

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	4Q33
Title	:	Crystal Structure of Inosine 5'-monophosphate Dehydrogenase from Clostrid-
		ium perfringens Complexed with IMP and A110
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Deposited on	:	2014-04-10
Resolution	:	2.88 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 (i)) 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)

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 2.88 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	$2868 \ (2.90-2.86)$
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	363	% 77%	18%	5%
1	В	363	80%	13%	• 6%
1	С	363	78%	15%	• 6%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996) Validation Pipeline (wwPDB-VP) : 2.35.1



Mol	Chain	Length	Quality of chain		
1	D	363	76%	17%	• 6%
1	Е	363	% 72%	21%	• 6%
1	F	363	74%	20%	5%
1	G	363	76%	17%	• 5%
1	Н	363	80%	13%	• 5%

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	FMT	F	502	-	-	Х	-
6	SO4	Ē	503	-	-	-	Х



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 20930 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	Δ	244	Total	С	Ν	0	\mathbf{S}	0	4	0
1	A	044	2574	1615	446	493	20	0	4	0
1	р	249	Total	С	Ν	0	S	0	2	0
1	D	342	2539	1594	441	485	19	0	2	0
1	С	242	Total	С	Ν	0	S	0	1	0
1	U	343	2536	1593	438	486	19	0	L	0
1	а	249	Total	С	Ν	0	S	0	2	0
1	D	342	2534	1591	437	486	20	0	2	0
1	F	242	Total	С	Ν	0	S	0	2	0
1	Ľ	343	2552	1603	443	487	19	0	5	0
1	Б	244	Total	С	Ν	0	S	0	1	0
1	Г	044	2545	1601	440	485	19	0	L	0
1	C	944	Total	С	Ν	0	S	0	0	0
1	G	044	2535	1594	438	484	19	0	0	0
1	п	944	Total	С	Ν	0	S	0	1	0
	п	044	2544	1599	439	487	19	0		

• Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase.

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-2	SER	-	expression tag	UNP Q0TN42
А	-1	ASN	-	expression tag	UNP Q0TN42
А	0	ALA	-	expression tag	UNP Q0TN42
А	89	SER	-	linker	UNP Q0TN42
А	90	GLY	-	linker	UNP Q0TN42
А	91	GLY	-	linker	UNP Q0TN42
В	-2	SER	-	expression tag	UNP Q0TN42
В	-1	ASN	-	expression tag	UNP Q0TN42
В	0	ALA	-	expression tag	UNP Q0TN42
В	89	SER	-	linker	UNP Q0TN42
В	90	GLY	-	linker	UNP Q0TN42
В	91	GLY	-	linker	UNP Q0TN42
C	-2	SER	_	expression tag	UNP Q0TN42



Chain	Residue	Modelled	Actual	Comment	Reference
С	-1	ASN	-	expression tag	UNP Q0TN42
С	0	ALA	_	expression tag	UNP Q0TN42
С	89	SER	-	linker	UNP Q0TN42
С	90	GLY	-	linker	UNP Q0TN42
С	91	GLY	-	linker	UNP Q0TN42
D	-2	SER	-	expression tag	UNP Q0TN42
D	-1	ASN	-	expression tag	UNP Q0TN42
D	0	ALA	-	expression tag	UNP Q0TN42
D	89	SER	-	linker	UNP Q0TN42
D	90	GLY	-	linker	UNP Q0TN42
D	91	GLY	-	linker	UNP Q0TN42
Е	-2	SER	-	expression tag	UNP Q0TN42
Е	-1	ASN	-	expression tag	UNP Q0TN42
Е	0	ALA	-	expression tag	UNP Q0TN42
Е	89	SER	-	linker	UNP Q0TN42
Е	90	GLY	-	linker	UNP Q0TN42
Е	91	GLY	-	linker	UNP Q0TN42
F	-2	SER	-	expression tag	UNP Q0TN42
F	-1	ASN	-	expression tag	UNP Q0TN42
F	0	ALA	-	expression tag	UNP Q0TN42
F	89	SER	-	linker	UNP Q0TN42
F	90	GLY	-	linker	UNP Q0TN42
F	91	GLY	-	linker	UNP Q0TN42
G	-2	SER	-	expression tag	UNP Q0TN42
G	-1	ASN	-	expression tag	UNP Q0TN42
G	0	ALA	-	expression tag	UNP Q0TN42
G	89	SER	-	linker	UNP Q0TN42
G	90	GLY	-	linker	UNP Q0TN42
G	91	GLY	-	linker	UNP Q0TN42
Н	-2	SER	-	expression tag	UNP Q0TN42
Н	-1	ASN	-	expression tag	UNP Q0TN42
Н	0	ALA	-	expression tag	UNP Q0TN42
Н	89	SER	-	linker	UNP Q0TN42
Н	90	GLY	-	linker	UNP Q0TN42
H	91	GLY	-	linker	UNP Q0TN42

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• Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	Δ	1	Total C N O P	0	0
	Л	T	23 10 4 8 1	0	0
2	В	1	Total C N O P	0	0
2	D	T	23 10 4 8 1	0	0
2	С	1	Total C N O P	0	0
2	U	T	23 10 4 8 1	0	0
2	л	1	Total C N O P	0	0
2	D	T	23 10 4 8 1	0	0
2	E	1	Total C N O P	0	0
2		T	23 10 4 8 1	0	0
2	F	1	Total C N O P	0	0
2	L	I	23 10 4 8 1	0	0
2	G	1	Total C N O P	0	0
	G	1	23 10 4 8 1	0	
2	н	1	Total C N O P	0	
	11	1 I	$\begin{vmatrix} 23 & 10 & 4 & 8 & 1 \end{vmatrix}$	0	

• Molecule 3 is 4-[(1R)-1-[1-(4-chlorophenyl)-1,2,3-triazol-4-yl]ethoxy]-1-oxidanyl-quinoline (three-letter code: 2YA) (formula: $C_{19}H_{15}ClN_4O_2$).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
2	Λ	1	Total	С	Cl	Ν	Ο	0	0
Ð	A	1	26	19	1	4	2	0	0
2	В	1	Total	С	Cl	Ν	0	0	0
0	D	1	26	19	1	4	2	0	0
2	Р	1	Total	С	Cl	Ν	0	0	0
0	D	1	26	19	1	4	2	0	0
2	С	1	Total	С	Cl	Ν	0	0	0
0	U	1	26	19	1	4	2	0	0
3	F	1	Total	С	Cl	Ν	Ο	0	0
0	Ľ	1	26	19	1	4	2	0	0
3	F	1	Total	С	Cl	Ν	Ο	0	0
0	Г	1	26	19	1	4	2	0	0
3	С	1	Total	С	Cl	Ν	Ο	0	0
5	G	L	26	19	1	4	2	0	0
3	н	1	Total	С	Cl	Ν	0	0	0
0	11	L	26	19	1	4	2	0	U

• Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	O 2	0	0

• Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Е	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 3 1 2 \end{array}$	0	0
5	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 3 1 2 \end{array}$	0	0
5	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 3 1 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	\mathbf{F}	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 3 1 2 \end{array}$	0	0
5	G	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 3 1 2 \end{array}$	0	0
5	Н	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 3 1 2 \end{array}$	0	0
5	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0

• Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Ato	\mathbf{pms}		ZeroOcc	AltConf
6	Е	1	Total 5	0 4	S 1	0	0

• Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	16	Total O 16 16	0	0
8	В	15	Total O 15 15	0	0
8	С	16	Total O 16 16	0	0
8	D	17	Total O 17 17	0	0
8	Е	22	TotalO2222	0	0
8	F	23	TotalO2323	0	0
8	G	11	Total O 11 11	0	0
8	Н	17	Total O 17 17	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: Inosine-5'-monophosphate dehydrogenase





