

Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 08:40 AM EDT

PDB ID	:	6CIN
Title	:	Crystal structure of pyruvate:ferredoxin oxidoreductase from Moorella ther-
		moacetica
Authors	:	Chen, P.YT.; Drennan, C.L.
Deposited on	:	2018-02-24
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.60 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.



Motria	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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		
			6%		
1	А	1171	90%	9%	•
			6%		
1	В	1171	92%	7%	-
			8%		
1	С	1171	92%	8%	•
			3%		
1	D	1171	88%	11%	•
			9%		
1	Ε	1171	90%	10%	•



Mol	Chain	Length	Quality of chain		
			4%		_
1	F	1171	91%	8%	•

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
5	SO4	В	1207	-	-	Х	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 53870 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.

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
1	Λ	1163	Total	С	Ν	Ο	S	0	0	0
1	Л	1105	8871	5646	1509	1672	44	0	0	0
1	В	1160	Total	С	Ν	Ο	S	0	0	0
1	D	1109	8905	5668	1515	1678	44	0		0
1	С	1163	Total	С	Ν	Ο	S	0	0	0
1		1105	8862	5644	1506	1668	44	0	0	0
1	Л	1157	Total	С	Ν	Ο	S	0	0	0
1	D	1157	8788	5593	1494	1657	44	0	0	0
1	F	1165	Total	С	Ν	Ο	S	0	0	0
1		1105	8875	5650	1511	1670	44	0	0	0
1	1 F	1159	Total	С	Ν	Ο	S	0	0	0
		1158	8789	5594	1495	1657	43		U	0

• Molecule 1 is a protein called PYRUVATE-FERREDOXIN OXIDOREDUCTASE.

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





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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	TotalFeS844	0	0
2	А	1	TotalFeS844	0	0
2	А	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	С	1	TotalFeS844	0	0
2	С	1	TotalFeS844	0	0
2	С	1	TotalFeS844	0	0
2	D	1	TotalFeS844	0	0
2	D	1	TotalFeS844	0	0
2	D	1	TotalFeS844	0	0
2	Е	1	TotalFeS844	0	0
2	Е	1	TotalFeS844	0	0
2	Е	1	TotalFeS844	0	0
2	F	1	TotalFeS844	0	0
2	F	1	TotalFeS844	0	0
2	F	1	$\begin{array}{ccc} \text{Total} & \text{Fe} & \text{S} \\ 8 & 4 & 4 \end{array}$	0	0

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





Mol	Chain	Residues		Α	ton	IS			ZeroOcc	AltConf				
2	Λ	1	Total	С	Ν	0	Р	S	0	0				
0	A	1	26	12	4	7	2	1	0	0				
2	В	1	Total	С	Ν	0	Р	S	0	0				
0	D	1	26	12	4	7	2	1	0	0				
3	C	1	Total	С	Ν	0	Р	\mathbf{S}	0	0				
0	U	1	26	12	4	7	2	1	0	0				
3	Л	1	Total	С	Ν	0	Р	S	0	0				
0	D	1	26	12	4	7	2	1	0	0				
3	F	F	Б	Г	Б	1	Total	С	Ν	0	Р	S	0	Ο
	Ľ	L	26	12	4	7	2	1	0	0				
3	F	1	Total	С	N	0	Р	S	0	0				
	T,	1	26	12	4	7	2	1	0	0				

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Mg 1 1	0	0
4	В	1	Total Mg 1 1	0	0
4	С	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	Е	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0



• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	D	1	$\begin{array}{c cc} Total & O & S \\ 5 & 4 & 1 \end{array}$	0	0
5	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	F	1	$\begin{array}{c cc} Total & O & S \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	73	Total O 73 73	0	0
6	В	88	Total O 88 88	0	0
6	С	76	Total O 76 76	0	0
6	D	83	Total O 83 83	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Е	61	Total O 61 61	0	0
6	F	58	Total O 58 58	0	0



3 Residue-property plots (i)

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



• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	340.61Å 106.63Å 239.08Å	Depositor
a, b, c, α , β , γ	90.00° 109.31° 90.00°	Depositor
Bosolution (Å)	88.95 - 2.60	Depositor
Resolution (A)	88.95 - 2.60	EDS
% Data completeness	98.4 (88.95-2.60)	Depositor
(in resolution range)	98.4 (88.95-2.60)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	$2.36 (at 2.62 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
D D .	0.195 , 0.227	Depositor
n, n_{free}	0.195 , 0.227	DCC
R_{free} test set	12231 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	56.5	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 51.5	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	53870	wwPDB-VP
Average B, all atoms $(Å^2)$	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 46.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1496e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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



¹Intensities estimated from amplitudes.

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: SF4, SO4, MG, 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).

Mal	Chain	Bond lengths		Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.27	0/9063	0.44	0/12286
1	В	0.27	0/9099	0.45	0/12339
1	С	0.27	0/9055	0.44	0/12277
1	D	0.27	0/8978	0.44	0/12178
1	Е	0.26	0/9068	0.44	0/12294
1	F	0.26	0/8980	0.43	0/12183
All	All	0.27	0/54243	0.44	0/73557

There are no bond length outliers.

There are no bond angle outliers.

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	А	8871	0	8796	62	0
1	В	8905	0	8821	53	0
1	С	8862	0	8779	54	0
1	D	8788	0	8658	75	0
1	Е	8875	0	8788	66	0
1	F	8789	0	8666	59	0
2	А	24	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	24	0	0	0	0
2	С	24	0	0	0	0
2	D	24	0	0	0	0
2	Е	24	0	0	0	0
2	F	24	0	0	0	0
3	А	26	0	16	1	0
3	В	26	0	16	0	0
3	С	26	0	16	2	0
3	D	26	0	16	0	0
3	Е	26	0	16	0	0
3	F	26	0	16	1	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
4	С	1	0	0	0	0
4	D	1	0	0	0	0
4	Е	1	0	0	0	0
4	F	1	0	0	0	0
5	А	5	0	0	0	0
5	В	10	0	0	3	0
5	С	5	0	0	0	0
5	D	5	0	0	0	0
5	Ε	5	0	0	0	0
5	F	5	0	0	0	0
6	А	73	0	0	1	0
6	В	88	0	0	1	0
6	С	76	0	0	2	0
6	D	83	0	0	5	0
6	Е	61	0	0	1	0
6	F	58	0	0	0	0
All	All	53870	0	52604	344	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 3.

All (344) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:ARG:NH2	5:B:1207:SO4:S	2.55	0.80
1:D:1057:LEU:HD23	1:D:1069:ILE:HD13	1.66	0.75
1:C:506:ILE:HG12	1:C:536:LYS:HE3	1.70	0.73
1:E:802:LEU:HB2	1:E:822:THR:HB	1.71	0.73



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:706:ALA:HB2	1:E:781:LEU:HD21	1.71	0.71
1:D:1059:GLU:OE1	6:D:1301:HOH:O	2.09	0.71
1:B:243:GLN:NE2	6:B:1302:HOH:O	2.29	0.64
1:F:1057:LEU:HD23	1:F:1069:ILE:HD13	1.78	0.64
1:A:112:ARG:HH21	1:A:119:LEU:HD11	1.63	0.63
1:C:345:VAL:HB	1:D:334:LEU:HD21	1.81	0.63
1:F:81:THR:HG21	1:F:91:MET:HE1	1.81	0.63
1:C:1057:LEU:HD23	1:C:1069:ILE:HD13	1.81	0.63
1:F:1127:ARG:HE	1:F:1151:PHE:HB3	1.63	0.63
1:E:204:ARG:NH2	6:E:1301:HOH:O	2.31	0.62
1:C:52:LYS:NZ	1:D:889:THR:OG1	2.32	0.62
1:C:81:THR:HG21	1:C:91:MET:HE1	1.81	0.62
1:A:671:LYS:NZ	1:A:741:ASP:OD2	2.26	0.61
1:C:204:ARG:NH2	6:C:1304:HOH:O	2.34	0.61
1:D:1079:GLY:HA3	1:D:1134:ILE:HB	1.83	0.61
1:B:521:ARG:NH2	5:B:1207:SO4:O3	2.32	0.61
1:C:5:THR:OG1	1:C:436:LYS:HG2	2.01	0.61
1:A:334:LEU:HD21	1:B:345:VAL:HB	1.82	0.61
1:B:438:ILE:HD13	1:B:569:VAL:HG11	1.82	0.60
1:F:838:SER:HA	1:F:841:TRP:CE2	2.36	0.60
1:F:5:THR:HG22	1:F:180:LYS:HB2	1.84	0.60
1:E:5:THR:HG22	1:E:180:LYS:HB2	1.84	0.59
1:E:52:LYS:NZ	1:F:889:THR:OG1	2.33	0.59
1:F:893:LYS:HB3	1:F:945:LEU:HD11	1.84	0.59
1:E:1079:GLY:HA3	1:E:1134:ILE:HB	1.84	0.59
1:C:750:ASP:OD1	1:C:1087:ARG:NH2	2.34	0.59
1:C:387:LYS:NZ	1:D:348:GLU:OE1	2.36	0.58
1:E:81:THR:HG21	1:E:91:MET:HE1	1.83	0.58
1:B:1057:LEU:HD23	1:B:1069:ILE:HD13	1.85	0.58
1:B:592:ASP:O	1:B:596:ASN:ND2	2.35	0.58
1:C:1036:TYR:O	1:D:1025:LYS:NZ	2.36	0.57
1:D:838:SER:HA	1:D:841:TRP:CE2	2.39	0.57
1:D:802:LEU:HB2	1:D:822:THR:HB	1.85	0.57
1:C:802:LEU:HB2	1:C:822:THR:HB	1.86	0.57
1:E:345:VAL:HB	1:F:334:LEU:HD21	1.87	0.57
1:A:802:LEU:HB2	1:A:822:THR:HB	1.86	0.56
1:E:671:LYS:NZ	1:E:741:ASP:OD2	2.32	0.56
1:C:828:ARG:NH2	1:C:1061:GLU:OE2	2.38	0.56
1:E:1004:GLN:HA	1:E:1016:ARG:HB2	1.89	0.55
1:A:1076:ILE:HA	1:A:1082:MET:HE3	1.89	0.55
1:B:838:SER:HA	1:B:841:TRP:CE2	2.42	0.55



