



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:14 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

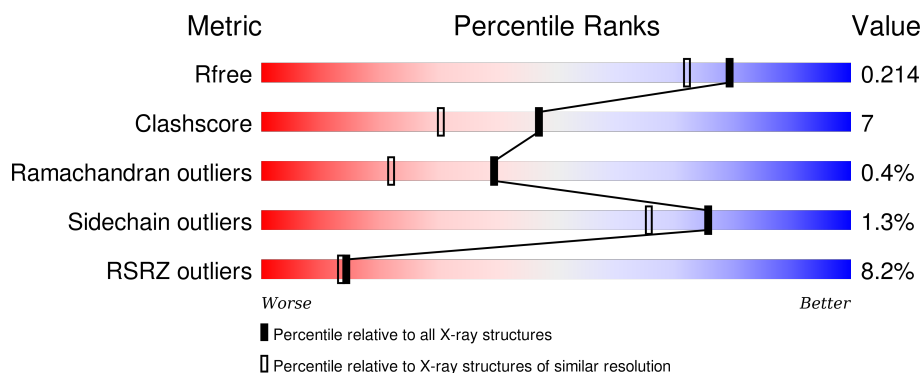
# 1 Overall quality at a glance

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))
$R_{free}$	91344	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (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](#)

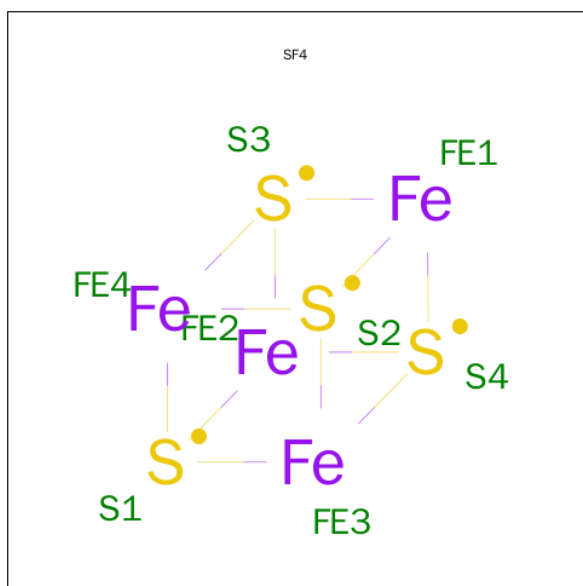
There are 7 unique types of molecules in this entry. The entry contains 20099 atoms, of which 0 are hydrogens and 0 are deuteriums.

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>).



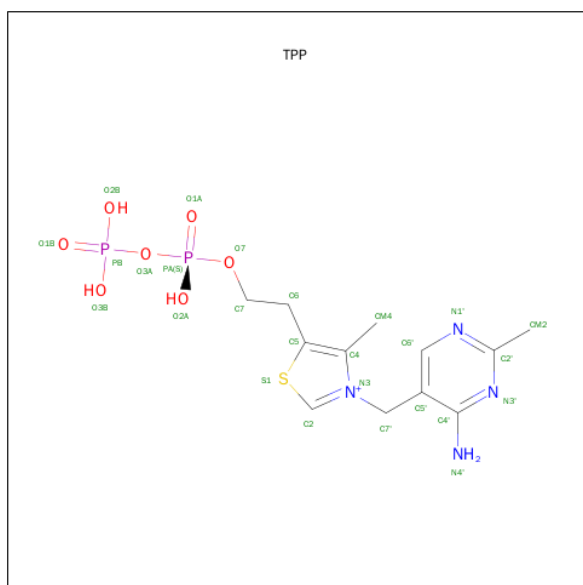
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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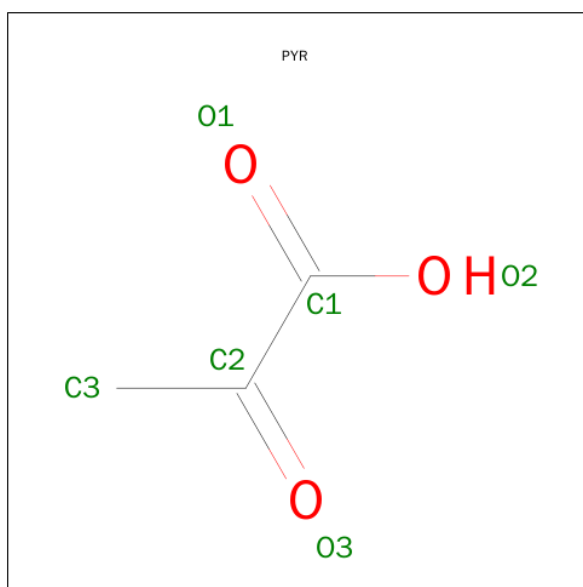
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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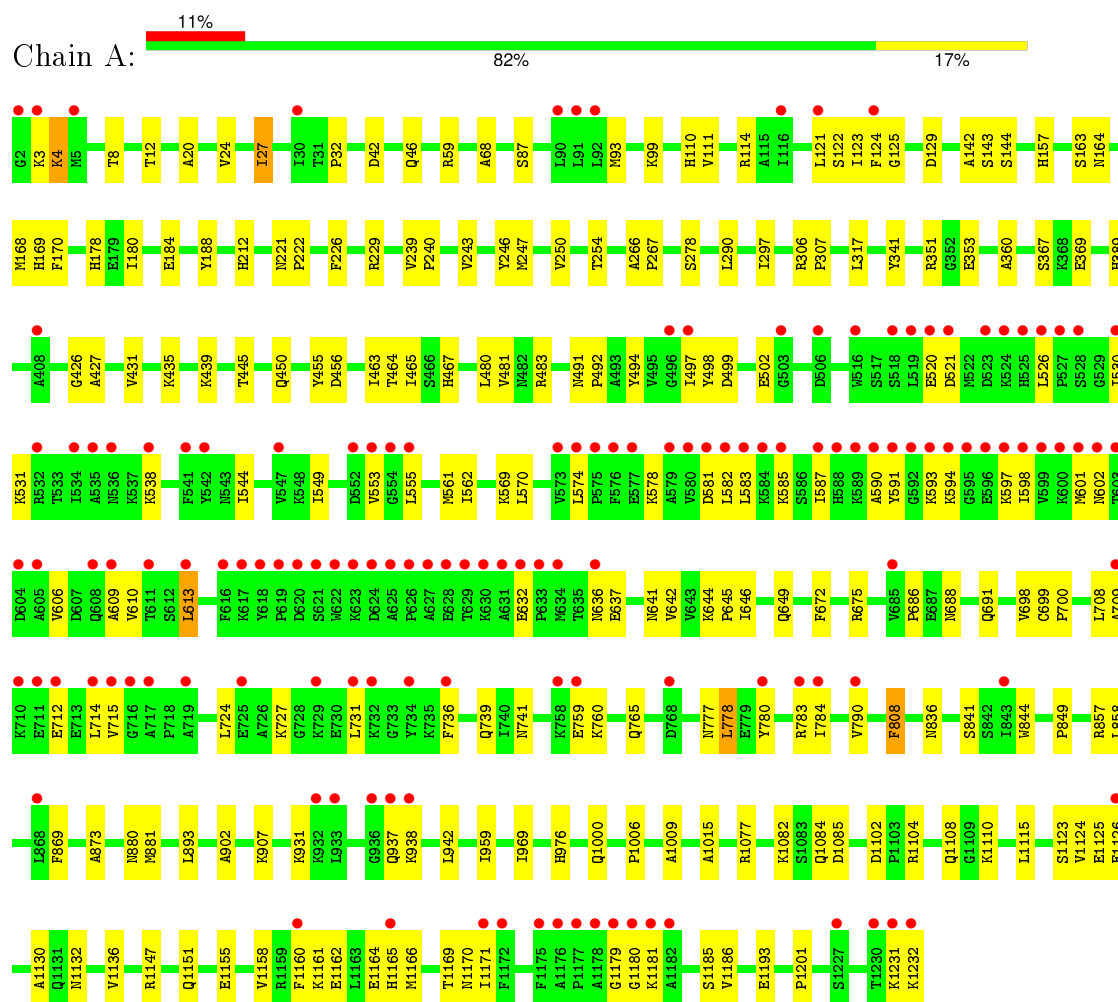
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	667	Total 667	O 667	0	0

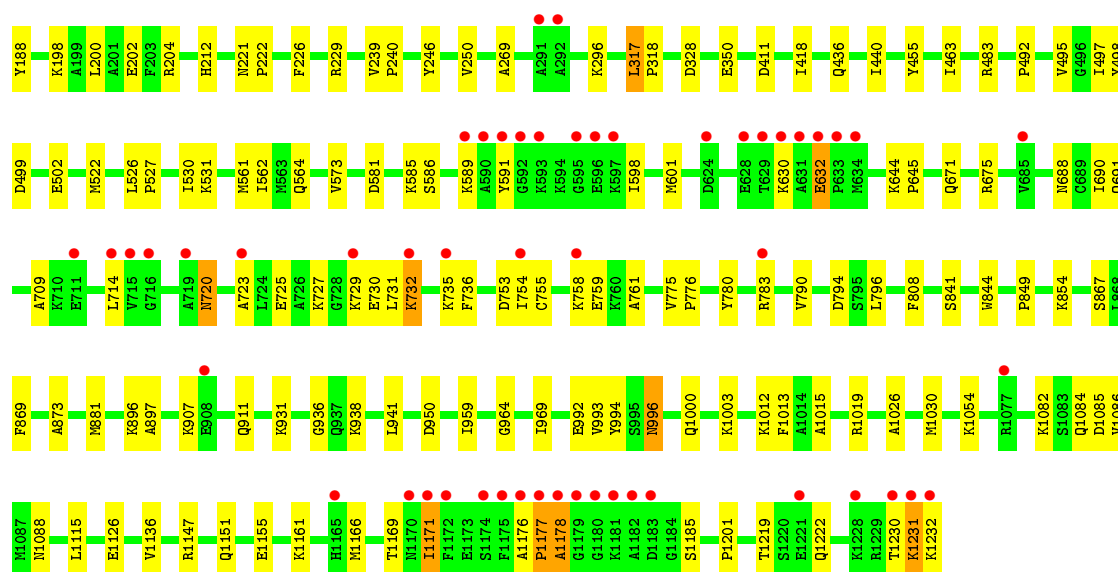
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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-FERREDONIN OXIDOREDUCTASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 241140 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:594:LYS:HB3	1:A:598:ILE:HD12	1.66	0.76
1:A:110:HIS:CE1	1:A:157:HIS:HE1	2.03	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:992:GLU:O	1:B:993:VAL:HG13	2.01	0.61
1:B:907:LYS:O	1:B:911:GLN:HG3	2.00	0.61
1:B:561:MET:HE1	1:B:564:GLN:HG2	1.83	0.61
1:B:527:PRO:HD2	1:B:530:ILE:HD12	1.81	0.61
1:B:1219:THR:OG1	1:B:1222:GLN:HG3	2.01	0.61
1:A:1181:LYS:HB2	1:A:1181:LYS:NZ	2.16	0.60
1:A:27:ILE:HB	7:A:2040:HOH:O	2.01	0.60
1:A:937:GLN:HG2	1:A:942:LEU:HB3	1.83	0.60
