



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 12:32 pm GMT

PDB ID : 2C3M  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

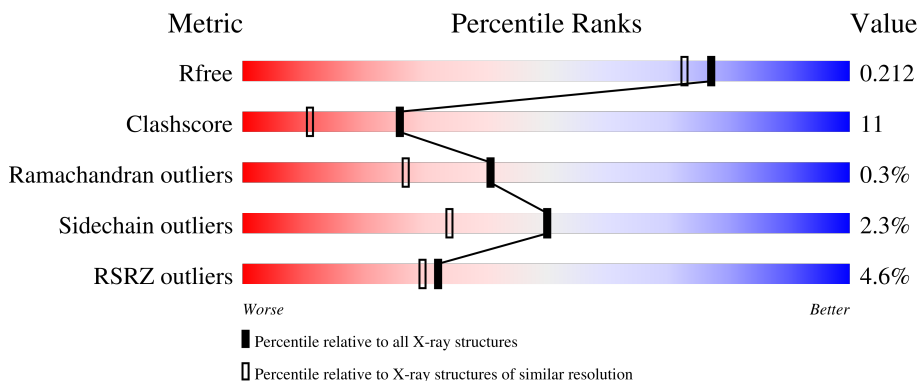
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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  $\geq 3$ , 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	 6% 79% 20% .
1	B	1231	 3% 81% 18% .

## 2 Entry composition [i](#)

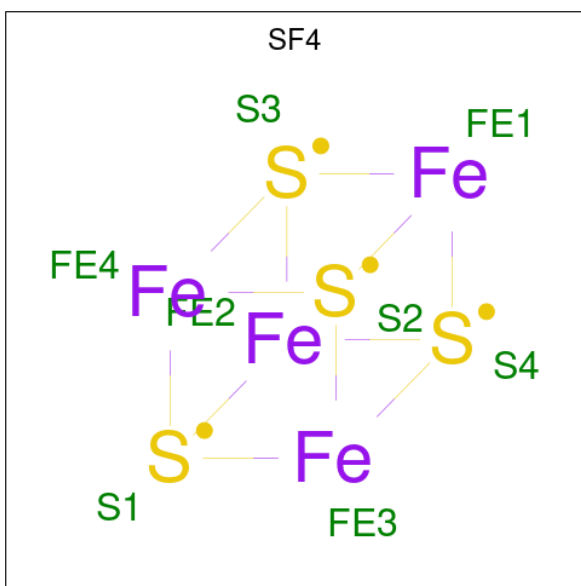
There are 7 unique types of molecules in this entry. The entry contains 20189 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



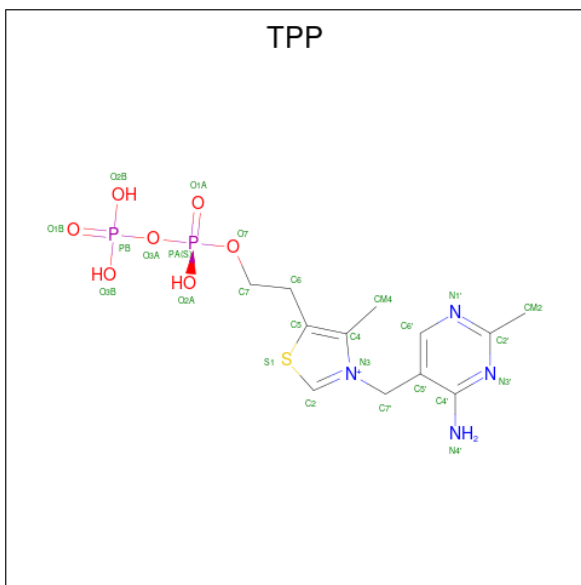
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	8	4	4	0	0
2	A	1	8	4	4	0	0
2	A	1	8	4	4	0	0
2	B	1	8	4	4	0	0