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:419:PHE:HB2	1:E:463:SER:HB2	1.88	0.55
1:E:1072:TYR:HB2	1:E:1098:TRP:CE2	2.41	0.55
1:F:85:SER:HA	1:F:127:ASP:HB3	1.89	0.55
1:D:5:THR:HG22	1:D:180:LYS:HB2	1.88	0.55
1:D:292:GLY:HA3	1:E:638:LYS:HE2	1.89	0.54
1:C:5:THR:HG22	1:C:180:LYS:HB2	1.88	0.54
1:D:356:VAL:HG13	1:D:386:ASN:HA	1.88	0.54
1:E:506:ILE:HG12	1:E:536:LYS:HE3	1.89	0.54
1:A:1060:ALA:HB1	1:A:1067:SER:HB3	1.90	0.54
1:A:1095:ALA:HB1	1:A:1126:PHE:HA	1.90	0.54
1:A:345:VAL:HB	1:B:334:LEU:HD21	1.90	0.53
1:A:1026:LYS:HZ3	1:A:1098:TRP:HZ3	1.54	0.53
1:C:838:SER:HA	1:C:841:TRP:CE2	2.43	0.53
1:A:1079:GLY:HA3	1:A:1134:ILE:HB	1.91	0.53
1:B:81:THR:HG21	1:B:91:MET:HE1	1.90	0.53
1:E:416:ARG:HG2	1:E:466:ARG:HG2	1.91	0.53
1:E:112:ARG:HH21	1:E:119:LEU:HD11	1.74	0.52
1:E:671:LYS:HD2	1:E:740:LEU:HB2	1.90	0.52
1:A:5:THR:HG22	1:A:180:LYS:HB2	1.90	0.52
1:C:1060:ALA:HB1	1:C:1067:SER:HB3	1.92	0.52
1:E:545:ILE:HG23	1:E:604:ARG:HD2	1.91	0.52
1:F:519:ASP:OD1	1:F:618:TRP:NE1	2.39	0.52
1:F:1072:TYR:HB2	1:F:1098:TRP:CE2	2.45	0.52
1:C:122:PHE:CE2	1:D:220:PRO:HD3	2.45	0.52
1:E:112:ARG:NH2	1:E:119:LEU:HD11	2.25	0.51
1:E:1076:ILE:HG22	1:E:1082:MET:HG3	1.91	0.51
1:B:1079:GLY:HA3	1:B:1134:ILE:HB	1.93	0.51
1:A:141:SER:OG	1:A:167:HIS:NE2	2.42	0.51
1:A:416:ARG:HG2	1:A:466:ARG:HG2	1.92	0.51
1:A:704:TYR:CE1	1:A:736:GLN:HB3	2.44	0.51
1:B:1060:ALA:HB1	1:B:1067:SER:HB3	1.93	0.51
1:D:793:VAL:HG21	1:D:1050:HIS:HB3	1.92	0.51
1:A:838:SER:HA	1:A:841:TRP:CE2	2.45	0.51
3:C:1204:TPP:H2	3:C:1204:TPP:HN42	1.75	0.51
1:E:1012:GLY:HA2	1:E:1150:LEU:HD13	1.92	0.51
1:C:85:SER:HA	1:C:127:ASP:HB3	1.93	0.50
1:F:1004:GLN:HG2	1:F:1017:PHE:CE2	2.45	0.50
1:F:1076:ILE:HG22	1:F:1082:MET:HG3	1.93	0.50
1:B:112:ARG:HH21	1:B:119:LEU:HD11	1.76	0.50
1:D:282:GLU:OE1	1:D:299:LYS:NZ	2.40	0.50
1:B:678:ILE:HD11	1:B:767:VAL:HG23	1.92	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:5:THR:HG22	1:B:180:LYS:HB2	1.93	0.50
1:B:85:SER:HA	1:B:127:ASP:HB3	1.94	0.50
1:C:695:VAL:HG11	1:C:751:VAL:HG21	1.94	0.50
1:D:136:PHE:CE2	1:D:164:PRO:HB2	2.46	0.50
1:A:85:SER:HA	1:A:127:ASP:HB3	1.94	0.49
1:D:506:ILE:HG12	1:D:536:LYS:HE3	1.94	0.49
1:D:671:LYS:NZ	1:D:741:ASP:OD2	2.40	0.49
1:C:356:VAL:HG13	1:C:386:ASN:HA	1.93	0.49
1:C:583:ILE:HD13	1:C:598:ASN:HB3	1.94	0.49
1:D:81:THR:HG21	1:D:91:MET:HE1	1.93	0.49
1:F:435:ILE:HD13	1:F:448:GLY:HA3	1.94	0.49
1:A:814:GLU:HB3	1:A:993:LEU:HD13	1.95	0.49
1:B:112:ARG:NH2	1:B:119:LEU:HD11	2.28	0.49
1:E:1010:GLN:HG3	1:E:1097:TYR:OH	2.13	0.49
1:A:1036:TYR:O	1:B:1025:LYS:NZ	2.46	0.48
1:C:694:LEU:HD22	1:C:793:VAL:HG13	1.94	0.48
1:B:112:ARG:NE	1:B:121:ILE:HA	2.28	0.48
1:C:996:GLU:HG2	1:C:1026:LYS:HZ2	1.77	0.48
1:A:112:ARG:NE	1:A:121:ILE:HA	2.28	0.48
1:C:455:LYS:HD3	1:C:672:ARG:CZ	2.42	0.48
1:E:747:ASN:ND2	1:E:1083:THR:O	2.46	0.48
1:E:967:ASP:HB3	1:E:994:ASP:HA	1.95	0.48
1:D:679:PRO:HD2	1:D:737:VAL:HG21	1.96	0.48
1:A:220:PRO:HD3	1:B:122:PHE:CE2	2.48	0.48
1:B:695:VAL:HG11	1:B:751:VAL:HG21	1.96	0.48
1:E:1060:ALA:HB1	1:E:1067:SER:HB3	1.95	0.48
1:A:480:GLN:HA	1:A:500:GLY:O	2.13	0.48
1:F:747:ASN:ND2	1:F:1083:THR:O	2.46	0.47
1:F:356:VAL:HG13	1:F:386:ASN:HA	1.95	0.47
1:E:189:MET:O	1:E:193:VAL:HG23	2.14	0.47
1:E:457:SER:O	1:E:672:ARG:NH1	2.36	0.47
1:E:719:VAL:O	1:E:734:ARG:NH2	2.46	0.47
1:F:802:LEU:HB2	1:F:822:THR:HB	1.95	0.47
1:A:59:MET:HG3	1:A:65:ALA:HA	1.97	0.47
1:B:583:ILE:HD13	1:B:598:ASN:HB3	1.97	0.47
1:D:1072:TYR:HB2	1:D:1098:TRP:CE2	2.49	0.47
1:A:313:LYS:HG3	1:A:314:VAL:HG13	1.97	0.47
1:A:590:LYS:HB3	1:A:594:ILE:HD12	1.97	0.47
1:B:665:GLY:N	1:B:850:TYR:O	2.47	0.47
1:C:733:PHE:HE1	1:C:735:ILE:HG12	1.80	0.47
1:A:998:TYR:CE1	1:A:1006:SER:HB2	2.50	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:523:PRO:O	1:C:527:LYS:HG3	2.15	0.47
1:C:1047:GLY:HA3	1:C:1089:ALA:HB3	1.97	0.47
1:E:855:GLN:N	1:E:855:GLN:OE1	2.48	0.46
1:F:1079:GLY:HA3	1:F:1134:ILE:HB	1.97	0.46
1:A:827:ASP:OD2	1:A:921:ARG:NH1	2.34	0.46
1:B:283:GLU:OE1	1:B:476:TYR:OH	2.24	0.46
1:F:136:PHE:CE2	1:F:164:PRO:HB2	2.51	0.46
1:C:358:GLY:HA3	1:C:388:PHE:CE1	2.51	0.46
1:D:85:SER:HA	1:D:127:ASP:HB3	1.98	0.46
1:B:826:GLY:HA2	1:B:829:MET:SD	2.56	0.46
1:C:334:LEU:HD21	1:D:345:VAL:HB	1.98	0.46
1:D:1127:ARG:HH22	1:D:1148:GLU:CD	2.18	0.46
1:E:334:LEU:HD21	1:F:345:VAL:HB	1.98	0.46
1:B:18:ALA:HB2	1:B:186:TYR:CZ	2.51	0.46
1:C:1030:GLY:O	1:C:1034:MET:HG3	2.16	0.46
1:D:1127:ARG:NH1	1:D:1148:GLU:OE2	2.47	0.46
1:F:18:ALA:HB2	1:F:186:TYR:CE1	2.50	0.46
3:F:1204:TPP:H2	3:F:1204:TPP:HN42	1.79	0.46
1:D:112:ARG:NE	1:D:121:ILE:HA	2.31	0.46
1:D:704:TYR:CE1	1:D:736:GLN:HB3	2.51	0.46
1:E:122:PHE:CE2	1:F:220:PRO:HD3	2.51	0.46
1:E:212:HIS:NE2	1:E:214:ARG:HD2	2.30	0.46
1:D:513:TRP:O	1:D:539:ASN:ND2	2.49	0.46
1:A:438:ILE:HD13	1:A:569:VAL:HG11	1.97	0.45
1:D:695:VAL:HG11	1:D:751:VAL:HG21	1.97	0.45
1:D:819:LYS:NZ	6:D:1320:HOH:O	2.48	0.45
1:A:790:PRO:HG3	1:A:799:ARG:NH2	2.31	0.45
1:C:479:ASP:OD1	6:C:1301:HOH:O	2.20	0.45
1:C:1119:TYR:HE2	1:C:1122:PRO:HA	1.80	0.45
1:F:18:ALA:HB2	1:F:186:TYR:CZ	2.51	0.45
1:F:935:ILE:HD13	1:F:947:LEU:HD23	1.97	0.45
1:A:1080:ILE:HG13	1:A:1082:MET:HE2	1.98	0.45
1:B:747:ASN:OD1	1:B:811:GLY:HA2	2.15	0.45
1:D:419:PHE:HB2	1:D:463:SER:HB2	1.97	0.45
1:C:426:GLY:HA3	1:C:556:ASN:HB3	1.99	0.45
1:E:590:LYS:HB3	1:E:594:ILE:HD12	1.97	0.45
1:A:426:GLY:HA3	1:A:556:ASN:HB3	1.99	0.45
1:E:817:TYR:CZ	1:E:1071:ALA:HB1	2.51	0.45
1:F:122:PHE:HB3	1:F:364:SER:HB2	1.97	0.45
1:C:506:ILE:HG21	1:C:566:ILE:HD12	1.99	0.45
1:A:112:ARG:NH2	1:A:119:LEU:HD11	2.30	0.45