• Molecule 1: Inosine-5'-monophosphate dehydrogenase







• Molecule 1: Inosine-5'-monophosphate dehydrogenase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	88.12Å 89.25Å 99.19Å	Deperitor
a, b, c, α , β , γ	70.82° 72.66° 79.30°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	37.21 - 2.88	Depositor
Resolution (A)	48.50 - 2.89	EDS
% Data completeness	97.6 (37.21-2.88)	Depositor
(in resolution range)	97.6 (48.50-2.89)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) > 1$	$1.98 (at 2.91 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1593)	Depositor
P. P.	0.185 , 0.243	Depositor
n, n_{free}	0.186 , 0.244	DCC
R_{free} test set	3015 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	52.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.34 , 53.6	EDS
L-test for $twinning^2$	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20930	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.10% 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: SO4, IMP, ACY, FMT, GOL, 2YA

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	0.21	0/2607	0.41	0/3515
1	В	0.22	0/2572	0.40	0/3470
1	С	0.22	0/2571	0.41	0/3469
1	D	0.22	0/2567	0.41	0/3464
1	Е	0.21	0/2585	0.41	0/3489
1	F	0.22	0/2578	0.42	0/3477
1	G	0.23	0/2568	0.42	0/3465
1	Н	0.23	0/2577	0.41	0/3477
All	All	0.22	0/20625	0.41	0/27826

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	2574	0	2637	25	0
1	В	2539	0	2602	29	0
1	С	2536	0	2604	28	0
1	D	2534	0	2592	33	0
1	Е	2552	0	2617	50	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2545	0	2619	43	0
1	G	2535	0	2605	41	0
1	Н	2544	0	2610	30	0
2	А	23	0	11	1	0
2	В	23	0	11	2	0
2	С	23	0	11	2	0
2	D	23	0	11	2	0
2	Е	23	0	11	3	0
2	F	23	0	11	2	0
2	G	23	0	11	2	0
2	Н	23	0	11	1	0
3	А	26	0	15	0	0
3	В	52	0	30	0	0
3	С	26	0	15	0	0
3	Е	26	0	15	0	0
3	F	26	0	15	0	0
3	G	26	0	15	0	0
3	Н	26	0	15	0	0
4	D	4	0	3	0	0
5	Е	3	0	1	0	0
5	F	9	0	3	2	0
5	G	3	0	1	1	0
5	Н	6	0	2	0	0
6	Е	5	0	0	0	0
7	F	12	0	16	0	0
8	А	16	0	0	0	0
8	В	15	0	0	0	0
8	С	16	0	0	0	0
8	D	17	0	0	0	0
8	Е	22	0	0	0	0
8	F	23	0	0	0	0
8	G	11	0	0	0	0
8	Н	17	0	0	0	0
All	All	20930	0	21120	248	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 6.

All (248) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



4Q33

Atom-1	Atom-2	Interatomic distance $(Å)$	Clash overlap (Å)
1·D·279·PRO·HB3	1.D.325[B].GLU.HG3	1.66	0.78
1:E:444:PRO:HD2	1:E:448:ASN:HD22	1.49	0.77
1:E:83:VAL:O	1:E:87:LYS:HG2	1.86	0.76
1:D:283:ABG:NH1	1:D:325[A]:GLU:OE2	2.21	0.72
1:B:272:ILE:HG12	1:B:292:CYS:HB3	1.74	0.68
1:E:247:THR:OG1	1:E:248:ALA:N	2.26	0.67
1:A:243:ILE:HG13	1:A:269:LEU:HD21	1.75	0.67
1:D:226:ASN:N	1:D:226:ASN:OD1	2.29	0.65
1:E:358:MET:HG2	1:E:361:ILE:HD12	1.79	0.65
1:B:263:LYS:NZ	1:B:269:LEU:O	2.27	0.65
1:B:56:LYS:HD2	1:B:367:GLU:HA	1.78	0.65
1:C:298:GLY:HA2	1:C:303:CYS:SG	2.38	0.64
1:A:409:VAL:HG21	1:C:432:GLY:HA3	1.80	0.64
1:D:244:VAL:HG12	1:D:272:ILE:HB	1.79	0.63
1:F:358:MET:HG2	1:F:361:ILE:HD12	1.79	0.63
1:E:87:LYS:HE3	1:E:87:LYS:HA	1.82	0.62
1:G:221:SER:HA	1:G:244:VAL:HG22	1.82	0.62
1:E:349:LEU:HD13	1:E:446:LEU:HD11	1.82	0.62
1:H:272:ILE:HG12	1:H:292:CYS:HB3	1.82	0.61
1:C:75:THR:HG22	1:C:77:GLU:H	1.65	0.61
1:G:249:HIS:HB3	5:G:502:FMT:H	1.82	0.61
1:E:384:ARG:HB3	1:E:414:GLU:HG3	1.82	0.60
1:H:298:GLY:N	1:H:299:PRO:HD3	2.16	0.60
1:A:272:ILE:HG12	1:A:292:CYS:HB3	1.82	0.60
1:E:432:GLY:HA3	1:F:409:VAL:HG21	1.82	0.60
1:A:283:ARG:HG2	1:A:329:LEU:HD11	1.84	0.59
1:C:336:ASP:OD2	2:C:500:IMP:O2'	2.20	0.59
1:E:461:ALA:HB2	5:F:502:FMT:H	1.83	0.59
1:G:272:ILE:HG12	1:G:292:CYS:HB3	1.85	0.58
1:A:70:ILE:HD13	1:A:82:GLU:HB3	1.85	0.58
1:A:64:GLU:HG2	1:A:427:ILE:HG21	1.85	0.58
1:B:244:VAL:HB	1:B:272:ILE:HB	1.84	0.58
1:E:298:GLY:HA2	1:E:303:CYS:SG	2.43	0.58
1:D:74:MET:O	1:D:231:ARG:NH1	2.35	0.58
1:E:389:LEU:HD13	1:E:410:PRO:HG3	1.86	0.58
1:G:336:ASP:OD2	2:G:500:IMP:O2'	2.21	0.58
1:C:384:ARG:HB3	1:C:414:GLU:HG3	1.86	0.57
1:B:246:ASP:OD1	1:B:246:ASP:N	2.36	0.57
1:D:298:GLY:HA2	1:D:303:CYS:SG	2.44	0.57
1:G:257:GLU:HA	1:G:260:LYS:HE2	1.86	0.57
1:G:302:ILE:HG22	1:H:471:ILE:HD12	1.87	0.57
1:F:64:GLU:HG2	1:F:427:ILE:HG21	1.87	0.56



