

Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 11:19 AM EDT

PDB ID	:	6CIQ
Title	:	Pyruvate:ferredoxin oxidoreductase from Moorella thermoacetica with coen-
		zyme A bound
Authors	:	Chen, P.YT.; Drennan, C.L.
Deposited on	:	2018-02-24
Resolution	:	3.30 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 3.30 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	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182(3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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		
1	А	1171	88%	11%	
1	В	1171	87%	13%	1
1	С	1171	3% 87%	12% •	i

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
2	SF4	В	1201	-	-	Х	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 26915 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	Atoms					ZeroOcc	AltConf	Trace
1	Λ	1160	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	I A	1109	8893	5659	1509	1682	43	0	0	
1	В	1166	Total	С	Ν	Ο	S	0	0	0
1	D	1100	8860	5643	1506	1668	43	0		0
1	С	1161	Total	С	Ν	Ο	S	0	0	0
		1101	8836	5628	1499	1665	44	0	0	U

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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	TotalFeS844	0	0
2	А	1	TotalFeS844	0	0
2	А	1	TotalFeS844	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	С	1	Total Fe S 8 4 4	0	0
2	С	1	TotalFeS844	0	0
2	С	1	TotalFeS844	0	0

• 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	Δ	1	Total	С	Ν	0	Р	\mathbf{S}	0	0
0	D A	L	26	12	4	7	2	1	0	0
3	В	1	Total	С	Ν	Ο	Р	\mathbf{S}	0	0
0	D	T	26	12	4	7	2	1	0	0
3	С	1	Total	С	N	0	Р	S	0	0
5	U	I	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

• Molecule 5 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Atoms					ZeroOcc	AltConf
5	Δ	A 1	Total	С	Ν	Ο	Р	S	0	0
0	A		48	21	7	16	3	1	0	0
5	В	1	Total	С	Ν	Ο	Р	S	0	0
0	D	D I	48	21	7	16	3	1	0	0
5	5 C	1	Total	С	Ν	Ο	Р	S	0	0
5		1	48	21	$\overline{7}$	16	3	1	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	12	Total O 12 12	0	0
6	В	9	Total O 9 9	0	0
6	С	8	Total O 8 8	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



P1994 P1994 R1016 F1016 F1016 A1018 A1055 L1057 L1057 L1057 L1058 F1069 F1069 F1120 F1120 F1120 F1122 F1126 F1166

•	Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE																																						
С	hε	ir	1 (C:	39	6													87	%														1	2%		•		
MET	P2	T5	101	P27	A75	<u>676</u>	T81		IAN	R112	A113	T116	H117	F1 22	G123	D124	R132	т136		P164	K180	0213		P220	F224	R227			E283	H310	R301	1701	L334	V345	L354	<mark>г367</mark>	N368 N368	5370 8370 M371	1
L379	K387		V390	F419	F420	G421	6423 G423	S424	V428	G429	A430	I435		1438	Y452	D453 S454	#0 70	S463 нлел	L465	R466	Y476	L477 T478	D479	1.483	I484	A485 C486	Q L L	F507	L508	T512	W513	H H D D	L522	A524	1530 •	T R36	K536	Y538	D541
A542	V543	1545		E548 1549	G550	L551	R554	I555		1558	E C J	F303 F564	K565	1566 A567	N568	V569 TEZO		E574	Y578	TE03	V584	1594	1595 L595	N598	F599	V602	1001	A608	L609	E611	I612 • K613 •	Y614	- Deo O	A621	ASP	GLU GLU	ALA	THR VAT	THR
E631	T636		L640	K671		I678	S693	t of t	P697		P703	F718		R734	D741	C742	0401	G746	M761	<u>11767</u>		N789 P790	A791	T792 V793		T807	G811	Y817		1822	N833 4834	FOOT	5838 5839	I840	N841	A879	L887	1935	L947
-	0952 K953	D954	2004	D967	D994		500T h	01010	R1016	F1017		F1023	T1024	K1025 K1026		S1035 V1036		V1039	H1050	V10FF		E1059 A1060		P1066 S1067		A10/1 Y1072	010 010 010	e TO LA	Y1097	960TM	R1127	M1131	T1134		ų1142	L1162	K1166	E1170 CIV	0F1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	337.71Å 106.99Å 120.47Å	Deneiten
a, b, c, α , β , γ	90.00° 109.85° 90.00°	Depositor
D ecolution (\hat{A})	80.25 - 3.30	Depositor
Resolution (A)	80.25 - 3.30	EDS
% Data completeness	96.5 (80.25-3.30)	Depositor
(in resolution range)	96.5 (80.25-3.30)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	0.16	Depositor
$< I/\sigma(I) > 1$	2.25 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
D D	0.184 , 0.223	Depositor
n, n_{free}	0.184 , 0.223	DCC
R_{free} test set	2951 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	76.8	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31 , 70.2	EDS
L-test for $twinning^2$	$< L > = 0.46, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.033 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26915	wwPDB-VP
Average B, all atoms $(Å^2)$	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.

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: COA, TPP, SF4, MG $\,$

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	0/9086	0.44	0/12325	
1	В	0.26	0/9054	0.44	0/12283	
1	С	0.26	0/9030	0.44	0/12251	
All	All	0.26	0/27170	0.44	0/36859	

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	8893	0	8795	78	0
1	В	8860	0	8740	93	0
1	С	8836	0	8726	89	0
2	А	24	0	0	0	0
2	В	24	0	0	2	0
2	С	24	0	0	0	0
3	А	26	0	16	0	0
3	В	26	0	16	2	0
3	С	26	0	16	0	0
4	A	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes				
4	В	1	0	0	0	0				
4	С	1	0	0	0	0				
5	А	48	0	32	2	0				
5	В	48	0	32	2	0				
5	С	48	0	32	4	0				
6	А	12	0	0	0	0				
6	В	9	0	0	1	0				
6	С	8	0	0	0	0				
All	All	26915	0	26405	250	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 5.