		Interatomic	Clash		
Atom-1	Atom-2	distance (\AA)	overlap (Å)		
1:B:212:HIS:NE2	1:B:214:ARG:HD2	2.31	0.45		
1:A:348:GLU:OE1	1:B:387:LYS:NZ	2.50	0.45		
1:D:826:GLY:HA2	1:D:829:MET:SD	2.57	0.45		
1:E:1004:GLN:HG2	1:E:1017:PHE:CE2	2.52	0.45		
1:A:81:THR:HG21	1:A:91:MET:HE1	1.98	0.45		
1:B:887:LEU:HD13	1:B:952:GLN:HB2	1.99	0.45		
1:C:18:ALA:HB2	1:C:186:TYR:CE1	2.52	0.45		
1:D:513:TRP:HE3	1:D:517:GLU:HG2	1.82	0.45		
1:F:1127:ARG:HH21	1:F:1151:PHE:HB3	1.81	0.45		
1:B:935:ILE:HD13	1:B:947:LEU:HD23	1.99	0.44		
1:D:1060:ALA:HB1	1:D:1067:SER:HB3	1.98	0.44		
1:E:85:SER:HA	1:E:127:ASP:HB3	1.99	0.44		
1:B:521:ARG:NH2	5:B:1207:SO4:O1	2.45	0.44		
1:A:681:TRP:CH2	1:A:734:ARG:HA	2.52	0.44		
1:C:879:ALA:HB3	1:D:75:ALA:HB3	2.00	0.44		
1:D:814:GLU:HB3	1:D:993:LEU:HD13	1.99	0.44		
1:A:1119:TYR:HE2	1:A:1122:PRO:HA	1.83	0.44		
1:B:802:LEU:HB2	1:B:822:THR:HB	1.99	0.44		
1:D:480:GLN:HA	1:D:500:GLY:O	2.17	0.44		
1:B:18:ALA:HB2	1:B:186:TYR:CE1	2.53	0.44		
1:F:124:ASP:HA	1:F:327:ARG:HD3	1.99	0.44		
1:A:838:SER:O	6:A:1301:HOH:O	2.21	0.44		
1:A:1004:GLN:HG2	1:A:1017:PHE:CE2	2.53	0.44		
1:A:1072:TYR:HB2	1:A:1098:TRP:CE2	2.52	0.44		
3:A:1204:TPP:H2	3:A:1204:TPP:HN42	1.83	0.44		
1:B:1102:ARG:NH1	1:B:1118:ASP:OD1	2.48	0.44		
1:F:1010:GLN:HG3	1:F:1097:TYR:OH	2.18	0.44		
1:D:122:PHE:HB3	1:D:364:SER:HB2	2.00	0.44		
1:E:583:ILE:HD13	1:E:598:ASN:HB3	2.00	0.44		
1:C:887:LEU:HD13	1:C:952:GLN:HB2	1.99	0.43		
1:B:258:LEU:HD22	1:B:310:HIS:CG	2.53	0.43		
1:C:814:GLU:HB3	1:C:993:LEU:HD13	2.00	0.43		
1:D:1030:GLY:O	1:D:1034:MET:HG3	2.18	0.43		
1:E:18:ALA:HB2	1:E:186:TYR:CE1	2.52	0.43		
1:A:419:PHE:HB2	1:A:463:SER:HB2	2.00	0.43		
1:A:1047:GLY:HA3	1:A:1089:ALA:HB3	1.99	0.43		
1:B:817:TYR:CZ	1:B:1071:ALA:HB1	2.53	0.43		
1:D:527:LYS:HD2	1:D:618:TRP:CE2	2.52	0.43		
1:D:671:LYS:HD2	1:D:740:LEU:HB2	1.99	0.43		
1:E:122:PHE:HB3	1:E:364:SER:HB2	1.99	0.43		
1:C:747:ASN:OD1	1:C:811:GLY:HA2	2.17	0.43		



