



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:49 am GMT

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

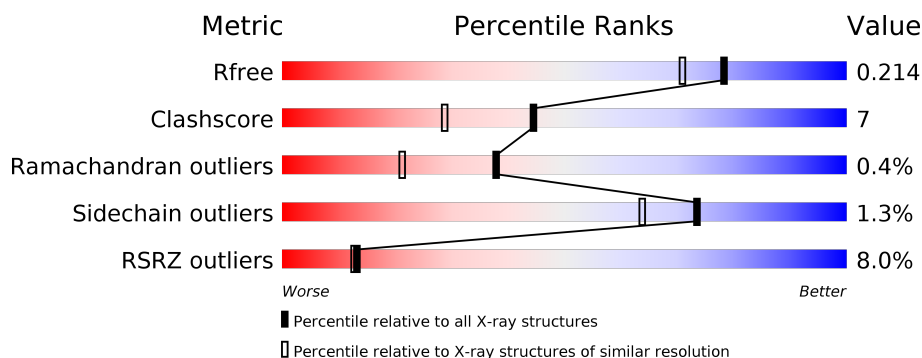
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	100719	7172 (1.80-1.76)
Clashscore	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>82%</div> <div>17%</div> </div>
1	B	1231	<div> <div>5%</div> <div>86%</div> <div>13%</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
4	PYR	B	3237	-	-	-	X
6	CA	A	3239	-	-	-	X

## 2 Entry composition [i](#)

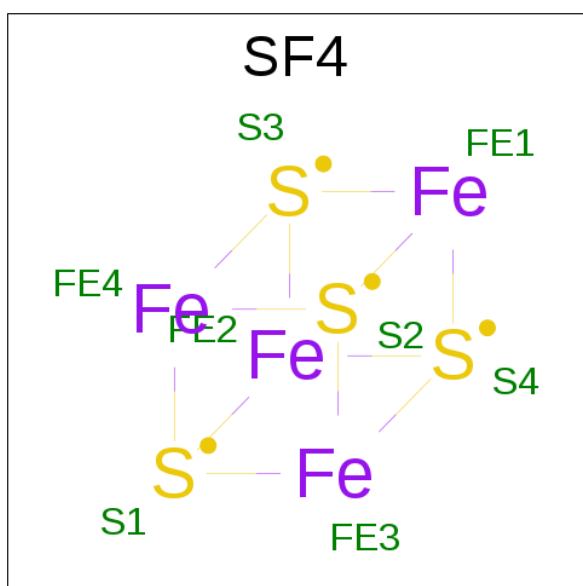
There are 7 unique types of molecules in this entry. The entry contains 20099 atoms, of which 0 are hydrogens and 0 are deuteriums.

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



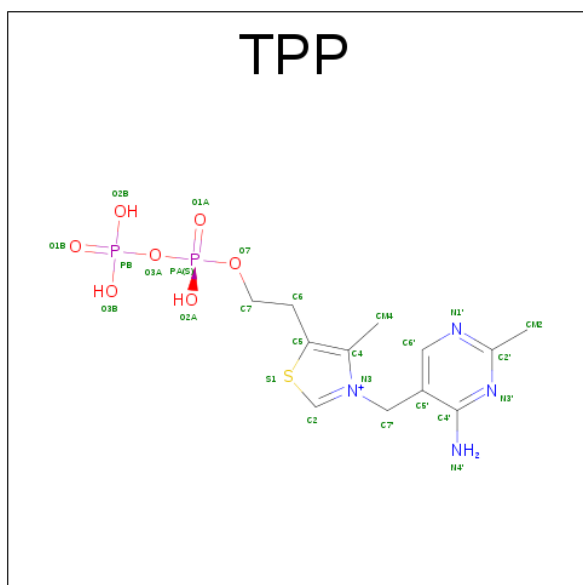
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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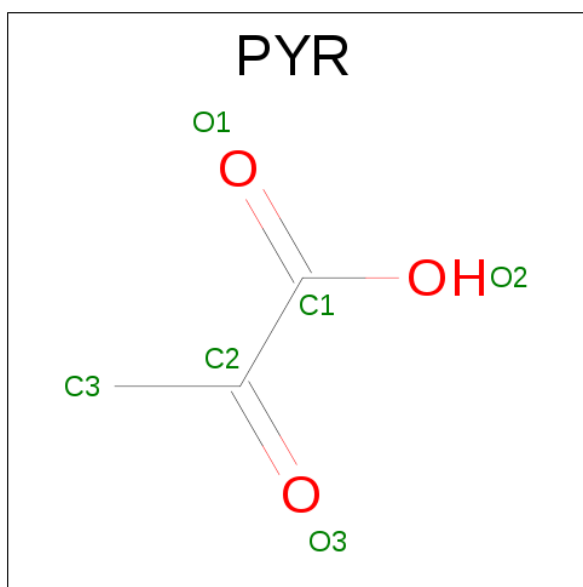
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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