All (250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 a ma 1		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:802:LEU:HB2	1:A:822:THR:HB	1.68	0.75
1:C:430:ALA:HB2	1:C:556:ASN:HB2	1.69	0.72
1:C:802:LEU:HB2	1:C:822:THR:HB	1.73	0.71
1:C:419:PHE:HB2	1:C:463:SER:HB2	1.73	0.69
1:B:419:PHE:HB2	1:B:463:SER:HB2	1.74	0.68
1:B:345:VAL:HB	1:C:334:LEU:HD21	1.75	0.68
1:B:427:THR:O	1:B:431:ASN:ND2	2.27	0.67
1:B:802:LEU:HB2	1:B:822:THR:HB	1.77	0.65
1:C:793:VAL:HG21	1:C:1050:HIS:HB3	1.80	0.64
1:B:348:GLU:OE1	1:C:387:LYS:NZ	2.32	0.63
1:B:588:GLY:HA2	1:B:595:LEU:HD21	1.82	0.62
1:A:290:GLU:OE2	1:B:412:LYS:HD3	2.01	0.61
1:A:141:SER:HG	1:A:167:HIS:HE2	1.49	0.60
1:A:1079:GLY:HA3	1:A:1134:ILE:HB	1.84	0.60
1:C:1055:LYS:HE2	1:C:1059:GLU:OE2	2.01	0.60
1:C:569:VAL:HG12	1:C:570:ILE:HG13	1.83	0.60
1:C:479:ASP:OD1	1:C:479:ASP:N	2.35	0.60
1:C:435:ILE:HD11	1:C:465:LEU:HB3	1.85	0.59
1:C:428:VAL:HG11	1:C:452:TYR:HE1	1.70	0.57
1:B:967:ASP:HB3	1:B:994:ASP:HA	1.87	0.57
1:A:1022:LYS:NZ	1:A:1024:THR:O	2.33	0.57
1:A:282:GLU:OE2	1:A:473:GLN:NE2	2.36	0.56
1:A:1026:LYS:HZ3	1:A:1098:TRP:HZ3	1.53	0.56
1:B:702:ARG:NH2	1:B:804:GLU:OE1	2.34	0.56
1:B:81:THR:HG21	1:B:91:MET:HE1	1.88	0.56



	a de pagem	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:B:479:ASP:OD1	1:B:479:ASP:N	2.36	0.55		
1:C:368:ASN:HB2	1:C:369:PRO:HD2	1.89	0.55		
1:B:553:SER:OG	1:B:554:ARG:NH1	2.39	0.55		
1:B:1060:ALA:HB1	1:B:1067:SER:HB3	1.88	0.55		
1:B:570:ILE:HG23	1:B:575:ALA:HB2	1.89	0.55		
1:A:967:ASP:HB3	1:A:994:ASP:HA	1.87	0.54		
1:C:466:ARG:NH1	1:C:478:ILE:HA	2.23	0.54		
1:B:513:TRP:HA	1:B:517:GLU:OE2	2.06	0.54		
1:B:883:ARG:NH1	1:C:76:GLY:O	2.41	0.54		
1:C:5:THR:HG22	1:C:180:LYS:HB2	1.90	0.54		
1:C:438:ILE:HD12	1:C:569:VAL:HG11	1.90	0.54		
1:A:1060:ALA:HB1	1:A:1067:SER:HB3	1.91	0.53		
1:B:678:ILE:HD11	1:B:767:VAL:HG23	1.91	0.53		
1:B:368:ASN:HB2	1:B:369:PRO:HD2	1.89	0.53		
1:A:1080:ILE:HG13	1:A:1082:MET:HE2	1.90	0.53		
1:A:81:THR:HG21	1:A:91:MET:HE1	1.91	0.53		
1:B:734:ARG:NH1	1:B:736:GLN:OE1	2.40	0.52		
1:A:112:ARG:HH21	1:A:119:LEU:HD11	1.73	0.52		
1:C:321:ARG:HB3	1:C:379:LEU:HD22	1.91	0.52		
1:C:1022:LYS:NZ	1:C:1024:THR:O	2.42	0.52		
1:B:502:LYS:HG2	1:B:503:PRO:HD2	1.92	0.52		
1:C:697:PRO:HG2	1:C:811:GLY:HA2	1.92	0.52		
1:B:695:VAL:HG11	1:B:751:VAL:HG21	1.92	0.52		
1:C:1004:GLN:HG2	1:C:1017:PHE:CE2	2.44	0.52		
1:A:1076:ILE:HA	1:A:1082:MET:HE3	1.92	0.51		
1:B:18:ALA:HB2	1:B:186:TYR:CZ	2.45	0.51		
1:C:935:ILE:HD13	1:C:947:LEU:HD23	1.93	0.51		
1:B:879:ALA:HB3	1:C:75:ALA:HB3	1.92	0.51		
1:A:479:ASP:N	1:A:479:ASP:OD1	2.42	0.51		
1:C:599:PHE:O	1:C:602:VAL:HG22	2.11	0.51		
1:C:1060:ALA:HB1	1:C:1067:SER:HB3	1.93	0.51		
1:B:556:ASN:OD1	1:B:557:VAL:N	2.43	0.51		
1:C:746:GLY:HA2	1:C:761:MET:HE3	1.93	0.51		
1:B:1004:GLN:HG2	1:B:1017:PHE:CE2	2.46	0.50		
1:C:321:ARG:HG2	1:C:354:LEU:HB3	1.92	0.50		
1:A:793:VAL:HG21	1:A:1050:HIS:HB3	1.94	0.50		
1:B:212:HIS:NE2	1:B:214:ARG:NH1	2.55	0.50		
1:C:967:ASP:HB3	1:C:994:ASP:HA	1.93	0.50		
1:A:482:ASP:OD1	1:A:502:LYS:HE2	2.11	0.50		
1:A:576:ILE:HD13	1:A:606:LEU:HD11	1.94	0.50		
1:B:140:SER:HB2	1:B:168:PHE:CZ	2.47	0.49		