1:A:902:ALA:O	1:A:907:LYS:HE3	2.02	0.60
1:A:636:ASN:ND2	1:A:672:PHE:HE1	2.00	0.59
1:A:526:LEU:HD11	1:A:530:ILE:HG21	1.83	0.59
1:B:780:TYR:HD1	1:B:783:ARG:HH21	1.50	0.59
1:A:731:LEU:HD23	1:A:790:VAL:HG11	1.84	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: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:B:723:ALA:HB1	1:B:735:LYS:HG2	1.86	0.57
1:A:553:VAL:HG23	1:A:555:LEU:HG	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:B:727:LYS:HA	1:B:727:LYS:HE2	1.88	0.56
1:A:1123:SER:O	1:A:1126:GLU:HG2	2.05	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:497:ILE:HG13	1:A:498:TYR:CD1	2.42	0.55
1:A:142:ALA:HB2	1:A:170:PHE:CZ	2.41	0.55
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:1115:LEU:HD21	1:A:1160:PHE:CZ	2.42	0.54
1:A:1015:ALA:HB1	1:B:1185:SER:HB2	1.88	0.54
1:A:520:GLU:HG3	1:A:521:ASP:N	2.23	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:465:ILE:HD11	1:A:649:GLN:HE22	1.73	0.52
1:A:562:ILE:HD12	1:A:562:ILE:N	2.25	0.52
1:A:1132:ASN:O	1:A:1136:VAL:HG12	2.10	0.52
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.39	0.52

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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:1161:LYS:CB	1:B:1171:ILE:HD12	2.39	0.51
1:A:1015:ALA:CB	1:B:1185:SER:HB2	2.41	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:B:1231:LYS:HG3	1:B:1232:LYS:N	2.23	0.51
1:A:637:GLU:HG3	1:A:641:ASN:ND2	2.26	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:729:LYS:O	1:B:732:LYS:HG3	2.11	0.50
1:B:20:ALA:HB2	1:B:188:TYR:CZ	2.47	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:741:ASN:CG	1:A:778:LEU:HD11	2.33	0.49
1:A:8:THR:OG1	1:A:12:THR:HB	2.11	0.49
1:A:1186:VAL:HG21	1:B:1136:VAL:HG22	1.94	0.49
1:A:494:TYR:HD2	1:A:497:ILE:HD11	1.76	0.49
1:B:873:ALA:HA	1:B:959:ILE:HD13	1.94	0.49
