

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	$6 \mathrm{MJF}$
Title	:	Catalytic Domain of dbOphMA
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Deposited on	:	2018-09-20
$\operatorname{Resolution}$:	2.20 Å(reported)
Deposited on Resolution	:	2018-09-20 2.20 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 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	:	2.11
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	$7.0.044 \ (Gargrove)$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$		
R_{free}	130704	4898 (2.20-2.20)		
Clashscore	141614	$5594 \ (2.20-2.20)$		
Ramachandran outliers	138981	$5503 \ (2.20-2.20)$		
Sidechain outliers	138945	5504 (2.20-2.20)		
RSRZ outliers	127900	4800 (2.20-2.20)		

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 >=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	
			4%	
1	А	386	85%	10% • •
			6%	
1	В	386	83%	12% • •
			7%	
1	C	386	82%	13% • •
			8%	
1	D	386	83%	13% •
			6%	
1	E	386	72%	23% • •
			9%	
1	F	386	70%	24% • •



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18111 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		At	oms			ZeroOcc	AltConf	Trace
1	Δ	271	Total	С	Ν	Ο	S	0	0	0
	A	371	2896	1846	487	545	18	0	0	0
1	р	270	Total	С	Ν	Ο	S	0	0	0
	D	570	2889	1841	486	544	18	0	0	0
1	C	271	Total	С	Ν	Ο	S	0	0	0
		371	2892	1843	486	545	18			
1	р	370	Total	С	Ν	Ο	S	0	0	0
		570	2889	1841	486	544	18	0	0	
1	Б	260	Total	С	Ν	Ο	S	0	0	0
		509	2881	1837	485	541	18	0	0	
1	Б	270	Total	С	Ν	Ο	S	0	0	0
	L L	370	2889	1841	486	544	18	0		

• Molecule 1 is a protein called dbOphM.

• Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
0	Δ	1	Total	С	Ν	Ο	S	0	0	
	A	L	26	14	6	5	1	0	0	
0	р	1	Total	С	Ν	Ο	S	0	0	
	D	L	26	14	6	5	1	0		
0	C	1	Total	С	Ν	Ο	S	0	0	
		L	26	14	6	5	1	0	U	
0	р	1	Total	С	Ν	Ο	S	0	0	
		L	26	14	6	5	1	0	0	
0	Б	1	Total	С	Ν	Ο	S	0	0	
	L L		26	14	6	5	1	0		

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	146	Total O 146 146	0	0
3	В	131	Total O 131 131	0	0
3	С	137	Total O 137 137	0	0
3	D	102	Total O 102 102	0	0
3	Е	61	Total O 61 61	0	0
3	F	68	Total O 68 68	0	0



3 Residue-property plots (i)

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



• Molecule 1: dbOphM



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants	109.54Å 109.54 Å 167.62 Å	Deneiten
$\mathrm{a,b,c,\alpha,\beta,\gamma}$	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	45.64 - 2.20	Depositor
Resolution (A)	45.64 - 2.20	EDS
% Data completeness	99.0 (45.64-2.20)	Depositor
(in resolution range $)$	$99.0 \ (45.64 - 2.20)$	EDS
R_{merge}	0.10	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) > 1$	$2.17 (at 2.20 \text{\AA})$	Xtriage
Refinement program	PHENIX (???)	Depositor
B B.	0.231 , 0.267	Depositor
n, n_{free}	0.234 , 0.269	DCC
R_{free} test set	5842 reflections $(5.15%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	35.8	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 22.4	EDS
L-test for twinning ²	$< L > = 0.46, < L^2 > = 0.28$	Xtriage
	0.029 for -h,-k,l	
Estimated twinning fraction	0.366 for h,-h-k,-l	Xtriage
	0.034 for -k,-h,-l	
F_o, F_c correlation	0.95	EDS
Total number of atoms	18111	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.73% 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: SAH

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		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.26	0/2969	0.42	0/4042	
1	В	0.25	0/2961	0.42	0/4031	
1	С	0.25	0/2965	0.42	0/4038	
1	D	0.26	0/2961	0.42	0/4031	
1	Е	0.28	0/2952	0.46	0/4017	
1	F	0.27	0/2961	0.45	0/4031	
All	All	0.26	0/17769	0.43	0/24190	