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

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

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

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

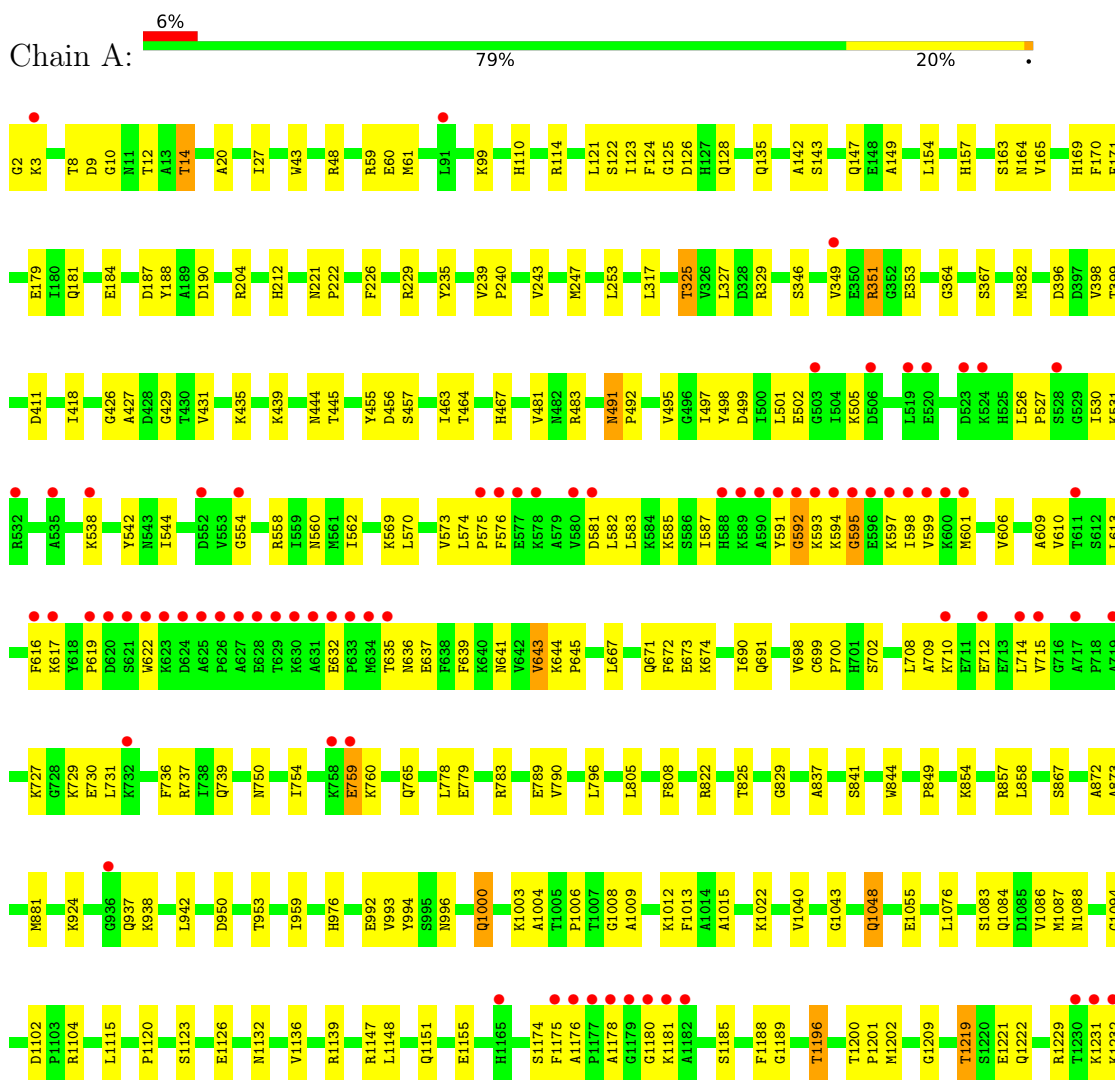
- Molecule 7 is water.

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

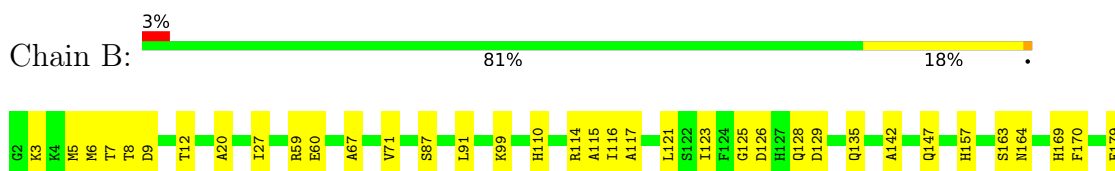
### 3 Residue-property plots [i](#)

