



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:27 am BST

PDB ID : 2C3P  
Title : CRYSTAL STRUCTURE OF THE FREE RADICAL INTERMEDIATE 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 : 2.33 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.

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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 : 1.8.5 (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

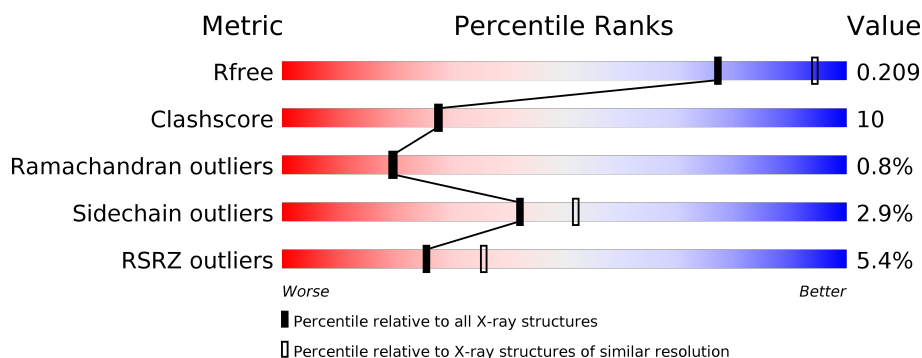
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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  $\geq 3$ , 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	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>23%</div> </div> <div></div> </div>
1	B	1231	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>16%</div> </div> <div></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1TP	A	2236	X	-	-	-
3	1TP	B	2236	X	-	-	-

## 2 Entry composition [i](#)

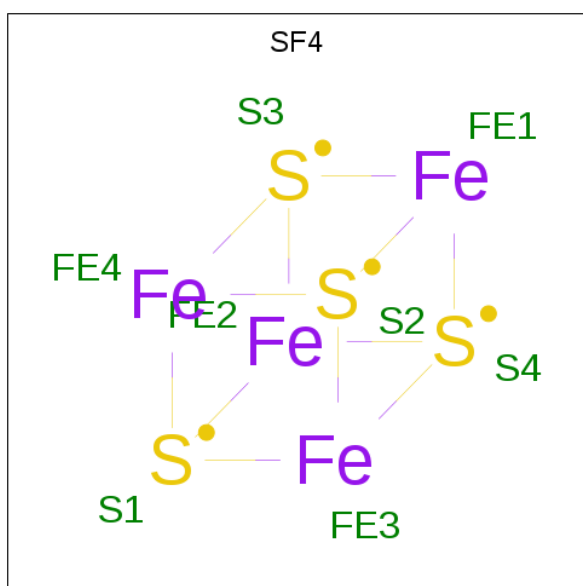
There are 6 unique types of molecules in this entry. The entry contains 19733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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<sub>4</sub>S<sub>4</sub>).



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

- # 1TP

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

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

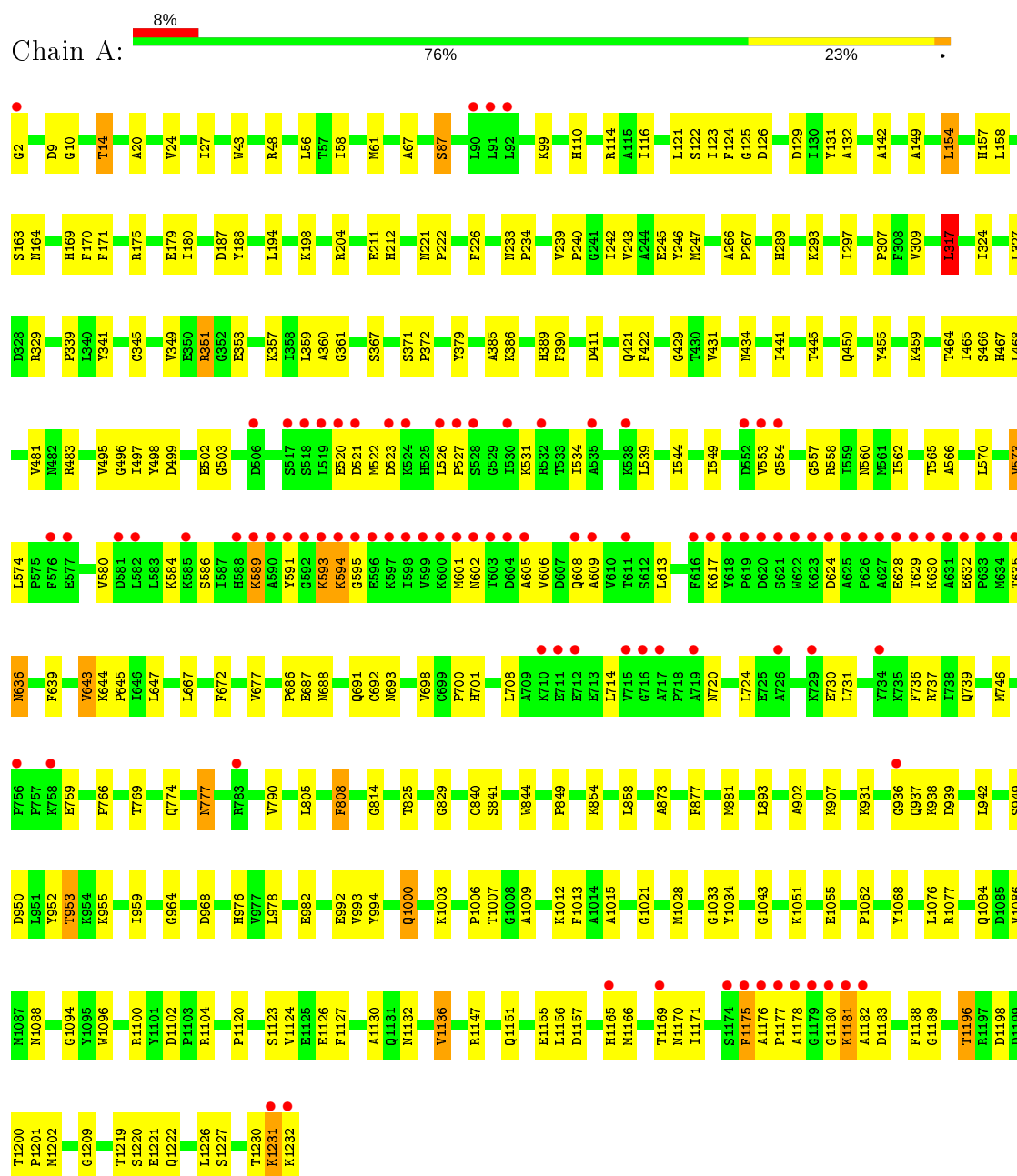
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	379	Total 379	O 379	0	0
6	B	472	Total 472	O 472	0	0

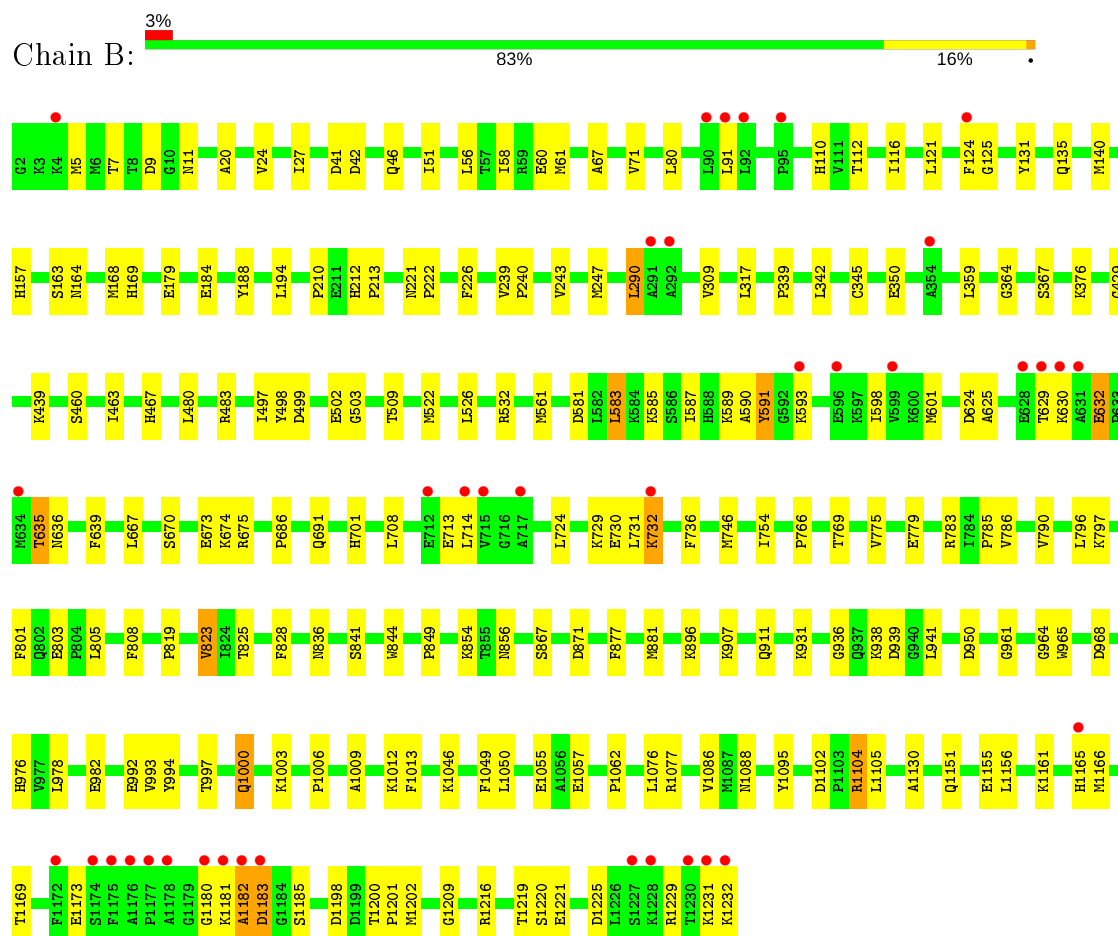
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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-FERREDONIN OXIDOREDUCTASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.97Å 145.84Å 210.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.37 – 2.33 47.37 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.37-2.33) 98.4 (47.37-2.33)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.55 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.171 , 0.223 0.157 , 0.209	Depositor DCC
$R_{free}$ test set	5637 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: MG, CA, SF4, 1TP

