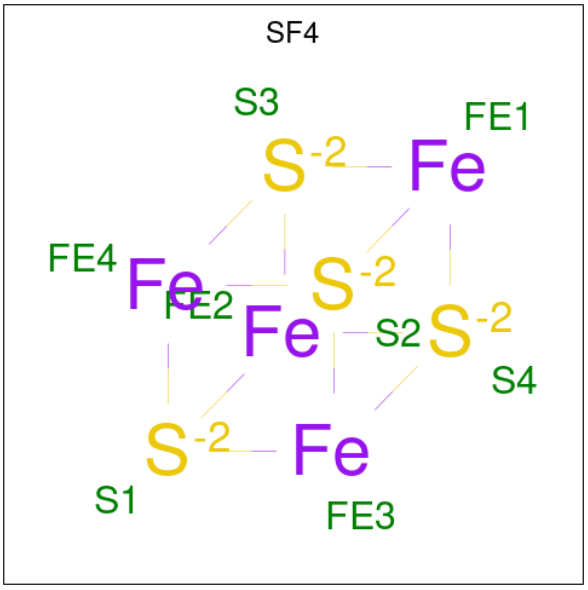
There are 7 unique types of molecules in this entry. The entry contains 20099 atoms, of which 0 are hydrogens and 0 are deuteriums.

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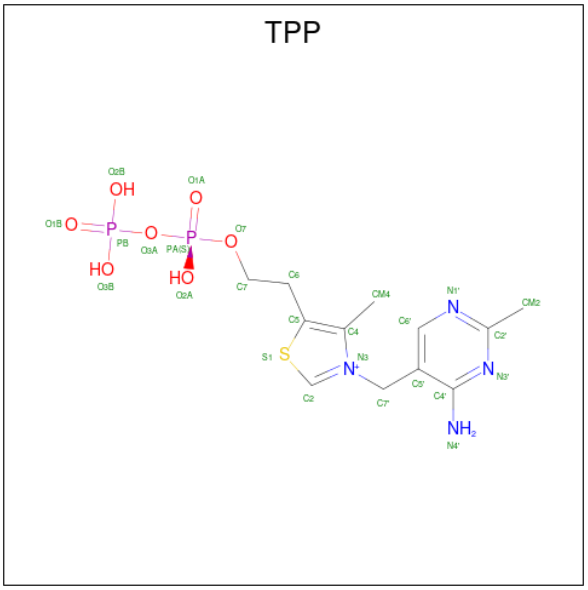
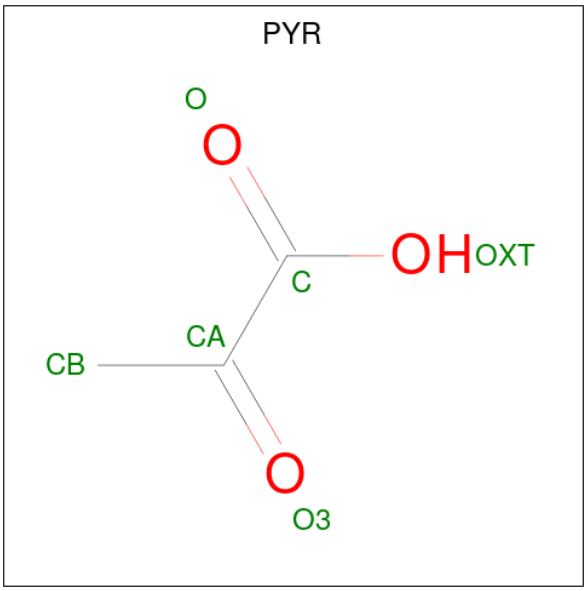
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	B	1	8	4	4	0	0
			Total	Fe	S		
2	B	1	8	4	4	0	0

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



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
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	550	Total O 550 550	0	0

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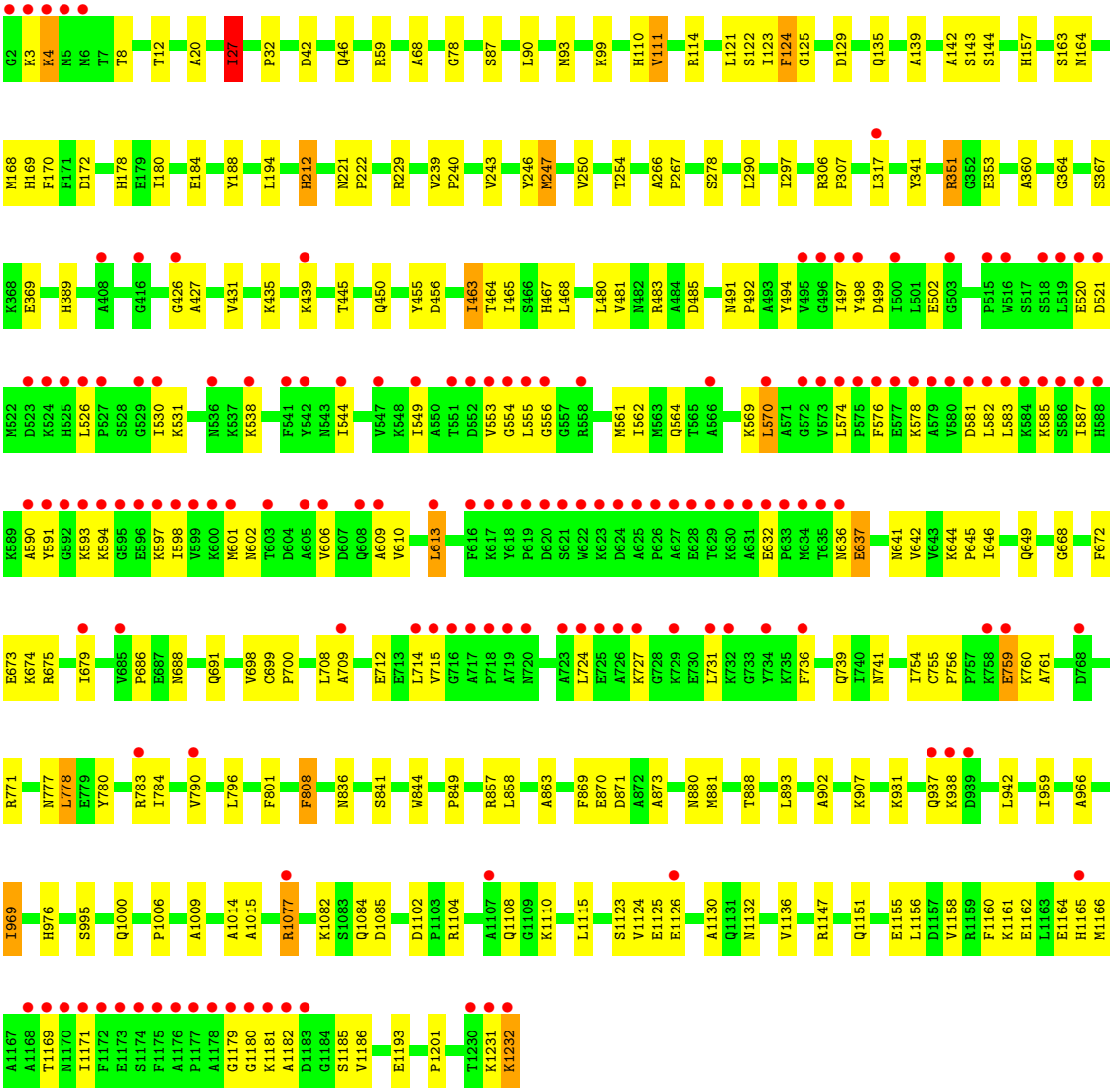
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	B	667	667	667	0	0

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.