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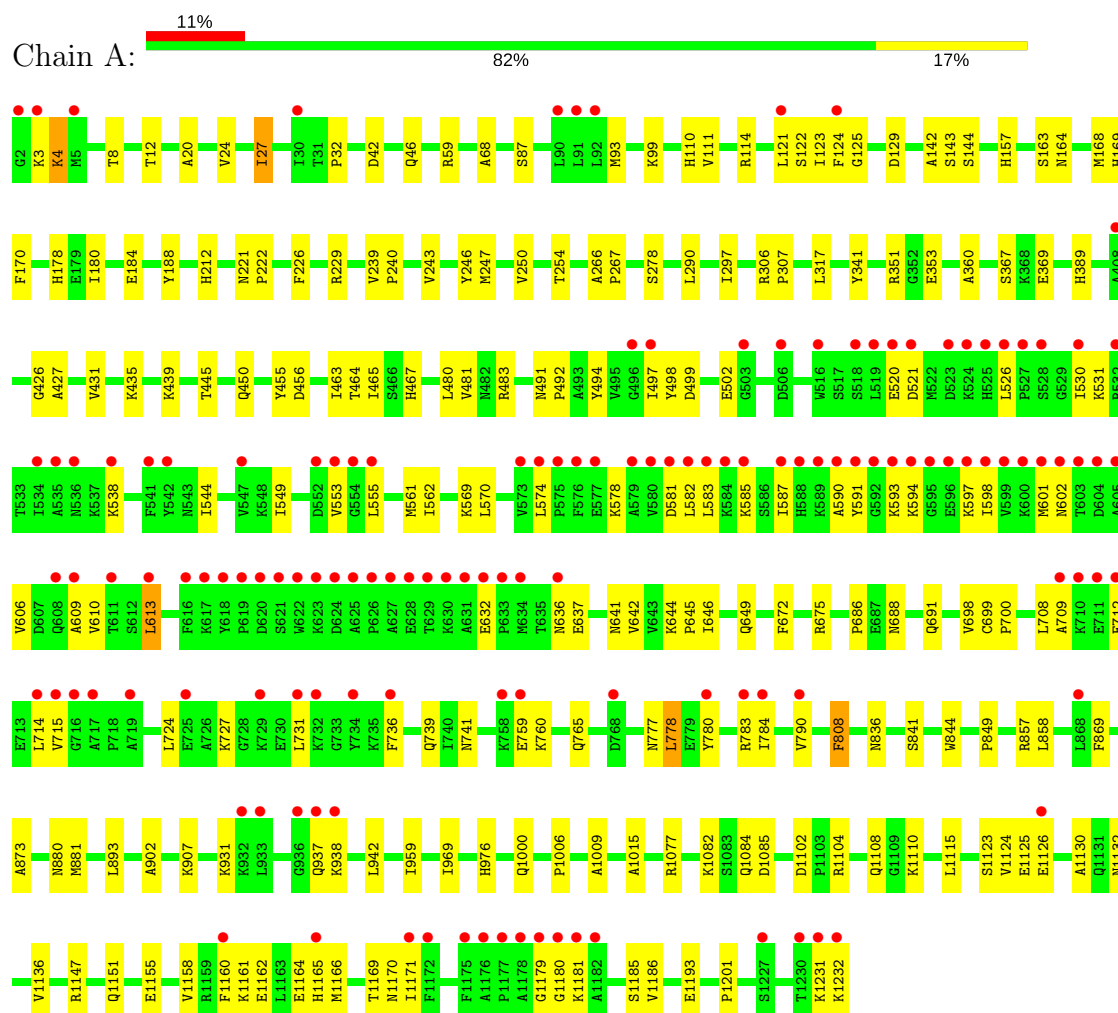
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	667	Total 667	O 667	0	0