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	0.44	0/9585	0.68	2/12954 (0.0%)
1	B	0.46	0/9585	0.69	4/12954 (0.0%)
All	All	0.45	0/19170	0.69	6/25908 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	GLY	N-CA-C	6.52	129.41	113.10
1	B	125	GLY	N-CA-C	5.85	127.73	113.10
1	B	1104	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	B	994	TYR	N-CA-C	-5.34	96.58	111.00
1	A	317	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	364	GLY	N-CA-C	5.15	125.97	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	232	0
1	B	9383	0	9262	157	0
2	A	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	24	0	0	0	0
3	A	32	0	21	7	0
3	B	32	0	21	8	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	379	0	0	3	0
6	B	472	0	0	6	0
All	All	19733	0	18566	374	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 10.

All (374) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2236:1TP:C15	3:A:2236:1TP:C25	1.79	1.59
3:B:2236:1TP:C25	3:B:2236:1TP:C15	1.82	1.56
3:B:2236:1TP:C2	3:B:2236:1TP:N3	1.67	1.48
3:B:2236:1TP:C2	3:B:2236:1TP:C15	1.93	1.44
3:A:2236:1TP:C15	3:A:2236:1TP:C2	2.09	1.29
1:B:1200:THR:HG22	1:B:1202:MET:H	1.17	1.07
1:A:1200:THR:HG22	1:A:1202:MET:H	1.25	1.02
1:A:639:PHE:HA	1:A:643:VAL:HG13	1.41	1.00
1:A:1231:LYS:HG3	1:A:1232:LYS:H	1.33	0.93
1:A:635:THR:HG22	1:A:636:ASN:H	1.35	0.90
1:A:877:PHE:HE1	1:A:982:GLU:HG3	1.36	0.90
1:B:110:HIS:HD2	1:B:169:HIS:CD2	1.92	0.88
1:A:1132:ASN:O	1:A:1136:VAL:HG22	1.77	0.85
3:A:2236:1TP:C15	3:A:2236:1TP:H2	2.06	0.85
1:B:1200:THR:HG22	1:B:1202:MET:N	1.91	0.85
1:B:877:PHE:HE1	1:B:982:GLU:HG3	1.39	0.84
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.20	0.84
1:A:566:ALA:HA	1:A:613:LEU:HD21	1.60	0.83
1:A:27:ILE:HD11	1:A:1013:PHE:CE2	2.15	0.82
1:A:1200:THR:HG22	1:A:1202:MET:N	1.93	0.82
1:B:110:HIS:CD2	1:B:169:HIS:HD2	1.97	0.82
1:A:976:HIS:HD2	1:B:1003:LYS:HZ2	1.25	0.81
1:A:110:HIS:HD2	1:A:169:HIS:HD2	1.28	0.81
1:B:877:PHE:CE1	1:B:982:GLU:HG3	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:LEU:HD13	1:A:1086:VAL:HG21	1.63	0.81
1:B:731:LEU:CD2	1:B:790:VAL:HG11	2.11	0.80
1:B:1151:GLN:O	1:B:1155:GLU:HG3	1.81	0.80
1:B:635:THR:HG23	1:B:639:PHE:HB3	1.64	0.80
1:A:1151:GLN:O	1:A:1155:GLU:HG3	1.83	0.78
1:A:544:ILE:HD12	1:A:613:LEU:HD13	1.65	0.76
1:A:639:PHE:HA	1:A:643:VAL:CG1	2.15	0.76
1:A:1231:LYS:HG3	1:A:1232:LYS:N	1.99	0.75
3:B:2236:1TP:C15	3:B:2236:1TP:H2	2.12	0.75
1:A:644:LYS:HB3	1:A:645:PRO:HD3	1.69	0.75
1:A:239:VAL:HG23	1:A:240:PRO:HD3	1.67	0.74
1:A:14:THR:HG22	1:A:149:ALA:HB1	1.69	0.74
1:A:239:VAL:CG2	1:A:240:PRO:HD3	2.18	0.74
1:A:10:GLY:O	1:A:14:THR:HG23	1.86	0.74
1:A:1102:ASP:OD1	1:A:1104:ARG:HG2	1.87	0.73
1:A:110:HIS:HD2	1:A:169:HIS:CD2	2.05	0.73
1:B:1198:ASP:OD2	1:B:1200:THR:HB	1.90	0.71
1:B:1219:THR:HG22	1:B:1221:GLU:H	1.54	0.71
1:B:598:ILE:HD13	1:B:601:MET:CE	2.20	0.70
1:A:1198:ASP:OD2	1:A:1200:THR:HB	1.91	0.70
1:A:708:LEU:HD21	1:A:731:LEU:HD22	1.74	0.70
1:A:731:LEU:HD23	1:A:790:VAL:HG11	1.73	0.70
1:A:730:GLU:CD	1:A:730:GLU:H	1.93	0.70
1:A:1230:THR:O	1:A:1232:LYS:HG2	1.92	0.70
1:B:1200:THR:CG2	1:B:1202:MET:H	1.99	0.69
1:B:635:THR:CG2	1:B:639:PHE:HB3	2.22	0.69
1:A:110:HIS:CD2	1:A:169:HIS:HD2	2.11	0.69
1:A:731:LEU:CD2	1:A:790:VAL:HG11	2.21	0.69
1:A:1200:THR:CG2	1:A:1202:MET:H	2.03	0.68
1:B:731:LEU:HD23	1:B:790:VAL:HG11	1.75	0.68
1:B:1102:ASP:OD1	1:B:1104:ARG:HG2	1.92	0.68
1:A:163:SER:HB2	1:A:239:VAL:HG12	1.75	0.68
1:B:691:GLN:HG2	1:B:736:PHE:CD2	2.29	0.67
1:A:483:ARG:HH11	1:A:483:ARG:HG2	1.59	0.67
1:B:41:ASP:HA	1:B:58:ILE:HD12	1.77	0.67
1:A:593:LYS:HG3	1:A:594:LYS:N	2.10	0.67
3:B:2236:1TP:C7'	3:B:2236:1TP:C2	2.71	0.67
1:B:630:LYS:HB2	1:B:632:GLU:HG3	1.77	0.66
1:B:591:TYR:C	1:B:593:LYS:H	1.97	0.66
1:A:1006:PRO:HG2	1:A:1009:ALA:HB2	1.76	0.66
1:A:558:ARG:HG2	1:A:560:ASN:HD21	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:MET:HE3	6:B:2373:HOH:O	1.96	0.66
1:A:467:HIS:HD2	1:A:481:VAL:H	1.41	0.66
1:A:635:THR:HG23	1:A:672:PHE:CG	2.30	0.66
1:A:431:VAL:CG2	1:A:464:THR:HG21	2.26	0.66
1:B:731:LEU:HD21	1:B:790:VAL:HG11	1.78	0.66
1:A:467:HIS:CD2	1:A:481:VAL:H	2.14	0.65
1:B:561:MET:HE1	1:B:583:LEU:HD21	1.78	0.65
1:B:713:GLU:OE1	1:B:785:PRO:HD2	1.97	0.65
1:A:877:PHE:CE1	1:A:982:GLU:HG3	2.26	0.65
1:A:1219:THR:HG22	1:A:1221:GLU:H	1.61	0.64
1:B:110:HIS:HE1	1:B:157:HIS:NE2	1.95	0.64
1:B:730:GLU:H	1:B:730:GLU:CD	2.01	0.64
1:A:602:ASN:O	1:A:606:VAL:HG23	1.99	0.63