	h h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:1113:ASN:ND2	1:A:1115:PHE:H	2.10	0.49
1:B:1031:LEU:HD23	1:C:1035:SER:HB2	1.94	0.49
1:C:464:HIS:HB3	1:C:478:ILE:HG13	1.94	0.49
1:A:838:SER:HA	1:A:841:TRP:CE2	2.47	0.49
1:B:112:ARG:HA	1:B:123:GLY:HA2	1.93	0.49
1:B:545:ILE:HG23	1:B:604:ARG:HD2	1.94	0.49
1:A:802:LEU:HD13	1:A:859:PRO:HD3	1.94	0.49
1:C:81:THR:HG21	1:C:91:MET:HE1	1.94	0.48
1:C:1079:GLY:HA3	1:C:1134:ILE:HB	1.95	0.48
1:B:18:ALA:HB2	1:B:186:TYR:CE1	2.48	0.48
1:C:1039:VAL:HG22	1:C:1066:PRO:HG2	1.95	0.48
1:B:900:SER:OG	1:B:934:GLU:OE2	2.18	0.48
1:A:887:LEU:HD13	1:A:952:GLN:HB2	1.94	0.48
1:C:574:GLU:HB3	1:C:578:TYR:CE2	2.49	0.48
1:A:112:ARG:NH2	1:A:119:LEU:HD11	2.28	0.48
1:B:693:SER:HB2	1:B:703:PRO:HD3	1.96	0.48
1:A:146:GLU:OE1	1:A:301:ARG:NH2	2.47	0.47
1:B:112:ARG:NH2	1:B:119:LEU:HD11	2.29	0.47
1:B:334:LEU:HD21	1:C:345:VAL:HB	1.96	0.47
1:C:551:LEU:O	1:C:554:ARG:HG2	2.13	0.47
1:B:1000:ASN:OD1	5:B:1206:COA:H21	2.14	0.47
1:A:583:ILE:HG22	1:A:595:LEU:HD22	1.96	0.47
1:A:85:SER:HB2	1:A:112:ARG:HB3	1.97	0.47
1:A:141:SER:HB2	1:A:169:PHE:HB3	1.96	0.47
1:A:1004:GLN:HG2	1:A:1017:PHE:CE2	2.50	0.47
1:B:527:LYS:HD2	1:B:618:TRP:CE2	2.49	0.47
1:A:570:ILE:HG13	1:A:575:ALA:HB2	1.97	0.47
1:B:838:SER:HA	1:B:841:TRP:CE2	2.50	0.47
1:C:545:ILE:O	1:C:549:ILE:HG13	2.15	0.47
1:B:802:LEU:HD13	1:B:859:PRO:HD3	1.96	0.46
1:C:1072:TYR:HB2	1:C:1098:TRP:CE2	2.50	0.46
1:C:671:LYS:NZ	1:C:741:ASP:OD2	2.33	0.46
1:B:27:PRO:HB3	1:B:1017:PHE:HE2	1.80	0.46
1:B:321:ARG:HB3	1:B:379:LEU:HD22	1.97	0.46
1:C:554:ARG:HD2	5:C:1206:COA:C4A	2.46	0.46
1:C:678:ILE:HD11	1:C:767:VAL:HG23	1.96	0.46
5:C:1206:COA:H8A	5:C:1206:COA:H52A	1.97	0.46
1:A:189:MET:O	1:A:193:VAL:HG23	2.16	0.46
1:A:453:ASP:OD1	1:A:454:SER:N	2.48	0.46
1:B:416:ARG:HG2	1:B:466:ARG:HG2	1.98	0.46
1:B:641:ARG:HB2	1:B:642:PRO:HD3	1.98	0.46