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	2896	0	2852	25	0
1	В	2889	0	2844	35	0
1	С	2892	0	2841	39	0
1	D	2889	0	2844	30	0
1	Ε	2881	0	2839	77	0
1	F	2889	0	2844	77	0
2	А	26	0	19	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	26	0	19	0	0
2	С	26	0	19	0	0
2	D	26	0	19	0	0
2	F	26	0	19	0	0
3	А	146	0	0	2	0
3	В	131	0	0	5	0
3	С	137	0	0	5	0
3	D	102	0	0	2	0
3	Е	61	0	0	3	0
3	F	68	0	0	9	0
All	All	18111	0	17159	258	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 (258) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${f distance} \ ({ m \AA})$	overlap (Å)
1:C:355:THR:HG21	1:C:377:MET:CE	2.01	0.90
1:F:58:CYS:SG	3:F:614:HOH:O	2.30	0.90
1:E:99:HIS:HD2	1:E:101:GLY:H	1.22	0.84
1:E:260:ILE:HD13	1:F:156:ILE:HD12	1.62	0.82
1:E:345:ARG:H	1:E:345:ARG:HD2	1.48	0.79
1:E:156:ILE:HD12	1:F:260:ILE:HG12	1.67	0.77
1:E:109:ARG:HE	1:E:113:ILE:HD11	1.52	0.75
1:F:213:ALA:HB1	1:F:218:GLN:HG3	1.68	0.75
1:C:138:CYS:SG	3:D:695:HOH:O	2.45	0.74
1:C:355:THR:CG2	1:C:357:GLN:HE21	2.01	0.74
1:E:210:TYR:OH	1:E:212:ALA:HB2	1.89	0.73
1:E:260:ILE:HD11	1:E:265:PHE:HB2	1.71	0.72
1:F:163:VAL:HG13	1:F:250:LYS:HB3	1.70	0.72
1:E:138:CYS:SG	3:F:661:HOH:O	2.48	0.71
1:A:143:ASN:HD21	1:A:277:GLN:HE21	1.39	0.71
1:F:29:LEU:HD21	1:F:54:LYS:HE3	1.73	0.71
1:F:115:ARG:HG3	1:F:121:ALA:HB3	1.72	0.70
1:C:355:THR:HG23	1:C:357:GLN:HE21	1.57	0.69
1:B:195:ASP:OD1	1:B:231:ARG:NH2	2.22	0.69
1:B:223:ASP:OD2	1:B:238:ARG:NH2	2.27	0.68
1:B:327:MET:HG3	1:B:374:MET:HE2	1.76	0.68
1:C:355:THR:HG21	1:C:377:MET:HE1	1.74	0.68
1:E:189:LYS:NZ	1:F:262:LEU:O	2.25	0.68



Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlap(Å)		
1:F:291:LEU:HD12	1:F:292:PBO:HD2	1 77	0.67		
1:A:355:THR:HG22	1:A:358:GLU:H	1.61	0.66		
1:F:12:ILE:HB	1:F:93:VAL:HG22	1.77	0.65		
1:B:12:ILE:HB	1:B:93:VAL:HG22	1.77	0.65		
1:E:72:MET:N	1:E:72:MET:SD	2.71	0.64		
1:D:345:ARG:HG3	1:D:346:ALA:N	2.12	0.64		
1:F:224:LYS:NZ	3:F:606:HOH:O	2.31	0.63		
1:F:296:GLN:O	1:F:300:ALA:N	2.30	0.62		
1:A:351:VAL:O	1:A:359:ARG:NH2	2.31	0.62		
1:E:99:HIS:CD2	1:E:101:GLY:H	2.11	0.62		
1:C:355:THR:OG1	1:C:357:GLN:NE2	2.33	0.62		
1:F:167:LEU:HB3	1:F:247:ILE:HB	1.81	0.61		
1:C:138:CYS:SG	3:C:719:HOH:O	2.56	0.61		
1:C:167:LEU:HB3	1:C:247:ILE:HB	1.82	0.60		
1:E:257:THR:HA	1:E:260:ILE:HG22	1.83	0.60		
1:F:152:SEB:O	1:F:156:ILE:HG12	2.03	0.59		
1:C:355:THR:HG21	1:C:377:MET:HE3	1.81	0.59		
1:E:348:ALA:O	1:E:359:ARG:NH1	2.34	0.59		
1:E:345:ARG:HD2	1:E:345:ABG:N	2.16	0.58		
1:D:36:SER:HB2	1:D:90:LEU:HB3	1.83	0.58		
1:E:259:ILE:O	1:E:263:LEU:HD22	2.03	0.58		
1:E:115:ARG:HG3	1:E:121:ALA:HB3	1.84	0.58		
1:E:351:VAL:HB	1:E:354:LEU:HD11	1.85	0.58		
1:C:85:GLU:HB3	1:C:90:LEU:HD12	1.86	0.58		
1:E:261:ARG:NH2	1:E:262:LEU:HG	2.19	0.57		
1:D:277:GLN:HG3	1:D:290:THR:HG23	1.87	0.57		
1:A:28:ALA:O	1:A:32:ILE:HG12	2.05	0.56		
1:E:65:TYR:HB3	1:E:180:PHE:CE2	2.40	0.56		
1:D:28:ALA:O	1:D:32:ILE:HG12	2.06	0.56		
1:D:72:MET:SD	1:D:105:ASN:ND2	2.79	0.56		
1:F:162:ASN:HB3	3:F:633:HOH:O	2.06	0.56		
1:F:196:ARG:NH1	3:F:615:HOH:O	2.37	0.56		
1:E:162:ASN:ND2	3:E:408:HOH:O	2.39	0.55		
1:F:370:ILE:O	1:F:374:MET:HG3	2.06	0.55		
1:E:157:ARG:CZ	1:E:159:ARG:NH2	2.70	0.55		
1:D:283:GLN:NE2	3:D:609:HOH:O	2.40	0.55		
1:D:354:LEU:HB3	1:D:359:ARG:HG2	1.89	0.55		
1:D:32:ILE:HD13	1:D:93:VAL:HG11	1.89	0.54		
1:B:152:SER:OG	1:B:176:GLY:N	2.40	0.54		
1:D:188:SER:OG	1:D:189:LYS:NZ	2.40	0.54		
1:D:273:ASP:OD2	1:D:276:THR:HB	2.07	0.54		