1:A:1231:LYS:CG	1:A:1232:LYS:H	2.11	0.63
1:B:1219:THR:HG22	1:B:1221:GLU:N	2.14	0.62
3:A:2236:1TP:C35	3:A:2236:1TP:C25	2.74	0.62
1:B:907:LYS:O	1:B:911:GLN:HG3	2.00	0.62
1:B:140:MET:HG2	1:B:168:MET:HE2	1.81	0.62
1:B:708:LEU:HD21	1:B:731:LEU:HD22	1.82	0.62
1:A:636:ASN:ND2	1:A:639:PHE:H	1.99	0.61
1:A:1156:LEU:HD12	1:A:1157:ASP:N	2.16	0.61
1:A:937:GLN:HG2	1:A:942:LEU:HB3	1.83	0.61
1:A:1219:THR:HG22	1:A:1221:GLU:N	2.14	0.61
1:A:445:THR:HG21	1:A:574:LEU:HD21	1.83	0.60
1:A:686:PRO:HB2	1:A:724:LEU:HD21	1.82	0.60
1:B:775:VAL:O	1:B:779:GLU:HG2	2.00	0.60
1:B:1200:THR:CG2	1:B:1202:MET:HB2	2.31	0.60
1:A:691:GLN:HG2	1:A:736:PHE:CD2	2.36	0.60
1:A:349:VAL:HG21	1:B:345:CYS:SG	2.41	0.60
1:A:2:GLY:N	1:A:187:ASP:OD2	2.35	0.60
1:A:554:GLY:HA3	1:A:601:MET:HE2	1.83	0.60
1:B:239:VAL:HB	1:B:240:PRO:HD3	1.83	0.60
1:A:549:ILE:HG23	1:A:608:GLN:HG2	1.84	0.59
1:A:1033:GLY:C	1:A:1175:PHE:HZ	2.05	0.59
1:B:1200:THR:HG21	1:B:1202:MET:HB2	1.85	0.59
1:A:14:THR:HG21	1:A:171:PHE:CE2	2.38	0.58
1:B:992:GLU:O	1:B:993:VAL:HG13	2.03	0.58
1:A:936:GLY:O	1:A:938:LYS:HD3	2.04	0.58
1:B:110:HIS:CD2	1:B:169:HIS:CD2	2.79	0.58
1:A:609:ALA:O	1:A:613:LEU:HB2	2.03	0.58
1:A:1051:LYS:HE3	1:A:1100:ARG:NH1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:SER:O	1:A:164:ASN:HB2	2.04	0.58
1:A:243:VAL:O	1:A:247:MET:HG3	2.03	0.58
1:A:121:LEU:C	1:A:121:LEU:HD23	2.23	0.58
1:A:434:ASN:ND2	1:A:466:SER:OG	2.37	0.58
1:A:441:ILE:HD13	1:A:573:VAL:HG21	1.86	0.57
1:A:635:THR:HG22	1:A:636:ASN:N	2.12	0.57
1:A:1188:PHE:CE1	1:A:1196:THR:HG23	2.39	0.57
1:A:61:MET:HG3	1:A:67:ALA:HA	1.85	0.57
1:A:976:HIS:HD2	1:B:1003:LYS:NZ	2.01	0.57
1:A:1077:ARG:HG2	1:A:1130:ALA:O	2.05	0.57
1:A:739:GLN:NE2	1:A:777:ASN:HB3	2.20	0.57
1:A:635:THR:HG23	1:A:672:PHE:CD2	2.40	0.57
1:B:61:MET:HG3	1:B:67:ALA:HA	1.85	0.57
1:A:1226:LEU:O	1:A:1230:THR:HG22	2.05	0.56
1:B:1232:LYS:HB3	1:B:1232:LYS:HZ2	1.70	0.56
1:A:1188:PHE:HE1	1:A:1196:THR:HG23	1.71	0.56
1:B:497:ILE:HG13	1:B:498:TYR:CD1	2.40	0.56
1:A:591:TYR:C	1:A:593:LYS:H	2.08	0.56
1:B:7:THR:HG21	1:B:439:LYS:HA	1.86	0.56
1:A:56:LEU:HD23	1:A:58:ILE:HD11	1.87	0.56
1:B:729:LYS:O	1:B:732:LYS:HG3	2.05	0.56
1:A:142:ALA:HB2	1:A:170:PHE:CZ	2.41	0.56
1:A:522:MET:SD	1:A:526:LEU:HD22	2.46	0.56
1:B:483:ARG:HA	1:B:503:GLY:O	2.05	0.56
1:A:1123:SER:O	1:A:1126:GLU:HG2	2.06	0.56
1:A:1200:THR:HG23	1:A:1201:PRO:HD2	1.87	0.56
1:A:635:THR:HG21	1:A:639:PHE:CG	2.40	0.55
1:B:591:TYR:O	1:B:593:LYS:N	2.38	0.55
1:A:110:HIS:HE1	1:A:157:HIS:NE2	2.04	0.55
1:A:774:GLN:HA	1:A:777:ASN:HB2	1.88	0.55
1:B:803:GLU:OE1	1:B:856:ASN:HB2	2.07	0.55
1:A:14:THR:CG2	1:A:149:ALA:HB1	2.36	0.55
1:B:896:LYS:HB2	1:B:941:LEU:HD21	1.87	0.55
1:A:411:ASP:HB2	1:A:483:ARG:HD2	1.88	0.55
1:A:421:GLN:HA	1:A:466:SER:O	2.05	0.55
1:A:1171:ILE:HD12	1:B:1161:LYS:HD3	1.89	0.55
1:A:20:ALA:HB2	1:A:188:TYR:CE1	2.42	0.55
1:A:992:GLU:O	1:A:993:VAL:HG13	2.07	0.55
1:A:692:CYS:O	1:A:693:ASN:HB2	2.06	0.55
3:B:2236:1TP:N3	3:B:2236:1TP:H2	2.04	0.55
1:B:1219:THR:HG22	1:B:1220:SER:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ASP:O	1:B:46:GLN:HG3	2.07	0.54
1:A:242:ILE:O	1:A:245:GLU:HG2	2.07	0.54
1:A:1176:ALA:HB1	1:A:1177:PRO:HD2	1.90	0.54
1:A:737:ARG:HE	1:A:739:GLN:NE2	2.05	0.54
1:A:766:PRO:HB2	1:A:769:THR:HG23	1.90	0.54
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.38	0.53
1:A:483:ARG:NH1	1:A:483:ARG:HG2	2.24	0.53
1:A:1219:THR:CG2	1:A:1221:GLU:H	2.21	0.53
1:A:99:LYS:HE3	1:B:867:SER:O	2.08	0.53
1:B:27:ILE:HD12	1:B:1013:PHE:CE2	2.43	0.53
1:A:841:SER:HA	1:A:844:TRP:CE2	2.44	0.53
1:B:1219:THR:CG2	1:B:1220:SER:N	2.71	0.53
1:B:779:GLU:HB3	1:B:783:ARG:HH21	1.74	0.53
1:A:455:TYR:HB2	1:B:1201:PRO:HD3	1.90	0.53
1:B:1232:LYS:NZ	1:B:1232:LYS:HB3	2.23	0.53
1:B:691:GLN:O	1:B:797:LYS:HE3	2.09	0.53
1:A:1166:MET:O	1:A:1169:THR:HG22	2.08	0.52
1:A:805:LEU:HB2	1:A:825:THR:HB	1.91	0.52
1:A:1200:THR:CG2	1:A:1202:MET:HB2	2.39	0.52
1:A:180:ILE:O	1:A:450:GLN:HA	2.09	0.52
1:B:841:SER:HA	1:B:844:TRP:CE2	2.44	0.52
1:A:221:ASN:HB3	1:A:222:PRO:HD2	1.92	0.52
1:A:389:HIS:HE1	1:B:350:GLU:OE1	1.91	0.52
1:A:554:GLY:HA3	1:A:601:MET:CE	2.39	0.52
1:A:635:THR:HG21	1:A:639:PHE:HB3	1.91	0.52
1:B:221:ASN:HB3	1:B:222:PRO:CD	2.40	0.52
1:A:239:VAL:HG23	1:A:240:PRO:CD	2.37	0.51
1:A:341:TYR:CD1	1:A:360:ALA:HB2	2.46	0.51
1:A:239:VAL:CG2	1:A:307:PRO:HG2	2.40	0.51
3:A:2236:1TP:O35	1:B:1202:MET:HG2	2.11	0.51
1:A:523:ASP:HA	1:A:531:LYS:NZ	2.25	0.51