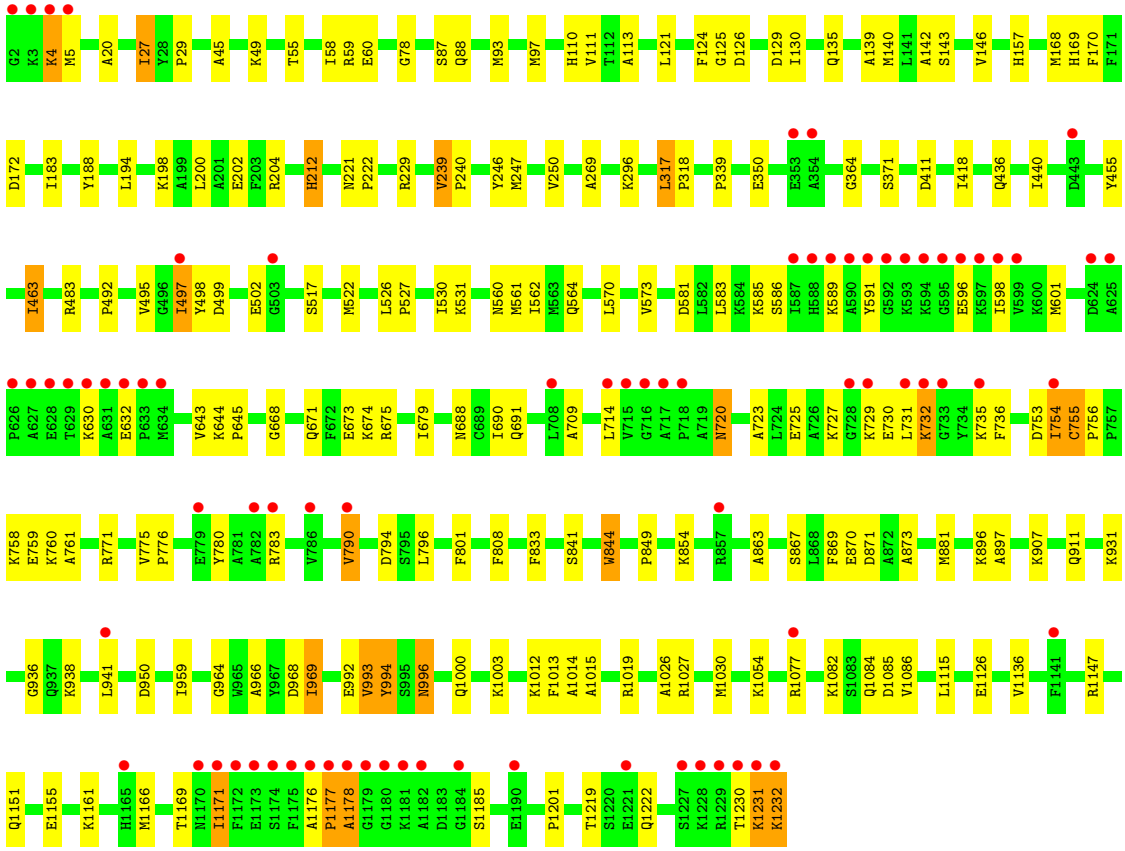
• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

Chain A: 12% 80% 19%



• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

Chain B: 6% 83% 15%


G2 K3 K4 M5 A20 I27 Y28 P29 A45 K49 T55 I58 R59 E60 G78 S87 Q88 M93 M97 H110 V111 T112 A113 L121 F124 G125 D126 D129 I130 Q135 A139 M140 L141 A142 S143 V146 H157 M168 H169 F170 F171
D172 I183 Y188 L194 K198 A199 L200 A201 E202 F203 R204 H212 N221 P222 R229 V239 P240 Y246 M247 V250 A269 K296 L317 P318 P339 E350 E353 A354 G364 S371 D411 I418 Q436 I440 D443 Y455
I463 R483 P492 V495 G496 I497 Y498 D499 E502 G503 S517 M522 L526 P527 I530 K531 N560 M561 I562 M563 Q564 L570 V573 D581 L582 L583 K584 K585 S586 I587 H588 K589 A590 Y591 G592 K593 K594 G595 E596 K597 I598 V599 K600 M601 D624 A625
P626 A627 E628 T629 K630 A631 E632 P633 M634 V643 K644 P645 G668 Q671 F672 E673 K674 R675 I679 N688 C689 I690 Q691 L708 A709 L714 V715 G716 A717 P718 A719 N720 A723 L724 E725 A726 K727 G728 K729 E730 L731 K732 G733 Y734 K735 F736 D753 I754 C755 P756 P757
K758 E759 K760 A761 R771 V775 P776 E779 Y780 A781 A782 R783 V786 V790 D794 S795 L796 F801 F808 F833 S841 W844 P849 K854 R857 A863 S867 L868 F869 E870 D871 A872 A873 M881 K896 A897 K907 Q911 K931
G936 Q937 K938 L941 D950 I959 G964 W965 A966 Y967 D968 I969 E992 V993 Y994 S995 N996 Q1000 K1003 K1012 F1013 A1014 A1015 R1019 A1026 R1027 M1030 K1054 R1077 K1082 S1083 Q1084 D1085 V1086 L1115 E1126 V1136 F1141 R1147
Q1151 E1155 K1161 H1165 M1166 T1169 N1170 I1171 F1172 E1173 S1174 F1175 A1176 P1177 A1178 G1179 G1180 K1181 A1182 D1183 G1184 S1185 E1190 P1201 T1219 S1220 E1221 Q1222 S1227 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	86.30Å 145.98Å 211.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.15 – 1.78 51.15 – 1.78	Depositor EDS
% Data completeness (in resolution range)	94.4 (51.15-1.78) 94.5 (51.15-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 1.78Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.219 0.188 , 0.211	Depositor DCC
R_{free} test set	12031 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.7	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	0.95	EDS
Total number of atoms	20099	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: PYR, SF4, MG, TPP, 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	0.34	0/9585	0.89	31/12954 (0.2%)
1	B	0.36	0/9585	0.90	40/12954 (0.3%)
All	All	0.35	0/19170	0.90	71/25908 (0.3%)

There are no bond length outliers.

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	125	GLY	N-CA-C	8.91	126.83	111.15
1	B	756	PRO	N-CA-C	8.34	120.88	110.70
1	B	125	GLY	N-CA-C	8.13	127.16	111.31
1	A	756	PRO	N-CA-C	7.93	120.38	110.70
1	B	139	ALA	N-CA-C	-7.42	100.04	110.50
1	B	969	ILE	N-CA-C	7.34	118.11	110.62
1	A	969	ILE	N-CA-C	7.16	117.93	110.62
1	B	993	VAL	CB-CA-C	-6.95	105.21	111.74
1	A	139	ALA	N-CA-C	-6.93	100.22	110.48
1	B	497	ILE	N-CA-C	6.91	117.92	112.12
1	A	771	ARG	N-CA-C	6.89	118.45	111.07
1	A	247	MET	N-CA-C	-6.76	103.99	111.36
1	B	771	ARG	N-CA-C	6.75	118.29	111.07
1	B	27	ILE	N-CA-C	6.64	118.49	108.80
1	B	517	SER	N-CA-C	6.58	118.11	111.07
1	B	1077	ARG	N-CA-C	6.38	119.05	111.71
1	B	247	MET	N-CA-C	-6.36	104.42	111.36
1	A	755	CYS	CA-C-N	6.34	126.91	120.38
1	A	755	CYS	C-N-CA	6.34	126.91	120.38
1	B	78	GLY	N-CA-C	6.33	124.83	115.08
1	B	560	ASN	N-CA-C	6.32	118.69	111.11
1	B	668	GLY	N-CA-C	6.24	124.51	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	485	ASP	N-CA-C	-6.18	105.88	113.41
1	B	111	VAL	N-CA-C	6.17	116.75	108.11
1	B	870	GLU	N-CA-C	6.03	120.37	112.89
1	A	1014	ALA	N-CA-C	-6.03	103.30	110.41
1	A	668	GLY	N-CA-C	5.88	123.47	115.30
1	B	871	ASP	N-CA-C	5.88	119.76	112.59
1	A	1077	ARG	N-CA-C	5.82	118.37	111.33
1	B	371	SER	N-CA-C	5.80	116.80	110.13
1	B	679	ILE	N-CA-C	-5.78	106.08	111.45
1	A	27	ILE	N-CA-C	5.73	117.09	108.96
1	A	871	ASP	N-CA-C	5.71	120.24	112.88
1	B	760	LYS	N-CA-C	5.69	118.32	110.35
1	B	801	PHE	N-CA-C	-5.67	105.67	112.59
1	B	570	LEU	N-CA-C	5.67	121.23	113.97
1	B	755	CYS	CA-C-N	5.61	126.16	120.38
1	B	755	CYS	C-N-CA	5.61	126.16	120.38
1	A	78	GLY	N-CA-C	5.59	124.26	114.76
1	B	212	HIS	CA-C-N	5.55	125.52	120.03
1	B	212	HIS	C-N-CA	5.55	125.52	120.03
1	A	124	PHE	N-CA-C	5.52	118.60	110.59
1	B	339	PRO	N-CA-C	5.52	123.83	112.47
1	B	833	PHE	N-CA-C	-5.51	101.18	109.95
1	A	1182	ALA	CB-CA-C	-5.50	110.21	116.54
1	A	995	SER	N-CA-C	5.47	117.10	111.03
1	A	801	PHE	N-CA-C	-5.46	105.83	112.88
1	B	966	ALA	N-CA-C	5.43	117.20	111.28
1	A	212	HIS	CA-C-N	5.43	125.33	119.85
1	A	212	HIS	C-N-CA	5.43	125.33	119.85
1	A	172	ASP	N-CA-C	5.42	118.17	110.10
1	B	968	ASP	N-CA-C	5.32	116.59	108.30
1	A	637	GLU	N-CA-C	-5.31	105.53	112.23
1	B	172	ASP	N-CA-C	5.29	117.98	110.10
1	B	994	TYR	N-CA-C	-5.27	99.16	108.23
1	A	679	ILE	N-CA-C	-5.26	106.00	111.58
1	B	124	PHE	N-CA-C	5.26	118.22	110.59
1	A	870	GLU	N-CA-C	5.26	119.54	113.18
1	B	239	VAL	CB-CA-C	-5.26	108.70	113.70
1	A	966	ALA	N-CA-C	5.24	116.99	111.28
1	B	844	TRP	N-CA-C	-5.22	106.41	112.89
1	B	364	GLY	N-CA-C	5.21	125.53	113.18
1	B	643	VAL	N-CA-C	5.19	115.34	110.30
1	A	761	ALA	N-CA-C	-5.18	106.65	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1014	ALA	N-CA-C	-5.16	101.83	109.83
1	A	888	THR	N-CA-C	-5.15	105.74	111.36
1	A	111	VAL	N-CA-C	5.15	115.31	108.11
1	A	364	GLY	N-CA-C	5.14	125.36	113.18
1	A	863	ALA	N-CA-C	-5.13	100.71	108.67
1	B	790	VAL	N-CA-C	5.13	116.59	111.00
1	B	863	ALA	N-CA-C	-5.12	100.73	108.67