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:63:GLN:NE2	3:B:611:HOH:O	2.40	0.54
1:F:174:CYS:HA	1:F:177:ILE:HD12	1.90	0.54
1:B:71:ARG:NH2	1:B:177:ILE:O	2.41	0.54
1:E:210:TYR:HA	1:E:221:VAL:O	2.08	0.54
1:C:355:THR:HG22	1:C:358:GLU:HB2	1.88	0.53
1:A:174:CYS:HA	1:A:177:ILE:HD12	1.91	0.53
1:B:278:ILE:HA	1:B:291:LEU:HD12	1.91	0.53
1:D:73:ASP:O	1:D:77:GLN:HG3	2.08	0.53
1:F:335:LYS:NZ	3:F:612:HOH:O	2.33	0.53
1:B:286:PRO:HB3	1:F:271:VAL:HG23	1.90	0.53
1:C:357:GLN:NE2	1:C:357:GLN:H	2.06	0.53
1:E:266:LEU:HD13	1:E:272:PRO:HB3	1.91	0.53
1:E:12:ILE:O	1:E:93:VAL:HA	2.09	0.52
1:F:226:THR:H	1:F:229:GLN:HE21	1.57	0.52
1:F:320:SER:HB3	1:F:377:MET:SD	2.49	0.52
1:B:251:ALA:HA	1:F:269:GLY:HA3	1.92	0.52
1:B:37:LYS:NZ	3:B:613:HOH:O	2.42	0.52
1:C:355:THR:O	1:C:359:ARG:HG3	2.08	0.52
1:E:157:ARG:CZ	1:E:159:ARG:HH22	2.22	0.52
1:E:214:MET:SD	1:E:214:MET:N	2.83	0.52
1:E:77:GLN:NE2	1:F:304:ARG:HD2	2.24	0.52
1:A:174:CYS:SG	3:A:727:HOH:O	2.59	0.52
1:B:298:GLU:O	1:B:302:ILE:HG12	2.10	0.52
1:C:76:THR:HG22	1:D:302:ILE:HD11	1.92	0.51
1:B:287:ASP:O	1:F:261:ARG:NH2	2.44	0.51
1:B:167:LEU:HB3	1:B:247:ILE:HB	1.93	0.51
1:F:33:GLU:HG2	1:F:54:LYS:HB3	1.93	0.51
1:E:305:LEU:HD21	1:F:77:GLN:HB3	1.92	0.51
1:B:28:ALA:O	1:B:32:ILE:HG12	2.11	0.51
1:C:357:GLN:CD	1:C:357:GLN:H	2.14	0.51
1:F:277:GLN:HG3	1:F:290:THR:HG23	1.92	0.50
1:D:278:ILE:HA	1:D:291:LEU:HD12	1.93	0.50
1:E:355:THR:HG22	1:E:357:GLN:H	1.76	0.50
1:A:12:ILE:O	1:A:93:VAL:HA	2.11	0.50
1:F:122:ARG:NH2	3:F:616:HOH:O	2.37	0.50
1:C:295:GLY:O	1:C:297:ASN:N	2.45	0.49
1:E:156:ILE:HD13	1:F:259:ILE:HG22	1.94	0.49
1:F:261:ARG:HH11	1:F:261:ARG:HG2	1.77	0.49
1:C:264:GLU:O	1:C:266:LEU:N	2.45	0.49
1:E:315:GLN:HB3	1:E:375:LYS:CG	2.43	0.48
1:A:45:PRO:HG2	1:B:371:ARG:HG2	1.94	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:F:317:LEU:HD12	1:F:374:MET:O	2.12	0.48
1:D:103:PHE:CE2	1:D:170:PHE:HB2	2.48	0.48
1:E:278:ILE:HA	1:E:291:LEU:HD12	1.95	0.48
1:E:63:GLN:HG2	1:F:314:TYR:CE1	2.49	0.48
1:F:296:GLN:HA	1:F:299:GLN:HB2	1.96	0.48
1:A:260:ILE:HG13	1:B:156:ILE:HD13	1.96	0.48
1:E:167:LEU:HB3	1:E:247:ILE:HB	1.95	0.48
1:E:223:ASP:OD2	3:E:401:HOH:O	2.20	0.48
1:E:109:ARG:NH2	1:F:293:PRO:O	2.47	0.48
1:D:12:ILE:HB	1:D:93:VAL:HG22	1.96	0.48
1:D:12:ILE:O	1:D:93:VAL:HA	2.14	0.48
1:A:156:ILE:HD11	1:B:263:LEU:HD12	1.94	0.48
1:F:109:ARG:O	1:F:113:ILE:HG13	2.14	0.48
1:E:157:ARG:NH1	1:E:159:ARG:NH2	2.62	0.47
1:F:150:GLU:HB3	1:F:153:ASP:HB3	1.96	0.47
1:F:12:ILE:O	1:F:93:VAL:HA	2.14	0.47
1:C:188:SER:O	3:C:601:HOH:O	2.20	0.47
1:F:226:THR:H	1:F:229:GLN:NE2	2.12	0.47
1:B:12:ILE:O	1:B:93:VAL:HA	2.15	0.47
1:F:20:SER:O	1:F:22:GLY:N	2.38	0.47
1:F:198:GLU:CD	1:F:231:ARG:HH21	2.18	0.47
1:A:146:CYS:HA	1:A:166:HIS:HB2	1.96	0.47
1:E:239:VAL:HG23	1:E:243:SER:CB	2.45	0.47
1:B:140:ASP:OD1	1:B:142:SER:OG	2.32	0.47
1:E:65:TYR:HB3	1:E:180:PHE:CD2	2.49	0.46
1:A:302:ILE:O	1:A:305:LEU:HB2	2.15	0.46
1:C:296:GLN:N	3:C:619:HOH:O	2.48	0.46
1:D:234:GLU:HA	1:D:237:LYS:HE2	1.98	0.46
1:E:36:SER:HB3	1:E:90:LEU:HD22	1.97	0.46
1:A:84:LYS:O	1:A:84:LYS:HD3	2.16	0.46
1:E:189:LYS:HD3	1:F:263:LEU:HA	1.98	0.46
1:F:323:MET:HA	1:F:326:VAL:HG12	1.97	0.46
1:B:218:GLN:NE2	3:B:608:HOH:O	2.38	0.46
1:E:192:ILE:HG12	1:F:262:LEU:HD22	1.97	0.46
1:F:71:ARG:NH1	1:F:75:TYR:OH	2.48	0.46
1:A:370:ILE:HG23	1:A:374:MET:HE3	1.98	0.46
1:C:174:CYS:HA	1:C:177:ILE:HD12	1.99	0.45
1:C:61:LEU:HD22	1:C:78:MET:HG2	1.99	0.45
1:D:65:TYR:HB3	1:D:180:PHE:CE2	2.52	0.45
1:E:149:TYR:HB2	1:E:169:LEU:HD23	1.99	0.45
1:E:87:ARG:NE	1:E:117:GLU:OE1	2.50	0.45