1:A:20:ALA:HB2	1:A:188:TYR:CZ	2.45	0.51
1:A:593:LYS:HG3	1:A:594:LYS:H	1.74	0.51
1:A:1189:GLY:CA	1:A:1196:THR:HG21	2.40	0.51
1:A:1000:GLN:HA	1:A:1012:LYS:HB2	1.93	0.50
1:B:1182:ALA:O	1:B:1183:ASP:C	2.49	0.50
1:A:317:LEU:HD21	1:A:324:ILE:HD11	1.93	0.50
1:A:1155:GLU:HG2	1:B:1173:GLU:OE2	2.12	0.50
1:B:91:LEU:HD11	1:B:116:ILE:HD12	1.93	0.50
1:B:1012:LYS:O	1:B:1013:PHE:HB2	2.11	0.50
1:A:558:ARG:HG2	1:A:560:ASN:ND2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:TRP:HB3	1:A:48:ARG:HD3	1.93	0.50
1:B:591:TYR:C	1:B:593:LYS:N	2.63	0.50
1:A:1051:LYS:HE3	1:A:1100:ARG:CZ	2.42	0.49
1:A:739:GLN:HE22	1:A:777:ASN:HB3	1.77	0.49
1:A:976:HIS:CD2	1:B:1003:LYS:HZ2	2.16	0.49
1:B:121:LEU:C	1:B:121:LEU:HD23	2.32	0.49
1:A:385:ALA:O	1:A:386:LYS:HB2	2.13	0.49
1:A:591:TYR:C	1:A:593:LYS:N	2.64	0.49
1:B:1225:ASP:O	1:B:1229:ARG:HG3	2.12	0.49
1:B:210:PRO:O	1:B:213:PRO:HD3	2.11	0.49
1:B:896:LYS:CB	1:B:941:LEU:HD21	2.41	0.49
1:A:565:THR:HG21	1:A:609:ALA:HB3	1.93	0.49
1:A:955:LYS:HD2	1:B:210:PRO:HG3	1.94	0.49
1:B:5:MET:SD	1:B:184:GLU:HG2	2.52	0.49
1:A:976:HIS:HE1	1:B:60:GLU:O	1.95	0.49
1:A:949:SER:HA	1:A:952:TYR:CE2	2.48	0.49
1:A:1094:GLY:HA3	1:A:1120:PRO:HG3	1.95	0.49
1:A:635:THR:CG2	1:A:639:PHE:HB3	2.42	0.49
1:A:964:GLY:O	1:A:968:ASP:HB2	2.13	0.49
1:A:1200:THR:HG21	1:A:1202:MET:HB2	1.95	0.48
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.96	0.48
1:A:635:THR:HG21	1:A:639:PHE:CB	2.43	0.48
1:B:779:GLU:HB3	1:B:783:ARG:NH2	2.28	0.48
1:A:212:HIS:HE1	1:B:950:ASP:OD2	1.96	0.48
1:B:1231:LYS:HG3	1:B:1232:LYS:N	2.29	0.48
1:B:522:MET:SD	1:B:526:LEU:HD13	2.53	0.48
1:B:936:GLY:O	1:B:938:LYS:HG2	2.13	0.48
1:B:1231:LYS:HG3	1:B:1232:LYS:H	1.78	0.48
1:A:1165:HIS:NE2	1:B:1165:HIS:CD2	2.82	0.48
1:B:805:LEU:HB2	1:B:825:THR:HB	1.95	0.48
1:A:1219:THR:HG21	6:B:2298:HOH:O	2.14	0.48
1:A:345:CYS:O	1:A:349:VAL:HG13	2.14	0.48
1:A:526:LEU:O	1:A:531:LYS:HE3	2.13	0.48
1:A:950:ASP:OD2	1:B:212:HIS:HE1	1.97	0.48
1:B:124:PHE:HB3	1:B:367:SER:HB2	1.95	0.48
1:B:499:ASP:OD2	1:B:502:GLU:HB2	2.14	0.48
1:A:1165:HIS:CD2	1:B:1165:HIS:NE2	2.82	0.48
1:A:593:LYS:CG	1:A:594:LYS:H	2.24	0.48
1:A:1200:THR:HG23	1:A:1202:MET:CE	2.43	0.47
1:A:698:VAL:HG13	6:A:2217:HOH:O	2.13	0.47
1:A:805:LEU:HD12	1:A:829:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:LYS:HE2	1:A:949:SER:HB2	1.95	0.47
1:A:994:TYR:HD2	3:A:2236:1TP:H5A1	1.78	0.47
1:A:9:ASP:HA	1:A:179:GLU:O	2.14	0.47
1:B:243:VAL:O	1:B:247:MET:HG3	2.14	0.47
1:B:766:PRO:HB2	1:B:769:THR:HG23	1.94	0.47
1:A:1015:ALA:CB	1:B:1185:SER:HB2	2.44	0.47
1:A:667:LEU:HB3	1:A:854:LYS:HA	1.95	0.47
1:A:1209:GLY:O	1:B:429:GLY:HA2	2.14	0.47
1:B:9:ASP:HA	1:B:179:GLU:O	2.14	0.47
1:B:590:ALA:O	1:B:591:TYR:C	2.51	0.47
1:B:581:ASP:O	1:B:585:LYS:HG2	2.15	0.47
1:A:434:ASN:ND2	1:A:466:SER:CB	2.78	0.46
1:A:499:ASP:OD2	1:A:502:GLU:HB2	2.16	0.46
1:B:630:LYS:HG3	1:B:632:GLU:OE2	2.15	0.46
1:A:351:ARG:HD3	1:A:353:GLU:HB2	1.97	0.46
1:A:222:PRO:HD3	1:B:124:PHE:CE2	2.50	0.46
1:A:1189:GLY:HA3	1:A:1196:THR:HG21	1.98	0.46
1:A:483:ARG:HA	1:A:503:GLY:O	2.14	0.46
1:B:701:HIS:CE1	1:B:746:MET:HG3	2.51	0.46
1:A:1227:SER:HA	1:A:1230:THR:HG22	1.96	0.46
1:A:520:GLU:HG3	1:A:521:ASP:N	2.30	0.46
1:A:297:ILE:HB	1:A:379:TYR:CE2	2.51	0.46
1:A:1068:TYR:HD1	1:A:1096:TRP:CE3	2.33	0.46
1:A:1230:THR:O	1:A:1231:LYS:C	2.55	0.46
1:A:116:ILE:HD11	1:A:129:ASP:HB3	1.98	0.46
1:A:233:ASN:HB2	1:A:234:PRO:HD3	1.97	0.46
1:B:1180:GLY:O	1:B:1182:ALA:N	2.38	0.46
1:A:873:ALA:HA	1:A:959:ILE:HD13	1.98	0.45
1:A:496:GLY:HA2	1:A:527:PRO:HG2	1.97	0.45
1:A:949:SER:HA	1:A:952:TYR:CZ	2.51	0.45
1:B:290:LEU:HD21	1:B:376:LYS:HD3	1.98	0.45
1:B:1077:ARG:HG3	1:B:1130:ALA:O	2.17	0.45
1:B:532:ARG:NH1	1:B:625:ALA:O	2.47	0.45
1:A:1232:LYS:NZ	1:A:1232:LYS:HB3	2.31	0.45
1:A:580:VAL:O	1:A:584:LYS:HG3	2.16	0.45
1:B:675:ARG:HD3	6:B:2271:HOH:O	2.16	0.45
1:A:110:HIS:CD2	1:A:169:HIS:CD2	2.94	0.45
1:A:635:THR:HG21	1:A:639:PHE:CD2	2.52	0.44
1:A:24:VAL:HG13	1:B:881:MET:HE1	1.98	0.44
1:B:56:LEU:HD23	1:B:58:ILE:HD11	1.98	0.44
1:A:1124:VAL:O	1:A:1127:PHE:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:HIS:CE1	1:A:746:MET:HG3	2.52	0.44
1:B:997:THR:HG21	3:B:2236:1TP:H4A3	1.99	0.44
1:B:460:SER:HB3	1:B:746:MET:CE	2.47	0.44
1:A:1219:THR:CG2	1:A:1220:SER:N	2.81	0.44
1:A:27:ILE:CD1	1:A:1013:PHE:CE2	2.96	0.44
1:B:467:HIS:CE1	1:B:480:LEU:HB3	2.53	0.43
1:B:670:SER:HA	1:B:673:GLU:OE1	2.17	0.43
1:A:1015:ALA:HB3	1:B:1185:SER:HB2	1.99	0.43