	t a second	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:556:ASN:OD1	1:C:557:VAL:N	2.48	0.46
1:A:263:GLY:HA3	1:A:296:GLY:HA2	1.98	0.46
1:B:279:GLU:OE1	1:B:473:GLN:HG2	2.16	0.46
1:B:453:ASP:OD1	1:B:454:SER:N	2.48	0.46
1:C:506:ILE:HG21	1:C:566:ILE:HG21	1.96	0.46
1:B:373:LYS:HE2	1:B:405:GLU:OE2	2.16	0.46
1:B:903:PHE:HB2	1:B:934:GLU:OE2	2.15	0.46
1:B:220:PRO:HD3	1:C:122:PHE:CE2	2.52	0.45
1:C:554:ARG:HD2	5:C:1206:COA:C5A	2.46	0.45
1:A:594:ILE:O	1:A:598:ASN:ND2	2.45	0.45
3:B:1204:TPP:H2	6:B:1308:HOH:O	2.15	0.45
1:A:424:SER:N	5:A:1206:COA:O4A	2.50	0.45
1:C:584:VAL:HA	1:C:595:LEU:HD11	1.98	0.45
1:B:206:LEU:HD23	1:B:212:HIS:CE1	2.52	0.45
1:A:1002:GLY:HA3	1:A:1016:ARG:NH1	2.32	0.45
1:B:501:ILE:HD13	1:B:535:LEU:HD13	1.98	0.45
1:B:506:ILE:HG21	1:B:566:ILE:HD12	1.97	0.45
1:B:435:ILE:HG23	1:B:446:ALA:HB1	1.96	0.45
1:C:484:ILE:O	1:C:507:PHE:HA	2.17	0.45
1:C:838:SER:HA	1:C:841:TRP:CE2	2.52	0.45
1:C:1127:ARG:O	1:C:1131:MET:HG2	2.17	0.45
1:B:75:ALA:HB3	1:C:879:ALA:HB3	1.99	0.45
1:B:836:GLY:HA2	3:B:1204:TPP:S1	2.57	0.45
1:A:422:LEU:N	1:A:425:ASP:OD2	2.49	0.45
1:B:514:SER:H	1:B:517:GLU:HG2	1.82	0.45
1:A:681:TRP:CD1	1:A:735:ILE:HB	2.52	0.44
1:B:91:MET:O	1:B:95:MET:HG3	2.17	0.44
1:B:834:ALA:O	1:B:839:SER:HB3	2.17	0.44
1:A:545:ILE:HB	1:A:558:ILE:HD13	1.98	0.44
1:B:718:PHE:HE1	1:B:778:ALA:HB2	1.82	0.44
1:C:113:ALA:HB2	1:C:124:ASP:OD2	2.17	0.44
1:A:519:ASP:OD1	1:A:527:LYS:NZ	2.50	0.44
1:A:18:ALA:HB2	1:A:186:TYR:CE1	2.53	0.44
1:A:419:PHE:HB2	1:A:463:SER:HB2	1.99	0.44
1:B:132:ARG:HH11	1:C:132:ARG:HH11	1.66	0.44
1:B:257:HIS:O	1:B:301:ARG:HG3	2.17	0.44
1:B:564:PHE:CD2	1:B:579:ILE:HD11	2.53	0.44
1:C:698:HIS:CE1	1:C:743:THR:HG21	2.52	0.44
1:C:834:ALA:O	1:C:839:SER:HB3	2.17	0.44
1:A:85:SER:HA	1:A:127:ASP:HB3	2.00	0.44
1:A:556:ASN:OD1	1:A:557:VAL:N	2.50	0.44



	the o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:116:THR:OG1	1:C:117:HIS:N	2.51	0.44
1:A:128:VAL:HG21	1:A:168:PHE:CD2	2.52	0.44
1:A:659:ASP:OD1	1:A:659:ASP:N	2.51	0.44
1:C:466:ARG:HH11	1:C:478:ILE:HA	1.83	0.44
1:B:1079:GLY:HA3	1:B:1134:ILE:HB	2.00	0.43
1:A:206:LEU:HD23	1:A:212:HIS:CE1	2.53	0.43
1:B:136:PHE:CE2	1:B:164:PRO:HB2	2.54	0.43
1:C:567:ALA:O	1:C:568:ASN:ND2	2.51	0.43
1:C:636:ILE:HA	1:C:640:LEU:HB3	2.00	0.43
1:A:556:ASN:ND2	1:A:587:TYR:OH	2.51	0.43
1:B:783:GLU:HB2	1:B:854:ARG:HD2	2.00	0.43
1:A:430:ALA:HB2	1:A:556:ASN:HB2	2.01	0.43
1:A:1139:LEU:HD21	1:A:1150:LEU:HD12	2.00	0.43
1:C:954:ASP:OD1	1:C:954:ASP:N	2.52	0.43
1:A:954:ASP:OD1	1:A:954:ASP:N	2.52	0.43
1:C:613:LYS:HA	1:C:613:LYS:HD3	1.76	0.43
1:C:1004:GLN:HG3	1:C:1016:ARG:HB2	2.00	0.43
1:C:1026:LYS:HZ3	1:C:1098:TRP:HZ3	1.66	0.43
1:A:32:SER:O	1:A:36:GLU:HG3	2.19	0.43
1:B:18:ALA:O	1:B:48:ASN:HB2	2.19	0.43
1:C:594:ILE:O	1:C:598:ASN:ND2	2.49	0.43
1:A:427:THR:O	1:A:431:ASN:ND2	2.52	0.43
1:A:136:PHE:CD2	1:A:166:VAL:HG23	2.54	0.43
1:B:122:PHE:CE2	1:C:220:PRO:HD3	2.53	0.43
1:C:371:MET:HB3	1:C:390:VAL:HG11	2.00	0.43
1:C:718:PHE:CZ	1:C:734:ARG:HD3	2.54	0.43
1:C:112:ARG:HA	1:C:123:GLY:HA2	2.00	0.43
1:A:326:ASP:CG	1:A:336:GLU:HB3	2.38	0.42
1:A:514:SER:O	1:A:518:MET:HG2	2.19	0.42
1:B:530:ILE:HA	1:B:535:LEU:HD12	2.01	0.42
1:B:867:GLU:OE1	1:B:867:GLU:N	2.50	0.42
5:A:1206:COA:C8A	5:A:1206:COA:H51A	2.49	0.42
1:B:50:PHE:CZ	1:B:78:LEU:HD12	2.54	0.42
1:B:489:PRO:HG3	1:B:510:ASN:O	2.20	0.42
1:B:523:PRO:O	1:B:527:LYS:HG3	2.19	0.42
1:B:687:ILE:HG12	2:B:1201:SF4:S3	2.59	0.42
1:C:422:LEU:HG	1:C:423:GLY:N	2.34	0.42
1:C:817:TYR:CZ	1:C:1071:ALA:HB1	2.54	0.42
1:A:998:TYR:CE1	1:A:1006:SER:HB2	2.54	0.42
1:A:781:LEU:O	1:A:854:ARG:NH2	2.52	0.42
1:C:693:SER:HB2	1:C:703:PRO:HD3	2.01	0.42