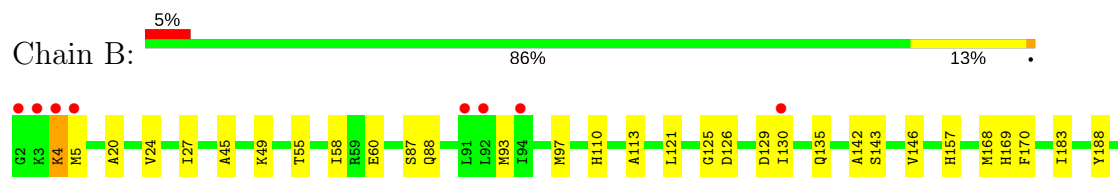
### 3 Residue-property plots

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.

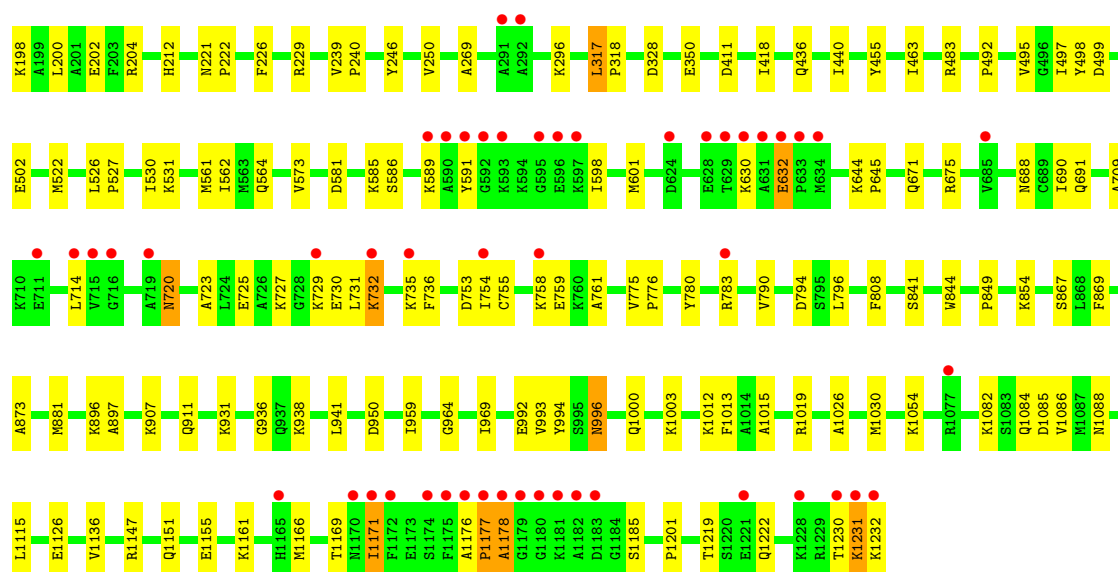
#### • Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE



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







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.30Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 1.78Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.195 , 0.219 0.191 , 0.214	Depositor DCC
$R_{free}$ test set	12031 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.0	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	20099	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 3.86% 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, 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%)	44	27
1	B	1229/1231 (100%)	1191 (97%)	33 (3%)	5 (0%)	38	21
All	All	2458/2462 (100%)	2365 (96%)	84 (3%)	9 (0%)	38	21