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:D:571:PRO:HB2	1:D:574:GLU:HG3	2.00	0.43	
1:D:718:PHE:CZ	1:D:734:ARG:HD3	2.53	0.43	
1:D:1102:ARG:HD2	6:D:1301:HOH:O	2.19	0.43	
1:E:75:ALA:HB3	1:F:879:ALA:HB3	2.01	0.43	
1:A:310:HIS:HA	1:A:313:LYS:CD	2.48	0.43	
1:B:1010:GLN:HG3	1:B:1097:TYR:OH	2.19	0.43	
1:C:583:ILE:HG23	1:C:587:TYR:HD2	1.84	0.43	
1:D:489:PRO:HG3	1:D:510:ASN:O	2.19	0.43	
1:E:356:VAL:HG13	1:E:386:ASN:HA	2.00	0.43	
1:F:426:GLY:HA3	1:F:556:ASN:HB3	2.01	0.43	
1:F:695:VAL:HG11	1:F:751:VAL:HG21	2.00	0.43	
1:F:720:THR:HG22	1:F:734:ARG:HB2	2.01	0.43	
1:B:891:ILE:HG12	1:B:949:ILE:HD12	2.01	0.43	
1:D:501:ILE:HD13	1:D:535:LEU:HD13	2.01	0.43	
1:E:356:VAL:HG12	1:E:388:PHE:HE1	1.83	0.43	
1:A:189:MET:O	1:A:193:VAL:HG23	2.19	0.43	
1:A:198:ILE:O	1:A:202:ARG:HG2	2.19	0.43	
1:D:435:ILE:HD13	1:D:448:GLY:HA3	2.00	0.43	
1:D:438:ILE:HD13	1:D:569:VAL:HG11	2.01	0.43	
1:D:1004:GLN:HG2	1:D:1017:PHE:CE2	2.54	0.43	
1:D:945:LEU:O	1:D:949:ILE:HG12	2.19	0.42	
1:F:83:THR:O	1:F:109:VAL:HA	2.19	0.42	
1:F:817:TYR:CZ	1:F:1071:ALA:HB1	2.53	0.42	
1:A:1010:GLN:HG3	1:A:1097:TYR:CZ	2.53	0.42	
1:B:489:PRO:HG3	1:B:510:ASN:O	2.19	0.42	
1:D:124:ASP:HA	1:D:327:ARG:HD3	2.00	0.42	
1:B:1031:LEU:HD21	1:B:1164:GLN:HE22	1.83	0.42	
1:C:802:LEU:HD13	1:C:859:PRO:HD3	2.00	0.42	
1:D:321:ARG:HG2	1:D:354:LEU:HB3	2.01	0.42	
1:D:511:SER:HB2	1:D:513:TRP:CD1	2.54	0.42	
1:F:97:LYS:HE3	1:F:97:LYS:HB3	1.86	0.42	
1:A:515:ALA:O	1:A:518:MET:HB2	2.19	0.42	
1:D:112:ARG:NH2	1:D:119:LEU:HD11	2.34	0.42	
1:A:1127:ARG:O	1:A:1131:MET:HG2	2.20	0.42	
1:B:389:THR:O	1:B:400:SER:HA	2.20	0.42	
1:D:96:TYR:CE1	1:D:134:THR:HA	2.55	0.42	
1:D:258:LEU:HD22	1:D:310:HIS:CG	2.54	0.42	
1:D:371:MET:HB3	1:D:390:VAL:CG1	2.49	0.42	
1:D:1062:LYS:HG3	6:D:1310:HOH:O	2.19	0.42	
1:F:480:GLN:HA	1:F:500:GLY:O	2.18	0.42	
1:C:7:ASP:HA	1:C:177:GLU:O	2.19	0.42	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:615:PRO:HG2	1:D:618:TRP:CD1	2.54	0.42
1:F:699:ALA:HB2	1:F:819:LYS:HD2	2.00	0.42
1:F:855:GLN:N	1:F:855:GLN:OE1	2.52	0.42
1:A:18:ALA:HB2	1:A:186:TYR:CE1	2.55	0.42
1:B:422:LEU:HD22	1:B:423:GLY:H	1.85	0.42
1:E:752:CYS:SG	1:E:758:ALA:HB3	2.59	0.42
1:F:827:ASP:OD2	1:F:921:ARG:NH1	2.29	0.42
1:A:75:ALA:HB3	1:B:879:ALA:HB3	2.02	0.42
1:A:1010:GLN:HE22	1:A:1161:ARG:HH12	1.68	0.42
1:A:1074:PRO:HA	1:A:1078:HIS:CE1	2.54	0.42
1:C:18:ALA:HB2	1:C:186:TYR:CZ	2.54	0.42
1:C:220:PRO:HD3	1:D:122:PHE:CE2	2.55	0.42
1:D:140:SER:HB2	1:D:168:PHE:CZ	2.54	0.42
1:E:998:TYR:CE1	1:E:1006:SER:HB2	2.54	0.42
1:F:112:ARG:NE	1:F:121:ILE:HA	2.35	0.42
1:F:112:ARG:NH2	1:F:119:LEU:HD11	2.34	0.42
1:F:841:TRP:O	1:F:849:PRO:HG3	2.20	0.42
1:A:356:VAL:HG13	1:A:386:ASN:HA	2.02	0.42
1:F:747:ASN:OD1	1:F:811:GLY:HA2	2.20	0.42
1:D:641:ARG:HB2	1:D:642:PRO:HD3	2.02	0.42
1:E:1155:GLU:HG2	1:E:1159:LYS:HE3	2.01	0.42
1:F:47:LYS:HD2	1:F:51:GLY:C	2.40	0.42
1:A:879:ALA:HB3	1:B:75:ALA:HB3	2.02	0.41
1:D:671:LYS:NZ	6:D:1314:HOH:O	2.42	0.41
1:F:826:GLY:HA2	1:F:829:MET:SD	2.60	0.41
1:D:373:LYS:HD2	1:D:407:ILE:HD13	2.02	0.41
1:D:803:LEU:HD12	1:D:849:PRO:HB2	2.02	0.41
1:F:1127:ARG:HH21	1:F:1151:PHE:CB	2.33	0.41
1:B:189:MET:O	1:B:193:VAL:HG23	2.21	0.41
1:E:565:LYS:HD3	1:E:606:LEU:HD22	2.02	0.41
1:E:1010:GLN:HG3	1:E:1097:TYR:CZ	2.55	0.41
1:C:567:ALA:HB1	1:C:569:VAL:HG23	2.03	0.41
1:D:447:GLN:OE1	1:D:466:ARG:NH2	2.42	0.41
1:E:220:PRO:HD3	1:F:122:PHE:CE2	2.56	0.41
1:E:482:ASP:OD1	1:E:502:LYS:HD2	2.21	0.41
1:E:641:ARG:HB2	1:E:642:PRO:HD3	2.02	0.41
1:A:1075:CYS:SG	1:A:1076:ILE:N	2.93	0.41
1:E:694:LEU:HD22	1:E:793:VAL:HG13	2.03	0.41
1:C:592:ASP:O	1:C:596:ASN:ND2	2.52	0.41
1:D:415:PHE:O	1:D:466:ARG:HA	2.21	0.41
1:E:826:GLY:HA2	1:E:829:MET:SD	2.61	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:841:TRP:O	1:E:849:PRO:HG3	2.20	0.41
1:F:1095:ALA:HB1	1:F:1126:PHE:HA	2.02	0.41
1:A:841:TRP:O	1:A:849:PRO:HG3	2.21	0.41
1:A:1035:SER:HB2	1:B:1031:LEU:HD23	2.03	0.41
1:B:26:TYR:HB3	1:B:62:GLU:HG3	2.03	0.41
1:B:945:LEU:O	1:B:949:ILE:HG12	2.21	0.41
1:D:747:ASN:ND2	1:D:1083:THR:O	2.52	0.41
1:E:692:CYS:HB2	1:E:748:CYS:HB2	2.02	0.41
1:C:136:PHE:CE2	1:C:164:PRO:HB2	2.55	0.41
1:E:426:GLY:HA3	1:E:556:ASN:HB3	2.03	0.41
1:A:435:ILE:HG23	1:A:446:ALA:HB1	2.03	0.41
1:A:523:PRO:HB2	1:A:525:ASP:OD1	2.21	0.41
1:A:641:ARG:HB2	1:A:642:PRO:HD3	2.01	0.41
1:A:747:ASN:ND2	1:A:1083:THR:O	2.53	0.41
1:C:641:ARG:HB2	1:C:642:PRO:HD3	2.03	0.41
1:D:692:CYS:HB2	1:D:748:CYS:HB2	2.03	0.41
1:D:1010:GLN:HG3	1:D:1097:TYR:CZ	2.56	0.41
1:E:21:GLU:OE2	1:E:202:ARG:NH1	2.42	0.41
1:E:50:PHE:CZ	1:E:78:LEU:HD12	2.55	0.41
1:E:649:ASP:OD1	1:F:221:ASP:HA	2.21	0.41
1:E:1031:LEU:HD23	1:F:1035:SER:HB2	2.02	0.41
1:A:935:ILE:HD13	1:A:947:LEU:HD23	2.03	0.41
1:B:521:ARG:HA	1:B:521:ARG:HD2	1.81	0.41
1:C:453:ASP:OD1	1:C:454:SER:N	2.52	0.41
1:C:855:GLN:OE1	1:C:855:GLN:N	2.54	0.41
1:D:85:SER:HB2	1:D:112:ARG:HB3	2.03	0.41
1:E:435:ILE:HG23	1:E:446:ALA:HB1	2.03	0.41
1:E:1075:CYS:SG	1:E:1076:ILE:N	2.94	0.41
1:F:815:THR:OG1	1:F:816:PRO:HD3	2.21	0.41
1:B:373:LYS:HE2	1:B:405:GLU:OE2	2.20	0.40
1:B:641:ARG:HB2	1:B:642:PRO:HD3	2.02	0.40
1:C:973:ILE:HD11	3:C:1204:TPP:HM23	2.02	0.40
1:D:212:HIS:NE2	1:D:214:ARG:HD2	2.37	0.40
1:A:132:ARG:HH11	1:B:132:ARG:HH11	1.69	0.40
1:C:348:GLU:OE1	1:D:387:LYS:NZ	2.54	0.40
1:D:143:SER:O	1:D:147:VAL:HG23	2.21	0.40
1:E:18:ALA:HB2	1:E:186:TYR:CZ	2.56	0.40
1:F:36:GLU:CD	1:F:1016:ARG:HD3	2.41	0.40
1:F:122:PHE:HB3	1:F:364:SER:CB	2.51	0.40
1:C:66:ALA:HB2	1:C:91:MET:HE2	2.02	0.40
1:E:838:SER:HA	1:E:841:TRP:CE2	2.56	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1060:ALA:HB1	1:F:1067:SER:HB3	2.02	0.40
1:C:122:PHE:HB3	1:C:364:SER:HB2	2.04	0.40
1:C:428:VAL:HG11	1:C:452:TYR:OH	2.22	0.40
1:E:879:ALA:HB3	1:F:75:ALA:HB3	2.03	0.40
1:E:883:ARG:NH2	1:E:886:GLU:OE1	2.41	0.40
1:F:249:ALA:HB1	1:F:255:HIS:CD2	2.56	0.40
1:F:1030:GLY:O	1:F:1034:MET:HG3	2.22	0.40
1:A:418:LYS:HA	1:A:463:SER:O	2.22	0.40
1:D:1010:GLN:HG3	1:D:1097:TYR:OH	2.21	0.40
1:E:91:MET:O	1:E:95:MET:HG3	2.22	0.40
1:F:524:ALA:HB3	1:F:623:ASP:HA	2.02	0.40
1:F:803:LEU:HD12	1:F:849:PRO:HB2	2.03	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	Perce	ntiles
1	А	1159/1171~(99%)	1142 (98%)	17 (2%)	0	100	100
1	В	1167/1171~(100%)	1148 (98%)	19 (2%)	0	100	100
1	С	1159/1171~(99%)	1143 (99%)	16 (1%)	0	100	100
1	D	$1151/1171 \ (98\%)$	1132~(98%)	19 (2%)	0	100	100
1	Ε	1161/1171~(99%)	1143~(98%)	18 (2%)	0	100	100
1	F	1154/1171~(98%)	1135~(98%)	19 (2%)	0	100	100
All	All	6951/7026~(99%)	6843~(98%)	108 (2%)	0	100	100