	the pagetti	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:464:HIS:CE1	1:A:477:LEU:HD22	2.55	0.42
1:C:887:LEU:HD13	1:C:952:GLN:HB2	2.00	0.42
1:A:694:LEU:HD22	1:A:793:VAL:HG13	2.01	0.42
1:A:1004:GLN:HG3	1:A:1016:ARG:HB2	2.01	0.42
1:A:1119:TYR:HE2	1:A:1122:PRO:HA	1.85	0.42
1:C:789:ASN:OD1	1:C:791:ALA:HB3	2.19	0.42
1:C:1162:LEU:HG	1:C:1166:LYS:HE3	2.01	0.42
1:B:1031:LEU:HD12	1:B:1034:MET:HE3	2.01	0.42
1:A:113:ALA:HB2	1:A:124:ASP:OD2	2.20	0.42
1:B:124:ASP:HA	1:B:327:ARG:HD3	2.01	0.42
1:B:178:VAL:O	1:B:447:GLN:HA	2.20	0.42
1:C:544:LYS:O	1:C:548:GLU:HG2	2.19	0.42
1:A:678:ILE:HD11	1:A:767:VAL:HG23	2.03	0.41
1:A:704:TYR:CE1	1:A:736:GLN:HB3	2.55	0.41
1:C:428:VAL:HG11	1:C:452:TYR:CE1	2.52	0.41
1:A:416:ARG:HG2	1:A:466:ARG:HG2	2.02	0.41
1:B:752:CYS:HA	2:B:1201:SF4:S1	2.61	0.41
1:B:1025:LYS:NZ	1:C:1036:TYR:O	2.44	0.41
1:B:935:ILE:HG12	1:B:946:LEU:HB3	2.01	0.41
1:C:136:PHE:CE2	1:C:164:PRO:HB2	2.55	0.41
1:C:283:GLU:OE2	1:C:476:TYR:OH	2.33	0.41
1:A:136:PHE:CE2	1:A:164:PRO:HB2	2.55	0.41
1:C:371:MET:HB3	1:C:390:VAL:CG1	2.50	0.41
1:C:1010:GLN:HG3	1:C:1097:TYR:CZ	2.55	0.41
1:A:1079:GLY:O	1:A:1134:ILE:HG13	2.20	0.41
1:C:583:ILE:HD13	1:C:598:ASN:HB3	2.02	0.41
1:A:416:ARG:HB3	1:A:478:ILE:HD12	2.01	0.41
1:A:480:GLN:HA	1:A:500:GLY:O	2.21	0.41
1:B:1004:GLN:HG3	1:B:1016:ARG:HB2	2.01	0.41
1:B:1057:LEU:HD23	1:B:1069:ILE:HD13	2.03	0.41
1:A:803:LEU:HD12	1:A:849:PRO:HB2	2.02	0.41
1:B:695:VAL:HG21	1:B:751:VAL:HG21	2.03	0.41
1:C:258:LEU:HD12	1:C:310:HIS:CG	2.56	0.41
1:A:422:LEU:HG	1:A:423:GLY:N	2.36	0.41
1:C:27:PRO:HB3	1:C:1017:PHE:HE2	1.84	0.41
1:B:416:ARG:HB3	1:B:478:ILE:HD13	2.03	0.41
1:B:429:GLY:N	5:B:1206:COA:O1A	2.46	0.41
1:B:434:SER:O	1:B:438:ILE:HG13	2.21	0.41
1:B:548:GLU:OE1	1:B:604:ARG:NH1	2.54	0.41
1:C:1072:TYR:HB2	1:C:1098:TRP:CD2	2.56	0.41
1:A:257:HIS:O	1:A:301:ARG:HG3	2.21	0.41



Atom-1	Atom-2	Interatomic $distance (\hat{\lambda})$	Clash
		distance (A)	overlap (A)
1:A:641:ARG:HB2	1:A:642:PRO:HD3	2.02	0.40
1:B:5:THR:HG22	1:B:180:LYS:HB2	2.02	0.40
1:B:1119:TYR:HE2	1:B:1122:PRO:HA	1.86	0.40
1:A:667:THR:HG22	1:A:847:ALA:HB1	2.03	0.40
1:B:861:TRP:HE3	1:C:213:GLN:HG3	1.86	0.40
1:C:524:ALA:HB1	1:C:622:VAL:HA	2.04	0.40
1:C:1010:GLN:HG3	1:C:1097:TYR:OH	2.20	0.40
1:A:790:PRO:HG3	1:A:799:ARG:NH2	2.37	0.40
1:A:903:PHE:HB2	1:A:934:GLU:OE2	2.21	0.40
1:B:786:VAL:HG13	1:B:788:PHE:H	1.85	0.40
1:B:954:ASP:OD1	1:B:954:ASP:N	2.49	0.40
1:A:112:ARG:HA	1:A:123:GLY:HA2	2.03	0.40
1:A:783:GLU:HB2	1:A:854:ARG:HD2	2.03	0.40
1:A:1080:ILE:HD13	1:A:1088:GLU:HG2	2.03	0.40
1:B:85:SER:HA	1:B:127:ASP:HB3	2.04	0.40
1:B:803:LEU:HD12	1:B:849:PRO:HB2	2.03	0.40
1:C:367:PHE:HA	1:C:371:MET:SD	2.61	0.40
1:C:424:SER:N	5:C:1206:COA:O5A	2.50	0.40
1:B:136:PHE:CD2	1:B:166:VAL:HG23	2.56	0.40
1:C:833:ASN:HD22	1:C:834:ALA:N	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	Perce	ntiles
1	А	1167/1171~(100%)	1143~(98%)	24 (2%)	0	100	100
1	В	1162/1171~(99%)	1135~(98%)	27 (2%)	0	100	100
1	С	$1157/1171 \ (99\%)$	1136~(98%)	21 (2%)	0	100	100
All	All	3486/3513~(99%)	3414 (98%)	72 (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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles			
1	А	918/932~(98%)	913 (100%)	5~(0%)	8	38	93	
1	В	911/932~(98%)	907~(100%)	4 (0%)	ĝ	91	95	
1	С	912/932~(98%)	909 (100%)	3~(0%)	ĝ	92	96	
All	All	2741/2796~(98%)	2729 (100%)	12 (0%)	ĝ	91	95	