1:A:686:PRO:HB2	1:A:724:LEU:HD21	1.95	0.49
1:B: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:B:1232:LYS:HB3	1:B:1232:LYS:HZ2	1.79	0.48
1:A:389:HIS:HD2	7:A:2059:HOH:O	1.96	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:869:PHE:CE2	1:B:969:ILE:HG21	2.48	0.47
1:B:775:VAL:N	1:B:776:PRO:HD2	2.29	0.47
1:B:630:LYS:O	1:B:630:LYS:HG3	2.13	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:1082:LYS:HE2	1:A:1085:ASP:OD1	2.14	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:N	1:B:730:GLU:OE1	2.47	0.47
1:B:436:GLN:O	1:B:440:ILE:HG13	2.15	0.47
1:B:4:LYS:HE2	1:B:4:LYS:HA	1.97	0.46
1:B:221:ASN:HB3	1:B:222:PRO:CD	2.45	0.46
1:A:212:HIS:HE1	1:B:950:ASP:OD2	1.97	0.46
1:B:714:LEU:N	1:B:714:LEU:HD22	2.31	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:A:121:LEU:C	1:A:121:LEU:HD23	2.34	0.46
1:A:937:GLN:C	1:A:938:LYS:HD2	2.36	0.46
1:A:246:TYR:O	1:A:250:VAL:HG23	2.15	0.46
1:A:675:ARG:HD3	7:A:2314:HOH:O	2.13	0.46
1:B:755:CYS:SG	1:B:761:ALA:HB3	2.56	0.46
1:B:897:ALA:HA	1:B:941:LEU:HD23	1.96	0.46
1:B:497:ILE:HG13	1:B:498:TYR:CD1	2.50	0.46
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.97	0.46
1:A:569:LYS:HB3	1:A:570:LEU:HD22	1.98	0.46
1:A:869:PHE:CE2	1:A:969:ILE:HG21	2.50	0.46
1:A:699:CYS:HA	1:A:700:PRO:HD3	1.82	0.46
1:B:723:ALA:CB	1:B:735:LYS:HG2	2.46	0.46
1:A:688:ASN:HB3	1:A:759:GLU:O	2.16	0.46
1:A:239:VAL:HB	1:A:240:PRO:HD3	1.97	0.46
1:A:1077:ARG:HG2	1:A:1130:ALA:O	2.16	0.45
1:A:976:HIS:CD2	1:B:1003:LYS:HZ2	2.34	0.45
1:A:808:PHE:CD2	1:A:808:PHE:N	2.85	0.45
1:A:1171:ILE:HD12	1:B:1161:LYS:HD3	1.98	0.45
1:B:996:ASN:ND2	3:B:3236:TPP:S1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:ASN:HB3	1:B:759:GLU:O	2.17	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: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: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:A:456:ASP:OD1	1:A:463:ILE:HG22	2.17	0.45