Interatomic Clash				
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:F:226:THR:OG1	1:F:229:GLN:HG3	2.16	0.45	
1:A:252:ARG:HH22	1:A:277:GLN:HE22	1.63	0.45	
1:E:326:VAL:HG21	1:E:351:VAL:HG21	1.98	0.45	
1:B:175:VAL:HB	3:B:620:HOH:O	2.16	0.45	
1:E:189:LYS:HZ2	1:F:264:GLU:HG3	1.81	0.45	
1:F:335:LYS:HD3	1:F:335:LYS:O	2.16	0.45	
1:C:12:ILE:O	1:C:93:VAL:HA	2.17	0.45	
1:F:274:LYS:HB3	1:F:274:LYS:HE3	1.75	0.45	
1:F:261:ARG:HH11	1:F:261:ARG:CG	2.31	0.44	
1:A:80:GLU:HG2	1:B:302:ILE:HD12	1.99	0.44	
1:E:105:ASN:N	1:E:106:PRO:HD2	2.33	0.44	
1:E:37:LYS:HD3	1:E:57:ASN:ND2	2.33	0.44	
1:D:266:LEU:HD13	1:D:272:PRO:HB3	1.98	0.44	
1:D:319:THR:OG1	1:D:320:SER:N	2.49	0.44	
1:E:360:ALA:O	1:E:364:LEU:HD23	2.18	0.44	
1:C:155:LEU:HD21	1:C:193:LEU:HA	1.99	0.44	
1:C:195:ASP:OD1	1:C:231:ARG:NH2	2.44	0.44	
1:D:302:ILE:O	1:D:305:LEU:HB2	2.17	0.44	
1:E:38:VAL:HA	1:E:93:VAL:O	2.18	0.44	
1:F:279:TYR:CG	1:F:280:PRO:HA	2.53	0.44	
1:F:355:THR:HG22	1:F:357:GLN:H	1.82	0.44	
1:B:375:LYS:HE3	1:B:375:LYS:HB2	1.78	0.44	
1:C:236:ALA:O	1:C:239:VAL:HG22	2.17	0.44	
1:F:335:LYS:HA	1:F:335:LYS:HE2	1.99	0.44	
1:F:177:ILE:HD13	1:F:185:PHE:HB3	1.99	0.44	
1:F:88:ASN:HB2	1:F:90:LEU:HD12	1.98	0.44	
1:B:83:LEU:O	1:B:87:ARG:HG3	2.18	0.44	
1:F:287:ASP:OD2	3:F:602:HOH:O	2.21	0.44	
1:E:81:LEU:HD21	1:F:305:LEU:HD11	2.00	0.44	
1:C:355:THR:HG23	1:C:358:GLU:H	1.83	0.43	
1:E:146:CYS:HA	1:E:166:HIS:HB2	2.00	0.43	
1:B:327:MET:HG3	1:B:374:MET:CE	2.46	0.43	
1:D:354:LEU:HD22	1:D:358:GLU:HB3	2.00	0.43	
1:F:143:ASN:HA	1:F:144:PRO:HA	1.72	0.43	
1:C:82:MET:O	1:C:86:VAL:HG23	2.18	0.43	
1:E:157:ARG:NH1	1:E:159:ARG:HH21	2.17	0.43	
1:E:279:TYR:CE2	1:E:293:PRO:HG3	2.54	0.43	
1:C:327:MET:HG3	1:C:374:MET:CE	2.48	0.43	
1:C:49:ALA:O	1:C:53:THR:HG23	2.19	0.43	
1:E:155:LEU:HD22	1:E:192:ILE:HG22	2.00	0.43	
1:E:40:TYR:HA	1:E:95:VAL:HB	2.00	0.43	