1:B:20:ALA:HB2	1:B:188:TYR:CZ	2.53	0.43
1:B:131:TYR:CE2	1:B:339:PRO:HB2	2.53	0.43
6:A:2024:HOH:O	1:B:871:ASP:HB3	2.17	0.43
1:A:1219:THR:HG22	1:A:1222:GLN:H	1.82	0.43
1:A:643:VAL:O	1:A:647:LEU:HG	2.17	0.43
1:B:1000:GLN:H	1:B:1000:GLN:NE2	2.16	0.43
1:B:240:PRO:HB3	1:B:309:VAL:HG21	2.00	0.43
1:B:828:PHE:CE2	1:B:1057:GLU:HG3	2.53	0.43
1:A:1180:GLY:O	1:A:1181:LYS:HB2	2.18	0.43
1:B:1006:PRO:HG3	1:B:1095:TYR:OH	2.19	0.43
1:B:808:PHE:N	1:B:808:PHE:CD2	2.85	0.43
1:B:598:ILE:HD13	1:B:601:MET:HE1	1.99	0.43
1:B:667:LEU:HB3	1:B:854:LYS:HA	2.00	0.43
1:A:422:PHE:O	1:A:465:ILE:HA	2.17	0.43
1:A:534:ILE:HG23	1:A:539:LEU:HB2	2.00	0.43
1:B:110:HIS:CE1	1:B:157:HIS:NE2	2.80	0.43
1:A:1156:LEU:HD12	1:A:1156:LEU:C	2.38	0.43
1:A:361:GLY:HA3	1:A:390:PHE:CZ	2.53	0.43
1:A:586:SER:O	1:A:589:LYS:HB3	2.18	0.43
1:B:1105:LEU:HD23	1:B:1105:LEU:HA	1.84	0.43
1:A:591:TYR:O	1:A:593:LYS:N	2.51	0.43
1:B:589:LYS:HE2	1:B:589:LYS:HB3	1.76	0.43
1:A:131:TYR:CE2	1:A:339:PRO:HB2	2.54	0.42
1:B:1166:MET:O	1:B:1169:THR:HG22	2.19	0.42
1:A:840:CYS:HB2	3:A:2236:1TP:O22	2.20	0.42
1:A:429:GLY:HA2	1:B:1209:GLY:O	2.18	0.42
1:A:953:THR:HG22	6:A:2294:HOH:O	2.19	0.42
1:B:1156:LEU:C	1:B:1156:LEU:HD12	2.39	0.42
1:B:1200:THR:HG23	1:B:1202:MET:CE	2.48	0.42
1:A:87:SER:HA	1:A:129:ASP:HB3	2.00	0.42
1:B:796:LEU:HA	1:B:1050:LEU:HD11	2.01	0.42
1:A:677:VAL:O	1:B:1216:ARG:HD2	2.19	0.42
1:A:560:ASN:H	1:A:560:ASN:HD22	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:ALA:O	1:A:907:LYS:HE3	2.19	0.42
3:B:2236:1TP:C35	3:B:2236:1TP:C2	2.89	0.42
1:A:1003:LYS:NZ	1:B:976:HIS:HD2	2.18	0.42
1:A:121:LEU:HD23	1:A:122:SER:N	2.35	0.42
1:A:497:ILE:HG13	1:A:498:TYR:CD1	2.54	0.42
1:A:700:PRO:HG2	1:A:814:GLY:HA2	2.01	0.42
1:A:808:PHE:CD2	1:A:808:PHE:N	2.85	0.42
1:A:953:THR:HG23	6:B:2077:HOH:O	2.19	0.42
1:B:673:GLU:O	1:B:674:LYS:C	2.57	0.42
1:A:1132:ASN:ND2	1:A:1136:VAL:HG13	2.34	0.42
1:B:27:ILE:HD12	1:B:1013:PHE:CZ	2.55	0.42
1:A:1007:THR:OG1	1:A:1021:GLY:HA2	2.20	0.42
1:A:978:LEU:O	1:A:1062:PRO:HG2	2.20	0.42
1:B:635:THR:HG22	1:B:636:ASN:O	2.20	0.42
1:A:371:SER:HB2	1:A:372:PRO:CD	2.50	0.42
1:B:1076:LEU:HD13	1:B:1086:VAL:HG21	2.01	0.42
1:A:240:PRO:HB3	1:A:309:VAL:HG21	2.02	0.41
1:A:467:HIS:C	1:A:468:LEU:HD23	2.40	0.41
1:A:245:GLU:HG3	1:A:246:TYR:N	2.35	0.41
1:A:688:ASN:HB3	1:A:759:GLU:O	2.20	0.41
1:B:27:ILE:CD1	1:B:1013:PHE:CE2	3.04	0.41
1:B:1046:LYS:HG3	6:B:2402:HOH:O	2.19	0.41
1:B:67:ALA:O	1:B:71:VAL:HG23	2.20	0.41
1:B:978:LEU:O	1:B:1062:PRO:HG2	2.20	0.41
1:A:110:HIS:CE1	1:A:157:HIS:NE2	2.85	0.41
1:A:422:PHE:HE1	1:A:468:LEU:HG	1.85	0.41
1:A:562:ILE:HD12	1:A:562:ILE:N	2.34	0.41
1:B:1055:GLU:O	1:B:1104:ARG:NH1	2.52	0.41
1:A:1043:GLY:HA3	1:A:1084:GLN:O	2.21	0.41
1:B:1006:PRO:HG2	1:B:1009:ALA:HB2	2.03	0.41
1:A:266:ALA:HA	1:A:267:PRO:HD3	1.89	0.41
1:A:544:ILE:O	1:A:544:ILE:HG23	2.20	0.41
1:B:11:ASN:HD21	1:B:112:THR:HG21	1.85	0.41
1:B:163:SER:O	1:B:164:ASN:HB2	2.19	0.41
1:B:632:GLU:O	1:B:632:GLU:CD	2.59	0.41
1:B:80:LEU:HA	1:B:80:LEU:HD23	1.86	0.41
1:A:1200:THR:HG23	1:A:1201:PRO:CD	2.49	0.41
1:A:126:ASP:HA	1:A:329:ARG:HD3	2.03	0.41
1:A:881:MET:HE1	1:B:24:VAL:HG13	2.02	0.41
1:B:819:PRO:O	1:B:823:VAL:HG13	2.21	0.41
1:A:553:VAL:HG21	1:A:605:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ALA:O	1:B:51:ILE:HG23	2.21	0.41
1:B:823:VAL:HG21	1:B:1049:PHE:CE2	2.56	0.41
1:B:961:GLY:HA3	1:B:965:TRP:CE3	2.55	0.41
1:A:465:ILE:HG22	1:A:467:HIS:CE1	2.56	0.41
1:B:1104:ARG:HB2	6:B:2429:HOH:O	2.20	0.41
1:B:587:ILE:O	1:B:590:ALA:O	2.39	0.41
1:B:786:VAL:HG12	1:B:801:PHE:O	2.21	0.41
1:A:1034:TYR:HB3	1:A:1175:PHE:CZ	2.57	0.40
1:A:239:VAL:HG22	1:A:240:PRO:HD3	2.00	0.40
1:A:691:GLN:HG2	1:A:736:PHE:CE2	2.56	0.40
1:A:1055:GLU:O	1:A:1104:ARG:NH1	2.53	0.40
1:A:459:LYS:HB3	1:B:1198:ASP:HB2	2.02	0.40
1:A:422:PHE:HD1	1:A:466:SER:HB2	1.86	0.40
1:B:439:LYS:NZ	1:B:439:LYS:HB2	2.36	0.40
1:B:686:PRO:HB2	1:B:724:LEU:HD21	2.04	0.40
1:A:114:ARG:NE	1:A:123:ILE:HA	2.36	0.40
1:A:132:ALA:HA	1:B:135:GLN:HE21	1.86	0.40
1:B:56:LEU:HG	1:B:58:ILE:HG12	2.02	0.40
1:B:964:GLY:O	1:B:968:ASP:HB2	2.21	0.40
1:A:154:LEU:HD22	1:A:158:LEU:CD1	2.51	0.40
1:A:289:HIS:CE1	1:A:293:LYS:HE2	2.57	0.40
1:A:357:LYS:HE3	1:A:359:LEU:HD21	2.03	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%)	1168 (95%)	47 (4%)	14 (1%)	14	13
1	B	1229/1231 (100%)	1183 (96%)	40 (3%)	6 (0%)	29	31
All	All	2458/2462 (100%)	2351 (96%)	87 (4%)	20 (1%)	19	20

