



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:27 am BST

PDB ID : 2C42
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

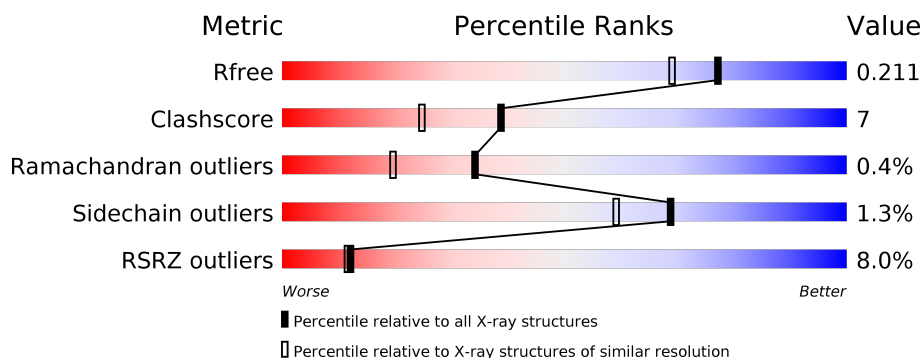
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1231	<div> <div>11%</div> <div> <div></div> <div>82%</div> <div>17%</div> </div> </div>
1	B	1231	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>13%</div> </div> </div>

2 Entry composition [i](#)

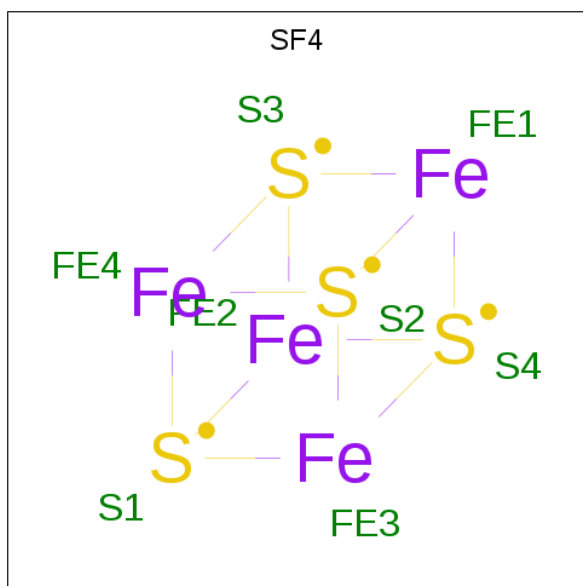
There are 7 unique types of molecules in this entry. The entry contains 20099 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



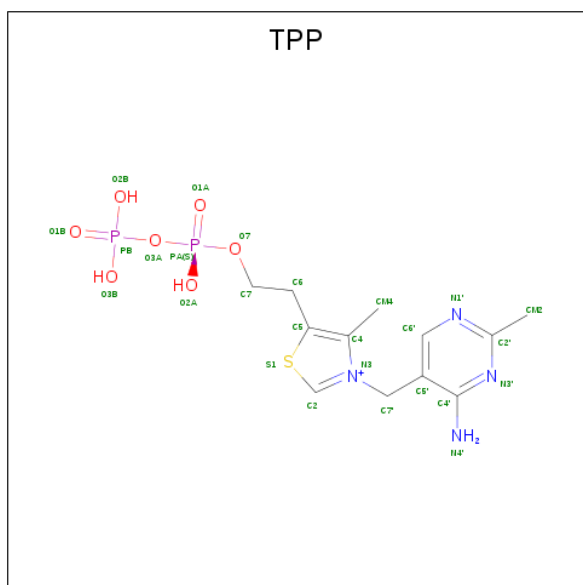
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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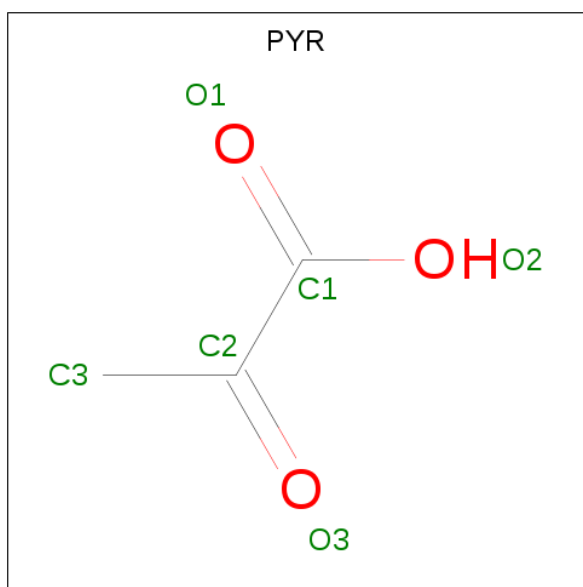
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0