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:341:LYS:HE3	1:F:341:LYS:HB3	1.66	0.43
1:C:187:ASN:HB3	3:C:669:HOH:O	2.18	0.43
1:D:298:GLU:O	1:D:302:ILE:HG12	2.18	0.43
1:F:257:THR:HG23	1:F:274:LYS:NZ	2.33	0.43
1:A:258:ASP:O	1:A:261:ARG:HG2	2.19	0.43
1:B:10:SER:HB2	1:B:120:GLN:HG3	1.99	0.43
1:C:375:LYS:O	3:C:602:HOH:O	2.21	0.43
1:F:27:GLN:O	1:F:31:TYR:HD1	2.02	0.43
1:E:210:TYR:CZ	1:E:212:ALA:HB2	2.53	0.43
1:E:259:ILE:O	1:E:262:LEU:HB2	2.19	0.43
1:A:252:ARG:HH22	1:A:277:GLN:NE2	2.17	0.43
1:C:20:SER:O	1:C:22:GLY:N	2.46	0.43
1:D:82:MET:O	1:D:86:VAL:HG23	2.18	0.43
1:F:207:VAL:HG13	1:F:225:PHE:HB2	2.01	0.43
1:C:103:PHE:CE2	1:C:170:PHE:HB2	2.54	0.42
1:E:330:LEU:HB3	1:F:216:PRO:HG2	2.01	0.42
1:F:261:ARG:HD2	1:F:261:ARG:HA	1.80	0.42
1:E:253:LYS:O	1:F:157:ARG:NH1	2.52	0.42
1:F:257:THR:HG23	1:F:274:LYS:HZ3	1.84	0.42
1:F:321:LYS:HD3	1:F:324:THR:HB	2.01	0.42
1:F:345:ARG:HG3	1:F:346:ALA:N	2.34	0.42
1:F:105:ASN:N	1:F:106:PRO:HD2	2.35	0.42
1:C:71:ARG:NH1	1:C:75:TYR:OH	2.49	0.42
1:D:299:GLN:O	1:D:303:THR:HG23	2.20	0.42
1:E:259:ILE:HG22	1:E:263:LEU:CD2	2.50	0.42
1:E:48:GLU:HG2	1:F:317:LEU:HD22	2.01	0.42
1:B:375:LYS:O	3:B:601:HOH:O	2.21	0.42
1:B:348:ALA:HA	1:B:362:LEU:HD23	2.02	0.42
1:E:255:ILE:HG13	1:F:157:ARG:NH1	2.35	0.42
1:F:186:ASP:HA	3:F:609:HOH:O	2.18	0.42
1:F:351:VAL:HA	1:F:352:PRO:HD3	1.90	0.42
1:B:103:PHE:CE2	1:B:170:PHE:HB2	2.55	0.42
1:D:20:SER:O	1:D:22:GLY:N	2.44	0.42
1:A:103:PHE:CE2	1:A:170:PHE:HB2	2.55	0.41
1:B:302:ILE:O	1:B:305:LEU:HB2	2.20	0.41
1:E:278:ILE:HG13	3:E:414:HOH:O	2.20	0.41
1:E:39:PHE:CD2	1:E:82:MET:HG2	2.55	0.41
1:E:298:GLU:HA	1:F:76:THR:HG21	2.03	0.41
1:B:213:ALA:HB1	1:B:218:GLN:HB2	2.02	0.41
1:E:259:ILE:HA	1:E:262:LEU:HD12	2.03	0.41
1:E:315:GLN:HB3	1:E:375:LYS:HE3	2.02	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:327:MET:HG3	1:C:374:MET:HE1	2.01	0.41
1:E:175:VAL:O	1:E:177:ILE:HG13	2.20	0.41
1:F:333:ASP:HB3	1:F:336:ALA:HB3	2.01	0.41
1:A:354:LEU:HD22	1:A:358:GLU:HB3	2.02	0.41
1:A:65:TYR:HB3	1:A:180:PHE:CD2	2.56	0.41
1:B:152:SER:O	1:B:156:ILE:HG13	2.20	0.41
3:A:604:HOH:O	1:B:138:CYS:SG	2.39	0.41
1:A:143:ASN:HD21	1:A:277:GLN:NE2	2.11	0.41
1:A:149:TYR:CE1	1:A:159:ARG:HD2	2.55	0.41
1:C:61:LEU:HB3	1:C:78:MET:SD	2.61	0.41
1:D:355:THR:HG23	1:D:356:PRO:HD2	2.03	0.41
1:E:327:MET:O	1:E:330:LEU:HB2	2.21	0.41
1:C:181:ASN:HB3	1:C:184:GLY:O	2.21	0.41
1:E:20:SER:O	1:E:22:GLY:N	2.40	0.41
1:E:210:TYR:OH	1:E:212:ALA:CB	2.65	0.41
1:A:278:ILE:HD12	1:A:279:TYR:O	2.21	0.41
1:E:232:GLU:HB2	1:E:235:ILE:HG12	2.03	0.41
1:E:361:ALA:HA	1:E:364:LEU:HB2	2.03	0.40
1:F:13:VAL:HG11	1:F:107:SER:HB2	2.03	0.40
1:B:174:CYS:HA	1:B:177:ILE:HD12	2.03	0.40
1:D:39:PHE:CD2	1:D:82:MET:HG2	2.56	0.40
1:C:355:THR:CG2	1:C:358:GLU:H	2.34	0.40
1:E:279:TYR:CG	1:E:280:PRO:HA	2.57	0.40
1:D:36:SER:CB	1:D:90:LEU:HB3	2.49	0.40
1:E:375:LYS:C	1:E:375:LYS:HD3	2.41	0.40
1:A:143:ASN:HA	1:A:144:PRO:HA	1.83	0.40
1:C:146:CYS:HA	1:C:166:HIS:HB2	2.02	0.40
1:D:146:CYS:HA	1:D:166:HIS:HB2	2.03	0.40
1:E:345:ARG:H	1:E:345:ARG:CD	2.27	0.40
1:F:15:GLY:HA3	1:F:100:PRO:HD3	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	369/386~(96%)	356~(96%)	12 (3%)	1 (0%)	41 46
1	В	368/386~(95%)	354~(96%)	13~(4%)	1~(0%)	41 46
1	С	369/386~(96%)	353~(96%)	15~(4%)	1 (0%)	41 46
1	D	368/386~(95%)	355~(96%)	13~(4%)	0	100 100
1	Е	365/386~(95%)	351~(96%)	14 (4%)	0	100 100
1	F	368/386~(95%)	354~(96%)	13~(4%)	1 (0%)	41 46
All	All	2207/2316~(95%)	2123~(96%)	80 (4%)	4 (0%)	47 55