1:A:431:VAL:CG2	1:A:464:THR:HG21	2.46	0.45
1:A:426:GLY:O	1:A:427:ALA:HB3	2.16	0.45
1:B:27:ILE:CD1	1:B:1013:PHE:CE2	3.00	0.45
1:A:42:ASP:O	1:A:46:GLN:HG3	2.17	0.45
1:B:644:LYS:HB3	1:B:645:PRO:HD3	1.99	0.45
1:B:691:GLN:NE2	1:B:727:LYS:HG2	2.32	0.44
1:A:3:LYS:O	1:A:4:LYS:HB2	2.17	0.44
1:B:897:ALA:CA	1:B:941:LEU:HD23	2.47	0.44
1:B:110:HIS:CE1	1:B:157:HIS:NE2	2.79	0.44
1:A:709:ALA:HB2	1:A:784:ILE:HG21	1.98	0.44
1:A:602:ASN:O	1:A:606:VAL:HG23	2.18	0.44
1:A:1124:VAL:HG13	1:A:1125:GLU:N	2.33	0.44
1:A: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:B:246:TYR:O	1:B:250:VAL:HG23	2.18	0.43
1:B:1147:ARG:HG3	1:B:1147:ARG:HH11	1.84	0.43
1:A:68:ALA:HB2	1:A:93:MET:HG2	2.01	0.43
1:B:130:ILE:HB	1:B:168:MET:HE1	1.99	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:20:ALA:HB2	1:A:188:TYR:CZ	2.54	0.43
1:A:114:ARG:NE	1:A:123:ILE:HA	2.33	0.43
1:A:306:ARG:HA	1:A:307:PRO:C	2.37	0.43
1:A:494:TYR:HA	1:A:497:ILE:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:PHE:O	1:A:1164:GLU:HG3	2.18	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:964:GLY:HA2	1:B:994:TYR:HE1	1.84	0.43
1:B:753:ASP:OD2	1:B:1085:ASP:OD2	2.37	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: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:A:317:LEU:HD11	7:A:2186:HOH:O	2.19	0.42
1:B:758:LYS:HB2	1:B:758:LYS:HE3	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:B:20:ALA:HB2	1:B:188:TYR:CE1	2.55	0.41
1:A:483:ARG:HH11	1:A:483:ARG:HG2	1.85	0.41
1:A:144:SER:O	1:A:278:SER:HA	2.20	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:896:LYS:HB3	1:B:941:LEU:HD21	2.02	0.41
1:B:754:ILE:HG12	7:B:2592:HOH:O	2.20	0.41
1:A:976:HIS:HE1	1:B:60:GLU:O	2.04	0.41
1:B:212:HIS:HD2	7:B:2104:HOH:O	2.04	0.41