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



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

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

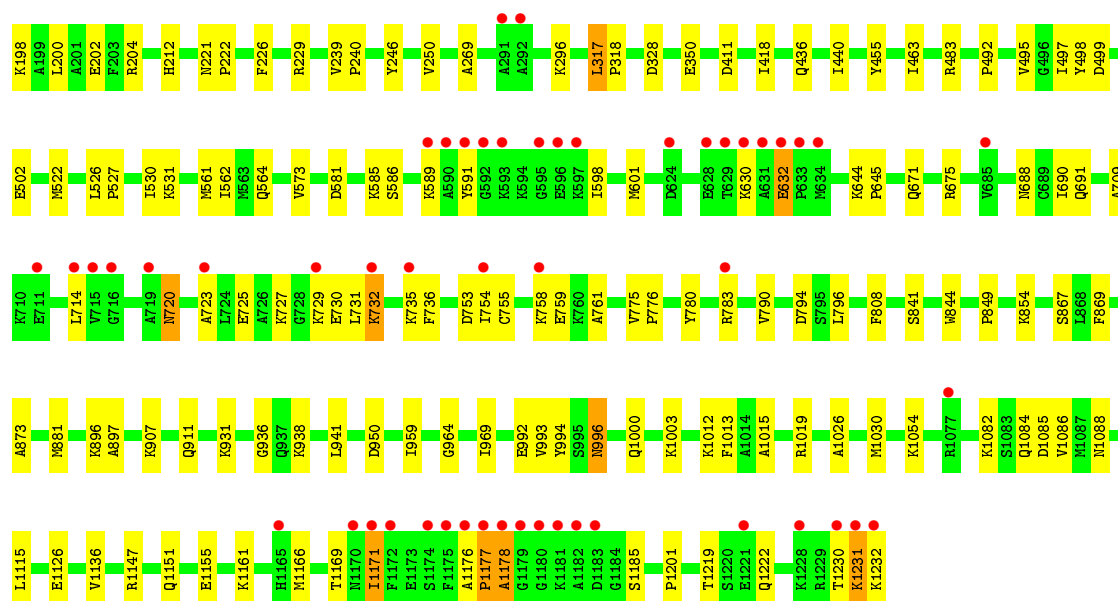
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	550	Total	O	0	0
			550	550		

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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.78Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.219 0.186 , 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)	0.35 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.30	0/9585	0.58	1/12954 (0.0%)
1	B	0.31	0/9585	0.59	1/12954 (0.0%)
All	All	0.31	0/19170	0.59	2/25908 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	GLY	N-CA-C	5.62	127.16	113.10
1	A	125	GLY	N-CA-C	5.49	126.83	113.10

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	169	0
1	B	9383	0	9262	134	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	1	0
4	A	6	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	3	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	18562	280	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 7.