Atom-1	Atom-2	Interatomic	Clash
	7100HI 2	distance (Å)	overlap (Å)
1:F:298:GLY:HA2	1:F:303:CYS:SG	2.45	0.56
1:G:233:ASP:HA	1:G:236:VAL:HB	1.88	0.56
1:H:384:ARG:HB3	1:H:414:GLU:HG3	1.86	0.56
1:C:272:ILE:HG12	1:C:292:CYS:HB3	1.86	0.56
1:E:32:THR:HG23	1:E:446:LEU:HD23	1.88	0.56
1:D:387:GLY:N	2:D:501:IMP:O6	2.36	0.56
1:A:372:ILE:HD13	1:A:381:LYS:HE2	1.88	0.56
1:G:59:ILE:HD11	1:G:86:VAL:HA	1.88	0.56
1:C:463:PHE:HZ	1:D:464:ARG:HH22	1.54	0.56
1:F:18:PRO:HG2	1:H:297:ILE:HD12	1.88	0.55
1:G:34:LEU:HD11	1:G:272:ILE:HD11	1.88	0.55
1:G:298:GLY:HA2	1:G:303:CYS:SG	2.47	0.55
1:C:235:VAL:HG21	1:C:243:ILE:HD11	1.89	0.54
1:E:455:PHE:HB2	1:F:4:ILE:HD13	1.88	0.54
1:D:57:MET:HE2	1:D:423:LEU:HD22	1.90	0.54
1:F:22:GLU:HG2	1:H:253:LYS:HB2	1.88	0.54
1:G:46:SER:HB2	1:G:61:MET:HG3	1.90	0.54
1:D:438:MET:HG2	1:D:449:LEU:HD13	1.88	0.54
1:F:461:ALA:HB1	1:H:12:ASP:HB2	1.90	0.54
1:C:346:VAL:HG22	1:C:434:ILE:HA	1.90	0.53
1:G:33:GLN:HG3	1:G:35:THR:O	2.09	0.53
1:D:225:THR:OG1	1:D:226:ASN:N	2.41	0.53
1:F:50:ASP:OD2	1:F:384:ARG:NH2	2.39	0.53
1:B:76:ILE:HG12	1:B:231[A]:ARG:HG2	1.89	0.53
1:E:340:LYS:HE2	1:G:469:HIS:CE1	2.43	0.53
1:E:315:GLN:NE2	1:E:336:ASP:O	2.42	0.53
1:G:233:ASP:HB3	1:G:266:TYR:OH	2.09	0.53
1:F:249:HIS:O	1:F:252:SER:OG	2.26	0.53
1:E:366:GLU:N	1:E:421:GLY:O	2.41	0.53
1:C:33:GLN:HG3	1:C:35:THR:O	2.09	0.52
1:H:10:THR:HG22	1:H:11:PHE:H	1.75	0.52
1:H:298:GLY:HA2	1:H:303:CYS:SG	2.50	0.52
1:E:478:PRO:HD2	1:F:410:PRO:HG2	1.92	0.52
1:A:336:ASP:OD2	2:A:500:IMP:O2'	2.28	0.52
1:B:286:ALA:HB2	1:B:331:ILE:HD13	1.92	0.52
1:D:250:GLY:HA2	1:D:255:VAL:HG21	1.91	0.52
1:E:440:TYR:HB3	1:F:311:VAL:HG11	1.92	0.52
1:F:329:LEU:HB2	1:F:331:ILE:HG22	1.91	0.52
1:E:23:VAL:HG23	1:E:27:GLU:HB2	1.91	0.51
1:E:466:SER:HA	1:F:306:ARG:HD2	1.93	0.51
1:B:432:GLY:HA3	1:D:409:VAL:HG21	1.93	0.51



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance (Å)	overlap (Å)
1:G:368:ALA:O	1:G:381:LYS:NZ	2.43	0.51
1:A:218:CYS:N	1:A:241:ASP:OD2	2.43	0.51
1:G:56:LYS:HD3	1:G:367:GLU:HA	1.93	0.51
1:F:336:ASP:OD2	2:F:500:IMP:O2'	2.29	0.50
1:G:83:VAL:HG11	1:G:240:VAL:HG23	1.93	0.50
1:G:235:VAL:HG13	1:G:240:VAL:HG21	1.93	0.50
1:C:294:LYS:HG3	1:C:334:ILE:HB	1.93	0.50
1:B:79[B]:GLN:HG3	1:B:231[B]:ARG:HH12	1.76	0.50
1:D:333:VAL:HG23	1:D:353:ALA:HA	1.93	0.50
1:H:243:ILE:HD11	1:H:262:ILE:HD13	1.94	0.49
1:A:33:GLN:NE2	1:A:35:THR:O	2.44	0.49
1:C:226:ASN:OD1	1:C:226:ASN:N	2.46	0.49
1:F:283:ARG:NH1	1:F:325:GLU:OE2	2.45	0.49
1:H:63:ARG:HG3	1:H:216:LEU:HD11	1.93	0.49
1:H:78:ASP:O	1:H:82:GLU:HG2	2.12	0.49
1:F:443:ALA:HA	1:F:448:ASN:HD22	1.78	0.49
1:D:419:TYR:CZ	1:D:421:GLY:HA2	2.48	0.49
1:H:472:ASN:OD1	1:H:472:ASN:N	2.46	0.49
1:C:221:SER:HB2	1:C:246:ASP:OD2	2.13	0.49
1:G:50:ASP:HA	1:G:71:HIS:CD2	2.48	0.49
1:A:323:ALA:O	1:A:327:LYS:HG2	2.13	0.48
1:B:440:TYR:HB3	1:D:311:VAL:HG11	1.95	0.48
1:H:55:SER:HB3	1:H:82:GLU:OE1	2.12	0.48
1:B:387:GLY:N	2:B:501:IMP:O6	2.37	0.48
1:F:466:SER:HA	1:H:306:ARG:HD2	1.95	0.48
1:A:384:ARG:HB3	1:A:414:GLU:HG3	1.94	0.48
1:F:56:LYS:HE2	1:F:367:GLU:HA	1.93	0.48
1:A:298:GLY:HA2	1:A:303:CYS:SG	2.53	0.48
1:F:384:ARG:HB3	1:F:414:GLU:HG3	1.96	0.48
1:C:250:GLY:HA2	1:C:255:VAL:HG21	1.95	0.48
1:F:12:ASP:OD2	1:F:340:LYS:NZ	2.34	0.48
1:B:243:ILE:HD13	1:B:269:LEU:HD21	1.96	0.48
1:D:389:LEU:HD13	1:D:410:PRO:HG3	1.95	0.48
1:C:298:GLY:N	1:C:299:PRO:HD3	2.29	0.47
1:G:283:ARG:HG2	1:G:329:LEU:HD11	1.95	0.47
1:C:408:PHE:HE2	1:D:25:PRO:HG2	1.78	0.47
1:C:224:VAL:HG22	1:C:245:LEU:HD22	1.95	0.47
1:D:361:ILE:HG21	1:D:430:LEU:HD11	1.96	0.47
1:F:6:LYS:HG2	1:F:7:THR:N	2.28	0.47
1:B:52:VAL:O	1:B:57:MET:HG3	2.15	0.47
1:C:34:LEU:HD11	1:C:272:ILE:HD11	1.96	0.47