1:A: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: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:B:630:LYS:C	1:B:632:GLU:H	2.24	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:581:ASP:OD2	1:B:585:LYS:HE3	2.20	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:113:ALA:HB1	1:B:126:ASP:O	2.20	0.41
1:B:418:ILE:HD12	1:B:573:VAL:HA	2.03	0.41
1:A:290:LEU:HB2	1:A:297:ILE:HD11	2.03	0.41
1:B:1176:ALA:HB1	1:B:1177:PRO:CD	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ASN:HA	1:A:492:PRO:HD2	1.96	0.40
1:B:4:LYS:HE2	1:B:5:MET:N	2.36	0.40
1:B:598:ILE:HD13	1:B:601:MET:CE	2.52	0.40
1:B:992:GLU:O	1:B:993:VAL:CG1	2.69	0.40
1:A:590:ALA:O	1:A:591:TYR:C	2.60	0.40
1:B:1151:GLN:O	1:B:1155:GLU:HG3	2.21	0.40
1:B:130:ILE:HB	1:B:168:MET:CE	2.51	0.40
1:B:720:ASN:H	1:B:720:ASN:ND2	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1229/1231 (100%)	1174 (96%)	51 (4%)	4 (0%)	46	28
1	B	1229/1231 (100%)	1191 (97%)	33 (3%)	5 (0%)	39	22
All	All	2458/2462 (100%)	2365 (96%)	84 (3%)	9 (0%)	39	22

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%)	78	69
1	B	978/978 (100%)	965 (99%)	13 (1%)	76	66
All	All	1956/1956 (100%)	1931 (99%)	25 (1%)	76	66

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	20,27,27	3.56	8 (40%)	31,40,40	1.55	7 (22%)
4	PYR	A	3237	-	2,5,5	1.11	0	2,6,6	1.44	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	20,27,27	3.05	8 (40%)	31,40,40	1.78	7 (22%)
4	PYR	B	3237	-	2,5,5	1.07	0	2,6,6	1.44	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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3236	TPP	O7-C7	-2.28	1.35	1.44
3	A	3236	TPP	C7'-C5'	-2.18	1.46	1.51
3	B	3236	TPP	PB-O3B	-2.14	1.47	1.54
3	B	3236	TPP	C6'-C5'	2.14	1.42	1.37
3	A	3236	TPP	C4'-N3'	3.41	1.40	1.35
3	A	3236	TPP	C2'-N3'	3.51	1.40	1.34