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	732	LYS
1	A	593	LYS
1	A	594	LYS
1	A	595	GLY
1	A	629	THR
1	A	630	LYS
1	B	629	THR
1	A	1178	ALA
1	A	1181	LYS
1	A	1182	ALA
1	A	1231	LYS
1	B	1183	ASP
1	B	591	TYR
1	A	87	SER
1	A	589	LYS
1	A	628	GLU
1	B	1182	ALA
1	B	1181	LYS
1	A	557	GLY
1	A	495	VAL

### 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%)	942 (96%)	36 (4%)	34	43
1	B	978/978 (100%)	957 (98%)	21 (2%)	53	65
All	All	1956/1956 (100%)	1899 (97%)	57 (3%)	42	52

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	154	LEU
1	A	175	ARG

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Mol	Chain	Res	Type
1	A	194	LEU
1	A	198	LYS
1	A	204	ARG
1	A	211	GLU
1	A	226	PHE
1	A	317	LEU
1	A	327	LEU
1	A	351	ARG
1	A	570	LEU
1	A	573	VAL
1	A	617	LYS
1	A	624	ASP
1	A	632	GLU
1	A	636	ASN
1	A	643	VAL
1	A	687	GLU
1	A	714	LEU
1	A	720	ASN
1	A	777	ASN
1	A	808	PHE
1	A	849	PRO
1	A	858	LEU
1	A	893	LEU
1	A	939	ASP
1	A	953	THR
1	A	1000	GLN
1	A	1088	ASN
1	A	1136	VAL
1	A	1147	ARG
1	A	1170	ASN
1	A	1175	PHE
1	A	1183	ASP
1	A	1196	THR
1	B	194	LEU
1	B	226	PHE
1	B	290	LEU
1	B	317	LEU
1	B	342	LEU
1	B	359	LEU
1	B	463	ILE
1	B	509	THR
1	B	583	LEU

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Mol	Chain	Res	Type
1	B	624	ASP
1	B	632	GLU
1	B	635	THR
1	B	714	LEU
1	B	754	ILE
1	B	823	VAL
1	B	836	ASN
1	B	849	PRO
1	B	931	LYS
1	B	939	ASP
1	B	1000	GLN
1	B	1088	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	46	GLN
1	A	110	HIS
1	A	169	HIS
1	A	212	HIS
1	A	289	HIS
1	A	389	HIS
1	A	434	ASN
1	A	467	HIS
1	A	513	ASN
1	A	560	ASN
1	A	602	ASN
1	A	636	ASN
1	A	641	ASN
1	A	739	GLN
1	A	777	ASN
1	A	836	ASN
1	A	866	ASN
1	A	976	HIS
1	A	1000	GLN
1	A	1088	ASN
1	A	1170	ASN
1	B	11	ASN
1	B	46	GLN
1	B	96	ASN
1	B	110	HIS

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Mol	Chain	Res	Type
1	B	169	HIS
1	B	212	HIS
1	B	434	ASN
1	B	602	ASN
1	B	688	ASN
1	B	750	ASN
1	B	777	ASN
1	B	866	ASN
1	B	976	HIS
1	B	1000	GLN
1	B	1047	GLN
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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SF4	A	2234	1	0,12,12	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	1TP	A	2236	4	24,33,33	5.01	12 (50%)	33,51,51	3.10	15 (45%)
2	SF4	B	2235	1	0,12,12	0.00	-	-		
2	SF4	A	2233	1	0,12,12	0.00	-	-		
3	1TP	B	2236	4	24,33,33	5.37	12 (50%)	33,51,51	3.79	13 (39%)
2	SF4	B	2234	1	0,12,12	0.00	-	-		
2	SF4	B	2233	1	0,12,12	0.00	-	-		
2	SF4	A	2235	1	0,12,12	0.00	-	-		

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	2234	1	-	-	0/6/5/5
3	1TP	A	2236	4	1/1/8/8	8/18/45/45	0/2/2/2
2	SF4	B	2235	1	-	-	0/6/5/5
2	SF4	A	2233	1	-	-	0/6/5/5
3	1TP	B	2236	4	1/1/8/8	5/18/45/45	0/2/2/2
2	SF4	B	2234	1	-	-	0/6/5/5
2	SF4	B	2233	1	-	-	0/6/5/5
2	SF4	A	2235	1	-	-	0/6/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2236	1TP	C35-C15	21.16	1.71	1.53
3	A	2236	1TP	C35-C15	15.63	1.66	1.53
3	A	2236	1TP	O25-C15	12.00	1.60	1.43
3	B	2236	1TP	C2'-N1'	8.78	1.48	1.34
3	A	2236	1TP	C2-S1	-7.61	1.68	1.83
3	B	2236	1TP	C5-S1	6.79	1.89	1.83
3	A	2236	1TP	C4A-C4	5.69	1.63	1.52
3	B	2236	1TP	C4'-N3'	4.95	1.42	1.35
3	A	2236	1TP	C4'-N3'	4.93	1.42	1.35
3	A	2236	1TP	C2'-N1'	4.15	1.41	1.34
3	B	2236	1TP	C5A-C5	4.15	1.62	1.52
3	A	2236	1TP	C5A-C5	4.10	1.62	1.52
3	B	2236	1TP	C7'-C5'	-3.83	1.45	1.51
3	A	2236	1TP	C6'-N1'	3.65	1.42	1.34
3	B	2236	1TP	P2-O23	-3.41	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2236	1TP	P2-O21	3.23	1.61	1.50
3	B	2236	1TP	O5G-C5B	-3.13	1.31	1.44
3	A	2236	1TP	P2-O22	-3.08	1.43	1.54
3	A	2236	1TP	C7'-N3	2.67	1.51	1.47
3	B	2236	1TP	C2-S1	2.55	1.88	1.83
3	B	2236	1TP	P2-O22	-2.33	1.45	1.54
3	B	2236	1TP	C2'-N3'	-2.21	1.30	1.34
3	B	2236	1TP	O25-C15	2.18	1.46	1.43
3	A	2236	1TP	C2'-N3'	-2.04	1.30	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2236	1TP	C2-S1-C5	-13.34	81.76	94.02
3	A	2236	1TP	C15-C2-N3	11.24	127.15	109.35
3	B	2236	1TP	C15-C2-N3	9.07	123.71	109.35
3	B	2236	1TP	C2A-C2'-N1'	7.94	125.88	117.14
3	B	2236	1TP	C4-C5-S1	6.79	114.88	104.81
3	A	2236	1TP	C2A-C2'-N1'	6.29	124.06	117.14
3	A	2236	1TP	N1'-C2'-N3'	-4.59	117.65	125.54
3	B	2236	1TP	N1'-C2'-N3'	-4.55	117.70	125.54
3	A	2236	1TP	C7'-N3-C4	4.20	122.40	114.45
3	A	2236	1TP	C2'-N3'-C4'	4.17	124.58	118.08
3	B	2236	1TP	C5A-C5-S1	-3.98	101.62	112.64
3	A	2236	1TP	O5G-C5B-C5A	3.82	122.19	109.09
3	A	2236	1TP	C5A-C5-C4	-3.52	111.27	116.14
3	B	2236	1TP	C2'-N3'-C4'	3.43	123.43	118.08
3	B	2236	1TP	O5G-C5B-C5A	3.25	120.23	109.09
3	A	2236	1TP	C5A-C5-S1	-2.90	104.62	112.64
3	B	2236	1TP	O23-P2-O22	2.77	118.21	107.64
3	A	2236	1TP	C5'-C7'-N3	-2.76	108.19	113.17
3	A	2236	1TP	O23-P2-O22	2.53	117.32	107.64
3	A	2236	1TP	C6'-N1'-C2'	2.49	120.19	115.96
3	A	2236	1TP	C5'-C4'-N4'	2.39	125.58	122.19
3	A	2236	1TP	C7'-C5'-C4'	2.30	124.89	122.56
3	B	2236	1TP	C5A-C5-C4	-2.26	113.02	116.14
3	B	2236	1TP	N4'-C4'-N3'	-2.18	113.95	117.03
3	B	2236	1TP	C5'-C4'-N4'	2.17	125.26	122.19
3	A	2236	1TP	N4'-C4'-N3'	-2.11	114.05	117.03
3	A	2236	1TP	O25-C15-C35	2.10	112.95	108.41
3	B	2236	1TP	C6'-N1'-C2'	2.10	119.54	115.96

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	2236	1TP	C4
3	B	2236	1TP	C4

All (13) torsion outliers are listed below:

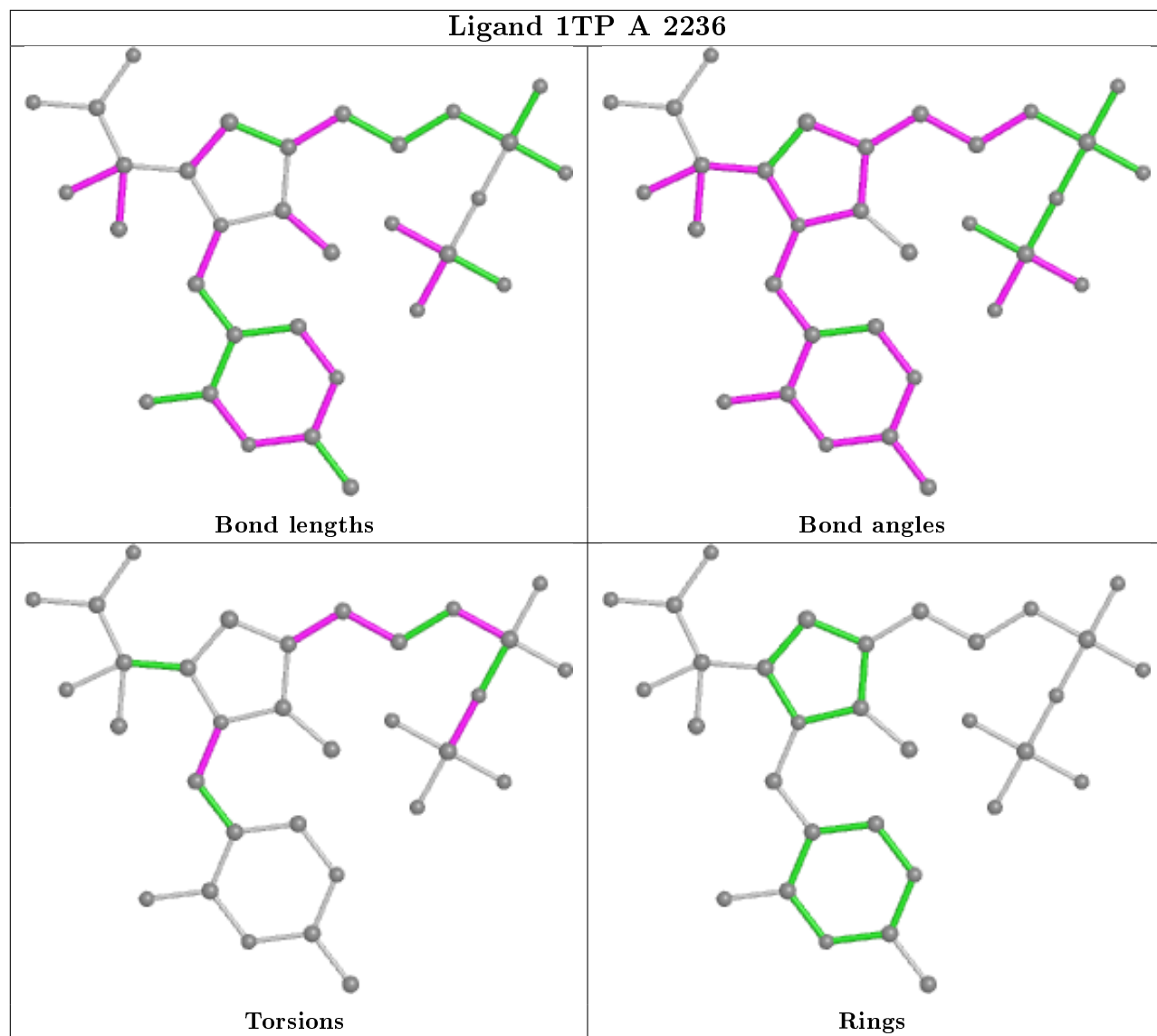
Mol	Chain	Res	Type	Atoms
3	A	2236	1TP	S1-C5-C5A-C5B
3	A	2236	1TP	C4-C5-C5A-C5B
3	A	2236	1TP	C5-C5A-C5B-O5G
3	A	2236	1TP	P1-O11-P2-O23
3	B	2236	1TP	S1-C5-C5A-C5B
3	B	2236	1TP	C4-C5-C5A-C5B
3	B	2236	1TP	C5'-C7'-N3-C4
3	A	2236	1TP	C5'-C7'-N3-C4
3	A	2236	1TP	C5'-C7'-N3-C2
3	B	2236	1TP	P1-O11-P2-O22
3	A	2236	1TP	C5B-O5G-P1-O11
3	B	2236	1TP	C5'-C7'-N3-C2
3	A	2236	1TP	C5B-O5G-P1-O12

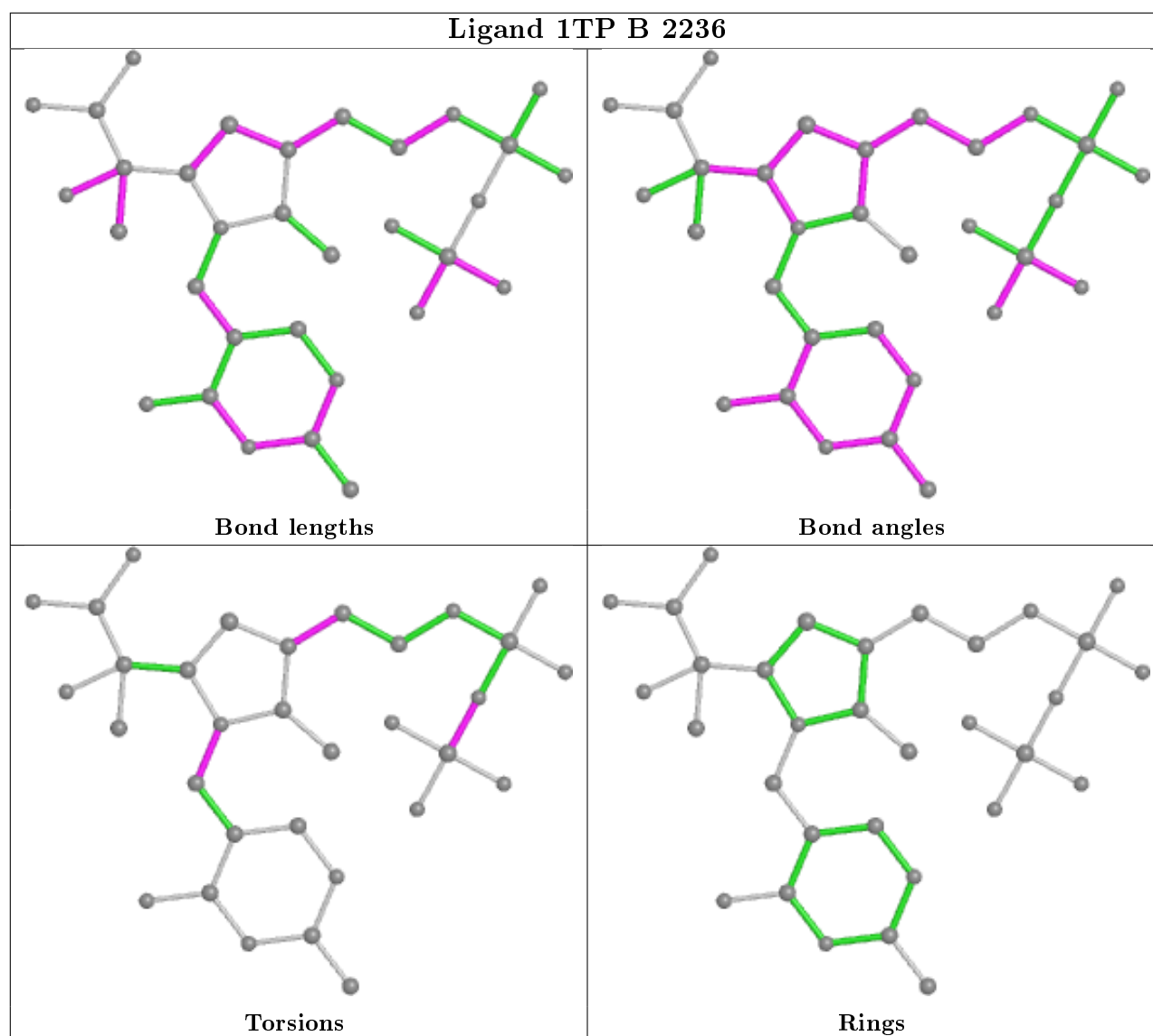
There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2236	1TP	7	0
3	B	2236	1TP	8	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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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(Å²)	Q<0.9	
1	A	1231/1231 (100%)	0.21	95 (7%)	13	20	7, 22, 62, 118	0
1	B	1231/1231 (100%)	-0.03	38 (3%)	49	59	7, 19, 46, 104	0
All	All	2462/2462 (100%)	0.09	133 (5%)	25	36	7, 20, 57, 118	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1232	LYS	8.7
1	B	631	ALA	8.3
1	A	1176	ALA	8.1
1	B	1176	ALA	8.1
1	A	1232	LYS	6.9
1	A	594	LYS	6.7
1	A	627	ALA	6.6
1	A	633	PRO	6.3
1	A	626	PRO	6.1
1	A	629	THR	6.0
1	A	628	GLU	5.6
1	A	619	PRO	5.5
1	A	1177	PRO	5.4
1	A	634	MET	5.4
1	A	1175	PHE	5.3
1	B	1231	LYS	4.9
1	B	1181	LYS	4.7
1	B	1183	ASP	4.7
1	A	625	ALA	4.6
1	A	576	PHE	4.6
1	A	631	ALA	4.5
1	A	596	GLU	4.4
1	A	535	ALA	4.3
1	A	598	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	621	SER	4.3
1	A	591	TYR	4.3
1	B	715	VAL	4.3
1	A	630	LYS	4.2
1	B	1165	HIS	4.2
1	A	1180	GLY	4.2
1	B	1178	ALA	4.1
1	A	1179	GLY	4.0
1	A	1231	LYS	4.0
1	A	593	LYS	3.8
1	A	600	LYS	3.7
1	A	1165	HIS	3.6
1	B	1228	LYS	3.6
1	B	1172	PHE	3.6
1	A	588	HIS	3.6
1	A	577	GLU	3.6
1	A	530	ILE	3.5
1	A	517	SER	3.5
1	A	518	SER	3.4
1	B	1174	SER	3.4
1	B	1180	GLY	3.4
1	A	553	VAL	3.4
1	A	620	ASP	3.4
1	A	618	TYR	3.3
1	A	595	GLY	3.3
1	A	597	LYS	3.3
1	A	624	ASP	3.3
1	B	291	ALA	3.2
1	A	632	GLU	3.2
1	A	554	GLY	3.2
1	B	1175	PHE	3.2
1	A	520	GLU	3.2
1	A	623	LYS	3.1
1	A	523	ASP	3.1
1	A	734	TYR	3.1
1	B	628	GLU	3.1
1	A	601	MET	3.0
1	B	1182	ALA	3.0
1	A	608	GLN	3.0
1	A	91	LEU	3.0
1	A	590	ALA	3.0
1	B	1230	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	552	ASP	2.9
1	A	599	VAL	2.9
1	A	1181	LYS	2.9
1	A	1174	SER	2.9
1	A	589	LYS	2.8
1	B	630	LYS	2.8
1	A	936	GLY	2.8
1	A	528	SER	2.8
1	A	532	ARG	2.8
1	A	611	THR	2.8
1	A	758	LYS	2.8
1	A	716	GLY	2.7
1	A	1178	ALA	2.7
1	B	292	ALA	2.7
1	A	729	LYS	2.7
1	A	592	GLY	2.7
1	A	605	ALA	2.7
1	A	622	TRP	2.6
1	A	712	GLU	2.6
1	A	616	PHE	2.6
1	B	629	THR	2.6
1	A	524	LYS	2.6
1	A	582	LEU	2.6
1	A	2	GLY	2.5
1	A	1169	THR	2.5
1	B	593	LYS	2.5
1	A	526	LEU	2.5
1	A	726	ALA	2.5
1	A	603	THR	2.5
1	B	91	LEU	2.5
1	A	581	ASP	2.5
1	A	90	LEU	2.5
1	A	506	ASP	2.4
1	A	527	PRO	2.4
1	B	1177	PRO	2.4
1	A	602	ASN	2.4
1	A	585	LYS	2.4
1	B	596	GLU	2.4
1	A	92	LEU	2.4
1	B	92	LEU	2.4
1	B	4	LYS	2.3
1	B	599	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	719	ALA	2.3
1	B	732	LYS	2.3
1	A	521	ASP	2.2
1	B	634	MET	2.2
1	A	710	LYS	2.2
1	A	635	THR	2.2
1	A	519	LEU	2.2
1	A	715	VAL	2.1
1	A	717	ALA	2.1
1	B	1227	SER	2.1
1	A	783	ARG	2.1
1	B	90	LEU	2.1
1	A	609	ALA	2.1
1	B	717	ALA	2.1
1	B	712	GLU	2.1
1	B	714	LEU	2.1
1	A	604	ASP	2.1
1	B	95	PRO	2.1
1	A	756	PRO	2.1
1	A	538	LYS	2.0
1	A	711	GLU	2.0
1	A	1182	ALA	2.0
1	B	354	ALA	2.0
1	B	124	PHE	2.0
1	A	617	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