Atom 1			Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:303:CYS:SG	2:E:500:IMP:H2	2.54	0.47	
1:F:232:VAL:O	1:F:236:VAL:HG12	2.13	0.47	
1:E:336:ASP:OD1	2:E:500:IMP:O3'	2.33	0.47	
1:E:298:GLY:HA3	1:E:306:ARG:HG3	1.96	0.47	
1:H:16:LEU:HD22	1:H:441:LEU:HD21	1.96	0.47	
1:C:78:ASP:O	1:C:82:GLU:HG2	2.14	0.46	
1:D:283:ARG:HG2	1:D:329:LEU:HD11	1.98	0.46	
1:F:87:LYS:HA	1:F:87:LYS:HD2	1.76	0.46	
1:E:16:LEU:HD13	1:E:441:LEU:HD21	1.98	0.46	
1:B:50:ASP:HA	1:B:71:HIS:CD2	2.49	0.46	
1:G:51:THR:O	1:G:51:THR:OG1	2.33	0.46	
1:B:479:ASN:ND2	1:D:410:PRO:HD2	2.30	0.46	
1:C:468:PRO:HD2	1:C:480:TYR:CZ	2.51	0.46	
1:E:298:GLY:N	1:E:299:PRO:HD3	2.31	0.46	
1:E:22:GLU:HG2	1:F:253:LYS:HB2	1.98	0.46	
1:F:55:SER:N	1:F:82:GLU:OE1	2.44	0.46	
1:A:84:ASP:O	1:A:88:ARG:HG2	2.16	0.45	
1:E:59:ILE:HG13	1:E:86:VAL:HG22	1.98	0.45	
1:G:48:SER:OG	1:G:246:ASP:OD1	2.34	0.45	
1:F:32:THR:HB	1:F:446:LEU:HD12	1.97	0.45	
1:F:469:HIS:ND1	1:F:470:ASP:OD2	2.31	0.45	
1:E:441:LEU:HD23	1:E:449:LEU:HD11	1.97	0.45	
1:G:303:CYS:SG	2:G:500:IMP:H2	2.56	0.45	
1:G:263:LYS:NZ	1:G:269:LEU:O	2.33	0.45	
1:A:455:PHE:HB2	1:B:4:ILE:HG12	1.99	0.45	
1:A:50:ASP:HA	1:A:71:HIS:CD2	2.52	0.45	
1:A:458[B]:GLN:OE1	1:A:466:SER:OG	2.34	0.45	
1:E:245:LEU:HD12	1:E:255:VAL:HG13	1.98	0.45	
1:E:387:GLY:N	2:E:500:IMP:O6	2.33	0.45	
1:B:461:ALA:HB1	1:D:12:ASP:HB2	1.99	0.44	
1:G:232:VAL:O	1:G:236:VAL:N	2.47	0.44	
1:B:298:GLY:HA2	1:B:303:CYS:SG	2.58	0.44	
1:D:263:LYS:HA	1:D:263:LYS:HD2	1.78	0.44	
1:C:72:LYS:HB3	1:C:221:SER:O	2.17	0.44	
1:D:384:ARG:HB3	1:D:414:GLU:HG3	2.00	0.44	
1:E:19:ASN:ND2	1:E:452:ASN:O	2.48	0.44	
1:B:19:ASN:ND2	1:B:452:ASN:O	2.51	0.44	
1:B:55:SER:O	1:B:59:ILE:HG13	2.18	0.44	
1:E:380:TYR:CG	1:E:416:ARG:HD3	2.52	0.44	
1:H:336:ASP:OD2	2:H:500:IMP:O2'	2.32	0.44	
1:E:306:ARG:NH2	1:G:465:GLU:OE1	2.48	0.44	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:30:LEU:HB3	1:F:43:PRO:HD3	1.99	0.44
1:G:69:ILE:HD13	1:G:219:GLY:HA3	1.99	0.44
1:B:46:SER:OG	1:B:61:MET:HG3	2.18	0.44
1:G:243:ILE:HG13	1:G:269:LEU:HD21	1.99	0.44
1:C:249:HIS:CE1	1:C:251:HIS:HB3	2.53	0.43
1:E:306:ARG:HD2	1:G:466:SER:HA	1.99	0.43
1:G:30:LEU:HB3	1:G:43:PRO:HD3	2.00	0.43
1:G:408:PHE:CZ	1:H:25:PRO:HG2	2.53	0.43
1:E:62:ALA:HB1	1:E:216:LEU:HB3	1.99	0.43
1:F:440:TYR:HB3	1:H:311:VAL:HG11	1.99	0.43
1:G:285:LEU:HD12	1:G:285:LEU:HA	1.83	0.43
1:H:293:VAL:HG23	1:H:333:VAL:HG12	1.99	0.43
1:C:331:ILE:HA	1:C:332:PRO:HD3	1.84	0.43
1:D:409:VAL:HA	1:D:410:PRO:HD3	1.69	0.43
1:G:407:LYS:HB2	1:G:407:LYS:HE2	1.67	0.43
1:E:286:ALA:HB2	1:E:331:ILE:HD13	1.99	0.43
1:F:19:ASN:ND2	1:F:452:ASN:O	2.48	0.43
1:D:79:GLN:NE2	1:D:221:SER:H	2.17	0.43
1:F:87:LYS:HG2	1:F:239:LYS:HB3	2.01	0.43
1:A:301:SER:HB2	1:C:469:HIS:O	2.19	0.42
1:B:78:ASP:O	1:B:82:GLU:HG2	2.19	0.42
1:G:10:THR:OG1	1:H:465:GLU:OE2	2.32	0.42
1:E:72:LYS:HB3	1:E:221:SER:O	2.19	0.42
1:E:32:THR:HG21	1:E:354:CYS:O	2.19	0.42
1:E:323:ALA:O	1:E:327:LYS:HG2	2.18	0.42
1:H:46:SER:HB3	1:H:53:THR:OG1	2.19	0.42
1:B:336:ASP:OD2	2:B:501:IMP:O2'	2.28	0.42
1:F:438:MET:HG2	1:F:449:LEU:HD22	2.00	0.42
1:G:243:ILE:HG12	1:G:269:LEU:HD11	2.01	0.42
1:D:303:CYS:SG	2:D:501:IMP:H2	2.59	0.42
1:G:59:ILE:HD13	1:G:86:VAL:HG13	2.01	0.42
1:A:293:VAL:HG23	1:A:333:VAL:HG12	2.01	0.42
1:A:298:GLY:N	1:A:299:PRO:HD3	2.34	0.42
1:E:388:SER:O	1:E:392:MET:HG2	2.20	0.42
1:F:46:SER:OG	1:F:53:THR:OG1	2.20	0.42
1:F:331:ILE:HA	1:F:332:PRO:HD3	1.82	0.42
1:H:26:ASN:ND2	1:H:27:GLU:HG3	2.34	0.42
1:A:324:GLU:HG2	1:A:328:LYS:HE3	2.00	0.42
1:E:444:PRO:HD2	1:E:448:ASN:ND2	2.27	0.42
1:D:220:ALA:O	1:D:244:VAL:HG22	2.20	0.42
1:E:389:LEU:HD22	1:G:478:PRO:HD3	2.02	0.42



Atom 1			Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:333:VAL:HG23	1:C:353:ALA:HA	2.01	0.42	
1:E:459:THR:OG1	1:F:13:ASP:OD1	2.28	0.42	
1:F:303:CYS:SG	2:F:500:IMP:H2	2.59	0.42	
1:H:84:ASP:O	1:H:88:ARG:HG2	2.20	0.42	
1:G:43:PRO:HG3	1:G:446:LEU:HD11	2.02	0.41	
1:A:17:VAL:HA	1:A:18:PRO:HD3	1.92	0.41	
1:H:40:LEU:HD21	1:H:67:ILE:HB	2.02	0.41	
1:A:80:ALA:HB2	1:A:234:ALA:HB1	2.01	0.41	
1:C:311:VAL:HG21	1:D:440:TYR:HB2	2.02	0.41	
1:D:50:ASP:HA	1:D:71:HIS:CD2	2.55	0.41	
1:F:440:TYR:OH	1:H:248:ALA:HB1	2.19	0.41	
1:G:32:THR:HG21	1:G:354:CYS:O	2.19	0.41	
1:G:79:GLN:OE1	1:G:231:ARG:NH1	2.45	0.41	
1:E:461:ALA:HB2	5:F:502:FMT:C	2.47	0.41	
1:E:389:LEU:HD12	1:E:389:LEU:HA	1.82	0.41	
1:C:70:ILE:H	1:C:70:ILE:HG12	1.70	0.41	
1:F:247:THR:OG1	1:F:248:ALA:N	2.54	0.41	
1:G:34:LEU:HD13	1:G:35:THR:HG23	2.02	0.41	
1:C:303:CYS:SG	2:C:500:IMP:H2	2.61	0.41	
1:D:42:ILE:HA	1:D:43:PRO:HD3	1.85	0.41	
1:E:272:ILE:HG12	1:E:292:CYS:HB3	2.02	0.41	
1:B:384:ARG:HD2	1:B:391:ALA:HB2	2.02	0.41	
1:B:388:SER:O	1:B:392:MET:HG3	2.21	0.41	
1:E:245:LEU:HD22	1:E:245:LEU:HA	1.85	0.41	
1:F:361:ILE:HG21	1:F:430:LEU:HD11	2.03	0.41	
1:H:10:THR:HG22	1:H:11:PHE:N	2.35	0.41	
1:B:468:PRO:HD2	1:B:480:TYR:CZ	2.56	0.41	
1:H:56:LYS:HD2	1:H:367:GLU:HA	2.02	0.41	
1:A:457:VAL:HB	1:B:7:THR:HA	2.03	0.40	
1:E:364:GLY:HA3	1:E:420:LYS:HE2	2.03	0.40	
1:F:11:PHE:O	1:F:347:LYS:NZ	2.41	0.40	
1:F:394:LYS:HB2	1:F:394:LYS:NZ	2.36	0.40	
1:B:231[B]:ARG:O	1:B:235:VAL:HG22	2.20	0.40	
1:D:479:ASN:OD1	1:D:479:ASN:N	2.54	0.40	
1:E:48:SER:HB3	1:E:69:ILE:HB	2.03	0.40	
1:H:298:GLY:N	1:H:299:PRO:CD	2.81	0.40	
1:A:30:LEU:HB3	1:A:43:PRO:HD3	2.04	0.40	
1:B:36:LYS:HE2	1:B:36:LYS:HB3	1.97	0.40	
1:D:43:PRO:HG3	1:D:446:LEU:HD11	2.03	0.40	
1:E:46:SER:HB3	1:E:53:THR:OG1	2.21	0.40	
1:F:365:CYS:O	1:F:381:LYS:NZ	2.42	0.40	