All (280) 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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:110:HIS:HE1	1:B:157:HIS:NE2	1.95	0.65
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:561:MET:HE1	1:B:564:GLN:HG2	1.83	0.61
1:B:1219:THR:OG1	1:B:1222:GLN:HG3	2.01	0.61
1:B:527:PRO:HD2	1:B:530:ILE:HD12	1.81	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: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:526:LEU:O	1:A:531:LYS:HE3	2.01	0.59
1:A:465:ILE:HD11	1:A:649:GLN:NE2	2.17	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:HD22	1:A:570:LEU:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:B:727:LYS:HE2	1.88	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:759:GLU:H	1:A:759:GLU:CD	2.08	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:1115:LEU:HD21	1:A:1160:PHE:CZ	2.42	0.54
1:A:27:ILE:H	1:A:27:ILE:HD13	1.72	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: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: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:1132:ASN:O	1:A:1136:VAL:HG12	2.10	0.52
1:A:562:ILE:HD12	1:A:562:ILE:N	2.25	0.52
1:A:465:ILE:HD11	1:A:649:GLN:HE22	1.73	0.52
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:841:SER:HA	1:B:844:TRP:CE2	2.45	0.51
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:B:731:LEU:CD2	1:B:790:VAL:HG11	2.41	0.51
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:561:MET:O	1:A:561:MET:HE2	2.12	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:741:ASN:CG	1:A:778:LEU:HD11	2.33	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:269:ALA:HA	1:B:296:LYS:HB3	1.95	0.49
1:A:1181:LYS:HZ2	1:A:1181:LYS:HB2	1.76	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: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:HZ2	1:A:1232:LYS:HB3	1.79	0.48
1:A:1180:GLY:O	1:A:1181:LYS:HB2	2.14	0.48
1:A:389:HIS:HD2	7:A:2059:HOH:O	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:NZ	1:A:1232:LYS:HB3	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:A:3:LYS:HZ3	1:A:254:THR:HA	1.80	0.47
1:B:730:GLU:OE1	1:B:730:GLU:N	2.47	0.47
1:B:436:GLN:O	1:B:440:ILE:HG13	2.15	0.47
1:B:221:ASN:HB3	1:B:222:PRO:CD	2.45	0.46
1:B:4:LYS:HE2	1:B:4:LYS:HA	1.97	0.46
1:A:212:HIS:HE1	1:B:950:ASP:OD2	1.97	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:121:LEU:C	1:A:121:LEU:HD23	2.34	0.46
1:A:246:TYR:O	1:A:250:VAL:HG23	2.15	0.46
1:A:937:GLN:C	1:A:938:LYS:HD2	2.36	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:723:ALA:CB	1:B:735:LYS:HG2	2.46	0.46
1:A:1077:ARG:HG2	1:A:1130:ALA:O	2.16	0.45
1:A:808:PHE:CD2	1:A:808:PHE:N	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:688:ASN:HB3	1:B:759:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:163:SER:O	1:A:164:ASN:HB2	2.17	0.45
1:A:32:PRO:HB2	1:A:178:HIS:CE1	2.51	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:426:GLY:O	1:A:427:ALA:HB3	2.16	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: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:1124:VAL:HG13	1:A:1125:GLU:N	2.33	0.44
1:A:602:ASN:O	1:A:606:VAL:HG23	2.18	0.44
1:A:881:MET:HE1	1:B:24:VAL:HG13	1.99	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:B:1082:LYS:O	1:B:1086:VAL:HG23	2.18	0.44
1:B:796:LEU:HD23	1:B:796:LEU:C	2.37	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:A:68:ALA:HB2	1:A:93:MET:HG2	2.01	0.43
1:B:1147:ARG:HG3	1:B:1147:ARG:HH11	1.84	0.43
1:B:130:ILE:HB	1:B:168:MET:HE1	1.99	0.43
1:B:246:TYR:O	1:B:250:VAL:HG23	2.18	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:690:ILE:HG12	2:B:3233:SF4:S2	2.58	0.43
1:B:671:GLN:NE2	1:B:854:LYS:HD2	2.33	0.43
1:B:754:ILE:HD13	1:B:1084:GLN:HB2	1.99	0.43
1:A:114:ARG:NE	1:A:123:ILE:HA	2.33	0.43
1:A:20:ALA:HB2	1:A:188:TYR:CZ	2.54	0.43
1:A:306:ARG:HA	1:A:307:PRO:C	2.37	0.43
1:A:1160:PHE:O	1:A:1164:GLU:HG3	2.18	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:B:936:GLY:O	1:B:938:LYS:HG2	2.19	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:184:GLU:HG2	7:A:2079:HOH:O	2.18	0.42
1:A:87:SER:HA	1:A:129:ASP:HB3	2.00	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:B:87:SER:HA	1:B:129:ASP:HB3	2.01	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:B:562:ILE:HD12	1:B:562:ILE:N	2.35	0.42
1:B:758:LYS:HE3	1:B:758:LYS:HB2	1.89	0.42
1:A:714:LEU:N	1:A:714:LEU:HD12	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: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:24:VAL:HG13	1:B:881:MET:HE2	2.01	0.41
1:A:266:ALA:HA	1:A:267:PRO:HD3	1.90	0.41
1:B:212:HIS:HD2	7:B:2104:HOH:O	2.04	0.41
1:A:976:HIS:HE1	1:B:60:GLU: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
1:A:111:VAL:HG21	1:A:168:MET:HE2	2.02	0.41
1:A:1193:GLU:N	1:A:1193:GLU:OE2	2.54	0.41
1:A:243:VAL:O	1:A:247:MET:HG3	2.21	0.41
1:B:630:LYS:C	1:B:632:GLU:H	2.24	0.41
1:A:642:VAL:O	1:A:646:ILE:HG13	2.21	0.41
1:B:121:LEU:C	1:B:121:LEU:HD23	2.41	0.41
1:B:581:ASP:OD2	1:B:585:LYS:HE3	2.20	0.41
1:B:113:ALA:HB1	1:B:126:ASP:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:590:ALA:O	1:A:591:TYR:C	2.60	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