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

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	377	MET
1	С	265	PHE
1	В	175	VAL
1	F	144	PRO

5.3.2 Protein sidechains (i)

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	А	314/327~(96%)	307~(98%)	7 (2%)	52 65
1	В	313/327~(96%)	306~(98%)	7(2%)	52 65
1	С	313/327~(96%)	306 (98%)	7 (2%)	52 65
1	D	313/327~(96%)	312~(100%)	1 (0%)	92 97
1	Е	312/327~(95%)	306 (98%)	6 (2%)	57 71
1	F	313/327~(96%)	307~(98%)	6 (2%)	57 71
All	All	1878/1962~(96%)	1844 (98%)	34 (2%)	59 72

All (34) residues with a non-rotameric sidechain are listed below:



Mol	Chain	\mathbf{Res}	Type
1	А	237	LYS
1	А	239	VAL
1	А	261	ARG
1	А	296	GLN
1	А	321	LYS
1	А	345	ARG
1	А	355	THR
1	В	142	SER
1	В	237	LYS
1	В	239	VAL
1	В	247	ILE
1	В	344	HIS
1	В	366	ASP
1	В	376	ASN
1	С	179	ASP
1	С	234	GLU
1	С	237	LYS
1	С	296	GLN
1	С	353	ASP
1	С	357	GLN
1	С	367	SER
1	D	239	VAL
1	Ε	37	LYS
1	Ε	73	ASP
1	Е	189	LYS
1	Ε	214	MET
1	Е	254	ASP
1	Ε	341	LYS
1	F	261	ARG
1	F	266	LEU
1	F	270	LYS
1	F	304	ARG
1	F	321	LYS
1	F	335	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	277	GLN
1	А	349	GLN
1	В	376	ASN
1	С	357	GLN
1	D	77	GLN



Continued from previous page...