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	224	PHE
1	А	452	TYR
1	А	467	PHE
1	А	833	ASN
1	А	1113	ASN
1	В	224	PHE
1	В	452	TYR
1	В	467	PHE
1	В	833	ASN
1	С	224	PHE
1	С	227	ARG
1	С	833	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	247	GLN
1	А	560	GLN
1	А	1113	ASN
1	А	1142	GLN
1	В	247	GLN
1	В	560	GLN



Continued from previous page...

Mol	Chain	Res	Type
1	В	833	ASN
1	С	247	GLN
1	С	480	GLN
1	С	560	GLN
1	С	568	ASN
1	С	833	ASN

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 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 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).

Mal	Turne	Chain	Dog	Res Link	Bo	ond leng	\mathbf{ths}	B	ond ang	gles
	туре		nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	SF4	С	1203	1	$0,\!12,\!12$	-	-	-		
2	SF4	С	1202	1	$0,\!12,\!12$	-	-	-		
3	TPP	С	1204	4	22,27,27	2.13	6 (27%)	29,40,40	1.89	7 (24%)
2	SF4	А	1202	1	0,12,12	-	-	-		
2	SF4	А	1201	1	0,12,12	-	-	-		
3	TPP	А	1204	4	22,27,27	2.08	6 (27%)	29,40,40	1.89	7 (24%)
5	COA	C	1206	-	41,50,50	0.83	1 (2%)	52,75,75	1.19	3 (5%)



Mal	Turne	Chain	Bos	Link	Bo	Bond lengths			Bond angles		
IVIOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ # Z > 2		
2	SF4	В	1202	1	0,12,12	-	-	-			
2	SF4	А	1203	1	0,12,12	-	-	-			
2	SF4	С	1201	1	0,12,12	-	-	-			
3	TPP	В	1204	4	22,27,27	1.96	6 (27%)	29,40,40	1.62 7 (24%)		
5	COA	А	1206	-	41,50,50	0.80	1 (2%)	52,75,75	1.31 $5(9\%)$		
2	SF4	В	1203	1	0,12,12	-	-	-			
5	COA	В	1206	-	41,50,50	0.83	1 (2%)	52,75,75	1.25 $6 (11\%)$		
2	SF4	В	1201	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	С	1203	1	-	-	0/6/5/5
3	TPP	С	1204	4	-	2/16/17/17	0/2/2/2
2	SF4	С	1202	1	-	-	0/6/5/5
2	SF4	А	1202	1	-	-	0/6/5/5
2	SF4	А	1201	1	-	-	0/6/5/5
3	TPP	А	1204	4	-	2/16/17/17	0/2/2/2
5	COA	С	1206	-	-	11/44/64/64	0/3/3/3
2	SF4	А	1203	1	-	-	0/6/5/5
2	SF4	В	1202	1	-	-	0/6/5/5
2	SF4	С	1201	1	-	-	0/6/5/5
3	TPP	В	1204	4	-	1/16/17/17	0/2/2/2
5	COA	А	1206	-	-	10/44/64/64	0/3/3/3
2	SF4	В	1203	1	-	-	0/6/5/5
5	COA	В	1206	-	-	4/44/64/64	0/3/3/3
2	SF4	В	1201	1	-	-	0/6/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
3	С	1204	TPP	C4-N3	-5.12	1.35	1.39
3	А	1204	TPP	C4-N3	-4.78	1.35	1.39
3	В	1204	TPP	C4-N3	-4.02	1.36	1.39
3	А	1204	TPP	C6-C5	3.87	1.52	1.50
3	С	1204	TPP	C6-C5	3.86	1.52	1.50
3	С	1204	TPP	C4'-N4'	3.74	1.43	1.34