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	186	0
1	B	9383	0	9262	147	0
2	A	24	0	0	0	0
2	B	24	0	0	1	0
3	A	26	0	16	0	0
3	B	26	0	16	2	0
4	A	6	0	0	0	0
4	B	6	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	550	0	0	8	0
7	B	667	0	0	7	0
All	All	20099	0	18556	308	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 8.

All (308) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:LYS:HG3	1:A:594:LYS:H	1.27	0.99
1:A:110:HIS:HD2	1:A:169:HIS:HD2	1.15	0.95
1:B:27:ILE:HD13	1:B:58:ILE:HD11	1.48	0.94
1:B:723:ALA:HB3	1:B:735:LYS:HE2	1.57	0.87
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.18	0.86
1:B:1176:ALA:HB1	1:B:1177:PRO:HD2	1.59	0.85
1:A:110:HIS:HE1	1:A:157:HIS:HE1	1.23	0.84
1:A:1180:GLY:HA3	1:B:1019:ARG:HH12	1.45	0.81
1:A:1231:LYS:HG3	1:A:1232:LYS:H	1.44	0.81
1:A:351:ARG:HD3	1:A:353:GLU:HB2	1.61	0.80
1:A:110:HIS:HD2	1:A:169:HIS:CD2	2.02	0.78
1:A:110:HIS:CE1	1:A:157:HIS:HE1	2.03	0.76
1:A:594:LYS:HB3	1:A:598:ILE:HD12	1.66	0.76
1:A:1102:ASP:OD1	1:A:1104:ARG:HG2	1.85	0.76
1:B:110:HIS:HD2	1:B:169:HIS:CD2	2.03	0.74
1:B:1231:LYS:HG3	1:B:1232:LYS:H	1.54	0.73
1:A:110:HIS:HE1	1:A:157:HIS:CE1	2.06	0.72
1:A:780:TYR:O	1:A:783:ARG:HG2	1.90	0.71
1:A:561:MET:HE1	1:A:583:LEU:HD11	1.71	0.71
1:A:644:LYS:HB3	1:A:645:PRO:HD3	1.72	0.71
1:A:1161:LYS:HB3	1:B:1171:ILE:HD12	1.73	0.69
1:A:111:VAL:HG21	1:A:168:MET:HE2	1.74	0.69
1:A:709:ALA:HB3	1:A:714:LEU:HD11	1.74	0.69
1:B:198:LYS:O	1:B:202:GLU:HG3	1.94	0.68
1:A:1108:GLN:HE21	1:A:1110:LYS:HD2	1.59	0.67
1:B:1230:THR:O	1:B:1232:LYS:HG2	1.95	0.67
1:A:597:LYS:O	1:A:601:MET:HG3	1.95	0.67
1:A:110:HIS:CD2	1:A:169:HIS:HD2	2.06	0.67
1:A:463:ILE:HD13	1:A:494:TYR:CE1	2.30	0.67
1:A:708:LEU:HD21	1:A:731:LEU:HD22	1.77	0.67
1:A:691:GLN:HG2	1:A:736:PHE:CD2	2.30	0.66
1:A:739:GLN:NE2	1:A:777:ASN:HB3	2.10	0.66
1:A:739:GLN:HE22	1:A:777:ASN:HB3	1.59	0.66
1:B:143:SER:OG	1:B:169:HIS:HE1	1.78	0.65
1:A:881:MET:HE3	1:B:59:ARG:HG2	1.77	0.65
1:B:463:ILE:HD11	1:B:498:TYR:OH	1.96	0.65
1:A:593:LYS:HG3	1:A:594:LYS:N	2.06	0.65
1:B:561:MET:HE1	1:B:583:LEU:HD11	1.76	0.65
1:A:1166:MET:O	1:A:1169:THR:HG22	1.97	0.65
1:B:691:GLN:HG2	1:B:736:PHE:CD2	2.32	0.65
1:A:90:LEU:HD21	1:A:168:MET:HE1	1.78	0.65
1:B:110:HIS:HE1	1:B:157:HIS:NE2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:HIS:CD2	1:B:1171:ILE:HG21	2.32	0.64
1:B:581:ASP:O	1:B:585:LYS:HG2	1.96	0.64
1:A:1151:GLN:O	1:A:1155:GLU:HG3	1.97	0.64
1:A:976:HIS:HD2	1:B:1003:LYS:NZ	1.96	0.63
1:A:583:LEU:O	1:A:587:ILE:HG13	1.98	0.63
1:A:1231:LYS:HG3	1:A:1232:LYS:N	2.14	0.62
1:B:110:HIS:CD2	1:B:169:HIS:HD2	2.09	0.62
1:A:1147:ARG:HB3	1:B:1178:ALA:O	1.98	0.62
1:A:445:THR:HG21	1:A:574:LEU:HD21	1.81	0.62
1:A:1185:SER:HB2	1:B:1015:ALA:HB1	1.82	0.61
1:B:907:LYS:O	1:B:911:GLN:HG3	2.00	0.61
1:B:992:GLU:O	1:B:993:VAL:HG13	2.01	0.61
1:B:527:PRO:HD2	1:B:530:ILE:HD12	1.81	0.61
1:B:1219:THR:OG1	1:B:1222:GLN:HG3	2.01	0.61
1:A:1181:LYS:HB2	1:A:1181:LYS:NZ	2.16	0.60
1:A:27:ILE:HB	7:A:2040:HOH:O	2.01	0.60
1:A:937:GLN:HG2	1:A:942:LEU:HB3	1.83	0.60
1:A:902:ALA:O	1:A:907:LYS:HE3	2.02	0.60
1:A:759:GLU:CD	1:A:759:GLU:H	2.08	0.60
1:B:561:MET:HE3	1:B:564:GLN:HB3	1.84	0.60
1:A:526:LEU:HD11	1:A:530:ILE:HG21	1.83	0.59
1:A:636:ASN:ND2	1:A:672:PHE:HE1	2.00	0.59
1:B:780:TYR:HD1	1:B:783:ARG:HH21	1.50	0.59
1:A:465:ILE:HD11	1:A:649:GLN:NE2	2.17	0.59
1:A:526:LEU:O	1:A:531:LYS:HE3	2.01	0.59
1:A:731:LEU:HD23	1:A:790:VAL:HG11	1.84	0.59
1:A:27:ILE:HD13	1:A:59:ARG:O	2.02	0.59
1:A:435:LYS:O	1:A:439:LYS:HD3	2.03	0.59
1:A:110:HIS:CE1	1:A:157:HIS:CE1	2.87	0.59
1:B:714:LEU:HG	1:B:735:LYS:HD3	1.85	0.58
1:A:570:LEU:N	1:A:570:LEU:HD22	2.19	0.58
1:A:544:ILE:HD12	1:A:613:LEU:HD22	1.85	0.58
1:B:731:LEU:HD23	1:B:790:VAL:HG11	1.85	0.58
1:A:553:VAL:HG23	1:A:555:LEU:HG	1.86	0.57
1:B:723:ALA:HB1	1:B:735:LYS:HG2	1.86	0.57
1:A:143:SER:OG	1:A:169:HIS:HE1	1.87	0.57
1:A:351:ARG:HD2	7:A:2205:HOH:O	2.04	0.57
1:B:931:LYS:HD2	7:B:2525:HOH:O	2.04	0.57
1:A:499:ASP:OD2	1:A:502:GLU:HB2	2.04	0.56
1:A:1123:SER:O	1:A:1126:GLU:HG2	2.05	0.56
1:B:727:LYS:HE2	1:B:727:LYS:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:MET:HE3	1:B:59:ARG:CG	2.35	0.56
1:A:931:LYS:HD2	7:A:2421:HOH:O	2.05	0.56
1:B:1166:MET:O	1:B:1169:THR:HG22	2.05	0.56
1:A:731:LEU:CD2	1:A:790:VAL:HG11	2.36	0.56
1:A:3:LYS:NZ	1:A:254:THR:HA	2.20	0.56
1:B:794:ASP:OD1	1:B:1054:LYS:HD2	2.06	0.55
1:A:609:ALA:O	1:A:613:LEU:HD23	2.07	0.55
1:A:142:ALA:HB2	1:A:170:PHE:CZ	2.41	0.55
1:A:497:ILE:HG13	1:A:498:TYR:CD1	2.42	0.55
1:A:27:ILE:HD13	1:A:27:ILE:H	1.72	0.54
1:A:1115:LEU:HD21	1:A:1160:PHE:CZ	2.42	0.54
1:B:142:ALA:HB2	1:B:170:PHE:CZ	2.43	0.54
1:A:520:GLU:HG3	1:A:521:ASP:N	2.23	0.54
1:A:1015:ALA:HB1	1:B:1185:SER:HB2	1.88	0.54
1:B:130:ILE:HB	1:B:168:MET:HE1	1.89	0.54