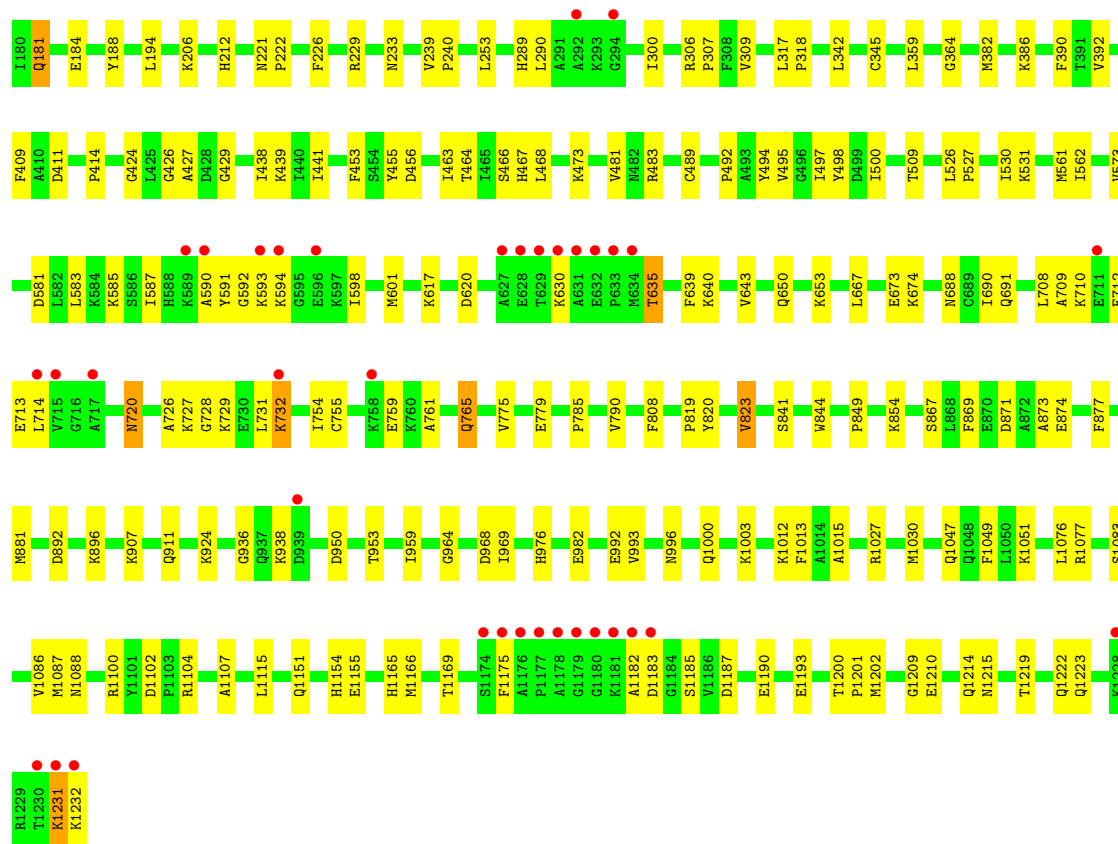
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE



#### • Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 93.6 (51.12-1.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.95 (at 1.84Å)	Xtrriage
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 <sup>2</sup> )	17.1	Xtrriage
Anisotropy	0.426	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, CL, TPP, MG, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/9585	0.59	2/12954 (0.0%)
1	B	0.32	0/9585	0.60	2/12954 (0.0%)
All	All	0.31	0/19170	0.60	4/25908 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	GLY	N-CA-C	5.44	126.70	113.10
1	B	364	GLY	N-CA-C	5.30	126.35	113.10
1	B	125	GLY	N-CA-C	5.24	126.19	113.10
1	A	364	GLY	N-CA-C	5.09	125.83	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	234	0
1	B	9383	0	9262	189	0
2	A	24	0	0	1	0
2	B	24	0	0	1	0
3	A	26	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	20189	0	18556	394	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 (394) 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: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: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:591:TYR:C	1:B:593:LYS:H	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:731:LEU:HD23	1:B:790:VAL:HG11	1.72	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: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:759:GLU:CD	1:A:759:GLU:H	1.98	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:992:GLU:O	1:B:993:VAL:HG13	1.97	0.65
1:A:591:TYR:C	1:A:593:LYS:H	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1166:MET:O	1:B:1169:THR:HG22	1.98	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:3:LYS:HD3	1:A:184:GLU:CD	2.22	0.61
1:A:445:THR:HG21	1:A:574:LEU:HD21	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: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:B:5:MET:HE1	1:B:184:GLU:HB3	1.84	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:635:THR:HG23	1:A:672:PHE:CG	2.38	0.59
1:B:1231:LYS:O	1:B:1232:LYS:HB2	2.03	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: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: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
1:A:142:ALA:HB2	1:A:170:PHE:CZ	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:164:ASN:HD22	1:B:206:LYS:HZ1	1.51	0.56
1:B:635:THR:HG21	1:B:639:PHE:HD2	1.69	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:B:598:ILE:HD13	1:B:601:MET:HE2	1.87	0.55
1:A:953:THR:HG21	7:B:2118:HOH:O	2.05	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:554:GLY:HA3	1:A:601:MET:HE2	1.88	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:59:ARG:HB2	1:B:881:MET:HE3	1.88	0.54
1:A:467:HIS:CD2	1:A:481:VAL:H	2.25	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:591:TYR:C	1:B:593:LYS:N	2.61	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:A:730:GLU:CD	1:A:730:GLU:H	2.15	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
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:121:LEU:HD23	1:A:121:LEU:C	2.32	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:841:SER:HA	1:A:844:TRP:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:PHE:CE1	1:B:392:VAL:HG23	2.47	0.49
1:B:561:MET:HE3	1:B:561:MET:O	2.12	0.49
1:A:1200:THR:HG21	1:A:1202:MET:CE	2.43	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:976:HIS:HD2	1:B:1003:LYS:HZ2	1.61	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:6:MET:HE2	1:B:8:THR:OG1	2.13	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
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:796:LEU:HD23	1:A:796:LEU:C	2.34	0.48
1:B:121:LEU:C	1:B:121:LEU:HD23	2.34	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:TYR:C	1:A:593:LYS:N	2.68	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: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: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:1132:ASN:CG	1:A:1136:VAL:HG13	2.36	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: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: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:1219:THR:CG2	1:B:1222:GLN:HG3	2.47	0.45
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:881:MET:HE3	1:B:59:ARG:HB2	1.97	0.45
1:B:590:ALA:O	1:B:591:TYR:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:VAL:HG23	1:A:399:THR:H	1.82	0.45
1:A:754:ILE:C	1:A:754:ILE:HD12	2.38	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:163:SER:O	1:A:164:ASN:HB2	2.17	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: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:A:1043:GLY:HA3	1:A:1087:MET:HB2	1.99	0.44
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:698:VAL:HG12	1:A:698:VAL:O	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:710:LYS:HB2	1:A:710:LYS:HZ2	1.83	0.42
1:A:730:GLU:CD	1:A:730:GLU:N	2.73	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:453:PHE:HD2	1:B:466:SER:HG	1.67	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:1200:THR:HG21	1:A:1202:MET:HE3	2.00	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:B:1027:ARG:HA	1:B:1030:MET:HE3	2.00	0.42
1:A:691:GLN:HG2	1:A:736:PHE:CD2	2.54	0.42
1:B:306:ARG:HA	1:B:307:PRO:C	2.40	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:778:LEU:HD13	1:A:778:LEU:C	2.40	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:1102:ASP:CG	1:A:1104:ARG:HE	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:673:GLU:O	1:A:674:LYS:C	2.58	0.41
1:A:729:LYS:HB3	1:A:730:GLU:OE2	2.21	0.41
1:A:976:HIS:CD2	1:B:1003:LYS:HZ2	2.39	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:759:GLU:CD	1:A:759:GLU:N	2.72	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:A:937:GLN:C	1:A:938:LYS:HD2	2.40	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: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: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:575:PRO:O	1:A:576:PHE:C	2.59	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:673:GLU:O	1:B:674:LYS:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1219:THR:HG22	1:B:1222:GLN:CD	2.42	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%)	41	27
1	B	1229/1231 (100%)	1184 (96%)	41 (3%)	4 (0%)	41	27
All	All	2458/2462 (100%)	2365 (96%)	85 (4%)	8 (0%)	41	27

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%)	49	32
1	B	978/978 (100%)	956 (98%)	22 (2%)	52	36
All	All	1956/1956 (100%)	1911 (98%)	45 (2%)	50	34