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)		
1:H:448:ASN:O	1:H:452:ASN:ND2	2.55	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	entiles
1	А	344/363~(95%)	333~(97%)	11 (3%)	0	100	100
1	В	340/363~(94%)	328 (96%)	12 (4%)	0	100	100
1	С	340/363~(94%)	325 (96%)	15 (4%)	0	100	100
1	D	340/363~(94%)	324 (95%)	16 (5%)	0	100	100
1	Е	342/363~(94%)	331 (97%)	11 (3%)	0	100	100
1	F	341/363~(94%)	325~(95%)	16 (5%)	0	100	100
1	G	340/363~(94%)	326 (96%)	14 (4%)	0	100	100
1	Н	341/363~(94%)	329 (96%)	12 (4%)	0	100	100
All	All	2728/2904 (94%)	2621 (96%)	107 (4%)	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 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.



4Q33

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	270/282~(96%)	248 (92%)	22 (8%)	11	31
1	В	266/282~(94%)	254~(96%)	12 (4%)	27	59
1	\mathbf{C}	267/282~(95%)	247~(92%)	20 (8%)	13	35
1	D	266/282~(94%)	238~(90%)	28 (10%)	7	19
1	Ε	268/282~(95%)	247 (92%)	21 (8%)	12	33
1	F	267/282~(95%)	255~(96%)	12 (4%)	27	59
1	G	266/282~(94%)	247~(93%)	19 (7%)	14	38
1	Η	267/282~(95%)	248~(93%)	19 (7%)	14	38
All	All	2137/2256~(95%)	1984 (93%)	153 (7%)	14	37

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1	MET
1	А	3	ARG
1	А	4	ILE
1	А	5	LEU
1	А	13	ASP
1	А	14	VAL
1	А	28	VAL
1	А	32	THR
1	А	34	LEU
1	А	63	ARG
1	А	221	SER
1	А	242	VAL
1	А	268	GLU
1	А	287	GLU
1	А	339	LEU
1	А	366	GLU
1	А	372	ILE
1	А	375	TYR
1	А	408	PHE
1	А	441	LEU
1	A	460	SER
1	А	481	SER
1	В	14	VAL
1	В	28	VAL
1	В	34	LEU
1	В	57	MET
1	В	72	LYS



Mol	Chain	Res	Type
1	В	243	ILE
1	В	244	VAL
1	В	245	LEU
1	В	246	ASP
1	В	257	GLU
1	В	304	THR
1	В	321	ASP
1	С	5	LEU
1	С	14	VAL
1	С	28	VAL
1	С	70	ILE
1	С	72	LYS
1	С	236	VAL
1	С	240	VAL
1	С	244	VAL
1	С	245	LEU
1	С	247	THR
1	С	255	VAL
1	С	261	ARG
1	С	268	GLU
1	С	280	GLU
1	С	340	LYS
1	С	358	MET
1	С	409	VAL
1	С	441	LEU
1	С	456	VAL
1	С	460	SER
1	D	4	ILE
1	D	5	LEU
1	D	6	LYS
1	D	24	LEU
1	D	32	THR
1	D	34	LEU
1	D	39	GLN
1	D	52	VAL
1	D	57	MET
1	D	63	ARG
1	D	73	ASN
1	D	85	ARG
1	D	225	THR
1	D	226	ASN
1	D	229	MET



Mol	Chain	\mathbf{Res}	Type
1	D	237	LYS
1	D	245	LEU
1	D	263	LYS
1	D	285	LEU
1	D	287	GLU
1	D	354[A]	CYS
1	D	354[B]	CYS
1	D	374	ILE
1	D	389	LEU
1	D	392	MET
1	D	420	LYS
1	D	456	VAL
1	D	464	ARG
1	Е	14	VAL
1	Е	32	THR
1	Е	34	LEU
1	Е	36	LYS
1	Е	39	GLN
1	Е	50	ASP
1	Е	55	SER
1	Е	63	ARG
1	Е	87	LYS
1	Е	217	LEU
1	Е	237	LYS
1	Е	245	LEU
1	Ε	247	THR
1	Ε	249	HIS
1	E	321	ASP
1	E	373	GLU
1	Е	378	ARG
1	E	408	PHE
1	E	441	LEU
1	Е	456	VAL
1	E	471	ILE
1	F	10	THR
1	F	14	VAL
1	F	34	LEU
1	F	37	LYS
1	F	77	GLU
1	F	86	VAL
1	F	88	ARG
1	F	285	LEU



Mol	Chain	Res	Type
1	F	366	GLU
1	F	394	LYS
1	F	441	LEU
1	F	475	LYS
1	G	4	ILE
1	G	14	VAL
1	G	26	ASN
1	G	32	THR
1	G	39	GLN
1	G	51	THR
1	G	77	GLU
1	G	233	ASP
1	G	235	VAL
1	G	244	VAL
1	G	246	ASP
1	G	247	THR
1	G	276	ILE
1	G	285	LEU
1	G	294	LYS
1	G	324	GLU
1	G	382	VAL
1	G	426	THR
1	G	441	LEU
1	Н	5	LEU
1	Н	14	VAL
1	Н	32	THR
1	Н	34	LEU
1	Н	55	SER
1	Н	67	ILE
1	Н	243	ILE
1	Н	244	VAL
1	Н	245	LEU
1	Н	247	THR
1	Н	293	VAL
1	Н	358	MET
1	Н	407	LYS
1	Н	408	PHE
1	Н	420	LYS
1	Н	452	ASN
1	Н	460	SER
1	Н	471	ILE
1	Н	472	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	С	452	ASN
1	С	454	ASN
1	D	422	HIS
1	Ε	448	ASN
1	F	448	ASN
1	F	452	ASN
1	G	39	GLN
1	G	452	ASN
1	G	458	GLN
1	Н	33	GLN
1	Н	39	GLN
1	Н	452	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)

27 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	Turne	Chain	Dec	Tink	Bond lengths			Bond angles		
	туре	Unam	nes	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
7	GOL	F	503	-	$5,\!5,\!5$	0.38	0	$5,\!5,\!5$	0.27	0