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	1204	TPP	C4'-N4'	3.73	1.43	1.34
3	В	1204	TPP	C4'-N4'	3.71	1.43	1.34
3	В	1204	TPP	C7'-N3	-3.34	1.42	1.48
3	В	1204	TPP	C6-C5	3.33	1.52	1.50
3	С	1204	TPP	C7'-N3	-3.28	1.42	1.48
3	А	1204	TPP	C7'-N3	-3.25	1.42	1.48
3	А	1204	TPP	C7'-C5'	3.19	1.57	1.51
3	В	1204	TPP	C7'-C5'	3.15	1.57	1.51
3	С	1204	TPP	C7'-C5'	3.08	1.57	1.51
5	А	1206	COA	P2A-O6A	2.73	1.70	1.59
5	В	1206	COA	P2A-O6A	2.62	1.69	1.59
5	С	1206	COA	P2A-O6A	2.54	1.69	1.59
3	С	1204	TPP	C6'-C5'	2.26	1.42	1.37
3	A	1204	TPP	C6'-C5'	2.20	1.42	1.37
3	B	1204	TPP	C6'-C5'	2.17	1.42	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	С	1204	TPP	C6-C5-C4	-5.94	122.66	127.43
3	А	1204	TPP	C6-C5-C4	-5.77	122.80	127.43
5	С	1206	COA	N3A-C2A-N1A	-4.60	121.49	128.68
5	А	1206	COA	N3A-C2A-N1A	-4.52	121.61	128.68
5	В	1206	COA	N3A-C2A-N1A	-4.38	121.84	128.68
3	В	1204	TPP	C6-C5-C4	-3.59	124.55	127.43
3	С	1204	TPP	N4'-C4'-N3'	3.30	121.69	117.03
5	В	1206	COA	C3P-N4P-C5P	3.20	128.78	122.84
3	В	1204	TPP	C6'-N1'-C2'	3.16	121.34	115.96
5	А	1206	COA	C7P-N8P-C9P	3.14	128.20	122.59
3	С	1204	TPP	C6'-N1'-C2'	3.06	121.16	115.96
3	А	1204	TPP	C6'-N1'-C2'	3.03	121.12	115.96
3	А	1204	TPP	N4'-C4'-N3'	3.01	121.29	117.03
3	В	1204	TPP	C5'-C6'-N1'	-2.81	119.14	123.82
3	А	1204	TPP	C5'-C6'-N1'	-2.77	119.21	123.82
5	А	1206	COA	O4B-C1B-C2B	-2.74	102.92	106.93
3	С	1204	TPP	C5'-C6'-N1'	-2.73	119.27	123.82
3	В	1204	TPP	PA-O3A-PB	-2.71	123.53	132.83
3	С	1204	TPP	PA-O3A-PB	-2.63	123.81	132.83
3	В	1204	TPP	CM4-C4-N3	2.59	125.84	122.53
3	А	1204	TPP	PA-O3A-PB	-2.54	124.10	132.83
5	A	1206	COA	C3P-N4P-C5P	2.52	127.52	122.84
5	A	1206	COA	C3B-C2B-C1B	2.50	105.43	99.89



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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$				
5	В	1206	COA	C7P-N8P-C9P	2.30	126.70	122.59				
5	С	1206	COA	C3P-N4P-C5P	2.26	127.03	122.84				
3	В	1204	TPP	N4'-C4'-N3'	2.22	120.17	117.03				
3	С	1204	TPP	C5'-C4'-N4'	-2.21	119.05	122.19				
5	В	1206	COA	O6A-CCP-CBP	-2.17	107.06	110.55				
3	А	1204	TPP	CM4-C4-N3	2.15	125.27	122.53				
5	В	1206	COA	CDP-CBP-CAP	2.12	112.50	108.82				
5	С	1206	COA	CEP-CBP-CAP	2.07	112.41	108.82				
3	В	1204	TPP	N1'-C2'-N3'	-2.06	122.00	125.54				
3	С	1204	TPP	N1'-C2'-N3'	-2.04	122.03	125.54				
5	В	1206	COA	CEP-CBP-CAP	2.03	112.34	108.82				
3	А	1204	TPP	N1'-C2'-N3'	-2.02	122.06	125.54				

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	1206	COA	C3B-C4B-C5B-O5B
5	А	1206	COA	C5B-O5B-P1A-O3A
5	А	1206	COA	CCP-O6A-P2A-O4A
5	А	1206	COA	S1P-C2P-C3P-N4P
5	С	1206	COA	CCP-O6A-P2A-O4A
5	С	1206	COA	CCP-O6A-P2A-O5A
5	А	1206	COA	O4B-C4B-C5B-O5B
5	А	1206	COA	O5P-C5P-C6P-C7P
3	С	1204	TPP	PB-O3A-PA-O7
5	С	1206	COA	P2A-O3A-P1A-O5B
5	С	1206	COA	P1A-O3A-P2A-O6A
5	С	1206	COA	C3B-O3B-P3B-O8A
5	А	1206	COA	C5B-O5B-P1A-O1A
5	А	1206	COA	CCP-O6A-P2A-O5A
5	А	1206	COA	N4P-C5P-C6P-C7P
3	А	1204	TPP	PA-O3A-PB-O1B
5	С	1206	COA	P1A-O3A-P2A-O4A
5	С	1206	COA	C3B-O3B-P3B-O7A
5	В	1206	COA	C2P-C3P-N4P-C5P
5	А	1206	COA	CCP-O6A-P2A-O3A
5	В	1206	COA	C3B-O3B-P3B-O8A
5	В	1206	COA	C3B-O3B-P3B-O9A
5	С	1206	COA	C3B-O3B-P3B-O9A
5	С	1206	COA	CCP-O6A-P2A-O3A
5	В	1206	COA	P2A-O3A-P1A-O2A



	U	-	1 0	
Mol	Chain	Res	Type	Atoms
5	С	1206	COA	C6P-C7P-N8P-C9P
5	С	1206	COA	O4B-C4B-C5B-O5B
3	А	1204	TPP	C4-C5-C6-C7
3	В	1204	TPP	C4-C5-C6-C7
3	С	1204	TPP	C4-C5-C6-C7