5.3.1 Protein backbone

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%)	41	25
1	B	1229/1231 (100%)	1191 (97%)	33 (3%)	5 (0%)	34	19
All	All	2458/2462 (100%)	2365 (96%)	84 (3%)	9 (0%)	34	19

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 ⓘ

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%)	966 (99%)	12 (1%)	71	62
1	B	978/978 (100%)	965 (99%)	13 (1%)	69	59
All	All	1956/1956 (100%)	1931 (99%)	25 (1%)	69	59

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	226	PHE
1	A	632	GLU
1	A	765	GLN
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	1170	ASN
1	B	4	LYS
1	B	226	PHE
1	B	317	LEU
1	B	328	ASP
1	B	632	GLU
1	B	720	ASN
1	B	808	PHE
1	B	849	PRO
1	B	996	ASN
1	B	1000	GLN
1	B	1088	ASN
1	B	1115	LEU
1	B	1171	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	110	HIS
1	A	157	HIS
1	A	169	HIS
1	A	212	HIS
1	A	389	HIS
1	A	421	GLN
1	A	434	ASN
1	A	467	HIS
1	A	536	ASN
1	A	543	ASN
1	A	636	ASN
1	A	683	GLN
1	A	688	ASN
1	A	739	GLN
1	A	765	GLN
1	A	777	ASN
1	A	937	GLN
1	A	976	HIS
1	A	1000	GLN
1	A	1108	GLN
1	A	1165	HIS
1	A	1170	ASN
1	B	46	GLN
1	B	54	GLN
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	434	ASN
1	B	683	GLN
1	B	688	ASN
1	B	720	ASN
1	B	836	ASN
1	B	866	ASN
1	B	996	ASN
1	B	1000	GLN
1	B	1088	ASN
1	B	1108	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SF4	B	3234	1	0,12,12	0.00	-	-		
2	SF4	B	3233	1	0,12,12	0.00	-	-		
2	SF4	A	3235	1	0,12,12	0.00	-	-		
4	PYR	B	3237	-	2,5,5	1.15	0	2,6,6	1.45	0
4	PYR	A	3237	-	2,5,5	1.18	0	2,6,6	1.45	0
2	SF4	A	3234	1	0,12,12	0.00	-	-		
2	SF4	B	3235	1	0,12,12	0.00	-	-		
2	SF4	A	3233	1	0,12,12	0.00	-	-		
3	TPP	A	3236	5	22,27,27	4.22	10 (45%)	29,40,40	1.54	8 (27%)
3	TPP	B	3236	5	22,27,27	3.64	9 (40%)	29,40,40	1.78	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	B	3234	1	-	-	0/6/5/5
2	SF4	B	3233	1	-	-	0/6/5/5
2	SF4	A	3235	1	-	-	0/6/5/5
4	PYR	B	3237	-	-	0/0/4/4	-
4	PYR	A	3237	-	-	0/0/4/4	-
2	SF4	A	3234	1	-	-	0/6/5/5
2	SF4	B	3235	1	-	-	0/6/5/5
2	SF4	A	3233	1	-	-	0/6/5/5
3	TPP	A	3236	5	-	3/16/17/17	0/2/2/2
3	TPP	B	3236	5	-	3/16/17/17	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3236	TPP	C4-N3	12.27	1.50	1.39
3	A	3236	TPP	C6-C5	10.80	1.55	1.50
3	B	3236	TPP	C4-N3	8.70	1.47	1.39
3	B	3236	TPP	C6-C5	8.54	1.54	1.50
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	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	O7-C7	-2.29	1.35	1.44
3	A	3236	TPP	C7'-C5'	-2.23	1.46	1.51
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	PB-O3B	-2.03	1.47	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3236	TPP	C6'-N1'-C2'	4.47	123.56	115.96
3	B	3236	TPP	CM4-C4-N3	3.58	127.10	122.53
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	A	3236	TPP	N1'-C2'-N3'	-2.56	121.14	125.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3236	TPP	C6'-N1'-C2'	2.48	120.18	115.96
3	A	3236	TPP	CM4-C4-N3	2.47	125.69	122.53
3	A	3236	TPP	C7'-N3-C2	-2.42	120.98	125.35
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	C6-C5-C4	2.16	129.17	127.43
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 (6) torsion outliers are listed below:

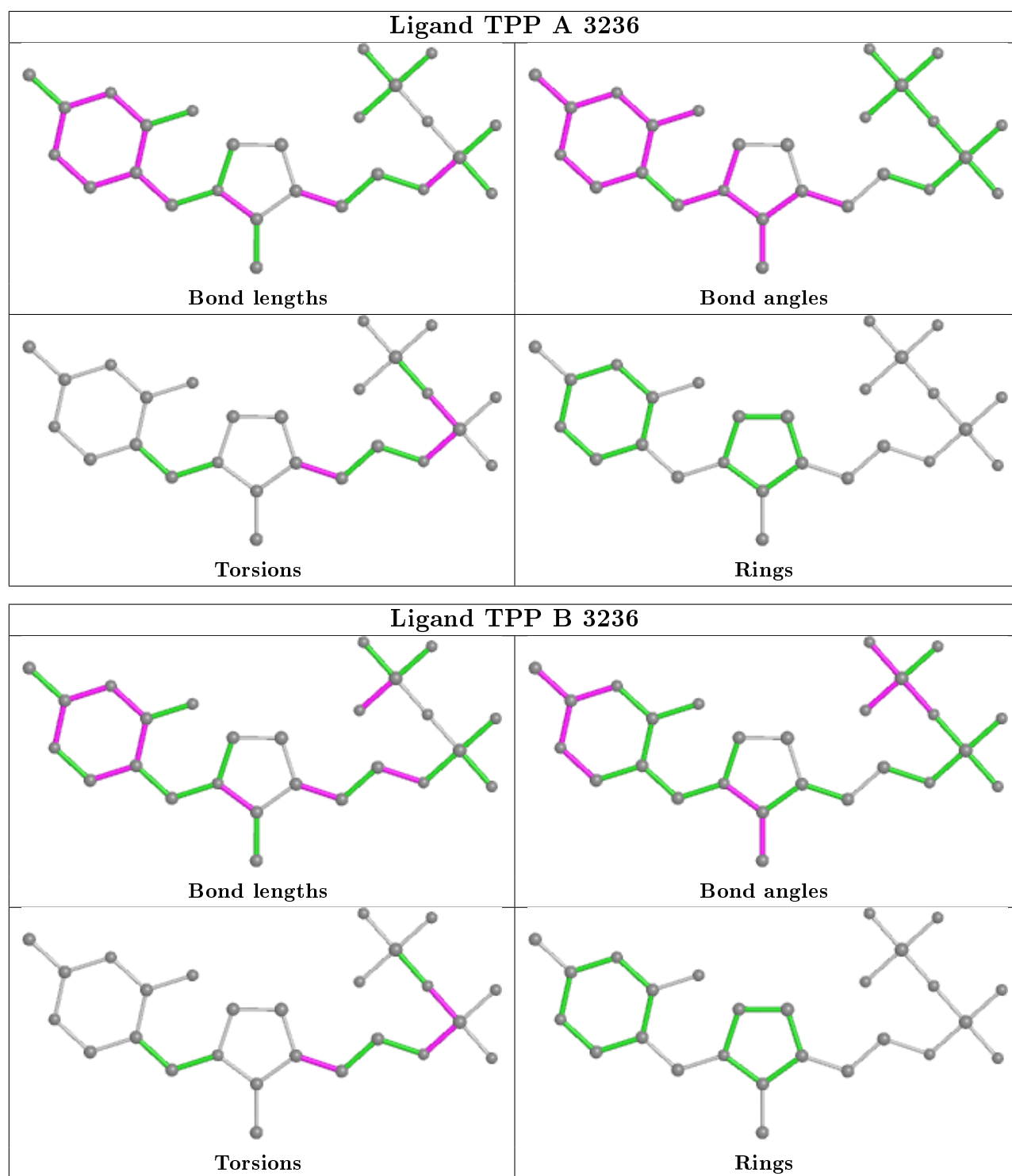
Mol	Chain	Res	Type	Atoms
3	A	3236	TPP	PB-O3A-PA-O7
3	B	3236	TPP	PB-O3A-PA-O7
3	A	3236	TPP	C4-C5-C6-C7
3	B	3236	TPP	C4-C5-C6-C7
3	A	3236	TPP	C7-O7-PA-O1A
3	B	3236	TPP	C7-O7-PA-O1A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3233	SF4	1	0
3	B	3236	TPP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1231/1231 (100%)	0.58	140 (11%) 5 4	9, 23, 64, 106	0
1	B	1231/1231 (100%)	0.27	58 (4%) 31 29	10, 19, 48, 96	0
All	All	2462/2462 (100%)	0.42	198 (8%) 12 11	9, 21, 58, 106	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	576	PHE	11.5
1	A	1182	ALA	9.5
1	A	594	LYS	8.9
1	A	591	TYR	8.4
1	A	630	LYS	8.3
1	B	631	ALA	7.8
1	A	629	THR	7.7
1	A	631	ALA	7.7
1	A	1232	LYS	7.3
1	B	1232	LYS	7.1
1	A	582	LEU	7.1
1	B	1177	PRO	7.1
1	A	593	LYS	7.1
1	A	1178	ALA	7.0
1	A	626	PRO	7.0
1	A	1179	GLY	6.5
1	B	2	GLY	6.5
1	A	1231	LYS	6.4
1	A	715	VAL	6.4
1	B	732	LYS	6.3
1	A	628	GLU	6.0
1	B	1176	ALA	6.0
1	B	1178	ALA	5.8
1	A	592	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	627	ALA	5.6
1	A	575	PRO	5.4
1	A	589	LYS	5.3
1	B	3	LYS	5.2
1	A	588	HIS	5.2
1	B	715	VAL	5.1
1	A	633	PRO	5.1
1	B	590	ALA	5.0
1	A	577	GLU	5.0
1	A	574	LEU	5.0
1	A	554	GLY	4.9
1	B	1175	PHE	4.8
1	B	630	LYS	4.8
1	A	621	SER	4.7
1	A	1175	PHE	4.7
1	B	592	GLY	4.6
1	A	597	LYS	4.6
1	A	1165	HIS	4.5
1	B	629	THR	4.5
1	B	628	GLU	4.5
1	A	625	ALA	4.5
1	A	595	GLY	4.4
1	A	518	SER	4.3
1	A	619	PRO	4.3
1	A	590	ALA	4.3
1	A	598	ILE	4.2
1	B	1171	ILE	4.2
1	A	1181	LYS	4.1
1	A	936	GLY	4.1
1	A	596	GLU	4.1
1	A	535	ALA	4.0
1	A	719	ALA	3.9
1	A	580	VAL	3.9
1	A	632	GLU	3.9
1	A	2	GLY	3.9
1	B	1231	LYS	3.8
1	B	632	GLU	3.8
1	A	585	LYS	3.7
1	A	714	LEU	3.7
1	A	599	VAL	3.7
1	A	520	GLU	3.6
1	A	1230	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1180	GLY	3.6
1	B	591	TYR	3.6
1	A	716	GLY	3.6
1	B	1228	LYS	3.6
1	A	519	LEU	3.6
1	A	634	MET	3.6
1	B	4	LYS	3.5
1	A	938	LYS	3.5
1	A	729	LYS	3.5
1	A	624	ASP	3.5
1	B	593	LYS	3.5
1	A	587	ILE	3.5
1	A	620	ASP	3.4
1	A	525	HIS	3.4
1	A	623	LYS	3.4
1	A	710	LYS	3.4
1	A	732	LYS	3.4
1	A	523	ASP	3.3
1	B	719	ALA	3.3
1	B	1165	HIS	3.3