There are no Ramachandran outliers to report.



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	А	918/932~(98%)	914 (100%)	4 (0%)	91	97
1	В	920/932~(99%)	915 (100%)	5 (0%)	88	96
1	С	916/932~(98%)	912~(100%)	4 (0%)	91	97
1	D	903/932~(97%)	898~(99%)	5 (1%)	86	95
1	Ε	916/932~(98%)	911 (100%)	5~(0%)	88	96
1	F	902/932~(97%)	899 (100%)	3 (0%)	92	98
All	All	5475/5592~(98%)	5449 (100%)	26~(0%)	88	96

All (26) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	224	PHE
1	А	390	VAL
1	А	518	MET
1	А	833	ASN
1	В	224	PHE
1	В	382	THR
1	В	518	MET
1	В	521	ARG
1	В	833	ASN
1	С	224	PHE
1	С	390	VAL
1	С	467	PHE
1	С	833	ASN
1	D	224	PHE
1	D	467	PHE
1	D	518	MET
1	D	833	ASN
1	D	926	ARG
1	Е	224	PHE
1	Е	326	ASP
1	Е	467	PHE
1	Е	518	MET



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Mol	Chain	Res	Type
1	Е	833	ASN
1	F	224	PHE
1	F	467	PHE
1	F	833	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	343	GLN
1	В	1164	GLN
1	D	547	GLN
1	F	255	HIS
1	F	433	ASN
1	F	560	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 6 are monoatomic - leaving 31 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).



6CIN

Mal	Tune	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	B	ond ang	gles
	Type	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	D	1201	1	0,12,12	-	-	-		
2	SF4	В	1203	1	0,12,12	-	-	-		
2	SF4	D	1202	1	0,12,12	-	-	-		
2	SF4	С	1202	1	$0,\!12,\!12$	-	-	-		
2	SF4	Ε	1202	1	$0,\!12,\!12$	-	-	-		
2	SF4	F	1202	1	$0,\!12,\!12$	-	-	-		
5	SO4	А	1206	-	4,4,4	0.16	0	6,6,6	0.04	0
2	SF4	Е	1201	1	$0,\!12,\!12$	-	-	-		
2	SF4	В	1202	1	0,12,12	-	-	-		
3	TPP	Е	1204	4	22,27,27	2.00	6 (27%)	29,40,40	1.61	8 (27%)
5	SO4	С	1206	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SF4	А	1203	1	$0,\!12,\!12$	-	-	-		
2	SF4	С	1201	1	$0,\!12,\!12$	-	-	-		
3	TPP	С	1204	4	$22,\!27,\!27$	1.96	6 (27%)	29,40,40	1.58	5 (17%)
2	SF4	В	1201	1	0,12,12	-	-	-		
5	SO4	F	1206	-	4,4,4	0.14	0	$6,\!6,\!6$	0.14	0
3	TPP	А	1204	4	22,27,27	1.94	6 (27%)	29,40,40	1.59	7 (24%)
2	SF4	А	1201	1	0,12,12	-	-	-		
2	SF4	С	1203	1	0,12,12	-	-	-		
3	TPP	D	1204	4	22,27,27	1.98	6 (27%)	29,40,40	1.67	8 (27%)
2	SF4	F	1203	1	0,12,12	-	-	-		
5	SO4	Е	1206	-	4,4,4	0.14	0	6,6,6	0.13	0
5	SO4	D	1206	-	$4,\!4,\!4$	0.15	0	$6,\!6,\!6$	0.14	0
3	TPP	F	1204	4	22,27,27	1.98	6 (27%)	29,40,40	1.78	7 (24%)
2	SF4	F	1201	1	0,12,12	-	-	-		
2	SF4	Е	1203	1	0,12,12	-	-	-		
5	SO4	В	1206	-	4,4,4	0.13	0	6,6,6	0.10	0
5	SO4	В	1207	-	4,4,4	0.13	0	6,6,6	0.12	0
3	TPP	В	1204	4	22,27,27	2.04	6 (27%)	29,40,40	1.60	7 (24%)
2	SF4	А	1202	1	0,12,12	-	-	-		
2	SF4	D	1203	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	D	1201	1	-	-	0/6/5/5
2	SF4	В	1203	1	-	-	0/6/5/5
2	SF4	D	1202	1	-	-	0/6/5/5



2

SF4

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Conti	nued fro	m nrevia	is nade					
Mol	Type	Chain	\mathbf{Res}	Link	Chirals	Torsions	Rings	
2	SF4	С	1202	1	-	-	0/6/5/5	
2	SF4	Е	1202	1	-	_	0/6/5/5	
2	SF4	F	1202	1	-	-	0/6/5/5	
2	SF4	Е	1201	1	-	-	0/6/5/5	
2	SF4	В	1202	1	-	-	0/6/5/5	
3	TPP	Е	1204	4	-	3/16/17/17	0/2/2/2	
2	SF4	А	1203	1	-	-	0/6/5/5	
3	TPP	С	1204	4	-	5/16/17/17	0/2/2/2	
2	SF4	С	1201	1	-	-	0/6/5/5	
2	SF4	В	1201	1	-	-	0/6/5/5	
3	TPP	А	1204	4	-	5/16/17/17	0/2/2/2	
2	SF4	А	1201	1	-	-	0/6/5/5	
2	SF4	С	1203	1	-	-	0/6/5/5	
3	TPP	D	1204	4	-	5/16/17/17	0/2/2/2	
2	SF4	F	1203	1	-	-	0/6/5/5	
3	TPP	F	1204	4	-	4/16/17/17	0/2/2/2	
2	SF4	F	1201	1	-	_	0/6/5/5	
2	SF4	Е	1203	1	-	-	0/6/5/5	
3	TPP	В	1204	4	-	2/16/17/17	0/2/2/2	
2	SF4	А	1202	1	-	-	0/6/5/5	

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0/6/5/5

All (36) bond length outli	ers are listed below:
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1203

1

D

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	В	1204	TPP	C4-N3	-4.85	1.35	1.39
3	F	1204	TPP	C4-N3	-4.55	1.35	1.39
3	С	1204	TPP	C4-N3	-4.46	1.35	1.39
3	Ε	1204	TPP	C4-N3	-4.46	1.35	1.39
3	А	1204	TPP	C4-N3	-4.26	1.36	1.39
3	Е	1204	TPP	C4'-N4'	3.91	1.43	1.34
3	D	1204	TPP	C4-N3	-3.83	1.36	1.39
3	D	1204	TPP	C6-C5	3.83	1.52	1.50
3	С	1204	TPP	C4'-N4'	3.82	1.43	1.34
3	F	1204	TPP	C4'-N4'	3.82	1.43	1.34
3	В	1204	TPP	C4'-N4'	3.82	1.43	1.34
3	А	1204	TPP	C4'-N4'	3.72	1.43	1.34
3	D	1204	TPP	C4'-N4'	3.69	1.43	1.34
3	A	1204	TPP	C7'-N3	-3.46	1.42	1.48
3	F	1204	TPP	C7'-N3	-3.45	1.42	1.48
3	C	1204	TPP	C7'-N3	-3.44	1.42	1.48