Mal	Turne	Chain	Dec	Tink	Bond lengths		$_{\rm ths}$	Bond angles		
WIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	FMT	Н	503	-	$2,\!2,\!2$	0.71	0	$1,\!1,\!1$	0.24	0
2	IMP	Ε	500	-	$21,\!25,\!25$	2.53	2 (9%)	24,38,38	1.29	4 (16%)
2	IMP	А	500	-	21,25,25	2.54	2 (9%)	24,38,38	1.18	2 (8%)
5	FMT	G	502	-	2,2,2	0.69	0	$1,\!1,\!1$	0.24	0
2	IMP	G	500	-	$21,\!25,\!25$	2.53	3 (14%)	24,38,38	1.19	2 (8%)
5	FMT	Н	502	-	2,2,2	0.72	0	$1,\!1,\!1$	0.24	0
3	2YA	В	503	-	26,29,29	1.75	7 (26%)	30,41,41	2.80	10 (33%)
3	2YA	Н	501	-	26,29,29	1.78	8 (30%)	30,41,41	2.87	10 (33%)
5	FMT	F	505	-	2,2,2	0.72	0	$1,\!1,\!1$	0.24	0
7	GOL	F	506	-	$5,\!5,\!5$	0.34	0	$5,\!5,\!5$	0.35	0
3	2YA	Е	501	-	$26,\!29,\!29$	1.76	8 (30%)	30,41,41	2.82	11 (36%)
5	FMT	F	504	-	2,2,2	0.70	0	1,1,1	0.24	0
5	FMT	F	502	-	2,2,2	0.72	0	1,1,1	0.21	0
2	IMP	С	500	-	$21,\!25,\!25$	2.54	2(9%)	24,38,38	1.18	2 (8%)
5	FMT	Е	502	-	2,2,2	0.72	0	1,1,1	0.24	0
3	2YA	В	502	-	26,29,29	1.76	7 (26%)	30,41,41	2.84	12 (40%)
6	SO4	Е	503	-	4,4,4	0.15	0	$6,\!6,\!6$	0.06	0
2	IMP	Η	500	-	$21,\!25,\!25$	2.55	2 (9%)	24,38,38	1.18	2 (8%)
2	IMP	D	501	-	21,25,25	2.88	3 (14%)	24,38,38	1.73	5 (20%)
4	ACY	D	502	-	3,3,3	0.77	0	3,3,3	0.82	0
3	2YA	А	501	-	26,29,29	1.74	8 (30%)	30,41,41	2.75	11 (36%)
3	2YA	G	501	-	26,29,29	1.75	7 (26%)	30,41,41	2.77	10 (33%)
2	IMP	F	500	-	21,25,25	2.54	2 (9%)	24,38,38	1.25	3 (12%)
3	2YA	С	501	-	26,29,29	1.76	7 (26%)	30,41,41	2.77	10 (33%)
3	2YA	F	501	-	26,29,29	1.75	8 (30%)	30,41,41	2.74	10 (33%)
2	IMP	В	501	-	21,25,25	2.53	3 (14%)	24,38,38	1.19	3 (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
7	GOL	F	503	-	-	2/4/4/4	-
7	GOL	F	506	-	-	2/4/4/4	-
2	IMP	Е	500	-	-	2/6/26/26	0/3/3/3
2	IMP	F	500	-	-	0/6/26/26	0/3/3/3
2	IMP	Н	500	-	-	0/6/26/26	0/3/3/3



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2YA	С	501	-	-	1/10/12/12	0/4/4/4
2	IMP	А	500	-	-	0/6/26/26	0/3/3/3
2	IMP	D	501	-	-	0/6/26/26	0/3/3/3
2	IMP	G	500	-	-	0/6/26/26	0/3/3/3
3	2YA	А	501	-	-	3/10/12/12	0/4/4/4
3	2YA	Е	501	-	-	2/10/12/12	0/4/4/4
3	2YA	G	501	-	-	4/10/12/12	0/4/4/4
2	IMP	С	500	-	-	2/6/26/26	0/3/3/3
3	2YA	В	503	-	-	4/10/12/12	0/4/4/4
3	2YA	F	501	-	-	2/10/12/12	0/4/4/4
3	2YA	Н	501	-	-	0/10/12/12	0/4/4/4
3	2YA	В	502	-	_	3/10/12/12	0/4/4/4
2	IMP	В	501	-	_	2/6/26/26	0/3/3/3

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	IMP	O6-C6	12.52	1.48	1.23
2	А	500	IMP	O6-C6	10.92	1.45	1.23
2	Н	500	IMP	O6-C6	10.91	1.45	1.23
2	F	500	IMP	O6-C6	10.91	1.45	1.23
2	С	500	IMP	O6-C6	10.90	1.45	1.23
2	В	501	IMP	O6-C6	10.85	1.45	1.23
2	G	500	IMP	O6-C6	10.84	1.45	1.23
2	Е	500	IMP	O6-C6	10.77	1.45	1.23
3	Н	501	2YA	N1-N2	3.75	1.41	1.34
3	В	502	2YA	N1-N2	3.72	1.41	1.34
3	С	501	2YA	N1-N2	3.65	1.41	1.34
3	В	503	2YA	N1-N2	3.64	1.41	1.34
3	Е	501	2YA	N1-N2	3.61	1.40	1.34
3	G	501	2YA	C16-N3	-3.57	1.33	1.44
3	С	501	2YA	C16-N3	-3.56	1.33	1.44
3	А	501	2YA	N1-N2	3.55	1.40	1.34
3	Ε	501	2YA	C16-N3	-3.54	1.34	1.44
3	F	501	2YA	N1-N2	3.52	1.40	1.34
3	В	503	2YA	C16-N3	-3.51	1.34	1.44
3	В	502	2YA	C16-N3	-3.49	1.34	1.44
3	А	501	2YA	C16-N3	-3.49	1.34	1.44
3	F	501	2YA	C16-N3	-3.48	1.34	1.44
3	G	501	2YA	N1-N2	3.47	1.40	1.34



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Н	501	2YA	C16-N3	-3.46	1.34	1.44
3	F	501	2YA	O2-N4	3.21	1.44	1.37
3	Е	501	2YA	C14-C11	-3.19	1.48	1.52
3	Н	501	2YA	C14-C11	-3.19	1.48	1.52
3	С	501	2YA	O2-N4	3.18	1.43	1.37
3	В	502	2YA	O2-N4	3.17	1.43	1.37
3	А	501	2YA	O2-N4	3.17	1.43	1.37
3	G	501	2YA	C14-C11	-3.16	1.48	1.52
3	С	501	2YA	C14-C11	-3.16	1.48	1.52
3	В	502	2YA	C14-C11	-3.15	1.48	1.52
3	Е	501	2YA	O2-N4	3.15	1.43	1.37
3	В	503	2YA	O2-N4	3.14	1.43	1.37
3	Н	501	2YA	O2-N4	3.14	1.43	1.37
3	G	501	2YA	O2-N4	3.11	1.43	1.37
3	В	503	2YA	C14-C11	-3.00	1.48	1.52
3	А	501	2YA	C14-C11	-2.96	1.48	1.52
3	F	501	2YA	C14-C11	-2.94	1.48	1.52
2	Е	500	IMP	C5-C6	-2.72	1.41	1.47
2	Н	500	IMP	C5-C6	-2.64	1.42	1.47
2	F	500	IMP	C5-C6	-2.64	1.42	1.47
2	В	501	IMP	C5-C6	-2.64	1.42	1.47
2	С	500	IMP	C5-C6	-2.63	1.42	1.47
3	Н	501	2YA	C19-CL1	2.62	1.80	1.74
2	А	500	IMP	C5-C6	-2.59	1.42	1.47
2	G	500	IMP	C5-C6	-2.53	1.42	1.47
3	А	501	2YA	C19-CL1	2.50	1.80	1.74
3	F	501	2YA	C19-CL1	2.47	1.79	1.74
3	В	503	2YA	C19-CL1	2.47	1.79	1.74
3	Ε	501	2YA	C19-CL1	2.46	1.79	1.74
3	В	502	2YA	C19-CL1	2.42	1.79	1.74
3	С	501	2YA	C19-CL1	2.42	1.79	1.74
3	G	501	2YA	C15-C14	2.31	1.39	1.36
3	F	501	2YA	C15-C14	2.31	1.39	1.36
2	D	501	IMP	O4'-C1'	2.31	1.44	1.41
3	А	501	2YA	C15-C14	2.30	1.39	1.36
3	G	501	2YA	C19-CL1	2.30	1.79	1.74
3	E	501	2YA	C15-C14	2.20	1.39	1.36
3	В	503	2YA	C15-C14	2.15	1.39	1.36
3	F	501	2YA	N2-N3	2.13	1.40	1.37
3	В	502	2YA	C15-C14	2.12	1.39	1.36
3	С	501	2YA	C15-C14	2.12	1.39	1.36
3	C	501	2YA	N2-N3	2.12	1.40	1.37