1:A:544:ILE:HD11	1:A:549:ILE:HD12	1.90	0.54
1:B:317:LEU:HD23	1:B:318:PRO:HD2	1.89	0.54
1:A:1158:VAL:O	1:A:1162:GLU:HG3	2.08	0.54
1:A:691:GLN:NE2	1:A:727:LYS:HG3	2.23	0.54
1:A:741:ASN:CG	1:A:778:LEU:HD11	2.33	0.54
1:B:1232:LYS:NZ	1:B:1232:LYS:HB3	2.23	0.54
1:A:99:LYS:HE3	1:B:867:SER:O	2.08	0.54
1:A:976:HIS:HD2	1:B:1003:LYS:HZ2	1.55	0.53
1:B:411:ASP:HB2	1:B:483:ARG:HD2	1.91	0.53
1:B:492:PRO:O	1:B:495:VAL:HG22	2.07	0.53
1:A:1231:LYS:CG	1:A:1232:LYS:H	2.18	0.53
1:A:857:ARG:HG3	1:A:858:LEU:CD1	2.39	0.53
1:B:1230:THR:O	1:B:1232:LYS:N	2.42	0.52
1:B:135:GLN:H	1:B:135:GLN:NE2	2.08	0.52
1:A:465:ILE:HD11	1:A:649:GLN:HE22	1.73	0.52
1:A:562:ILE:HD12	1:A:562:ILE:N	2.25	0.52
1:A:1132:ASN:O	1:A:1136:VAL:HG12	2.10	0.52
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.39	0.52
1:A:467:HIS:HD2	1:A:481:VAL:H	1.58	0.52
1:A:341:TYR:CD1	1:A:360:ALA:HB2	2.45	0.51
1:A:1015:ALA:CB	1:B:1185:SER:HB2	2.41	0.51
1:A:1161:LYS:CB	1:B:1171:ILE:HD12	2.39	0.51
1:A:606:VAL:O	1:A:610:VAL:HG23	2.10	0.51
1:A:1180:GLY:HA3	1:B:1019:ARG:NH1	2.22	0.51
1:B:140:MET:HE3	1:B:168:MET:HE1	1.93	0.51
1:B:841:SER:HA	1:B:844:TRP:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:ARG:HD3	7:B:2398:HOH:O	2.11	0.51
1:A:637:GLU:HG3	1:A:641:ASN:ND2	2.26	0.51
1:B:1231:LYS:HG3	1:B:1232:LYS:N	2.23	0.51
1:A:59:ARG:CG	1:B:881:MET:HE3	2.41	0.51
1:A:121:LEU:HD23	1:A:121:LEU:C	2.34	0.51
1:B:731:LEU:CD2	1:B:790:VAL:HG11	2.41	0.51
1:A:937:GLN:C	1:A:938:LYS:HD2	2.36	0.50
1:B:1177:PRO:O	1:B:1178:ALA:HB2	2.11	0.50
1:B:499:ASP:OD2	1:B:502:GLU:HB2	2.11	0.50
1:A:455:TYR:HB2	1:B:1201:PRO:HG3	1.94	0.50
1:B:586:SER:O	1:B:589:LYS:HB3	2.11	0.50
1:A:1006:PRO:HG2	1:A:1009:ALA:HB2	1.94	0.50
1:B:709:ALA:HB3	1:B:714:LEU:HD21	1.94	0.50
1:B:725:GLU:O	1:B:727:LYS:HE3	2.10	0.50
1:A:157:HIS:HD2	7:A:2004:HOH:O	1.94	0.50
1:B:20:ALA:HB2	1:B:188:TYR:CZ	2.47	0.50
1:B:729:LYS:O	1:B:732:LYS:HG3	2.11	0.50
1:A:581:ASP:OD2	1:A:585:LYS:HE3	2.12	0.49
1:A:8:THR:OG1	1:A:12:THR:HB	2.11	0.49
1:A:1186:VAL:HG21	1:B:1136:VAL:HG22	1.94	0.49
1:A:494:TYR:HD2	1:A:497:ILE:HD11	1.76	0.49
1:B:873:ALA:HA	1:B:959:ILE:HD13	1.94	0.49
1:A:686:PRO:HB2	1:A:724:LEU:HD21	1.95	0.49
1:B:49:LYS:HZ2	1:B:55:THR:HG23	1.77	0.49
1:B:269:ALA:HA	1:B:296:LYS:HB3	1.95	0.49
1:A:229:ARG:HD2	7:B:2059:HOH:O	2.13	0.49
1:A:389:HIS:HE1	1:B:350:GLU:OE1	1.96	0.48
1:B:796:LEU:C	1:B:796:LEU:HD23	2.37	0.48
1:A:578:LYS:O	1:A:582:LEU:HD13	2.14	0.48
1:A:467:HIS:CD2	1:A:481:VAL:H	2.32	0.48
1:B:239:VAL:HB	1:B:240:PRO:HD3	1.95	0.48
1:A:1232:LYS:HB3	1:A:1232:LYS:HZ2	1.79	0.48
1:A:306:ARG:HA	1:A:307:PRO:C	2.37	0.48
1:A:389:HIS:HD2	7:A:2059:HOH:O	1.96	0.48
1:A:1180:GLY:O	1:A:1181:LYS:HB2	2.14	0.48
1:B:1232:LYS:HB3	1:B:1232:LYS:HZ2	1.79	0.48
1:A:538:LYS:HD2	1:A:538:LYS:N	2.29	0.48
1:B:229:ARG:HD2	7:B:2125:HOH:O	2.13	0.48
1:B:526:LEU:O	1:B:531:LYS:HE3	2.14	0.47
1:A:593:LYS:CG	1:A:594:LYS:H	2.05	0.47
1:A:636:ASN:ND2	1:A:672:PHE:CE1	2.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:VAL:N	1:B:776:PRO:HD2	2.29	0.47
1:B:869:PHE:CE2	1:B:969:ILE:HG21	2.48	0.47
1:B:630:LYS:O	1:B:630:LYS:HG3	2.13	0.47
1:A:1082:LYS:HE2	1:A:1085:ASP:OD1	2.14	0.47
1:A:1232:LYS:HB3	1:A:1232:LYS:NZ	2.28	0.47
1:B:1126:GLU:HG3	7:B:2618:HOH:O	2.13	0.47
1:A:741:ASN:ND2	1:A:778:LEU:HD11	2.29	0.47
1:B:93:MET:O	1:B:97:MET:HG3	2.15	0.47
1:B:1231:LYS:O	1:B:1232:LYS:HB2	2.14	0.47
1:B:730:GLU:N	1:B:730:GLU:OE1	2.47	0.47
1:B:436:GLN:O	1:B:440:ILE:HG13	2.15	0.47
1:A:212:HIS:HE1	1:B:950:ASP:OD2	1.97	0.46
1:B:4:LYS:HE2	1:B:4:LYS:HA	1.97	0.46
1:B:221:ASN:HB3	1:B:222:PRO:CD	2.45	0.46
1:A:1201:PRO:HG3	1:B:455:TYR:HB2	1.97	0.46
1:B:49:LYS:NZ	1:B:55:THR:HG23	2.30	0.46
1:B:714:LEU:N	1:B:714:LEU:HD22	2.31	0.46
1:A:246:TYR:O	1:A:250:VAL:HG23	2.15	0.46
1:A:675:ARG:HD3	7:A:2314:HOH:O	2.13	0.46
1:B:755:CYS:SG	1:B:761:ALA:HB3	2.56	0.46
1:B:897:ALA:HA	1:B:941:LEU:HD23	1.96	0.46
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.97	0.46
1:B:497:ILE:HG13	1:B:498:TYR:CD1	2.50	0.46
1:A:569:LYS:HB3	1:A:570:LEU:HD22	1.98	0.46
1:A:699:CYS:HA	1:A:700:PRO:HD3	1.82	0.46
1:A:869:PHE:CE2	1:A:969:ILE:HG21	2.50	0.46
1:A:239:VAL:HB	1:A:240:PRO:HD3	1.97	0.46
1:A:688:ASN:HB3	1:A:759:GLU:O	2.16	0.46
1:B:630:LYS:C	1:B:632:GLU:H	2.24	0.46
1:B:723:ALA:CB	1:B:735:LYS:HG2	2.46	0.46
1:B:121:LEU:C	1:B:121:LEU:HD23	2.41	0.45
1:A:1077:ARG:HG2	1:A:1130:ALA:O	2.16	0.45
1:A:808:PHE:N	1:A:808:PHE:CD2	2.85	0.45
1:A:976:HIS:CD2	1:B:1003:LYS:HZ2	2.34	0.45
1:A:1171:ILE:HD12	1:B:1161:LYS:HD3	1.98	0.45
1:B:140:MET:HE3	1:B:168:MET:CE	2.46	0.45
1:B:688:ASN:HB3	1:B:759:GLU:O	2.17	0.45
1:B:996:ASN:ND2	3:B:3236:TPP:S1	2.90	0.45
1:A:121:LEU:HD23	1:A:122:SER:N	2.31	0.45
1:A:369:GLU:OE1	1:A:480:LEU:HG	2.17	0.45
1:A:59:ARG:HG2	1:B:881:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ALA:O	1:A:591:TYR:C	2.60	0.45