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	В	1204	TPP	C7'-N3	-3.34	1.42	1.48
3	Е	1204	TPP	C7'-N3	-3.30	1.42	1.48
3	D	1204	TPP	C7'-N3	-3.30	1.42	1.48
3	Ε	1204	TPP	C6-C5	3.29	1.52	1.50
3	С	1204	TPP	C7'-C5'	3.26	1.58	1.51
3	Ε	1204	TPP	C7'-C5'	3.24	1.58	1.51
3	В	1204	TPP	C6-C5	3.22	1.52	1.50
3	D	1204	TPP	C7'-C5'	3.21	1.57	1.51
3	А	1204	TPP	C7'-C5'	3.18	1.57	1.51
3	В	1204	TPP	C7'-C5'	3.17	1.57	1.51
3	F	1204	TPP	C7'-C5'	3.09	1.57	1.51
3	F	1204	TPP	C6-C5	3.08	1.52	1.50
3	А	1204	TPP	C6-C5	2.83	1.52	1.50
3	С	1204	TPP	C6-C5	2.39	1.52	1.50
3	А	1204	TPP	C6'-C5'	2.36	1.42	1.37
3	В	1204	TPP	C6'-C5'	2.31	1.42	1.37
3	С	1204	TPP	C6'-C5'	2.26	1.42	1.37
3	D	1204	TPP	C6'-C5'	2.25	1.42	1.37
3	F	1204	TPP	C6'-C5'	2.25	1.42	1.37
3	Ε	1204	TPP	C6'-C5'	2.24	1.42	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	F	1204	TPP	C6-C5-C4	-4.90	123.50	127.43
3	D	1204	TPP	C6-C5-C4	-4.35	123.94	127.43
3	В	1204	TPP	C6-C5-C4	-4.18	124.08	127.43
3	С	1204	TPP	C6-C5-C4	-3.90	124.30	127.43
3	Е	1204	TPP	C6-C5-C4	-3.79	124.39	127.43
3	А	1204	TPP	C6-C5-C4	-3.35	124.75	127.43
3	С	1204	TPP	C6'-N1'-C2'	3.33	121.63	115.96
3	F	1204	TPP	C6'-N1'-C2'	3.32	121.61	115.96
3	В	1204	TPP	C6'-N1'-C2'	3.17	121.36	115.96
3	D	1204	TPP	C6'-N1'-C2'	3.16	121.34	115.96
3	Ε	1204	TPP	C6'-N1'-C2'	3.15	121.33	115.96
3	А	1204	TPP	C6'-N1'-C2'	3.12	121.27	115.96
3	С	1204	TPP	C5'-C6'-N1'	-3.10	118.65	123.82
3	F	1204	TPP	C5'-C6'-N1'	-2.96	118.89	123.82
3	В	1204	TPP	C5'-C6'-N1'	-2.84	119.09	123.82
3	D	1204	TPP	C5'-C6'-N1'	-2.81	119.15	123.82
3	А	1204	TPP	C5'-C6'-N1'	-2.78	119.19	123.82
3	Е	1204	TPP	C5'-C6'-N1'	-2.72	119.29	123.82



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	1204	TPP	CM4-C4-N3	2.69	125.95	122.53
3	Е	1204	TPP	N4'-C4'-N3'	2.53	120.61	117.03
3	D	1204	TPP	CM4-C4-N3	2.44	125.64	122.53
3	F	1204	TPP	PA-O3A-PB	-2.37	124.69	132.83
3	А	1204	TPP	PA-O3A-PB	-2.31	124.89	132.83
3	С	1204	TPP	CM4-C4-N3	2.31	125.47	122.53
3	F	1204	TPP	CM4-C4-N3	2.30	125.47	122.53
3	F	1204	TPP	N1'-C2'-N3'	-2.29	121.60	125.54
3	Е	1204	TPP	PA-O3A-PB	-2.26	125.06	132.83
3	В	1204	TPP	PA-O3A-PB	-2.23	125.18	132.83
3	D	1204	TPP	N1'-C2'-N3'	-2.21	121.73	125.54
3	D	1204	TPP	PA-O3A-PB	-2.20	125.27	132.83
3	Е	1204	TPP	CM4-C4-N3	2.18	125.31	122.53
3	F	1204	TPP	N4'-C4'-N3'	2.16	120.09	117.03
3	D	1204	TPP	CM2-C2'-N1'	2.16	119.51	117.14
3	В	1204	TPP	N1'-C2'-N3'	-2.16	121.83	125.54
3	А	1204	TPP	N4'-C4'-N3'	2.10	120.00	117.03
3	Е	1204	TPP	N1'-C2'-N3'	-2.07	121.97	125.54
3	В	1204	TPP	N4'-C4'-N3'	2.07	119.96	117.03
3	D	1204	TPP	C2'-N3'-C4'	2.07	121.31	118.08
3	A	1204	TPP	N1'-C2'-N3'	-2.07	121.98	125.54
3	С	1204	TPP	N1'-C2'-N3'	-2.05	122.01	125.54
3	Е	1204	TPP	CM2-C2'-N3'	2.05	120.35	117.15
3	В	1204	TPP	C2'-N3'-C4'	2.01	121.22	118.08

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
3	А	1204	TPP	PA-O3A-PB-O1B
3	F	1204	TPP	PA-O3A-PB-O1B
3	А	1204	TPP	C5-C6-C7-O7
3	С	1204	TPP	C5-C6-C7-O7
3	D	1204	TPP	C5-C6-C7-O7
3	Ε	1204	TPP	C5-C6-C7-O7
3	С	1204	TPP	PA-O3A-PB-O3B
3	F	1204	TPP	PA-O3A-PB-O3B
3	В	1204	TPP	C4-C5-C6-C7
3	С	1204	TPP	C4-C5-C6-C7
3	Ε	1204	TPP	C4-C5-C6-C7
3	F	1204	TPP	C5-C6-C7-O7
3	А	1204	TPP	PA-O3A-PB-O3B



Mol	Chain	Res	Type	Atoms
3	В	1204	TPP	PA-O3A-PB-O3B
3	С	1204	TPP	PA-O3A-PB-O2B
3	D	1204	TPP	PA-O3A-PB-O2B
3	D	1204	TPP	PA-O3A-PB-O3B
3	Е	1204	TPP	PA-O3A-PB-O3B
3	А	1204	TPP	C7-O7-PA-O1A
3	С	1204	TPP	C7-O7-PA-O1A
3	D	1204	TPP	C7-O7-PA-O1A
3	A	1204	TPP	C4-C5-C6-C7
3	D	1204	TPP	C4-C5-C6-C7
3	F	1204	TPP	C4-C5-C6-C7

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There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	1204	TPP	2	0
3	А	1204	TPP	1	0
3	F	1204	TPP	1	0
5	В	1207	SO4	3	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 then 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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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	$OWAB(A^2)$	Q<0.9
1	А	$1163/1171 \ (99\%)$	0.31	68 (5%) 23 17	36, 66, 125, 151	0
1	В	$1169/1171 \ (99\%)$	0.26	68 (5%) 23 17	34, 66, 117, 171	0
1	С	1163/1171 (99%)	0.40	90 (7%) 13 10	36, 74, 130, 165	0
1	D	$1157/1171 \ (98\%)$	0.22	36 (3%) 49 42	45, 77, 130, 170	0
1	Е	$1165/1171 \ (99\%)$	0.46	108 (9%) 8 6	29, 77, 128, 161	0
1	F	1158/1171~(98%)	0.22	48 (4%) 37 30	37, 78, 132, 188	0
All	All	6975/7026~(99%)	0.31	418 (5%) 21 16	29, 73, 128, 188	0

All (418) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	1131	MET	7.8
1	Е	754	ALA	7.6
1	Е	788	PHE	7.3
1	В	1150	LEU	6.9
1	F	1018	ALA	6.1
1	Е	757	LYS	5.7
1	А	629	VAL	5.7
1	С	678	ILE	5.5
1	Е	755	LYS	5.4
1	С	1044	VAL	5.4
1	С	594	ILE	5.2
1	Е	607	GLU	5.1
1	А	1122	PRO	4.9
1	С	598	ASN	4.9
1	Е	687	ILE	4.8
1	A	1012	GLY	4.8
1	А	818	VAL	4.7
1	А	788	PHE	4.7
1	E	766	GLU	4.7