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Н	501	2YA	N2-N3	2.09	1.40	1.37
3	Н	501	2YA	C15-C14	2.09	1.39	1.36
3	В	503	2YA	N2-N3	2.07	1.40	1.37
3	Н	501	2YA	C6-C5	-2.07	1.39	1.42
2	D	501	IMP	C2-N3	2.07	1.33	1.29
3	G	501	2YA	N2-N3	2.05	1.40	1.37
3	Е	501	2YA	N2-N3	2.04	1.39	1.37
3	В	502	2YA	N2-N3	2.04	1.39	1.37
3	Е	501	2YA	C6-C5	-2.02	1.39	1.42
3	А	501	2YA	N2-N3	2.02	1.39	1.37
2	G	500	IMP	C2-N3	2.02	1.33	1.29
3	A	501	2YA	C6-C5	-2.01	1.39	1.42
2	В	501	IMP	C2-N3	2.01	1.33	1.29
3	F	501	2YA	C6-C5	-2.01	1.39	1.42

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Н	501	2YA	C15-C14-C11	-8.97	114.86	129.16
3	В	502	2YA	C15-C14-C11	-8.81	115.11	129.16
3	Е	501	2YA	C15-C14-C11	-8.79	115.14	129.16
3	С	501	2YA	C15-C14-C11	-8.67	115.33	129.16
3	В	503	2YA	C15-C14-C11	-8.50	115.60	129.16
3	G	501	2YA	C15-C14-C11	-8.34	115.86	129.16
3	F	501	2YA	C15-C14-C11	-8.23	116.03	129.16
3	А	501	2YA	C15-C14-C11	-8.17	116.13	129.16
3	Н	501	2YA	C11-C14-N1	7.36	132.27	120.30
3	В	502	2YA	C11-C14-N1	7.14	131.91	120.30
3	Е	501	2YA	C11-C14-N1	7.09	131.84	120.30
3	С	501	2YA	C11-C14-N1	6.97	131.64	120.30
3	В	503	2YA	C11-C14-N1	6.94	131.59	120.30
3	G	501	2YA	C11-C14-N1	6.68	131.17	120.30
3	F	501	2YA	C11-C14-N1	6.63	131.09	120.30
3	А	501	2YA	C11-C14-N1	6.58	131.00	120.30
3	G	501	2YA	C21-C16-N3	5.87	124.28	119.15
3	А	501	2YA	C21-C16-N3	5.20	123.70	119.15
3	F	501	2YA	C21-C16-N3	5.18	123.68	119.15
3	В	503	2YA	O1-C1-C6	5.03	120.83	114.22
3	Е	501	2YA	O1-C1-C6	4.87	120.62	114.22
3	В	502	2YA	O1-C1-C6	4.86	120.61	114.22
3	Н	501	2YA	O1-C1-C6	4.79	120.52	114.22
3	А	501	2YA	O1-C1-C6	4.78	120.50	114.22



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	503	2YA	C21-C16-N3	4.76	123.31	119.15
3	F	501	2YA	O1-C1-C6	4.72	120.42	114.22
3	G	501	2YA	O1-C1-C6	4.68	120.38	114.22
3	С	501	2YA	O1-C1-C6	4.53	120.18	114.22
3	Е	501	2YA	C21-C16-N3	4.53	123.11	119.15
3	С	501	2YA	C21-C16-N3	4.50	123.09	119.15
3	В	502	2YA	C21-C16-N3	4.39	122.99	119.15
2	D	501	IMP	C8-N7-C5	4.26	111.10	102.99
3	А	501	2YA	C21-C16-C17	-4.20	115.11	121.33
3	Н	501	2YA	C21-C16-C17	-4.16	115.17	121.33
3	В	502	2YA	C21-C16-C17	-4.09	115.27	121.33
3	F	501	2YA	C21-C16-C17	-4.07	115.31	121.33
3	Е	501	2YA	C21-C16-C17	-4.02	115.37	121.33
3	В	503	2YA	C21-C16-C17	-4.02	115.38	121.33
3	G	501	2YA	C21-C16-C17	-3.96	115.46	121.33
3	С	501	2YA	C21-C16-C17	-3.96	115.46	121.33
3	Н	501	2YA	C21-C16-N3	3.88	122.55	119.15
3	Н	501	2YA	C17-C16-N3	3.58	122.28	119.15
2	D	501	IMP	O6-C6-N1	-3.53	116.03	120.32
2	Е	500	IMP	C5-C6-N1	3.08	119.39	113.95
2	Е	500	IMP	C8-N7-C5	3.06	108.82	102.99
2	А	500	IMP	C8-N7-C5	2.99	108.69	102.99
3	В	502	2YA	C17-C16-N3	2.96	121.75	119.15
2	Н	500	IMP	C8-N7-C5	2.94	108.60	102.99
2	В	501	IMP	C5-C6-N1	2.94	119.14	113.95
2	G	500	IMP	C5-C6-N1	2.93	119.13	113.95
3	А	501	2YA	C18-C17-C16	2.93	123.33	119.07
2	G	500	IMP	C8-N7-C5	2.92	108.56	102.99
2	F	500	IMP	C8-N7-C5	2.90	108.52	102.99
2	С	500	IMP	C8-N7-C5	2.89	108.50	102.99
2	F	500	IMP	C5-C6-N1	2.88	119.04	113.95
2	Н	500	IMP	C5-C6-N1	2.88	119.03	113.95
3	F	501	2YA	C18-C17-C16	2.88	123.25	119.07
2	С	500	IMP	C5-C6-N1	2.87	119.03	113.95
2	В	501	IMP	C8-N7-C5	2.86	108.44	102.99
3	G	501	2YA	C18-C17-C16	2.82	123.17	119.07
2	А	500	IMP	C5-C6-N1	2.76	118.82	113.95
3	В	503	2YA	C18-C17-C16	2.75	123.07	119.07
3	В	502	2YA	C18-C17-C16	2.75	123.07	119.07
3	Н	501	2YA	C18-C17-C16	2.74	123.06	119.07
3	Е	501	2YA	C18-C17-C16	2.73	123.04	119.07
3	Н	501	2YA	C20-C21-C16	2.72	123.02	119.07