1:A:32:PRO:HB2	1:A:178:HIS:CE1	2.51	0.45
1:A:163:SER:O	1:A:164:ASN:HB2	2.17	0.45
1:B:27:ILE:HD12	1:B:1013:PHE:CE2	2.51	0.45
1:B:522:MET:SD	1:B:526:LEU:HG	2.57	0.45
1:A:456:ASP:OD1	1:A:463:ILE:HG22	2.17	0.45
1:A:431:VAL:CG2	1:A:464:THR:HG21	2.46	0.45
1:A:42:ASP:O	1:A:46:GLN:HG3	2.17	0.45
1:A:426:GLY:O	1:A:427:ALA:HB3	2.16	0.45
1:B:27:ILE:CD1	1:B:1013:PHE:CE2	3.00	0.45
1:B:644:LYS:HB3	1:B:645:PRO:HD3	1.99	0.45
1:A:3:LYS:O	1:A:4:LYS:HB2	2.17	0.44
1:B:691:GLN:NE2	1:B:727:LYS:HG2	2.32	0.44
1:B:897:ALA:CA	1:B:941:LEU:HD23	2.47	0.44
1:A:709:ALA:HB2	1:A:784:ILE:HG21	1.98	0.44
1:B:110:HIS:CE1	1:B:157:HIS:NE2	2.79	0.44
1:A:602:ASN:O	1:A:606:VAL:HG23	2.18	0.44
1:A:1124:VAL:HG13	1:A:1125:GLU:N	2.33	0.44
1:A:110:HIS:CD2	1:A:169:HIS:CD2	2.92	0.44
1:A:544:ILE:HD12	1:A:613:LEU:CD2	2.47	0.44
1:A:561:MET:HE3	1:A:561:MET:O	2.18	0.44
1:B:1082:LYS:O	1:B:1086:VAL:HG23	2.18	0.44
1:B:1027:ARG:HA	1:B:1030:MET:HE3	2.00	0.44
1:A:180:ILE:O	1:A:450:GLN:HA	2.18	0.44
1:A:841:SER:HA	1:A:844:TRP:CE2	2.53	0.44
1:A:594:LYS:HB3	1:A:598:ILE:CD1	2.43	0.43
1:B:29:PRO:O	3:B:3236:TPP:HM43	2.18	0.43
1:A:68:ALA:HB2	1:A:93:MET:HG2	2.01	0.43
1:A:759:GLU:CD	1:A:759:GLU:N	2.76	0.43
1:B:246:TYR:O	1:B:250:VAL:HG23	2.18	0.43
1:B:1147:ARG:HG3	1:B:1147:ARG:HH11	1.84	0.43
1:A:698:VAL:HG13	1:A:1084:GLN:NE2	2.32	0.43
1:A:712:GLU:O	1:A:715:VAL:HG23	2.19	0.43
1:B:671:GLN:NE2	1:B:854:LYS:HD2	2.33	0.43
1:B:690:ILE:HG12	2:B:3233:SF4:S2	2.58	0.43
1:A:591:TYR:C	1:A:593:LYS:N	2.75	0.43
1:B:754:ILE:HD13	1:B:1084:GLN:HB2	1.99	0.43
1:B:1230:THR:O	1:B:1231:LYS:C	2.62	0.43
1:A:20:ALA:HB2	1:A:188:TYR:CZ	2.54	0.43
1:A:114:ARG:NE	1:A:123:ILE:HA	2.33	0.43
1:A:673:GLU:O	1:A:674:LYS:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:TYR:HA	1:A:497:ILE:CG1	2.49	0.43
1:A:873:ALA:HA	1:A:959:ILE:HD13	2.01	0.43
1:A:1160:PHE:O	1:A:1164:GLU:HG3	2.18	0.43
1:A:1181:LYS:HB2	1:A:1181:LYS:HZ3	1.83	0.43
1:B:720:ASN:C	1:B:720:ASN:HD22	2.25	0.43
1:B:936:GLY:O	1:B:938:LYS:HG2	2.19	0.43
1:B:596:GLU:H	1:B:596:GLU:CD	2.27	0.43
1:B:753:ASP:OD2	1:B:1085:ASP:OD2	2.37	0.43
1:B:964:GLY:HA2	1:B:994:TYR:HE1	1.84	0.43
1:B:200:LEU:O	1:B:204:ARG:HG2	2.19	0.42
1:A:87:SER:HA	1:A:129:ASP:HB3	2.00	0.42
1:A:184:GLU:HG2	7:A:2079:HOH:O	2.18	0.42
1:A:1102:ASP:CG	1:A:1104:ARG:HE	2.26	0.42
1:B:1012:LYS:O	1:B:1013:PHE:HB2	2.20	0.42
1:A:698:VAL:O	1:A:698:VAL:HG12	2.19	0.42
1:A:754:ILE:C	1:A:754:ILE:HD12	2.45	0.42
1:B:87:SER:HA	1:B:129:ASP:HB3	2.01	0.42
1:A:135:GLN:H	1:A:135:GLN:CD	2.28	0.42
1:A:317:LEU:HD11	7:A:2186:HOH:O	2.19	0.42
1:A:494:TYR:HA	1:A:497:ILE:HG12	2.02	0.42
1:A:561:MET:HE3	1:A:564:GLN:HB3	2.02	0.42
1:B:562:ILE:HD12	1:B:562:ILE:N	2.35	0.42
1:A:1156:LEU:HD12	1:A:1156:LEU:C	2.45	0.42
1:B:673:GLU:O	1:B:674:LYS:C	2.62	0.42
1:B:758:LYS:HE3	1:B:758:LYS:HB2	1.89	0.42
1:A:714:LEU:HD12	1:A:714:LEU:N	2.35	0.42
1:A:221:ASN:HB3	1:A:222:PRO:HD2	2.01	0.41
1:A:144:SER:O	1:A:278:SER:HA	2.20	0.41
1:A:317:LEU:HD13	1:A:317:LEU:C	2.44	0.41
1:A:467:HIS:C	1:A:468:LEU:HD23	2.45	0.41
1:A:483:ARG:HH11	1:A:483:ARG:HG2	1.85	0.41
1:B:20:ALA:HB2	1:B:188:TYR:CE1	2.55	0.41
1:B:1026:ALA:O	1:B:1030:MET:HG3	2.20	0.41
1:B:146:VAL:HG12	1:B:183:ILE:HD13	2.02	0.41
1:B:754:ILE:HG12	7:B:2592:HOH:O	2.20	0.41
1:B:896:LYS:HB3	1:B:941:LEU:HD21	2.02	0.41
1:A:266:ALA:HA	1:A:267:PRO:HD3	1.90	0.41
1:A:976:HIS:HE1	1:B:60:GLU:O	2.04	0.41
1:B:212:HIS:HD2	7:B:2104:HOH:O	2.04	0.41
1:A:1185:SER:HB3	1:B:45:ALA:HB3	2.03	0.41
1:B:87:SER:OG	1:B:88:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:VAL:O	1:A:247:MET:HG3	2.21	0.41
1:A:576:PHE:CD1	1:A:576:PHE:C	2.98	0.41
1:A:1193:GLU:OE2	1:A:1193:GLU:N	2.54	0.41
1:A:553:VAL:O	1:A:601:MET:HE2	2.21	0.41
1:A:642:VAL:O	1:A:646:ILE:HG13	2.21	0.41
1:B:113:ALA:HB1	1:B:126:ASP:O	2.20	0.41
1:B:581:ASP:OD2	1:B:585:LYS:HE3	2.20	0.41
1:A:290:LEU:HB2	1:A:297:ILE:HD11	2.03	0.41
1:B:418:ILE:HD12	1:B:573:VAL:HA	2.03	0.41
1:A:491:ASN:HA	1:A:492:PRO:HD2	1.96	0.40
1:B:1176:ALA:HB1	1:B:1177:PRO:CD	2.43	0.40
1:B:4:LYS:HE2	1:B:5:MET:N	2.36	0.40
1:B:598:ILE:HD13	1:B:601:MET:CE	2.52	0.40
1:B:731:LEU:O	1:B:732:LYS:C	2.64	0.40
1:A:554:GLY:C	1:A:556:GLY:H	2.29	0.40
1:A:796:LEU:HD23	1:A:796:LEU:C	2.46	0.40
1:B:992:GLU:O	1:B:993:VAL:CG1	2.69	0.40
1:B:1151:GLN:O	1:B:1155:GLU:HG3	2.21	0.40
1:B:130:ILE:HB	1:B:168:MET:CE	2.51	0.40
1:B:720:ASN:H	1:B:720:ASN:ND2	2.20	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%)	1174 (96%)	51 (4%)	4 (0%)	36	22
1	B	1229/1231 (100%)	1191 (97%)	33 (3%)	5 (0%)	30	16
All	All	2458/2462 (100%)	2365 (96%)	84 (3%)	9 (0%)	30	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1231	LYS
1	A	760	LYS
1	A	613	LEU
1	B	591	TYR
1	B	1178	ALA
1	A	4	LYS
1	B	732	LYS
1	A	1179	GLY
1	B	1177	PRO