All (45) 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	204	ARG
1	A	226	PHE
1	A	317	LEU
1	A	325	THR
1	A	327	LEU
1	A	351	ARG
1	A	463	ILE
1	A	491	ASN
1	A	632	GLU
1	A	643	VAL
1	A	759	GLU
1	A	789	GLU
1	A	808	PHE
1	A	996	ASN
1	A	1000	GLN
1	A	1048	GLN
1	A	1088	ASN
1	A	1115	LEU
1	A	1196	THR
1	A	1219	THR
1	B	181	GLN
1	B	194	LEU
1	B	226	PHE
1	B	342	LEU
1	B	359	LEU
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	765	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	808	PHE
1	B	823	VAL
1	B	849	PRO
1	B	996	ASN
1	B	1000	GLN
1	B	1047	GLN
1	B	1088	ASN
1	B	1115	LEU
1	B	1165	HIS
1	B	1183	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	11	ASN
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
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	560	ASN
1	A	602	ASN
1	A	641	ASN
1	A	683	GLN
1	A	688	ASN
1	A	691	GLN
1	A	720	ASN
1	A	739	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	750	ASN
1	A	765	GLN
1	A	777	ASN
1	A	836	ASN
1	A	866	ASN
1	A	937	GLN
1	A	976	HIS
1	A	996	ASN
1	A	1000	GLN
1	A	1048	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	110	HIS
1	B	128	GLN
1	B	135	GLN
1	B	147	GLN
1	B	164	ASN
1	B	169	HIS
1	B	181	GLN
1	B	212	HIS
1	B	220	GLN
1	B	421	GLN
1	B	434	ASN
1	B	467	HIS
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	836	ASN
1	B	866	ASN
1	B	976	HIS
1	B	996	ASN
1	B	1000	GLN
1	B	1073	ASN
1	B	1084	GLN

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Mol	Chain	Res	Type
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 monosaccharides 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
3	TPP	B	2236	5	22,27,27	4.61	8 (36%)	29,40,40	1.61	7 (24%)
2	SF4	B	2234	1	0,12,12	-	-	-		
2	SF4	A	2233	1	0,12,12	-	-	-		
3	TPP	A	2236	5	22,27,27	3.47	10 (45%)	29,40,40	1.55	5 (17%)
2	SF4	A	2235	1	0,12,12	-	-	-		
2	SF4	B	2233	1	0,12,12	-	-	-		
2	SF4	A	2234	1	0,12,12	-	-	-		
2	SF4	B	2235	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	B	2236	5	-	2/16/17/17	0/2/2/2
2	SF4	B	2234	1	-	-	0/6/5/5
3	TPP	A	2236	5	-	2/16/17/17	0/2/2/2
2	SF4	A	2233	1	-	-	0/6/5/5
2	SF4	A	2235	1	-	-	0/6/5/5
2	SF4	B	2233	1	-	-	0/6/5/5
2	SF4	A	2234	1	-	-	0/6/5/5
2	SF4	B	2235	1	-	-	0/6/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2236	TPP	C6-C5	16.98	1.58	1.50
3	A	2236	TPP	C6-C5	9.17	1.54	1.50
3	B	2236	TPP	C4-N3	7.68	1.46	1.39
3	A	2236	TPP	C4-N3	7.01	1.45	1.39
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	4.16	1.58	1.49
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'	2.86	1.39	1.34
3	A	2236	TPP	C4'-N3'	2.75	1.39	1.35
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	B	2236	TPP	C6'-C5'	2.16	1.42	1.37
3	A	2236	TPP	C7'-N3	2.07	1.52	1.48

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	B	2236	TPP	N1'-C2'-N3'	-3.10	120.20	125.54
3	A	2236	TPP	CM4-C4-N3	2.56	125.80	122.53
3	A	2236	TPP	N1'-C2'-N3'	-2.54	121.17	125.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	CM4-C4-N3	2.35	125.53	122.53
3	A	2236	TPP	CM2-C2'-N3'	2.20	120.59	117.15
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	C5'-C6'-N1'	-2.07	120.37	123.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