Conti	nued from	n previo	ous page.	
\mathbf{Mol}	Chain	\mathbf{Res}	Type	RSRZ

1	В	1109	GLN	4.7
1	А	1136	TYR	4.6
1	Е	1136	TYR	4.6
1	Е	1123	THR	4.6
1	Е	1166	LYS	4.5
1	В	1139	LEU	4.5
1	С	788	PHE	4.5
1	С	706	ALA	4.5
1	А	1128	ASP	4.5
1	D	435	ILE	4.4
1	С	1126	PHE	4.4
1	Е	794	LYS	4.4
1	А	687	ILE	4.3
1	С	1123	THR	4.3
1	Е	1005	SER	4.2
1	А	716	GLU	4.2
1	F	522	LEU	4.2
1	В	1107	LEU	4.1
1	В	1128	ASP	4.1
1	С	605	ALA	4.1
1	В	1119	TYR	4.1
1	А	1129	PHE	4.1
1	Е	791	ALA	4.1
1	F	561	THR	4.1
1	Е	1019	ALA	4.1
1	Е	724	ILE	4.0
1	F	607	GLU	4.0
1	Е	635	PHE	4.0
1	Е	716	GLU	4.0
1	Е	759	LEU	3.9
1	А	821	VAL	3.9
1	С	716	GLU	3.9
1	С	735	ILE	3.9
1	Е	787	ASN	3.9
1	Е	1131	MET	3.9
1	В	1106	GLN	3.8
1	А	1127	ARG	3.8
1	С	1097	TYR	3.8
1	В	728	ALA	3.8
1	А	727	GLU	3.8
1	Е	761	MET	3.8
1	E	688	GLN	3.8



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733	PHE	3.6
798	PHE	3.6
765	GLU	3.6
758	ALA	3.6
.093	VAL	3.6
894	ALA	3.6
113	ASN	3.6
747	ASN	3.6
009	THR	3.5
598	ASN	3.5
125	SER	3.5
1.0.0	OT TT	~ ~

Continued from previous page... Mol Chain Res Type RSRZ

1097

728

1161

997

1126

674

1002

TYR

ALA

ARG

VAL

PHE

ILE

GLY

3.7

3.7

3.7

3.7

3.7

3.7

3.7

Е

С

А

Е

А

Е

Е

В

4	~	700	DITT	0.2
1	C	798	PHE	3.6
1	Е	765	GLU	3.6
1	Ε	758	ALA	3.6
1	С	1093	VAL	3.6
1	В	894	ALA	3.6
1	В	1113	ASN	3.6
1	Ε	747	ASN	3.6
1	А	1009	THR	3.5
1	D	598	ASN	3.5
1	Е	1125	SER	3.5
1	А	1163	GLU	3.5
1	Ε	691	GLN	3.5
1	В	710	ASP	3.5
1	С	762	VAL	3.5
1	Е	756	VAL	3.5
1	Е	821	VAL	3.4
1	В	1069	ILE	3.4
1	D	1153	LYS	3.4
1	Е	784	VAL	3.4
1	Е	606	LEU	3.4
1	В	1142	GLN	3.4
1	В	1151	PHE	3.4
1	С	1109	GLN	3.4
1	А	706	ALA	3.4
1	Е	751	VAL	3.4
1	С	1158	ALA	3.3
1	F	783	GLU	3.3
1	А	1109	GLN	3.3
1	А	1057	LEU	3.3
1	С	1150	LEU	3.3
1	Е	760	THR	3.3
1	Е	467	PHE	3.3
1	F	1159	LYS	3.3
1	С	551	LEU	3.3
	C	ontinue	d on nea	t page



110	0.2
AL	3.2
RG	3.2
AL	3.2
YS	3.2
LA	3.2
LE	3.2
LA	3.2
EU	3.2
EU	3.2

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Mol Chain Res Type RSRZ

	1			
1	D	629	VAL	3.3
1	С	404	LYS	3.3
1	Е	1072	TYR	3.3
1	С	1012	GLY	3.2
1	F	1017	PHE	3.2
1	В	1164	GLN	3.2
1	Е	1078	HIS	3.2
1	С	784	VAL	3.2
1	В	1127	ARG	3.2
1	В	1014	VAL	3.2
1	А	1159	LYS	3.2
1	С	1154	ALA	3.2
1	Е	540	ILE	3.2
1	С	1042	ALA	3.2
1	А	705	LEU	3.2
1	А	1031	LEU	3.2
1	С	1122	PRO	3.2
1	D	420	PHE	3.2
1	Е	1041	VAL	3.2
1	С	1119	TYR	3.2
1	А	1130	LEU	3.2
1	В	1121	THR	3.1
1	F	435	ILE	3.1
1	С	993	LEU	3.1
1	С	1121	THR	3.1
1	Е	739	PRO	3.1
1	А	777	PHE	3.1
1	В	1110	GLU	3.1
1	В	726	LYS	3.1
1	А	1103	TYR	3.1
1	С	1120	LYS	3.1
1	С	1157	ASP	3.1
1	F	1143	PHE	3.1
1	Е	542	ALA	3.1
1	Е	526	MET	3.0
1	F	718	PHE	3.0
1	Е	685	ASN	3.0
1	А	755	LYS	3.0
1	В	1108	ALA	3.0
1	В	686	CYS	3.0
1	F	433	ASN	3.0
1	В	788	PHE	3.0



Continued from previous page...

 Mol
 Chain
 Res
 Type
 RSRZ

			5	
1	В	910	TRP	3.0
1	В	1071	ALA	3.0
1	D	1017	PHE	3.0
1	А	1162	LEU	3.0
1	А	1156	ALA	3.0
1	В	730	GLY	3.0
1	Е	680	GLN	3.0
1	С	553	SER	3.0
1	В	1163	GLU	3.0
1	Е	711	LEU	2.9
1	Е	786	VAL	2.9
1	D	1097	TYR	2.9
1	С	590	LYS	2.9
1	F	626	ALA	2.9
1	F	627	ALA	2.9
1	В	1125	SER	2.9
1	В	1019	ALA	2.9
1	С	1071	ALA	2.9
1	F	854	ARG	2.9
1	Е	1100	LEU	2.9
1	D	565	LYS	2.9
1	Е	656	PHE	2.9
1	D	352	ASN	2.9
1	Е	762	VAL	2.8
1	Е	1014	VAL	2.8
1	А	1087	ARG	2.8
1	А	1149	GLN	2.8
1	С	1128	ASP	2.8
1	D	726	LYS	2.8
1	С	601	ALA	2.8
1	А	1049	SER	2.8
1	А	791	ALA	2.8
1	F	788	PHE	2.8
1	Е	717	THR	2.8
1	F	601	ALA	2.8
1	Е	1142	GLN	2.8
1	А	820	LEU	2.8
1	F	570	ILE	2.8
1	А	1097	TYR	2.8
1	Е	1126	PHE	2.8
1	F	420	PHE	2.8
1	С	1166	LYS	2.8



Mol

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В

В

С

С

А

D

Е

F

Е

А

D

Е

С

Е

${ m E}$	609	LEU	2.7	
D	1150	LEU	2.7	
F	1011	THR	2.7	
А	919	ARG	2.7	
А	1150	LEU	2.7	
Ε	1129	PHE	2.7	
В	1044	VAL	2.7	
С	1020	GLY	2.7	
А	1119	TYR	2.7	
Ε	564	PHE	2.7	
С	684	GLU	2.7	
\mathbf{F}	686	CYS	2.7	
С	935	ILE	2.7	
Ε	1083	THR	2.7	
А	1013	ALA	2.6	
Е	508	LEU	2.6	
Е	595	LEU	2.6	
С	1134	ILE	2.6	
Е	949	ILE	2.6	

Continued from previous page...

Res

1127

1142

1122

998

1161

1011

1047

717

1126

1111

1161

1080

787

1157

582

1012

684

695

949

561

677

852

793

PHE

GLY

ARG

ILE

ASN

ASP

SER

GLY

GLU

VAL

ILE

THR

ASN

VAL

2.6

2.6

2.6

2.6

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2.6

Type

ARG

GLN

PRO

TYR

ARG

THR

GLY

THR

RSRZ

2.8

2.7

2.7

2.7

2.7

2.7

2.7

2.7

Chain

Е

С

Е

Е

D

А

С

С



Mol

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	-	-
1159	LYS	2.5
689	CYS	2.5
51	GLY	2.5
1161	ARG	2.5
1126	PHE	2.5
789	ASN	2.5
1152	ALA	2.5
1100	LEU	2.5
1135	ARG	2.5
1125	SER	2.5
1012	GLY	2.5
1003	GLY	2.5
1017	PHE	2.5
710	ASP	2.5

2.5

2.5

2.5

2.5

2.5

2.5

 $\frac{2.5}{2.5}$

2.5

2.5

2.5

2.5

2.4

2.4

2.4

2.4

2.4

Continued from previous page...