1	A	613	LEU	3.3
1	A	524	LYS	3.3
1	A	547	VAL	3.3
1	A	553	VAL	3.2
1	A	611	THR	3.2
1	A	526	LEU	3.2
1	B	1174	SER	3.2
1	A	3	LYS	3.2
1	A	605	ALA	3.2
1	A	758	LYS	3.1
1	B	1172	PHE	3.1
1	A	584	LYS	3.1
1	A	616	PHE	3.1
1	A	532	ARG	3.0
1	B	589	LYS	3.0
1	A	581	ASP	3.0
1	A	91	LEU	3.0
1	A	516	TRP	3.0
1	A	734	TYR	3.0
1	A	552	ASP	3.0
1	B	714	LEU	3.0
1	B	291	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	596	GLU	2.9
1	A	92	LEU	2.9
1	B	1230	THR	2.9
1	A	1177	PRO	2.9
1	A	573	VAL	2.9
1	B	595	GLY	2.9
1	A	538	LYS	2.8
1	A	731	LEU	2.8
1	A	530	ILE	2.8
1	B	92	LEU	2.8
1	A	534	ILE	2.7
1	A	783	ARG	2.7
1	A	30	ILE	2.7
1	A	618	TYR	2.7
1	A	602	ASN	2.7
1	A	1176	ALA	2.7
1	A	622	TRP	2.7
1	A	759	GLU	2.7
1	B	633	PRO	2.7
1	B	716	GLY	2.7
1	A	608	GLN	2.7
1	B	292	ALA	2.6
1	B	1179	GLY	2.6
1	B	1180	GLY	2.6
1	A	497	ILE	2.6
1	B	1077	ARG	2.6
1	A	583	LEU	2.6
1	B	758	LYS	2.6
1	A	408	ALA	2.6
1	A	601	MET	2.6
1	A	541	PHE	2.6
1	A	527	PRO	2.6
1	A	579	ALA	2.6
1	A	528	SER	2.5
1	B	754	ILE	2.5
1	A	603	THR	2.5
1	A	1172	PHE	2.5
1	A	555	LEU	2.5
1	A	790	VAL	2.5
1	B	94	ILE	2.5
1	A	90	LEU	2.5
1	A	600	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	121	LEU	2.4
1	A	617	LYS	2.4
1	A	542	TYR	2.4
1	A	609	ALA	2.4
1	B	1182	ALA	2.4
1	A	932	LYS	2.4
1	B	91	LEU	2.4
1	B	1183	ASP	2.3
1	A	717	ALA	2.3
1	A	636	ASN	2.3
1	A	933	LEU	2.3
1	A	736	PHE	2.3
1	A	536	ASN	2.3
1	B	1181	LYS	2.3
1	A	712	GLU	2.3
1	A	1171	ILE	2.3
1	A	711	GLU	2.3
1	B	1221	GLU	2.2
1	B	597	LYS	2.2
1	B	729	LYS	2.2
1	B	735	LYS	2.2
1	B	624	ASP	2.2
1	A	784	ILE	2.2
1	A	937	GLN	2.2
1	B	1170	ASN	2.2
1	B	685	VAL	2.2
1	A	604	ASP	2.2
1	A	503	GLY	2.2
1	A	1126	GLU	2.2
1	B	634	MET	2.2
1	A	709	ALA	2.2
1	A	5	MET	2.1
1	A	780	TYR	2.1
1	A	725	GLU	2.1
1	B	711	GLU	2.1
1	A	124	PHE	2.1
1	A	1227	SER	2.1
1	B	130	ILE	2.1
1	A	506	ASP	2.1
1	A	868	LEU	2.1
1	A	1160	PHE	2.0
1	B	783	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	116	ILE	2.0
1	A	843	ILE	2.0
1	B	723	ALA	2.0
1	A	685	VAL	2.0
1	A	768	ASP	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 carbohydrates 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.