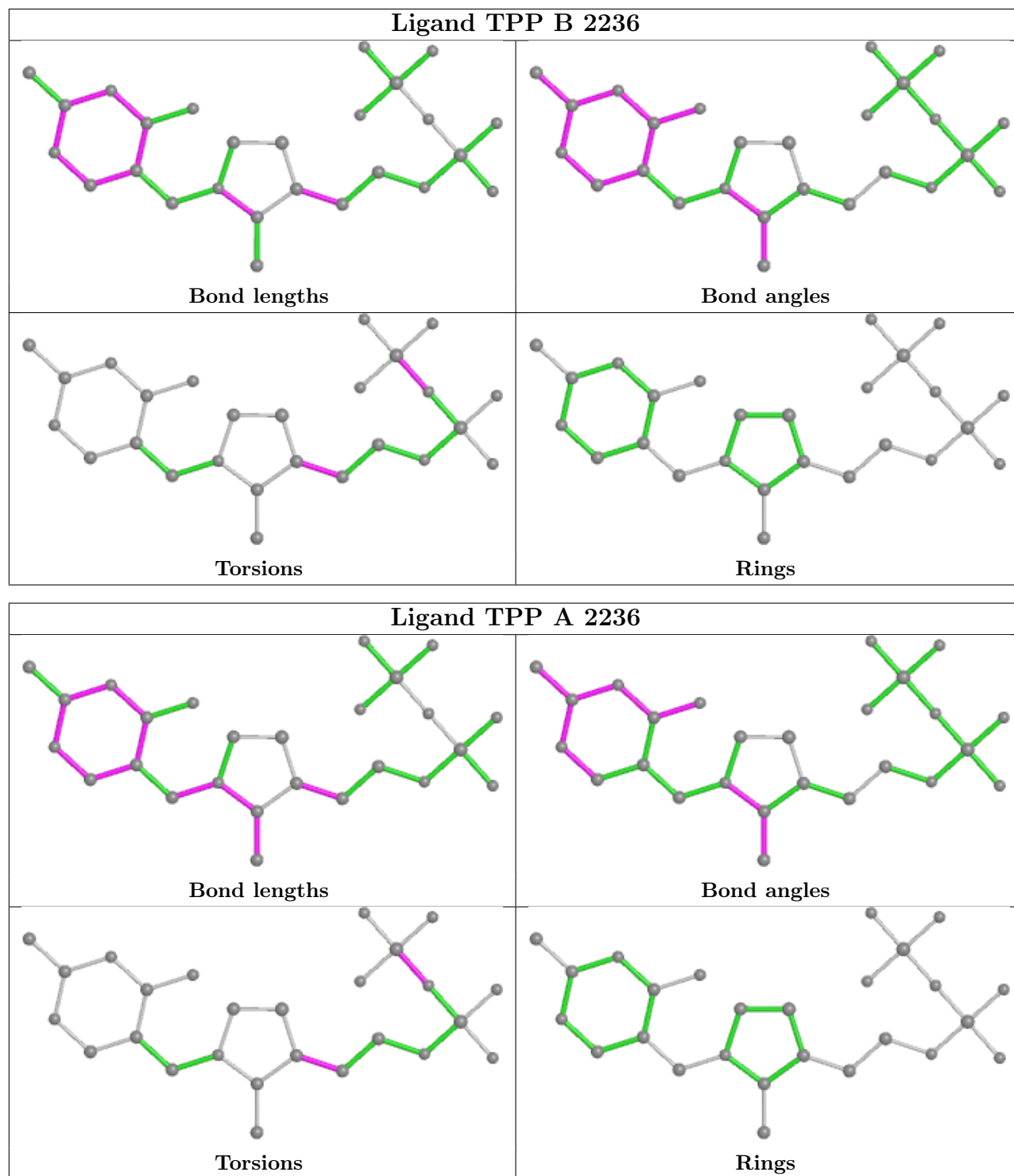
Mol	Chain	Res	Type	Atoms
3	A	2236	TPP	C4-C5-C6-C7
3	A	2236	TPP	PA-O3A-PB-O2B
3	B	2236	TPP	PA-O3A-PB-O2B
3	B	2236	TPP	C4-C5-C6-C7