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%)	963 (98%)	15 (2%)	57	41
1	B	978/978 (100%)	965 (99%)	13 (1%)	61	46
All	All	1956/1956 (100%)	1928 (99%)	28 (1%)	59	44

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	194	LEU
1	A	351	ARG
1	A	463	ILE
1	A	570	LEU
1	A	632	GLU
1	A	759	GLU
1	A	778	LEU
1	A	808	PHE
1	A	836	ASN
1	A	849	PRO
1	A	880	ASN
1	A	893	LEU
1	A	1000	GLN
1	A	1232	LYS

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Mol	Chain	Res	Type
1	B	4	LYS
1	B	194	LEU
1	B	317	LEU
1	B	463	ILE
1	B	720	ASN
1	B	754	ILE
1	B	808	PHE
1	B	849	PRO
1	B	996	ASN
1	B	1000	GLN
1	B	1115	LEU
1	B	1171	ILE
1	B	1232	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	96	ASN
1	A	110	HIS
1	A	157	HIS
1	A	164	ASN
1	A	169	HIS
1	A	197	GLN
1	A	212	HIS
1	A	389	HIS
1	A	421	GLN
1	A	434	ASN
1	A	467	HIS
1	A	476	GLN
1	A	536	ASN
1	A	543	ASN
1	A	608	GLN
1	A	641	ASN
1	A	649	GLN
1	A	683	GLN
1	A	688	ASN
1	A	739	GLN
1	A	765	GLN
1	A	976	HIS
1	A	1000	GLN
1	A	1073	ASN

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Mol	Chain	Res	Type
1	A	1084	GLN
1	A	1108	GLN
1	A	1165	HIS
1	A	1170	ASN
1	B	46	GLN
1	B	96	ASN
1	B	110	HIS
1	B	135	GLN
1	B	164	ASN
1	B	169	HIS
1	B	197	GLN
1	B	212	HIS
1	B	220	GLN
1	B	221	ASN
1	B	434	ASN
1	B	602	ASN
1	B	671	GLN
1	B	683	GLN
1	B	688	ASN
1	B	720	ASN
1	B	996	ASN
1	B	1000	GLN
1	B	1073	ASN
1	B	1088	ASN
1	B	1108	GLN

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, 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	3234	1	0,12,12	-	-	-		
2	SF4	A	3233	1	0,12,12	-	-	-		
2	SF4	A	3235	1	0,12,12	-	-	-		
4	PYR	A	3237	-	5,5,5	1.14	0	3,6,6	2.11	1 (33%)
4	PYR	B	3237	-	5,5,5	1.13	0	3,6,6	2.06	1 (33%)
2	SF4	B	3234	1	0,12,12	-	-	-		
3	TPP	A	3236	5	25,27,27	2.53	10 (40%)	37,40,40	1.49	8 (21%)
3	TPP	B	3236	5	25,27,27	2.54	9 (36%)	37,40,40	1.69	9 (24%)
2	SF4	B	3233	1	0,12,12	-	-	-		
2	SF4	B	3235	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
2	SF4	A	3234	1	-	-	0/6/5/5
2	SF4	A	3233	1	-	-	0/6/5/5
2	SF4	A	3235	1	-	-	0/6/5/5
4	PYR	A	3237	-	-	0/4/4/4	-
4	PYR	B	3237	-	-	0/4/4/4	-
2	SF4	B	3234	1	-	-	0/6/5/5
3	TPP	A	3236	5	-	6/17/17/17	0/2/2/2
3	TPP	B	3236	5	-	6/17/17/17	0/2/2/2
2	SF4	B	3233	1	-	-	0/6/5/5
2	SF4	B	3235	1	-	-	0/6/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3236	TPP	C5'-C4'	6.70	1.54	1.42
3	B	3236	TPP	C4'-N3'	5.59	1.43	1.35
3	B	3236	TPP	C2'-N1'	5.04	1.42	1.34
3	A	3236	TPP	C5'-C4'	4.89	1.51	1.42
3	A	3236	TPP	C4-N3	4.85	1.50	1.39
3	A	3236	TPP	C2'-N1'	4.22	1.41	1.34
3	A	3236	TPP	C6'-C5'	4.17	1.46	1.37
3	B	3236	TPP	C2'-N3'	3.85	1.40	1.34
3	A	3236	TPP	C6'-N1'	3.79	1.42	1.34
3	A	3236	TPP	C2'-N3'	3.74	1.40	1.34
3	A	3236	TPP	C4'-N3'	3.68	1.40	1.35
3	B	3236	TPP	C4-N3	3.42	1.47	1.39
3	A	3236	TPP	C6-C5	2.55	1.55	1.50
3	A	3236	TPP	C7'-C5'	-2.29	1.46	1.51
3	B	3236	TPP	O7-C7	-2.29	1.35	1.44
3	B	3236	TPP	C6'-C5'	2.22	1.42	1.37
3	A	3236	TPP	PA-O7	-2.18	1.50	1.59
3	B	3236	TPP	C6-C5	2.03	1.54	1.50
3	B	3236	TPP	PB-O3B	-2.03	1.47	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	3236	TPP	C6'-N1'-C2'	4.47	123.56	115.96
4	A	3237	PYR	OXT-C-CA	3.38	123.22	113.97
4	B	3237	PYR	OXT-C-CA	3.32	123.06	113.97
3	B	3236	TPP	CM2-C2'-N3'	3.31	122.32	117.15
3	A	3236	TPP	N4'-C4'-N3'	-2.96	112.84	117.03
3	B	3236	TPP	N1'-C2'-N3'	-2.88	120.58	125.54
3	B	3236	TPP	CM4-C4-N3	2.75	127.10	120.52
3	B	3236	TPP	C4-C5-S1	2.73	115.01	110.56
3	B	3236	TPP	C5-C4-N3	-2.59	106.78	111.69
3	A	3236	TPP	N1'-C2'-N3'	-2.56	121.14	125.54
3	A	3236	TPP	C6'-N1'-C2'	2.48	120.18	115.96
3	A	3236	TPP	C4-C5-S1	2.42	114.50	110.56
3	A	3236	TPP	CM2-C2'-N1'	2.38	119.75	117.14
3	B	3236	TPP	O2B-PB-O3A	-2.32	96.84	104.64
3	A	3236	TPP	C5-C4-N3	-2.27	107.39	111.69
3	A	3236	TPP	CM4-C4-N3	2.16	125.69	120.52
3	B	3236	TPP	C6-C5-S1	-2.05	115.96	120.89
3	A	3236	TPP	C6'-C5'-C4'	-2.03	112.96	115.72
3	B	3236	TPP	O3B-PB-O2B	2.00	115.29	107.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