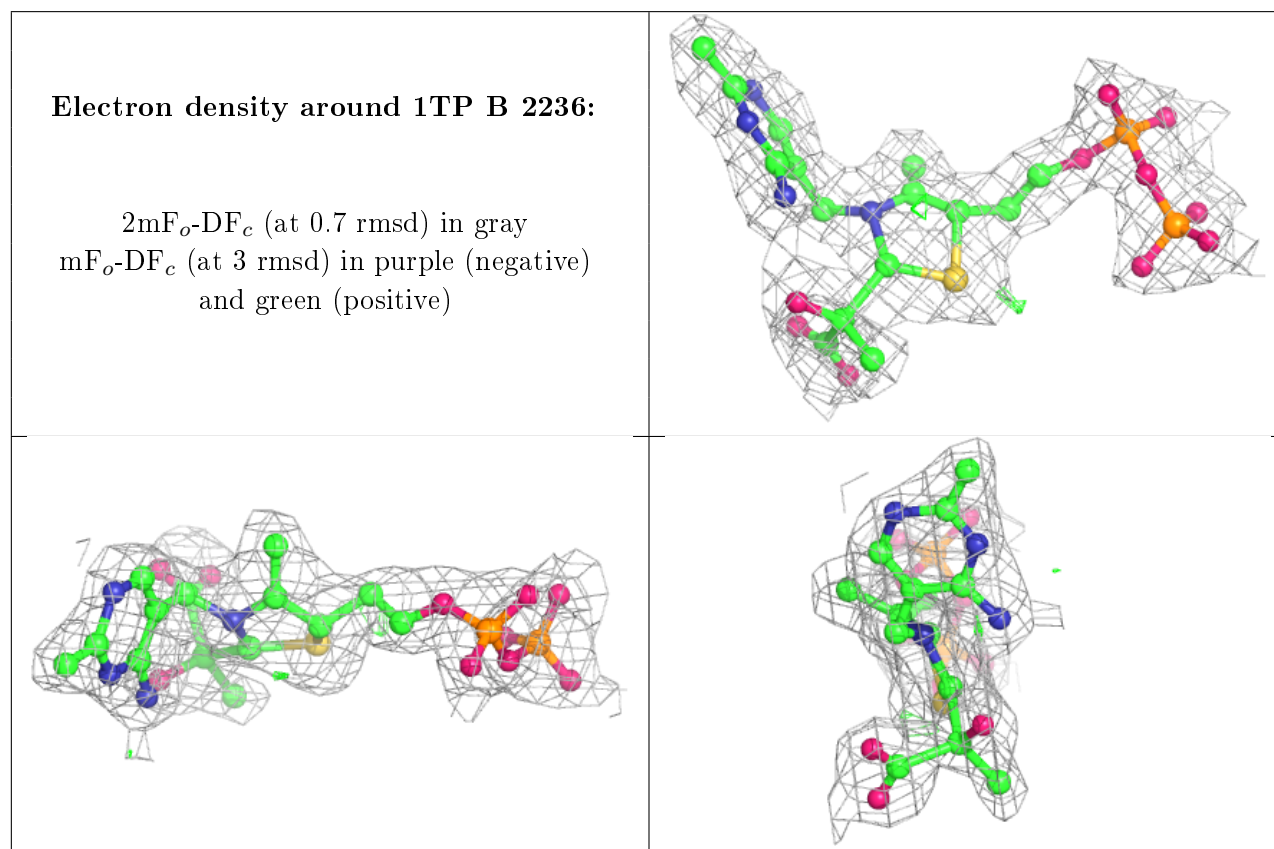
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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.

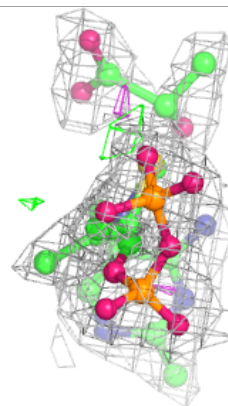
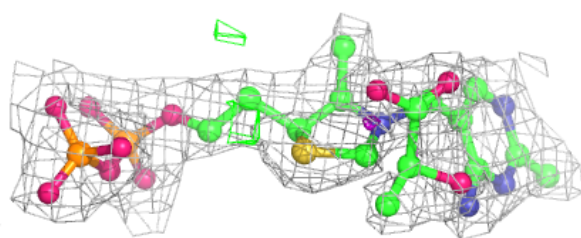
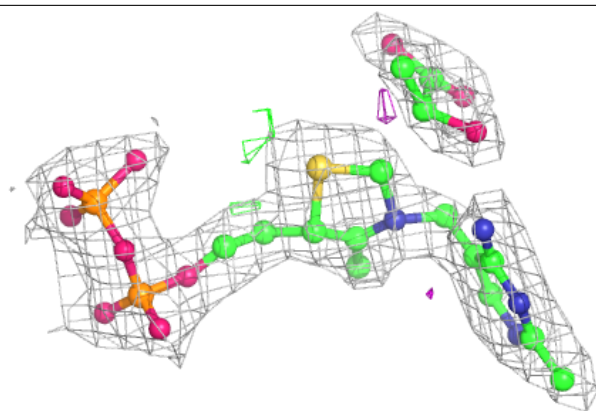
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	B	2238	1/1	0.96	0.10	46,46,46,46	0
5	CA	A	2238	1/1	0.96	0.15	57,57,57,57	0
3	1TP	B	2236	32/32	0.97	0.16	6,15,32,32	0
3	1TP	A	2236	32/32	0.97	0.18	14,20,39,43	0
2	SF4	B	2233	8/8	0.97	0.07	19,20,21,23	0
2	SF4	A	2235	8/8	0.97	0.05	15,18,19,20	0
4	MG	A	2237	1/1	0.98	0.08	9,9,9,9	0
2	SF4	A	2234	8/8	0.98	0.05	22,25,25,27	0
2	SF4	B	2234	8/8	0.98	0.05	13,14,15,17	0
2	SF4	B	2235	8/8	0.98	0.06	10,12,13,13	0
2	SF4	A	2233	8/8	0.98	0.09	27,31,32,33	0
4	MG	B	2237	1/1	0.99	0.10	4,4,4,4	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 1TP 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.