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2236	TPP	1	0
2	A	2233	SF4	1	0
3	A	2236	TPP	1	0
2	B	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1231/1231 (100%)	0.19	77 (6%) 20 17	10, 20, 60, 92	0
1	B	1231/1231 (100%)	-0.03	36 (2%) 51 49	8, 18, 41, 90	0
All	All	2462/2462 (100%)	0.08	113 (4%) 32 29	8, 19, 51, 92	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	631	ALA	11.9
1	A	1177	PRO	11.1
1	B	1178	ALA	10.1
1	B	1232	LYS	9.1
1	A	1176	ALA	8.9
1	A	1182	ALA	8.5
1	B	1176	ALA	8.1
1	B	1182	ALA	7.1
1	B	1175	PHE	7.0
1	A	631	ALA	6.9
1	A	633	PRO	6.9
1	B	1183	ASP	6.8
1	A	629	THR	6.6
1	A	1178	ALA	6.6
1	A	594	LYS	6.6
1	A	1232	LYS	6.6
1	A	630	LYS	6.2
1	B	1177	PRO	6.2
1	A	576	PHE	6.1
1	A	1180	GLY	6.0
1	A	634	MET	5.9
1	B	1179	GLY	5.9
1	A	595	GLY	5.7
1	A	1179	GLY	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	630	LYS	5.5
1	A	628	GLU	5.3
1	A	597	LYS	5.3
1	A	1231	LYS	5.1
1	A	627	ALA	5.1
1	A	593	LYS	5.0
1	A	1175	PHE	4.8
1	A	715	VAL	4.7
1	B	629	THR	4.6
1	A	577	GLU	4.3
1	B	1231	LYS	4.2
1	B	1180	GLY	4.2
1	A	632	GLU	4.1
1	A	623	LYS	4.0
1	A	624	ASP	4.0
1	B	1174	SER	3.9
1	A	626	PRO	3.8
1	A	588	HIS	3.8
1	B	1181	LYS	3.8
1	A	619	PRO	3.7
1	A	620	ASP	3.7
1	A	714	LEU	3.7
1	A	1181	LYS	3.5
1	B	596	GLU	3.5
1	B	632	GLU	3.5
1	A	596	GLU	3.5
1	A	600	LYS	3.4
1	A	732	LYS	3.4
1	B	593	LYS	3.3
1	A	758	LYS	3.2
1	A	523	ASP	3.1
1	B	732	LYS	3.1
1	B	714	LEU	3.1
1	A	575	PRO	3.0
1	A	554	GLY	3.0
1	B	633	PRO	3.0
1	A	538	LYS	3.0
1	A	1165	HIS	3.0
1	A	621	SER	3.0
1	A	617	LYS	3.0
1	B	717	ALA	3.0
1	A	519	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1228	LYS	2.9
1	A	532	ARG	2.9
1	A	589	LYS	2.9
1	A	598	ILE	2.8
1	A	625	ALA	2.8
1	A	1230	THR	2.8
1	A	717	ALA	2.7
1	A	591	TYR	2.7
1	A	3	LYS	2.6
1	A	599	VAL	2.6
1	A	590	ALA	2.6
1	A	580	VAL	2.6
1	B	715	VAL	2.6
1	A	936	GLY	2.6
1	A	524	LYS	2.6
1	A	506	ASP	2.6
1	A	535	ALA	2.5
1	B	292	ALA	2.5
1	A	635	THR	2.5
1	B	594	LYS	2.5
1	B	590	ALA	2.5
1	B	628	GLU	2.4
1	B	294	GLY	2.4
1	A	578	LYS	2.4
1	B	1230	THR	2.4
1	A	601	MET	2.3
1	A	710	LYS	2.3
1	B	627	ALA	2.3
1	B	634	MET	2.3
1	A	552	ASP	2.3
1	A	581	ASP	2.3
1	A	616	PHE	2.3
1	A	528	SER	2.3
1	B	758	LYS	2.3
1	A	622	TRP	2.2
1	B	939	ASP	2.2
1	A	503	GLY	2.2
1	A	91	LEU	2.2
1	A	592	GLY	2.2
1	A	759	GLU	2.2
1	A	611	THR	2.1
1	A	719	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	589	LYS	2.1
1	A	520	GLU	2.1
1	A	712	GLU	2.1
1	A	349	VAL	2.1
1	B	711	GLU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