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Е	501	2YA	C17-C16-N3	2.71	121.52	119.15
3	С	501	2YA	C18-C17-C16	2.69	122.98	119.07
2	D	501	IMP	N1-C2-N3	-2.67	118.89	125.87
3	В	502	2YA	C20-C21-C16	2.66	122.94	119.07
3	С	501	2YA	C17-C16-N3	2.63	121.45	119.15
3	Е	501	2YA	C20-C21-C16	2.61	122.86	119.07
3	С	501	2YA	C20-C21-C16	2.58	122.83	119.07
2	F	500	IMP	O3P-P-O2P	2.58	117.49	107.64
3	А	501	2YA	C20-C21-C16	2.57	122.81	119.07
3	В	503	2YA	C20-C21-C16	2.56	122.80	119.07
3	F	501	2YA	C20-C21-C16	2.49	122.69	119.07
3	В	503	2YA	C17-C16-N3	2.46	121.31	119.15
2	D	501	IMP	O3P-P-O5'	2.45	113.26	106.73
3	G	501	2YA	C20-C21-C16	2.43	122.61	119.07
3	В	503	2YA	O1-C1-C2	-2.35	120.34	124.59
3	А	501	2YA	C17-C16-N3	2.33	121.19	119.15
3	Н	501	2YA	C16-N3-N2	2.32	121.91	117.19
2	D	501	IMP	C4-N3-C2	2.27	124.75	115.55
3	В	502	2YA	O1-C1-C2	-2.24	120.53	124.59
3	Е	501	2YA	O1-C1-C2	-2.21	120.59	124.59
3	В	502	2YA	C16-N3-N2	2.21	121.67	117.19
2	Е	500	IMP	C3'-C2'-C1'	2.19	104.27	100.98
3	А	501	2YA	O1-C1-C2	-2.16	120.68	124.59
3	Н	501	2YA	O1-C1-C2	-2.15	120.69	124.59
3	G	501	2YA	O1-C1-C2	-2.13	120.73	124.59
3	F	501	2YA	C17-C16-N3	2.12	121.01	119.15
3	С	501	2YA	C16-N3-N2	2.10	121.45	117.19
3	Е	501	2YA	C16-N3-N2	2.10	121.45	117.19
3	G	501	2YA	C7-C6-C5	2.08	120.43	118.17
3	F	501	2YA	O1-C1-C2	-2.07	120.84	124.59
3	F	501	2YA	C7-C6-C5	2.06	120.42	118.17
3	С	501	2YA	C15-C14-N1	2.04	113.03	110.14
3	А	501	2YA	C7-C6-C5	2.04	120.39	118.17
3	Е	501	2YA	C15-C14-N1	2.04	113.02	110.14
3	В	502	2YA	C7-C6-C5	2.02	120.38	118.17
2	Е	500	IMP	O6-C6-C5	-2.02	120.43	124.37
3	А	501	2YA	O1-C11-C12	2.01	109.63	105.53
3	В	503	2YA	C16-N3-N2	2.01	121.27	117.19
3	В	502	2YA	C15-C14-N1	2.01	112.97	110.14
2	В	501	IMP	O6-C6-C5	-2.00	120.46	124.37
3	G	501	2YA	C15-C14-N1	2.00	112.97	110.14

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
3	В	502	2YA	C21-C16-N3-C15
3	Е	501	2YA	C17-C16-N3-C15
3	Е	501	2YA	C21-C16-N3-C15
7	F	506	GOL	O1-C1-C2-O2
7	F	506	GOL	O1-C1-C2-C3
7	F	503	GOL	O1-C1-C2-O2
3	А	501	2YA	C17-C16-N3-C15
3	В	502	2YA	C17-C16-N3-C15
3	F	501	2YA	C17-C16-N3-C15
3	F	501	2YA	C21-C16-N3-C15
7	F	503	GOL	O1-C1-C2-C3
2	Е	500	IMP	C3'-C4'-C5'-O5'
3	А	501	2YA	C21-C16-N3-C15
2	В	501	IMP	C5'-O5'-P-O2P
2	С	500	IMP	C5'-O5'-P-O2P
3	В	503	2YA	C21-C16-N3-N2
3	G	501	2YA	C21-C16-N3-N2
2	Е	500	IMP	O4'-C4'-C5'-O5'
2	В	501	IMP	C5'-O5'-P-O1P
2	С	500	IMP	C5'-O5'-P-O1P
3	В	503	2YA	C17-C16-N3-N2
3	G	501	2YA	C17-C16-N3-N2
3	А	501	2YA	C12-C11-C14-C15
3	В	502	2YA	C12-C11-C14-C15
3	С	501	2YA	C12-C11-C14-C15
3	В	503	2YA	C17-C16-N3-C15
3	В	503	2YA	C21-C16-N3-C15
3	G	501	2YA	C17-C16-N3-C15
3	G	501	2YA	C21-C16-N3-C15

All (29) torsion outliers are listed below:

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Е	500	IMP	3	0
2	А	500	IMP	1	0
5	G	502	FMT	1	0
2	G	500	IMP	2	0
5	F	502	FMT	2	0
2	С	500	IMP	2	0
2	Н	500	IMP	1	0



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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	IMP	2	0
2	F	500	IMP	2	0
2	В	501	IMP	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 sufficient 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	344/363~(94%)	-0.17	4 (1%) 79 78	36, 53, 73, 90	7(2%)
1	В	342/363~(94%)	-0.17	2 (0%) 89 89	38, 59, 80, 97	12 (3%)
1	С	343/363~(94%)	-0.33	0 100 100	31, 48, 69, 83	4 (1%)
1	D	342/363~(94%)	-0.14	0 100 100	37, 58, 78, 95	15 (4%)
1	Е	343/363~(94%)	-0.19	4 (1%) 79 78	30, 54, 78, 92	13 (3%)
1	F	344/363~(94%)	-0.35	0 100 100	31, 46, 64, 79	2 (0%)
1	G	344/363~(94%)	-0.24	1 (0%) 94 94	35, 54, 77, 85	6 (1%)
1	Н	344/363~(94%)	-0.26	1 (0%) 94 94	30, 49, 71, 90	9(2%)
All	All	2746/2904 (94%)	-0.23	12 (0%) 92 92	30, 53, 76, 97	68 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Н	407	LYS	3.7
1	А	375	TYR	3.2
1	В	233	ASP	2.9
1	Е	89	SER	2.8
1	А	246	ASP	2.5
1	А	285	LEU	2.2
1	G	407	LYS	2.2
1	В	269	LEU	2.1
1	Е	90	GLY	2.1
1	Е	408	PHE	2.1
1	А	1	MET	2.1
1	Е	363	ALA	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	RSR	$B-factors(Å^2)$	Q<0.9
6	SO4	Е	503	5/5	0.77	0.42	30,34,35,35	5
5	FMT	Е	502	3/3	0.81	0.16	53,53,53,54	0
5	FMT	F	504	3/3	0.87	0.20	71,71,72,73	0
5	FMT	F	502	3/3	0.87	0.16	56,56,60,64	0
7	GOL	F	506	6/6	0.88	0.26	67,76,80,80	0
5	FMT	F	505	3/3	0.89	0.15	57,57,61,63	0
3	2YA	В	503	26/26	0.90	0.20	58,66,78,79	0
4	ACY	D	502	4/4	0.91	0.24	69,70,72,72	0
7	GOL	F	503	6/6	0.91	0.21	66,68,70,72	0
5	FMT	Н	503	3/3	0.91	0.15	58,58,59,60	0
3	2YA	Е	501	26/26	0.92	0.28	62,70,77,79	0
3	2YA	Н	501	26/26	0.93	0.27	53,66,74,77	0
3	2YA	А	501	26/26	0.93	0.21	49,60,68,79	0
3	2YA	G	501	26/26	0.93	0.24	59,66,76,80	0
5	FMT	Н	502	3/3	0.93	0.18	74,74,78,83	0
3	2YA	С	501	26/26	0.94	0.28	59,65,77,91	0
5	FMT	G	502	3/3	0.95	0.17	36,36,44,49	0
3	2YA	F	501	26/26	0.95	0.20	41,46,62,66	0
3	2YA	В	502	26/26	0.95	0.26	59,65,81,83	0
2	IMP	С	500	23/23	0.96	0.13	$26,\!36,\!55,\!61$	0
2	IMP	G	500	23/23	0.96	0.16	35,43,52,54	0
2	IMP	В	501	23/23	0.96	0.14	31,39,46,48	0
2	IMP	Н	500	23/23	0.97	0.13	29,37,46,47	0
2	IMP	D	501	23/23	0.97	0.13	32,42,47,50	0
2	IMP	Е	500	23/23	0.97	0.12	40,50,54,55	0
2	IMP	F	500	23/23	0.97	0.14	24,36,44,46	0
2	IMP	A	500	23/23	0.97	0.14	24,40,49,52	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.