Mol	Chain	\mathbf{Res}	Type
1	D	171	GLN
1	D	315	GLN
1	Е	99	HIS
1	Е	120	GLN
1	Е	344	HIS
1	F	229	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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	True	Chain	Dec	Timle	Bo	ond leng	$_{\rm sths}$	B	ond ang	les
MOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAH	В	500	-	21,28,28	1.17	2 (9%)	20,40,40	1.70	2(10%)
2	SAH	С	500	-	21,28,28	1.20	2 (9%)	20,40,40	1.64	2(10%)
2	SAH	А	500	-	21,28,28	1.18	2 (9%)	20,40,40	1.63	2(10%)
2	SAH	F	500	-	21,28,28	1.18	2 (9%)	20,40,40	1.73	2(10%)
2	SAH	D	500	-	21,28,28	1.18	2 (9%)	20,40,40	1.68	2 (10%)



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	SAH	В	500	-	-	1/7/31/31	0/3/3/3
2	SAH	С	500	-	-	0/7/31/31	0/3/3/3
2	SAH	А	500	-	-	1/7/31/31	0/3/3/3
2	SAH	F	500	-	-	0/7/31/31	0/3/3/3
2	SAH	D	500	-	-	1/7/31/31	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
2	С	500	SAH	C2-N3	3.85	1.38	1.32
2	А	500	SAH	C2-N3	3.81	1.38	1.32
2	D	500	SAH	C2-N3	3.80	1.38	1.32
2	F	500	SAH	C2-N3	3.78	1.38	1.32
2	В	500	SAH	C2-N3	3.74	1.38	1.32
2	С	500	SAH	C2-N1	2.44	1.38	1.33
2	В	500	SAH	C2-N1	2.39	1.38	1.33
2	D	500	SAH	C2-N1	2.37	1.38	1.33
2	А	500	SAH	C2-N1	2.37	1.38	1.33
2	F	500	SAH	C2-N1	2.30	1.38	1.33

All ((10)	bond	angle	outliers	are	listed	below:
· · · · /	. - ~ /	Sona	~	outitors	or c	motour	0010111

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	F	500	SAH	N3-C2-N1	-5.78	119.64	128.68
2	В	500	SAH	N3-C2-N1	-5.69	119.78	128.68
2	D	500	SAH	N3-C2-N1	-5.69	119.78	128.68
2	С	500	SAH	N3-C2-N1	-5.64	119.87	128.68
2	А	500	SAH	N3-C2-N1	-5.59	119.93	128.68
2	F	500	SAH	C5'-SD-CG	-3.75	91.03	102.27
2	D	500	SAH	C5'-SD-CG	-3.72	91.11	102.27
2	В	500	SAH	C5'-SD-CG	-3.68	91.23	102.27
2	С	500	SAH	C5'-SD-CG	-3.66	91.27	102.27
2	A	500	SAH	C5'-SD-CG	-3.51	91.72	102.27

There are no chirality outliers.

All (3) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	В	500	SAH	C3'-C4'-C5'-SD
2	А	500	SAH	C3'-C4'-C5'-SD
2	D	500	SAH	C3'-C4'-C5'-SD

There are no ring outliers.

No monomer is involved in short contacts.

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	$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9
1	А	371/386~(96%)	0.28	15 (4%) 38 36	20, 38, 65, 146	0
1	В	370/386~(95%)	0.41	24 (6%) 18 17	20, 40, 78, 159	0
1	С	371/386~(96%)	0.35	26 (7%) 16 15	22, 39, 76, 166	0
1	D	370/386~(95%)	0.49	29 (7%) 13 11	22, 42, 76, 146	0
1	Е	369/386~(95%)	0.72	24 (6%) 18 17	38, 61, 88, 200	0
1	F	370/386~(95%)	0.80	33 (8%) 9 8	38, 60, 103, 220	0
All	All	2221/2316~(95%)	0.51	151 (6%) 17 16	20, 47, 89, 220	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	268	ALA	29.2
1	С	271	VAL	19.1
1	D	271	VAL	18.3
1	D	268	ALA	18.1
1	Е	268	ALA	17.4
1	D	265	PHE	16.1
1	Е	267	PRO	15.7
1	Е	266	LEU	15.5
1	D	266	LEU	14.5
1	С	265	PHE	14.4
1	А	267	PRO	14.2
1	F	378	PRO	14.0
1	А	266	LEU	13.5
1	Е	265	PHE	13.0
1	С	272	PRO	12.9
1	F	267	PRO	12.7
1	F	271	VAL	12.4
1	В	378	PRO	12.3
1	F	275	HIS	11.7