3	A	3236	TPP	C5'-C4'	3.55	1.51	1.42
3	B	3236	TPP	C2'-N3'	3.61	1.40	1.34
3	A	3236	TPP	C6'-N1'	3.71	1.42	1.34
3	A	3236	TPP	C2'-N1'	3.94	1.41	1.34
3	A	3236	TPP	C6'-C5'	3.95	1.46	1.37
3	B	3236	TPP	C2'-N1'	4.70	1.42	1.34
3	B	3236	TPP	C5'-C4'	4.86	1.54	1.42
3	B	3236	TPP	C4'-N3'	5.16	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 (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3236	TPP	C6-C5-S1	-3.05	115.96	120.24
3	A	3236	TPP	N4'-C4'-N3'	-2.83	112.84	116.95
3	A	3236	TPP	C6-C5-S1	-2.80	116.33	120.24
3	B	3236	TPP	N1'-C2'-N3'	-2.72	120.58	125.60
3	A	3236	TPP	N1'-C2'-N3'	-2.41	121.14	125.60
3	B	3236	TPP	O3B-PB-O2B	2.08	115.29	107.38
3	B	3236	TPP	O3A-PA-O7	2.15	108.64	102.94
3	A	3236	TPP	CM2-C2'-N1'	2.27	119.75	117.03
3	A	3236	TPP	CM4-C4-N3	2.32	125.69	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	3236	TPP	C6'-N1'-C2'	2.52	120.18	115.77
3	A	3236	TPP	O3A-PA-O7	2.82	110.42	102.94
3	B	3236	TPP	CM2-C2'-N3'	3.01	122.32	117.20
3	B	3236	TPP	CM4-C4-N3	3.38	127.10	122.59
3	B	3236	TPP	C6'-N1'-C2'	4.46	123.56	115.77

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%)	0.60	141 (11%) 6 6	9, 23, 64, 106	0
1	B	1231/1231 (100%)	0.29	61 (4%) 32 30	10, 19, 48, 96	0
All	All	2462/2462 (100%)	0.45	202 (8%) 14 13	9, 21, 58, 106	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	576	PHE	11.3
1	A	1182	ALA	9.6
1	A	594	LYS	8.8
1	A	630	LYS	8.3
1	A	591	TYR	8.3
1	B	631	ALA	8.0
1	A	631	ALA	7.8
1	A	629	THR	7.7
1	A	582	LEU	7.2
1	A	1232	LYS	7.2
1	B	1177	PRO	7.2
1	B	1232	LYS	7.1
1	A	593	LYS	7.0
1	A	626	PRO	7.0
1	A	1178	ALA	7.0
1	A	1179	GLY	6.5
1	A	1231	LYS	6.5
1	A	715	VAL	6.4
1	B	2	GLY	6.4
1	B	732	LYS	6.3
1	B	1176	ALA	6.1
1	A	628	GLU	6.1
1	B	1178	ALA	6.0
1	A	592	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	627	ALA	5.6
1	A	575	PRO	5.4
1	A	588	HIS	5.3