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There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	С	1206	COA	4	0
3	В	1204	TPP	2	0
5	А	1206	COA	2	0
5	В	1206	COA	2	0
2	В	1201	SF4	2	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	$OWAB(Å^2)$	Q<0.9
1	А	1169/1171~(99%)	-0.02	16 (1%) 75 75	40, 79, 150, 187	0
1	В	1166/1171~(99%)	0.21	52 (4%) 33 32	36, 90, 178, 253	0
1	С	1161/1171 (99%)	0.08	36 (3%) 49 48	48, 89, 172, 259	0
All	All	3496/3513~(99%)	0.09	104 (2%) 50 49	36, 86, 169, 259	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	537	PHE	6.2
1	С	612	ILE	5.4
1	С	507	PHE	4.9
1	С	535	LEU	4.3
1	С	508	LEU	4.1
1	В	705	LEU	4.1
1	С	513	TRP	4.0
1	В	683	PRO	3.9
1	В	708	PRO	3.9
1	А	811	GLY	3.8
1	С	420	PHE	3.8
1	С	614	TYR	3.8
1	С	522	LEU	3.7
1	С	514	SER	3.7
1	В	518	MET	3.6
1	В	733	PHE	3.6
1	В	788	PHE	3.5
1	В	707	LYS	3.5
1	В	706	ALA	3.5
1	С	563	PHE	3.4
1	В	587	TYR	3.4
1	В	784	VAL	3.4
1	С	613	LYS	3.4



Mol

1 1

1

1

1

1

1

1

1

С	1142	GLN	3.0
С	543	VAL	2.9
С	608	ALA	2.9
С	538	TYR	2.9
С	541	ASP	2.9
С	530	ILE	2.8
А	1119	TYR	2.8
В	1018	ALA	2.8
А	906	ALA	2.8
В	553	SER	2.8
А	1011	THR	2.8
В	710	ASP	2.7
С	512	THR	2.7
В	703	PRO	2.7
В	513	TRP	2.7
А	1112	LYS	2.7
В	1074	PRO	2.7
В	619	ALA	2.7
С	484	ILE	2.7
В	551	LEU	2.6
А	1105	PRO	2.6
В	545	ILE	2.6
В	422	LEU	2.6
В	755	LYS	2.5
В	588	GLY	2.5

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В

В

С

В

В

С

В

С

А

А

В

С

В

А

В

В

В

1

1

1

1

1

1

1

1

1

 \mathbf{Res}

609

956

609

786

798

485

735

565

Type

LEU

LEU

LEU

VAL

PHE

ALA

ILE

LYS

RSRZ

3.2

3.2

3.2

3.1

3.1

3.1

3.1

3.0

PHE Continued on next page...

TYR

LYS

SER

ALA

PHE

VAL

PHE

LEU

1072 1120

511

542

1126

988

777

1150

1143

2.4

2.4

2.4

2.4

2.4

2.4

2.3

2.3

2.3



Mol

1 1

1

1

1

1

1

1 1

1

В

А

С

В

В

С

С

В

512

1155

454

785

964

483

523

1110

THR

GLU

SER

LYS

ILE

LEU

PRO

GLU

2.0

2.0

2.0

2.0

2.0

2.0

2.0

2.0

1	В	751	VAL	2.3	
1	С	558	ILE	2.3	
1	В	729	ALA	2.3	
1	В	684	GLU	2.3	
1	В	569	VAL	2.2	
1	С	598	ASN	2.2	
1	В	1086	GLN	2.2	
1	С	607	GLU	2.2	
1	С	620	ASP	2.2	
1	В	484	ILE	2.2	
1	В	687	ILE	2.2	
1	С	419	PHE	2.2	
1	С	486	CYS	2.2	
1	В	824	LEU	2.2	
1	В	754	ALA	2.1	
1	С	506	ILE	2.1	
1	С	551	LEU	2.1	
1	А	1095	ALA	2.1	
1	В	598	ASN	2.1	
1	А	1126	PHE	2.1	
1	А	1151	PHE	2.1	
1	В	737	VAL	2.1	
1	А	1012	GLY	2.1	
1	С	611	GLU	2.1	
1	В	563	PHE	2.1	
1	В	1105	PRO	2.1	
1	В	549	ILE	2.1	
1	В	692	CYS	2.0	
1	А	628	THR	2.0	

$\alpha \cdot \cdot \cdot \cdot$	C	•	
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Res

1057

709

Type | RSRZ

2.3

2.3

LEU

ALA

Chain

А

В



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	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
5	COA	А	1206	48/48	0.83	0.26	123,131,141,141	0
5	COA	В	1206	48/48	0.84	0.24	118,130,138,138	0
5	COA	С	1206	48/48	0.88	0.22	102,112,136,137	0
4	MG	А	1205	1/1	0.96	0.09	$35,\!35,\!35,\!35$	0
4	MG	В	1205	1/1	0.97	0.06	30,30,30,30	0
3	TPP	С	1204	26/26	0.97	0.17	54,63,67,71	0
3	TPP	В	1204	26/26	0.98	0.15	53,63,65,70	0
3	TPP	А	1204	26/26	0.98	0.19	68,74,79,82	0
4	MG	С	1205	1/1	0.98	0.06	19,19,19,19	0
2	SF4	С	1202	8/8	0.99	0.20	70,72,74,98	0
2	SF4	А	1201	8/8	0.99	0.13	91,110,112,126	0
2	SF4	В	1201	8/8	0.99	0.13	126,156,197,211	0
2	SF4	В	1202	8/8	0.99	0.15	97,107,117,169	0
2	SF4	С	1201	8/8	0.99	0.19	81,85,96,104	0
2	SF4	А	1202	8/8	1.00	0.18	74,81,107,115	0
2	SF4	А	1203	8/8	1.00	0.16	60,73,84,89	0
2	SF4	С	1203	8/8	1.00	0.17	61,63,65,65	0
2	SF4	В	1203	8/8	1.00	0.14	63,78,80,97	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.















6.5 Other polymers (i)

There are no such residues in this entry.