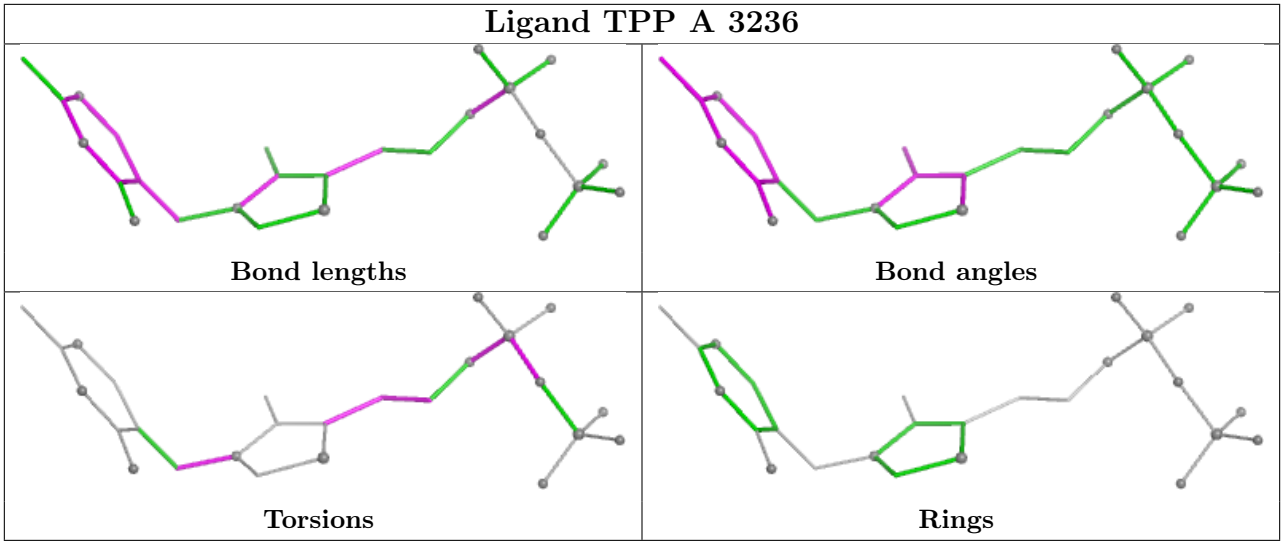
Mol	Chain	Res	Type	Atoms
3	B	3236	TPP	S1-C5-C6-C7
3	A	3236	TPP	PB-O3A-PA-O7
3	B	3236	TPP	PB-O3A-PA-O7
3	B	3236	TPP	C4-C5-C6-C7
3	B	3236	TPP	C5'-C7'-N3-C2
3	A	3236	TPP	S1-C5-C6-C7
3	A	3236	TPP	C4-C5-C6-C7
3	B	3236	TPP	C5'-C7'-N3-C4
3	A	3236	TPP	C5-C6-C7-O7
3	A	3236	TPP	C5'-C7'-N3-C2
3	A	3236	TPP	C7-O7-PA-O1A
3	B	3236	TPP	C7-O7-PA-O1A

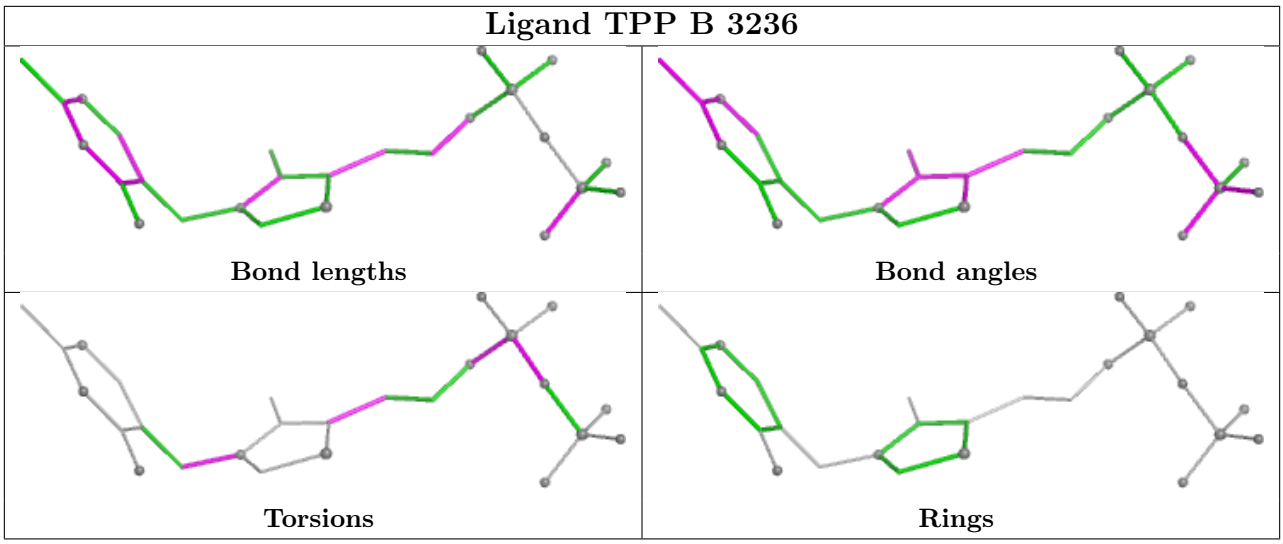
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3236	TPP	2	0
2	B	3233	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.