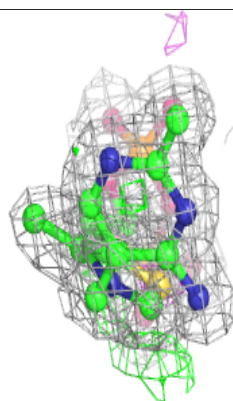
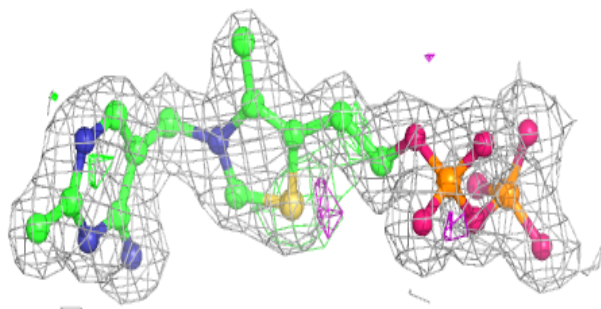
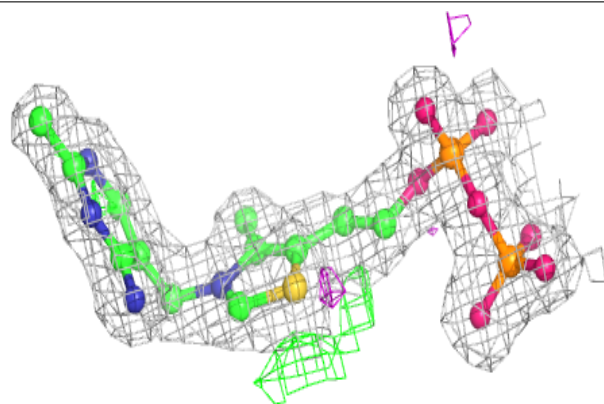
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PYR	B	3237	6/6	0.92	0.21	16,19,24,26	0
4	PYR	A	3237	6/6	0.95	0.15	21,25,28,29	0
2	SF4	A	3233	8/8	0.96	0.06	27,30,32,33	0
2	SF4	B	3233	8/8	0.97	0.07	20,23,25,26	0
2	SF4	A	3234	8/8	0.98	0.06	23,24,24,25	0
3	TPP	A	3236	26/26	0.98	0.13	12,15,27,34	0
3	TPP	B	3236	26/26	0.98	0.12	7,13,24,30	0
5	MG	A	3238	1/1	0.99	0.10	12,12,12,12	0
2	SF4	A	3235	8/8	0.99	0.07	16,18,18,18	0
2	SF4	B	3234	8/8	0.99	0.06	16,17,19,19	0
6	CA	B	3239	1/1	0.99	0.09	44,44,44,44	0
6	CA	A	3239	1/1	0.99	0.11	40,40,40,40	0
2	SF4	B	3235	8/8	1.00	0.07	12,13,14,15	0
5	MG	B	3238	1/1	1.00	0.11	9,9,9,9	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