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%)	75	67
1	B	978/978 (100%)	965 (99%)	13 (1%)	73	64
All	All	1956/1956 (100%)	1931 (99%)	25 (1%)	73	64

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	A	3233	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	3234	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	3235	1	0,12,12	0.00	-	0,24,24	0.00	-
3	TPP	A	3236	5	21,27,27	3.64	10 (47%)	25,40,40	1.50	7 (28%)
4	PYR	A	3237	-	2,5,5	1.13	0	2,6,6	1.47	0
2	SF4	B	3233	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	3234	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	3235	1	0,12,12	0.00	-	0,24,24	0.00	-
3	TPP	B	3236	5	21,27,27	3.02	7 (33%)	25,40,40	1.79	4 (16%)
4	PYR	B	3237	-	2,5,5	1.10	0	2,6,6	1.47	0

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	3233	1	-	0/0/48/48	0/6/5/5
2	SF4	A	3234	1	-	0/0/48/48	0/6/5/5
2	SF4	A	3235	1	-	0/0/48/48	0/6/5/5
3	TPP	A	3236	5	-	0/16/17/17	0/2/2/2
4	PYR	A	3237	-	-	0/0/4/4	0/0/0/0
2	SF4	B	3233	1	-	0/0/48/48	0/6/5/5
2	SF4	B	3234	1	-	0/0/48/48	0/6/5/5
2	SF4	B	3235	1	-	0/0/48/48	0/6/5/5
3	TPP	B	3236	5	-	0/16/17/17	0/2/2/2
4	PYR	B	3237	-	-	0/0/4/4	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3236	TPP	O7-C7	-2.40	1.35	1.44
3	A	3236	TPP	C7'-C5'	-2.23	1.46	1.51
3	A	3236	TPP	PA-O7	-2.04	1.50	1.59
3	B	3236	TPP	C6'-C5'	2.22	1.42	1.37
3	A	3236	TPP	C4'-N3'	3.47	1.40	1.35
3	A	3236	TPP	C5'-C4'	3.61	1.51	1.42
3	A	3236	TPP	C2'-N3'	3.63	1.40	1.34
3	A	3236	TPP	C6'-N1'	3.72	1.42	1.34
3	B	3236	TPP	C2'-N3'	3.74	1.40	1.34
3	A	3236	TPP	C2'-N1'	4.06	1.41	1.34
3	A	3236	TPP	C6'-C5'	4.11	1.46	1.37
3	A	3236	TPP	PB-O3A	4.56	1.67	1.60
3	B	3236	TPP	C2'-N1'	4.85	1.42	1.34
3	B	3236	TPP	C5'-C4'	4.95	1.54	1.42
3	B	3236	TPP	C4'-N3'	5.27	1.43	1.35
3	B	3236	TPP	C4-N3	8.70	1.47	1.39
3	A	3236	TPP	C4-N3	12.27	1.50	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3236	TPP	N1'-C2'-N3'	-2.90	120.58	125.59
3	A	3236	TPP	N4'-C4'-N3'	-2.82	112.84	117.00
3	A	3236	TPP	N1'-C2'-N3'	-2.57	121.14	125.59
3	A	3236	TPP	C6'-C5'-C4'	-2.04	112.96	115.68
3	A	3236	TPP	C6-C5-C4	2.16	129.17	127.43
3	A	3236	TPP	CM2-C2'-N1'	2.38	119.75	117.06
3	A	3236	TPP	CM4-C4-N3	2.47	125.69	122.53
3	A	3236	TPP	C6'-N1'-C2'	2.49	120.18	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3236	TPP	CM2-C2'-N3'	3.13	122.32	117.20
3	B	3236	TPP	CM4-C4-N3	3.58	127.10	122.53
3	B	3236	TPP	C6'-N1'-C2'	4.44	123.56	115.88

There are no chirality outliers.

There are no torsion outliers.