 \mathbf{Res}

569

682

1062

753

678

589

1147

575

1139

Type

VAL

GLN

LYS

PRO

ILE

LYS

ALA

ALA

LEU

RSRZ

2.6

2.6

2.6

2.6

2.6

2.6

2.5

2.5

2.5

Chain

F

F

В

Е

F

С

В

F

С

С

Е

D

 $\overline{\mathbf{C}}$

В

Е

Е

А

Е

С

D

F

А

А

С

D

Е

С

С

В

В

 $\overline{\mathbf{C}}$

А

А

В

Е

С

F

В

В

Е

701

437

1010

457

764

1097

782

766

724

754

1165

1165

630

618

1055

1124

1121

ILE

ILE

GLN

SER

LEU

TYR

PRO

GLU

ILE

ALA

TYR

TYR

THR

TRP

LYS

ALA

THR

 C
 1130
 LEU
 2.4

 E
 1139
 LEU
 2.4

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 Mol
 Chain
 Res
 Type
 RSRZ

1.101	Onam	1000	-380	100101
1	С	620	ASP	2.4
1	D	716	GLU	2.4
1	В	590	LYS	2.4
1	D	485	ALA	2.4
1	А	946	LEU	2.4
1	В	1162	LEU	2.4
1	С	606	LEU	2.4
1	В	682	GLN	2.4
1	С	537	PHE	2.4
1	D	1023	PHE	2.4
1	В	876	MET	2.4
1	D	1009	THR	2.4
1	F	755	LYS	2.4
1	А	998	TYR	2.4
1	А	1018	ALA	2.4
1	С	1100	LEU	2.4
1	Е	694	LEU	2.4
1	В	679	PRO	2.4
1	С	1011	THR	2.4
1	С	1014	VAL	2.4
1	F	733	PHE	2.4
1	В	727	GLU	2.4
1	С	680	GLN	2.4
1	А	726	LYS	2.4
1	С	593	LYS	2.4
1	Е	565	LYS	2.4
1	F	1166	LYS	2.4
1	D	602	VAL	2.4
1	F	1023	PHE	2.4
1	С	1029	LEU	2.3
1	В	684	GLU	2.3
1	В	1116	ILE	2.3
1	С	1163	GLU	2.3
1	Е	1117	LEU	2.3
1	Е	558	ILE	2.3
1	F	583	ILE	2.3
1	А	1014	VAL	2.3
1	В	765	GLU	2.3
1	В	993	LEU	2.3
1	Е	684	GLU	2.3
1	Е	655	THR	2.3
1	С	576	ILE	2.3



6CIN

Mol	Chain	Res	Type	RSRZ
1	А	707	LYS	2.3
1	Е	1023	PHE	2.3
1	В	716	GLU	2.3
1	А	717	THR	2.3
1	В	678	ILE	2.3
1	D	1006	SER	2.3
1	В	1159	LYS	2.3
1	D	1014	VAL	2.3
1	Е	672	ARG	2.3
1	D	1168	LEU	2.3
1	Е	640	LEU	2.3
1	С	760	THR	2.3
1	С	734	ARG	2.3
1	В	755	LYS	2.3
1	Е	589	LYS	2.3
1	D	988	VAL	2.3
1	С	511	SER	2.2
1	С	1010	GLN	2.2
1	В	1131	MET	2.2
1	В	1129	PHE	2.2
1	С	733	PHE	2.2
1	Е	1128	ASP	2.2
1	А	913	GLY	2.2
1	А	1108	ALA	2.2
1	D	575	ALA	2.2
1	А	607	GLU	2.2
1	Е	352	ASN	2.2
1	Е	618	TRP	2.2
1	C	1054	MET	2.2
1	C	1129	PHE	2.2
1	В	569	VAL	2.2
1	С	724	ILE	2.2
1	C	1053	LEU	2.2
1	Е	512	THR	2.2
1	E	710	ASP	2.2
1	В	1010	GLN	2.2
1	D	1142	GLN	2.2
1	В	1072	TYR	2.2
1	F	467	PHE	2.2
1	F	564	PHE	2.2
1	F	508	LEU	2.2
1	А	766	GLU	2.2



Mol

1

1

1

1

1

1

1

1

1

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1

1

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1

991	LEU	2.2
794	LYS	2.2
811	GLY	2.2
518	MET	2.2
1092	ALA	2.2
546	ALA	2.2
1016	ARG	2.2
587	TYR	2.1
737	VAL	2.1
1074	PRO	2.1
759	LEU	2.1
706	ALA	2.1
607	GLU	2.1

Continued from previous page...

 \mathbf{Res}

1157

730

1015

467

604

735

569

908

1112

Type

ASP

GLY

ALA

PHE

ARG

ILE

VAL

GLU

LYS

RSRZ

2.2

2.2

2.2

2.2

2.2

 $\frac{2.2}{2.2}$

2.2

2.2

Chain

В

 $\overline{\mathbf{C}}$

F

D

Е

В

D

А

А

В

F

Е

C E

F

F

 $\frac{C}{C}$

A F

Е

С

SER 1 Е 2.11085F 1 22 VAL 2.11 Е ALA 625 2.1Е THR 1 7432.11 А 569 VAL 2.11 С 462 ILE 2.1 1 D 711 LEU 2.11 F 785LYS 2.1675 ALA 1 $\overline{\mathbf{C}}$ 2.11 А 1120 LYS 2.11 В 891 ILE 2.1С ASP 1 1118 2.1PRO 1 А 11142.1ALA 1 Е 723 2.1THR 1 D 1121 2.1GLY 1 А 1111 2.11 Е 727 GLU 2.1С 1 1043 SER 2.1457 2.1 Е 1 SER 1 F 159LEU 2.1



6CIN

Mol	Chain	Res	Type	RSRZ
1	Е	1084	TYR	2.1
1	F	708	PRO	2.1
1	F	721	LYS	2.1
1	В	1012	GLY	2.1
1	D	570	ILE	2.1
1	В	1169	ALA	2.1
1	Е	1124	ALA	2.1
1	А	750	ASP	2.1
1	D	1143	PHE	2.1
1	С	1090	LYS	2.0
1	С	1162	LEU	2.0
1	F	483	LEU	2.0
1	Е	750	ASP	2.0
1	F	680	GLN	2.0
1	А	1160	ALA	2.0
1	В	1013	ALA	2.0
1	С	1033	ALA	2.0
1	D	755	LYS	2.0
1	Е	749	ALA	2.0
1	В	720	THR	2.0
1	F	252	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	\mathbf{RSR}	B-factors(Å ²)	Q < 0.9
4	MG	F	1205	1/1	0.94	0.13	$35,\!35,\!35,\!35$	0
5	SO4	D	1206	5/5	0.94	0.15	87,89,90,92	0



6CIN

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	Е	1206	5/5	0.94	0.13	79,80,82,83	0
5	SO4	В	1207	5/5	0.95	0.15	87,87,88,89	0
3	TPP	С	1204	26/26	0.95	0.18	57,70,80,87	0
2	SF4	С	1203	8/8	0.95	0.10	73,87,107,124	0
5	SO4	F	1206	5/5	0.95	0.10	101,101,103,103	0
4	MG	С	1205	1/1	0.96	0.06	31,31,31,31	0
3	TPP	А	1204	26/26	0.96	0.17	52,75,86,95	0
5	SO4	А	1206	5/5	0.96	0.14	88,89,89,89	0
5	SO4	В	1206	5/5	0.96	0.17	93,95,95,96	0
3	TPP	В	1204	26/26	0.96	0.16	59,70,83,87	0
2	SF4	А	1203	8/8	0.96	0.13	70,85,115,169	0
3	TPP	Е	1204	26/26	0.96	0.15	44,70,77,82	0
4	MG	А	1205	1/1	0.96	0.07	44,44,44,44	0
2	SF4	D	1202	8/8	0.97	0.25	73,82,95,121	0
2	SF4	D	1203	8/8	0.97	0.14	59,67,72,78	0
3	TPP	D	1204	26/26	0.97	0.15	58,64,73,82	0
2	SF4	Е	1203	8/8	0.97	0.11	63,95,138,162	0
2	SF4	F	1201	8/8	0.97	0.16	88,92,105,106	0
2	SF4	В	1203	8/8	0.97	0.12	60,79,85,96	0
4	MG	Е	1205	1/1	0.97	0.08	44,44,44,44	0
2	SF4	А	1202	8/8	0.98	0.16	75,81,86,88	0
2	SF4	Е	1202	8/8	0.98	0.11	80,88,105,113	0
2	SF4	А	1201	8/8	0.98	0.11	95,103,122,123	0
2	SF4	D	1201	8/8	0.98	0.16	73,76,81,84	0
3	TPP	F	1204	26/26	0.98	0.14	48,68,71,77	0
5	SO4	С	1206	5/5	0.98	0.12	75,75,78,78	0
2	SF4	F	1203	8/8	0.98	0.15	61,66,85,103	0
2	SF4	В	1202	8/8	0.98	0.13	68,71,72,73	0
4	MG	D	1205	1/1	0.98	0.14	32,32,32,32	0
4	MG	В	1205	1/1	0.99	0.09	32,32,32,32	0
2	SF4	В	1201	8/8	0.99	0.10	83,88,93,104	0
2	SF4	F	1202	8/8	0.99	0.19	75,79,85,88	0
2	SF4	Е	1201	8/8	0.99	0.09	95,97,110,115	0
2	SF4	С	1201	8/8	0.99	0.09	96,100,109,122	0
2	SF4	С	1202	8/8	0.99	0.10	72,76,81,82	0

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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.















6.5 Other polymers (i)

There are no such residues in this entry.