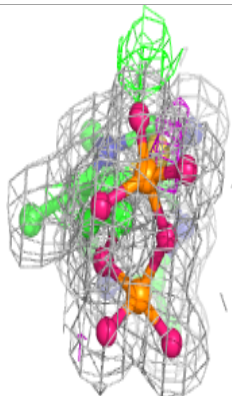
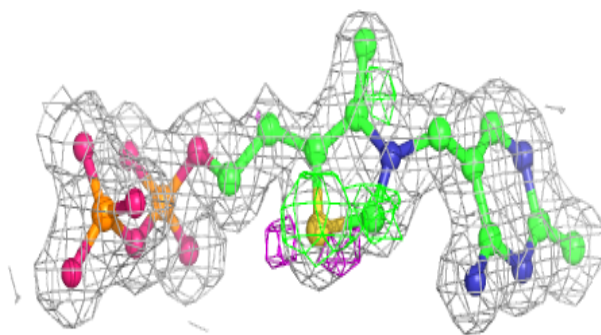
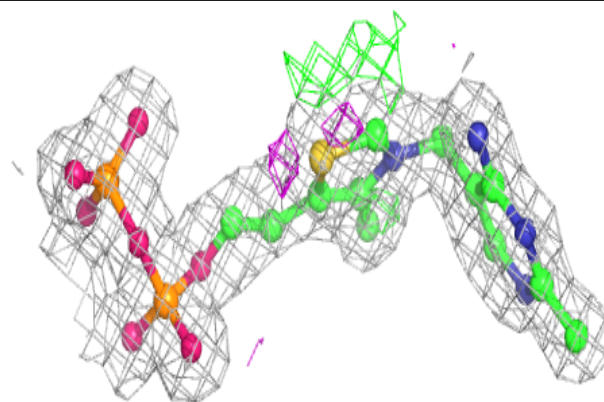
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

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

There are no such residues in this entry.