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

## 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(Å <sup>2</sup> )	Q<0.9
1	A	1231/1231 (100%)	0.58	138 (11%) <b>6</b> <b>5</b>	9, 23, 64, 106	0
1	B	1231/1231 (100%)	0.27	58 (4%) <b>32</b> <b>31</b>	10, 19, 48, 96	0
All	All	2462/2462 (100%)	0.42	196 (7%) <b>13</b> <b>13</b>	9, 21, 58, 106	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	576	PHE	11.4
1	A	1182	ALA	9.5
1	A	594	LYS	8.9
1	A	630	LYS	8.3
1	A	591	TYR	8.3
1	B	631	ALA	7.9
1	A	631	ALA	7.7
1	A	629	THR	7.6
1	A	1232	LYS	7.2
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	626	PRO	7.0
1	A	1178	ALA	6.9
1	A	1231	LYS	6.5
1	A	715	VAL	6.4
1	A	1179	GLY	6.4
1	B	2	GLY	6.4
1	B	732	LYS	6.4
1	A	628	GLU	6.1
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	A	588	HIS	5.3
1	B	3	LYS	5.3
1	A	633	PRO	5.1
1	B	715	VAL	5.1
1	A	577	GLU	5.0
1	A	574	LEU	5.0
1	B	590	ALA	4.9
1	A	554	GLY	4.8
1	B	1175	PHE	4.8
1	A	621	SER	4.7
1	A	1175	PHE	4.7
1	B	630	LYS	4.7
1	B	592	GLY	4.7
1	A	597	LYS	4.6
1	A	625	ALA	4.5
1	A	1165	HIS	4.5
1	B	629	THR	4.5
1	B	628	GLU	4.5
1	A	590	ALA	4.4
1	A	595	GLY	4.3
1	A	518	SER	4.3
1	A	619	PRO	4.3
1	A	598	ILE	4.2
1	B	1171	ILE	4.2
1	A	936	GLY	4.1
1	A	596	GLU	4.1
1	A	535	ALA	4.1
1	A	1181	LYS	4.1
1	A	2	GLY	4.0
1	A	719	ALA	4.0
1	A	580	VAL	3.9
1	A	632	GLU	3.9
1	B	1231	LYS	3.9
1	B	632	GLU	3.8
1	A	714	LEU	3.7
1	A	585	LYS	3.7
1	A	520	GLU	3.7
1	A	599	VAL	3.6
1	A	1230	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	634	MET	3.6
1	B	591	TYR	3.6
1	A	716	GLY	3.6
1	B	1228	LYS	3.6
1	B	4	LYS	3.5
1	A	1180	GLY	3.5
1	A	587	ILE	3.5
1	A	519	LEU	3.5
1	A	729	LYS	3.5
1	A	938	LYS	3.5
1	B	593	LYS	3.5
1	A	620	ASP	3.5
1	A	624	ASP	3.5
1	A	525	HIS	3.4
1	A	623	LYS	3.4
1	A	710	LYS	3.4
1	B	719	ALA	3.4
1	A	732	LYS	3.4
1	A	523	ASP	3.3
1	A	613	LEU	3.3
1	B	1165	HIS	3.3
1	A	524	LYS	3.3
1	A	547	VAL	3.3
1	B	1174	SER	3.2
1	A	611	THR	3.2
1	A	3	LYS	3.2
1	A	553	VAL	3.2
1	A	605	ALA	3.2
1	A	526	LEU	3.2
1	A	758	LYS	3.1
1	A	584	LYS	3.1
1	B	1172	PHE	3.1
1	A	532	ARG	3.1
1	A	91	LEU	3.0
1	A	616	PHE	3.0
1	B	589	LYS	3.0
1	A	581	ASP	3.0
1	A	734	TYR	3.0
1	A	1177	PRO	3.0
1	A	516	TRP	3.0
1	A	552	ASP	3.0
1	B	596	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	1230	THR	2.9
1	A	92	LEU	2.9