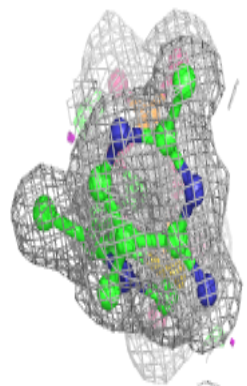
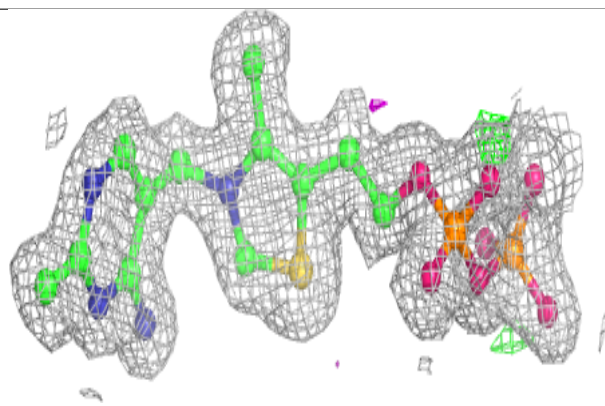
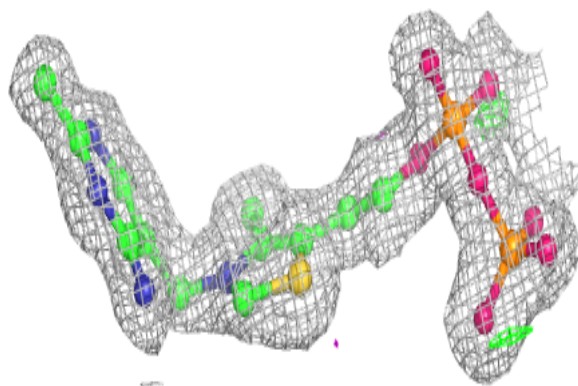
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SF4	A	2233	8/8	0.97	0.06	23,24,25,25	0
3	TPP	A	2236	26/26	0.98	0.12	8,12,14,16	0
2	SF4	A	2235	8/8	0.99	0.07	15,15,16,17	0
2	SF4	B	2233	8/8	0.99	0.05	17,18,19,20	0
2	SF4	B	2234	8/8	0.99	0.06	13,15,16,16	0
2	SF4	A	2234	8/8	0.99	0.06	18,20,21,22	0
3	TPP	B	2236	26/26	0.99	0.12	7,9,13,14	0
4	CL	A	2237	1/1	0.99	0.09	21,21,21,21	0
4	CL	B	2237	1/1	0.99	0.10	20,20,20,20	0
6	CA	A	2239	1/1	0.99	0.06	45,45,45,45	0
6	CA	B	2239	1/1	0.99	0.08	40,40,40,40	0
5	MG	B	2238	1/1	1.00	0.12	5,5,5,5	0
2	SF4	B	2235	8/8	1.00	0.07	9,11,12,12	0
5	MG	A	2238	1/1	1.00	0.15	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.

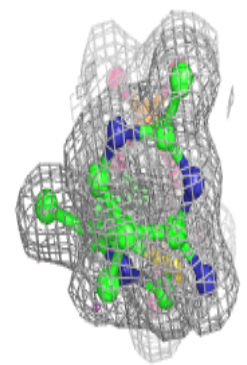
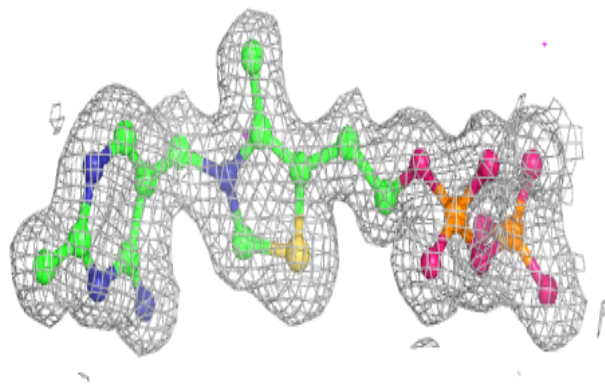
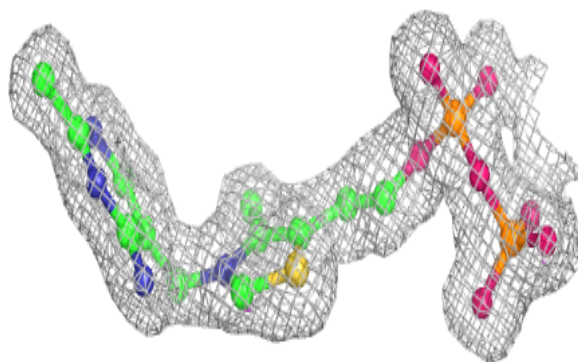


**Electron density around TPP A 2236:**

$2mF_o-DF_c$  (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.