1	A	589	LYS	5.3
1	B	3	LYS	5.2
1	A	633	PRO	5.2
1	B	715	VAL	5.1
1	A	574	LEU	5.1
1	A	577	GLU	5.0
1	B	590	ALA	5.0
1	A	554	GLY	4.9
1	A	621	SER	4.8
1	B	1175	PHE	4.8
1	A	1175	PHE	4.7
1	B	592	GLY	4.7
1	B	630	LYS	4.7
1	A	625	ALA	4.6
1	A	597	LYS	4.6
1	B	629	THR	4.5
1	A	1165	HIS	4.5
1	B	628	GLU	4.5
1	A	590	ALA	4.4
1	A	595	GLY	4.4
1	A	518	SER	4.3
1	A	619	PRO	4.3
1	B	1171	ILE	4.2
1	A	598	ILE	4.2
1	A	936	GLY	4.1
1	A	535	ALA	4.1
1	A	596	GLU	4.1
1	A	2	GLY	4.1
1	A	1181	LYS	4.1
1	A	719	ALA	4.0
1	A	580	VAL	4.0
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	3.7
1	A	716	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1230	THR	3.6
1	B	591	TYR	3.6
1	A	634	MET	3.6
1	A	587	ILE	3.6
1	A	1180	GLY	3.6
1	A	519	LEU	3.6
1	B	1228	LYS	3.6
1	B	4	LYS	3.5
1	A	620	ASP	3.5
1	A	624	ASP	3.5
1	A	729	LYS	3.5
1	A	938	LYS	3.5
1	B	593	LYS	3.5
1	A	525	HIS	3.5
1	B	719	ALA	3.4
1	A	613	LEU	3.4
1	A	623	LYS	3.4
1	A	710	LYS	3.4
1	A	732	LYS	3.4
1	A	523	ASP	3.3
1	B	1165	HIS	3.3
1	A	547	VAL	3.3
1	A	524	LYS	3.3
1	B	1174	SER	3.3
1	A	553	VAL	3.2
1	A	605	ALA	3.2
1	A	611	THR	3.2
1	A	3	LYS	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	91	LEU	3.1
1	A	532	ARG	3.1
1	A	616	PHE	3.0
1	A	516	TRP	3.0
1	A	734	TYR	3.0
1	B	589	LYS	3.0
1	A	581	ASP	3.0
1	A	1177	PRO	3.0
1	A	92	LEU	3.0
1	A	552	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	291	ALA	3.0
1	B	596	GLU	3.0
1	B	1230	THR	3.0
1	B	714	LEU	3.0
1	A	573	VAL	2.9
1	B	595	GLY	2.9
1	A	538	LYS	2.9
1	A	530	ILE	2.9
1	A	731	LEU	2.8
1	B	92	LEU	2.8
1	A	30	ILE	2.8
1	A	534	ILE	2.8
1	A	497	ILE	2.7
1	A	783	ARG	2.7
1	B	1179	GLY	2.7
1	B	1180	GLY	2.7
1	A	622	TRP	2.7
1	A	1176	ALA	2.7
1	A	618	TYR	2.7
1	A	602	ASN	2.7
1	A	759	GLU	2.7
1	A	583	LEU	2.7
1	B	633	PRO	2.7
1	A	408	ALA	2.7
1	B	292	ALA	2.7
1	B	758	LYS	2.7
1	A	608	GLN	2.7
1	B	716	GLY	2.6
1	A	541	PHE	2.6