1	B	291	ALA	2.9
1	A	573	VAL	2.9
1	B	714	LEU	2.9
1	A	538	LYS	2.9
1	B	595	GLY	2.9
1	A	530	ILE	2.8
1	A	731	LEU	2.8
1	A	534	ILE	2.7
1	B	92	LEU	2.7
1	A	783	ARG	2.7
1	A	30	ILE	2.7
1	A	497	ILE	2.7
1	A	618	TYR	2.7
1	A	759	GLU	2.7
1	B	1179	GLY	2.7
1	B	1180	GLY	2.7
1	A	602	ASN	2.7
1	A	1176	ALA	2.7
1	A	622	TRP	2.7
1	B	758	LYS	2.7
1	A	608	GLN	2.7
1	B	633	PRO	2.6
1	B	716	GLY	2.6
1	A	541	PHE	2.6
1	B	1077	ARG	2.6
1	A	583	LEU	2.6
1	A	408	ALA	2.6
1	B	292	ALA	2.6
1	A	601	MET	2.6
1	A	527	PRO	2.6
1	A	528	SER	2.6
1	A	1172	PHE	2.5
1	A	579	ALA	2.5
1	A	790	VAL	2.5
1	B	94	ILE	2.5
1	B	754	ILE	2.5
1	A	600	LYS	2.5
1	A	603	THR	2.5
1	A	90	LEU	2.5
1	A	555	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	542	TYR	2.4
1	A	617	LYS	2.4
1	A	121	LEU	2.4
1	A	932	LYS	2.4
1	A	609	ALA	2.4
1	B	1182	ALA	2.4
1	B	91	LEU	2.4
1	B	1183	ASP	2.3
1	B	1181	LYS	2.3
1	A	536	ASN	2.3
1	A	636	ASN	2.3
1	A	711	GLU	2.3
1	A	933	LEU	2.3
1	A	784	ILE	2.3
1	A	717	ALA	2.3
1	A	736	PHE	2.3
1	B	597	LYS	2.3
1	A	712	GLU	2.2
1	B	1221	GLU	2.2
1	A	937	GLN	2.2
1	A	1171	ILE	2.2
1	A	604	ASP	2.2
1	B	1170	ASN	2.2
1	A	1126	GLU	2.2
1	B	735	LYS	2.2
1	A	503	GLY	2.2
1	A	709	ALA	2.2
1	A	780	TYR	2.2
1	B	624	ASP	2.2
1	B	634	MET	2.2
1	B	685	VAL	2.2
1	B	729	LYS	2.2
1	A	124	PHE	2.1
1	A	725	GLU	2.1
1	B	711	GLU	2.1
1	A	1227	SER	2.1
1	B	130	ILE	2.1
1	A	506	ASP	2.1
1	A	5	MET	2.1
1	B	5	MET	2.1
1	A	496	GLY	2.1
1	A	868	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	783	ARG	2.0
1	A	768	ASP	2.0
1	A	1160	PHE	2.0
1	A	521	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PYR	B	3237	6/6	0.92	0.21	3.76	16,19,24,26	0
6	CA	A	3239	1/1	0.99	0.11	3.46	40,40,40,40	0
6	CA	B	3239	1/1	0.99	0.09	-0.17	44,44,44,44	0
5	MG	B	3238	1/1	1.00	0.11	-0.18	9,9,9,9	0
3	TPP	A	3236	26/26	0.98	0.13	-0.47	12,15,27,34	0
5	MG	A	3238	1/1	0.99	0.10	-0.66	12,12,12,12	0
3	TPP	B	3236	26/26	0.98	0.12	-0.82	7,13,24,30	0
4	PYR	A	3237	6/6	0.95	0.15	-1.42	21,25,28,29	0
2	SF4	B	3235	8/8	1.00	0.07	-1.59	12,13,14,15	0
2	SF4	A	3235	8/8	0.99	0.07	-1.70	16,18,18,18	0
2	SF4	B	3233	8/8	0.97	0.07	-1.96	20,23,25,26	0
2	SF4	A	3234	8/8	0.98	0.06	-2.23	23,24,24,25	0
2	SF4	A	3233	8/8	0.96	0.06	-2.92	27,30,32,33	0
2	SF4	B	3234	8/8	0.99	0.06	-3.12	16,17,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.