6MJF

Mol	Chain	Res	Type	RSRZ
1	D	378	PRO	11.1
1	В	268	ALA	10.9
1	F	269	GLY	10.8
1	D	269	GLY	10.5
1	А	265	PHE	10.5
1	С	266	LEU	10.2
1	С	275	HIS	9.6
1	А	270	LYS	8.9
1	В	269	GLY	8.8
1	F	377	MET	8.8
1	С	378	PRO	8.8
1	D	272	PRO	8.7
1	В	377	MET	8.4
1	В	265	PHE	8.1
1	А	268	ALA	7.7
1	В	275	HIS	7.6
1	А	378	PRO	7.6
1	D	270	LYS	7.5
1	С	273	ASP	7.5
1	D	267	PRO	7.4
1	Е	271	VAL	7.4
1	С	268	ALA	7.2
1	Е	272	PRO	6.9
1	С	276	THR	6.7
1	F	265	PHE	6.5
1	С	267	PRO	6.3
1	F	266	LEU	6.3
1	В	266	LEU	6.2
1	В	274	LYS	6.2
1	В	271	VAL	6.0
1	С	269	GLY	5.7
1	Е	269	GLY	5.7
1	Е	185	PHE	5.6
1	F	376	ASN	5.5
1	D	275	HIS	5.4
1	Е	377	MET	5.4
1	A	269	GLY	5.2
1	С	270	LYS	5.1
1	Е	270	LYS	5.1
1	D	377	MET	5.0
1	E	378	PRO	4.7
1	С	274	LYS	4.6



6MJF

Mol	Chain	Res	Type	RSRZ
1	В	267	PRO	4.6
1	F	272	PRO	4.5
1	D	288	VAL	4.5
1	D	178	ALA	4.4
1	F	270	LYS	4.4
1	F	273	ASP	4.4
1	F	274	LYS	4.2
1	В	273	ASP	4.2
1	Е	180	PHE	4.1
1	В	272	PRO	4.1
1	А	377	MET	4.1
1	В	288	VAL	4.0
1	D	68	GLY	3.9
1	F	277	GLN	3.8
1	A	274	LYS	3.8
1	F	368	TRP	3.7
1	F	278	ILE	3.7
1	D	276	THR	3.6
1	А	264	GLU	3.6
1	D	345	ARG	3.5
1	Ε	376	ASN	3.5
1	F	296	GLN	3.5
1	D	185	PHE	3.5
1	В	270	LYS	3.4
1	F	289	PRO	3.3
1	E	86	VAL	3.3
1	D	177	ILE	3.3
1	D	278	ILE	3.3
1	В	177	ILE	3.2
1	С	277	GLN	3.2
1	F	300	ALA	3.2
1	С	307	ALA	3.2
1	В	290	THR	3.1
1	E	342	ALA	3.1
1	F	261	ARG	3.1
1	В	185	PHE	3.1
1	С	278	ILE	3.1
1	D	274	LYS	3.1
1	C	377	MET	3.0
1	A	271	VAL	2.9
1	С	349	GLN	2.9
1	F	291	LEU	2.9



6MJF

Mol	Chain	Res	Type	RSRZ	
1	F	276	THR	2.9	
1	С	300	ALA	2.9	
1	А	275	HIS	2.8	
1	В	276	THR	2.8	
1	F	257 THR		2.8	
1	Е	264 GLU		2.8	
1	С	312	GLU	2.8	
1	В	296	GLN	2.8	
1	D	289	PRO	2.8	
1	Е	90	LEU	2.8	
1	В	376	ASN	2.7	
1	Е	345	ARG	2.7	
1	С	303	THR	2.7	
1	С	306	GLU	2.7	
1	Е	306	GLU	2.7	
1	F	304	ARG	2.6	
1	F	313	GLU	2.6	
1	Е	255	ILE	2.6	
1	Е	138	CYS	2.6	
1	В	355	THR	2.5	
1	D	364	LEU	2.5	
1	В	289	PRO	2.5	
1	Е	364	LEU	2.4	
1	D	115	ARG	2.4	
1	А	272	PRO	2.4	
1	D	264	GLU	2.4	
1	С	185	PHE	2.4	
1	Е	352	PRO	2.4	
1	F	138	CYS	2.4	
1	Е	304	ARG	2.4	
1	A	296	GLN	2.3	
1	F	346	ALA	2.3	
1	F	360	ALA	2.3	
1	D	260	ILE	2.3	
1	В	349	GLN	2.2	
1	F	335	LYS	2.2	
1	F	287	ASP	2.2	
1	С	348	ALA	2.2	
1	D	56	LYS	2.2	
1	D	90	LEU	2.2	
1	С	296	GLN	2.2	
1	D	179	ASP	2.1	



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Mol	Chain	Res Type		RSRZ
1	С	354	LEU	2.1
1	В	179	ASP	2.1
1	D	261	ARG	2.0
1	F	292	PRO	2.0
1	F	255	ILE	2.0
1	А	261	ARG	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. 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	B-factors(Å ²)	Q<0.9
2	SAH	F	500	26/26	0.94	0.11	$35,\!43,\!46,\!47$	0
2	SAH	А	500	26/26	0.95	0.10	15,22,29,30	0
2	SAH	В	500	26/26	0.96	0.11	15,23,29,30	0
2	SAH	С	500	26/26	0.96	0.08	17,24,29,31	0
2	SAH	D	500	26/26	0.96	0.08	17,24,30,30	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.