1	B	1077	ARG	2.6
1	A	528	SER	2.6
1	A	579	ALA	2.6
1	A	601	MET	2.6
1	A	527	PRO	2.6
1	A	1172	PHE	2.6
1	B	754	ILE	2.6
1	A	790	VAL	2.5
1	B	94	ILE	2.5
1	A	90	LEU	2.5
1	A	555	LEU	2.5
1	A	603	THR	2.5
1	A	121	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	542	TYR	2.5
1	A	600	LYS	2.5
1	A	617	LYS	2.4
1	A	609	ALA	2.4
1	B	91	LEU	2.4
1	B	1182	ALA	2.4
1	A	932	LYS	2.4
1	B	1183	ASP	2.4
1	A	536	ASN	2.3
1	B	1181	LYS	2.3
1	A	933	LEU	2.3
1	A	636	ASN	2.3
1	A	717	ALA	2.3
1	A	784	ILE	2.3
1	A	711	GLU	2.3
1	A	736	PHE	2.3
1	A	1171	ILE	2.3
1	A	712	GLU	2.3
1	B	597	LYS	2.2
1	B	1221	GLU	2.2
1	B	1170	ASN	2.2
1	A	709	ALA	2.2
1	A	604	ASP	2.2
1	A	503	GLY	2.2
1	A	937	GLN	2.2
1	B	685	VAL	2.2
1	A	1126	GLU	2.2
1	B	735	LYS	2.2
1	A	780	TYR	2.2
1	B	624	ASP	2.2
1	A	725	GLU	2.2
1	B	130	ILE	2.2
1	B	729	LYS	2.2
1	B	634	MET	2.2
1	A	124	PHE	2.1
1	B	711	GLU	2.1
1	A	1227	SER	2.1
1	A	868	LEU	2.1
1	A	506	ASP	2.1
1	A	496	GLY	2.1
1	A	5	MET	2.1
1	B	783	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	116	ILE	2.1
1	A	843	ILE	2.1
1	B	5	MET	2.0
1	B	723	ALA	2.0
1	A	768	ASP	2.0
1	A	1160	PHE	2.0
1	B	30	ILE	2.0
1	A	521	ASP	2.0
1	A	685	VAL	2.0
1	B	908	GLU	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(Å <sup>2</sup> )	Q<0.9
4	PYR	B	3237	6/6	0.92	0.21	3.78	16,19,24,26	0
6	CA	A	3239	1/1	0.99	0.11	3.49	40,40,40,40	0
6	CA	B	3239	1/1	0.99	0.09	-0.16	44,44,44,44	0
5	MG	B	3238	1/1	1.00	0.11	-0.17	9,9,9,9	0
3	TPP	A	3236	26/26	0.98	0.13	-0.46	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	-0.81	7,13,24,30	0
4	PYR	A	3237	6/6	0.95	0.15	-1.38	21,25,28,29	0
2	SF4	B	3235	8/8	1.00	0.07	-1.58	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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	-3.10	16,17,19,19	0

## 6.5 Other polymers

There are no such residues in this entry.