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%)	0.50	152 (12%)	8	9	9, 23, 64, 106	0
1	B	1231/1231 (100%)	0.19	78 (6%)	26	31	10, 19, 48, 96	0
All	All	2462/2462 (100%)	0.35	230 (9%)	14	16	9, 21, 58, 106	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1175	PHE	7.6
1	B	1175	PHE	7.6
1	B	1180	GLY	7.5
1	B	1176	ALA	7.3
1	B	1177	PRO	7.3
1	B	1178	ALA	7.2
1	A	1179	GLY	6.8
1	A	1182	ALA	6.7
1	B	590	ALA	6.7
1	B	591	TYR	6.4
1	B	1179	GLY	6.3
1	A	1178	ALA	6.1
1	B	631	ALA	6.0
1	B	629	THR	5.8
1	B	1182	ALA	5.8
1	A	580	VAL	5.7
1	A	1172	PHE	5.7
1	A	2	GLY	5.5
1	A	1180	GLY	5.3
1	A	1181	LYS	5.3
1	A	595	GLY	5.2
1	B	630	LYS	5.2
1	B	1171	ILE	5.1
1	B	1172	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	598	ILE	5.1
1	B	1174	SER	5.0
1	B	592	GLY	4.9
1	B	1165	HIS	4.9
1	A	633	PRO	4.8
1	A	1174	SER	4.8
1	B	2	GLY	4.8
1	B	1173	GLU	4.8
1	A	1165	HIS	4.8
1	A	587	ILE	4.7
1	B	633	PRO	4.7
1	A	576	PHE	4.7
1	B	589	LYS	4.7
1	A	1176	ALA	4.7
1	A	582	LEU	4.7
1	A	553	VAL	4.6
1	B	715	VAL	4.6
1	B	732	LYS	4.6
1	A	1171	ILE	4.6
1	A	631	ALA	4.6
1	B	627	ALA	4.6
1	A	591	TYR	4.4
1	B	595	GLY	4.3
1	A	1177	PRO	4.3
1	A	616	PHE	4.3
1	A	636	ASN	4.2
1	B	1230	THR	4.2
1	A	627	ALA	4.2
1	A	1173	GLU	4.2
1	A	592	GLY	4.2
1	B	4	LYS	4.1
1	A	593	LYS	4.1
1	B	593	LYS	4.0
1	A	590	ALA	4.0
1	B	3	LYS	4.0
1	A	3	LYS	3.9
1	A	1230	THR	3.9
1	A	594	LYS	3.9
1	B	1181	LYS	3.9
1	A	783	ARG	3.9
1	B	597	LYS	3.9
1	B	1231	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	714	LEU	3.8
1	A	629	THR	3.8
1	A	597	LYS	3.8
1	A	719	ALA	3.8
1	A	630	LYS	3.7
1	B	594	LYS	3.7
1	A	618	TYR	3.7
1	A	574	LEU	3.6
1	A	575	PRO	3.6
1	A	583	LEU	3.6
1	A	622	TRP	3.6
1	B	628	GLU	3.6
1	A	497	ILE	3.6
1	B	754	ILE	3.6
1	A	524	LYS	3.6
1	A	573	VAL	3.6
1	A	599	VAL	3.6
1	B	632	GLU	3.6
1	B	596	GLU	3.5
1	A	530	ILE	3.5
1	A	625	ALA	3.5
1	A	426	GLY	3.4
1	A	588	HIS	3.4
1	A	731	LEU	3.4
1	A	1231	LYS	3.4
1	B	598	ILE	3.4
1	A	555	LEU	3.4
1	A	626	PRO	3.3
1	B	1228	LYS	3.3
1	A	790	VAL	3.3
1	A	715	VAL	3.2
1	A	1170	ASN	3.2
1	A	685	VAL	3.2
1	A	716	GLY	3.2
1	A	542	TYR	3.1
1	A	552	ASP	3.1
1	A	620	ASP	3.1
1	A	723	ALA	3.1
1	A	1232	LYS	3.1
1	B	587	ILE	3.1
1	A	526	LEU	3.1
1	A	579	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	732	LYS	3.0
1	A	758	LYS	3.0
1	B	714	LEU	3.0
1	B	1221	GLU	3.0
1	A	635	THR	3.0
1	A	768	ASP	3.0
1	B	1232	LYS	3.0
1	A	554	GLY	3.0
1	A	759	GLU	3.0
1	B	733	GLY	3.0
1	A	603	THR	2.9
1	A	596	GLU	2.9
1	B	941	LEU	2.9
1	A	577	GLU	2.9
1	A	628	GLU	2.9
1	A	605	ALA	2.9
1	A	519	LEU	2.9
1	A	5	MET	2.9
1	A	634	MET	2.9
1	A	717	ALA	2.8
1	A	623	LYS	2.8
1	A	495	VAL	2.8
1	A	613	LEU	2.8
1	A	632	GLU	2.8
1	A	937	GLN	2.8
1	B	634	MET	2.8
1	B	625	ALA	2.7
1	A	736	PHE	2.7
1	A	1183	ASP	2.7
1	A	536	ASN	2.7
1	A	408	ALA	2.7
1	A	1168	ALA	2.7
1	A	516	TRP	2.7
1	B	857	ARG	2.7
1	A	584	LYS	2.7
1	A	729	LYS	2.7
1	A	496	GLY	2.6
1	A	609	ALA	2.6
1	A	523	ASP	2.6
1	B	497	ILE	2.6
1	A	586	SER	2.6
1	B	354	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	525	HIS	2.5
1	B	783	ARG	2.5
1	B	5	MET	2.5
1	A	606	VAL	2.5
1	A	619	PRO	2.5
1	A	718	PRO	2.5
1	B	790	VAL	2.5
1	A	938	LYS	2.5
1	B	735	LYS	2.5
1	A	624	ASP	2.5
1	A	578	LYS	2.5
1	A	1169	THR	2.5
1	A	621	SER	2.5
1	A	600	LYS	2.4
1	B	731	LEU	2.4
1	B	779	GLU	2.4
1	B	716	GLY	2.4
1	B	1077	ARG	2.4
1	B	624	ASP	2.4
1	A	439	LYS	2.4
1	B	1190	GLU	2.4
1	A	317	LEU	2.4
1	A	541	PHE	2.4
1	B	1170	ASN	2.4
1	A	939	ASP	2.4
1	B	588	HIS	2.4
1	A	572	GLY	2.4
1	B	718	PRO	2.4
1	B	1227	SER	2.4
1	A	581	ASP	2.4
1	A	4	LYS	2.4
1	B	626	PRO	2.3
1	B	443	ASP	2.3
1	A	556	GLY	2.3
1	A	734	TYR	2.3
1	B	353	GLU	2.3
1	A	558	ARG	2.3
1	B	1229	ARG	2.3
1	A	551	THR	2.2
1	A	725	GLU	2.2
1	A	709	ALA	2.2
1	A	608	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	786	VAL	2.2
1	A	724	LEU	2.2
1	A	416	GLY	2.2
1	A	529	GLY	2.2
1	A	520	GLU	2.2
1	A	726	ALA	2.2
1	A	503	GLY	2.2
1	B	708	LEU	2.2
1	A	727	LYS	2.2
1	A	6	MET	2.1
1	B	599	VAL	2.1
1	B	717	ALA	2.1
1	B	782	ALA	2.1
1	B	1184	GLY	2.1
1	A	538	LYS	2.1
1	A	527	PRO	2.1
1	A	547	VAL	2.1
1	B	729	LYS	2.1
1	B	1141	PHE	2.1
1	A	544	ILE	2.1
1	A	679	ILE	2.1
1	A	1107	ALA	2.1
1	A	617	LYS	2.1
1	A	498	TYR	2.1
1	A	549	ILE	2.1
1	B	728	GLY	2.0
1	A	1126	GLU	2.0
1	A	601	MET	2.0
1	A	521	ASP	2.0
1	A	570	LEU	2.0
1	A	515	PRO	2.0
1	A	585	LYS	2.0
1	A	720	ASN	2.0
1	B	503	GLY	2.0
1	A	500	ILE	2.0
1	A	1077	ARG	2.0
1	A	566	ALA	2.0
1	A	518	SER	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)

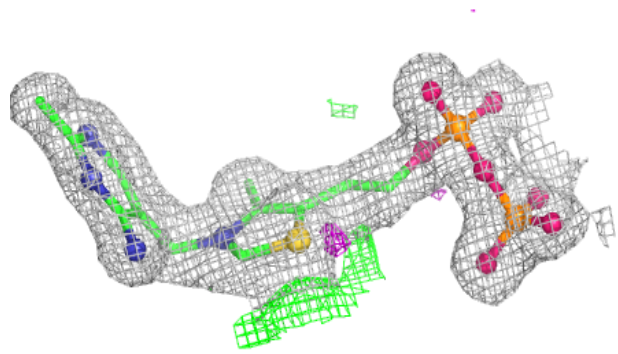
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

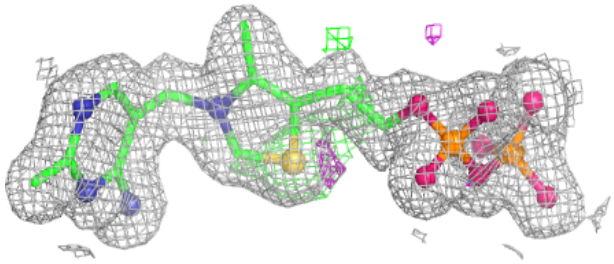
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PYR	B	3237	6/6	0.93	0.11	16,19,24,26	0
4	PYR	A	3237	6/6	0.94	0.10	21,25,28,29	0
2	SF4	A	3233	8/8	0.96	0.06	27,30,32,33	0
2	SF4	B	3233	8/8	0.96	0.06	20,23,25,26	0
3	TPP	A	3236	26/26	0.97	0.06	12,15,27,34	0
3	TPP	B	3236	26/26	0.98	0.06	7,13,24,30	0
2	SF4	B	3234	8/8	0.98	0.04	16,17,19,19	0
2	SF4	A	3234	8/8	0.98	0.04	23,24,24,25	0
6	CA	B	3239	1/1	0.98	0.20	44,44,44,44	0
2	SF4	B	3235	8/8	0.99	0.03	12,13,14,15	0
5	MG	A	3238	1/1	0.99	0.03	12,12,12,12	0
5	MG	B	3238	1/1	0.99	0.03	9,9,9,9	0
6	CA	A	3239	1/1	0.99	0.21	40,40,40,40	0
2	SF4	A	3235	8/8	0.99	0.02	16,18,18,18	0

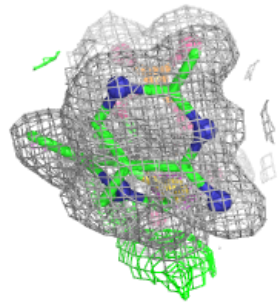
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 3236:

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

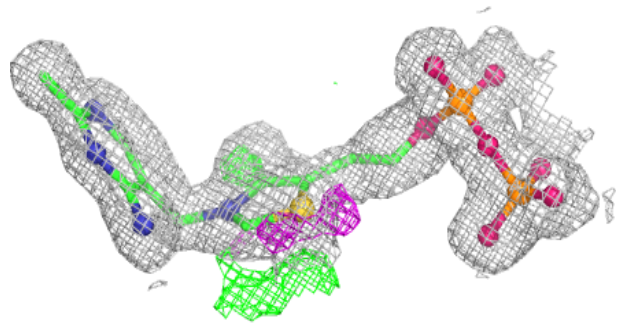


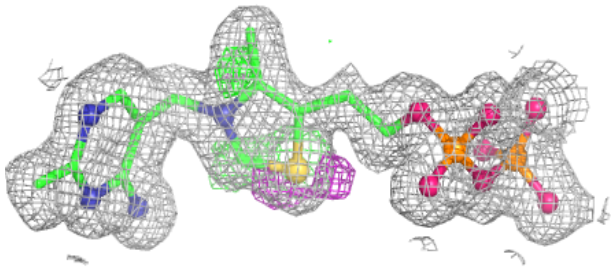


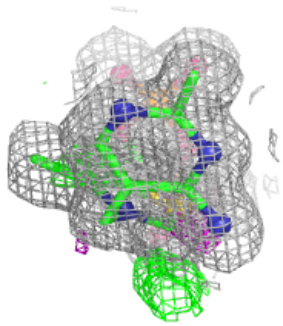


Electron density around TPP B 3236:

$2mF_o$-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.