

Full wwPDB X-ray Structure Validation Report (i)

Dec 6, 2023 – 01:01 PM JST

PDB ID	:	8K6U
Title	:	Serial Femtosecond X-ray structure of E.coli Cyanase with un-modeled density
		at active site
Authors	:	Kim, J.; Nam, K.H.; Cho, Y.
Deposited on	:	2023-07-25
Resolution	:	1.90 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	:	2.36
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)	:	2.36

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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%

Mol	Chain	Length	Quality of chain		
1	А	160	89%	9%	•
1	В	160	84% 13	3%	·
1	С	160	84% 13	3%	•••
1	D	160	89%	8%	••
1	Е	160	85% 12	2%	·
1	F	160	86%	12%	•
1	G	160	83% 14	%	••



Mol	Chain	Length	Quality of chain		
1	Н	160	86%	11%	·
1	Ι	160	87%	11%	·
1	J	160	91%	7%	·

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	SO4	D	201	-	-	Х	-



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12721 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	156	Total	С	Ν	0	S	0	9	0
1	Л	150	1210	778	200	227	5	0		0
1	В	156	Total	С	Ν	Ο	\mathbf{S}	0	1	Ο
1	D	150	1208	776	200	227	5	0	1	0
1	C	156	Total	С	Ν	Ο	\mathbf{S}	0	3	Ο
1	U	150	1215	782	201	227	5	0	5	0
1	П	156	Total	С	Ν	Ο	\mathbf{S}	0	1	Ο
1	D	150	1208	776	200	227	5	0	1	0
1	E	156	Total	С	Ν	Ο	\mathbf{S}	0	2	Ο
1	Ľ	150	1211	779	200	227	5	0	2	0
1	F	156	Total	С	Ν	Ο	\mathbf{S}	0	1	0
1	Ľ	100	1208	776	200	227	5	0	1	0
1	G	156	Total	С	Ν	Ο	\mathbf{S}	0	9	0
1	ŭ	150	1209	776	201	227	5	0		0
1	н	156	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	1	0
1	11	150	1208	776	200	227	5	0	1	0
1	т	156	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	1	Ο
		100	1208	776	200	227	5	0		0
1	T	156	Total	С	Ν	0	S	0	1	0
	J	100	1208	776	200	227	5	0		0

• Molecule 1 is a protein called Cyanate hydratase.

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-3	GLY	-	expression tag	UNP P00816
А	-2	SER	-	expression tag	UNP P00816
А	-1	HIS	-	expression tag	UNP P00816
А	0	MET	-	expression tag	UNP P00816
В	-3	GLY	-	expression tag	UNP P00816
В	-2	SER	-	expression tag	UNP P00816
В	-1	HIS	-	expression tag	UNP P00816
В	0	MET	-	expression tag	UNP P00816
C	-3	GLY	-	expression tag	UNP P00816



8 K6U

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP P00816
C	-1	HIS	-	expression tag	UNP P00816
C	0	MET	-	expression tag	UNP P00816
D	-3	GLY	-	expression tag	UNP P00816
D	-2	SER	-	expression tag	UNP P00816
D	-1	HIS	-	expression tag	UNP P00816
D	0	MET	-	expression tag	UNP P00816
E	-3	GLY	-	expression tag	UNP P00816
E	-2	SER	-	expression tag	UNP P00816
E	-1	HIS	-	expression tag	UNP P00816
E	0	MET	-	expression tag	UNP P00816
F	-3	GLY	-	expression tag	UNP P00816
F	-2	SER	-	expression tag	UNP P00816
F	-1	HIS	-	expression tag	UNP P00816
F	0	MET	-	expression tag	UNP P00816
G	-3	GLY	-	expression tag	UNP P00816
G	-2	SER	-	expression tag	UNP P00816
G	-1	HIS	-	expression tag	UNP P00816
G	0	MET	-	expression tag	UNP P00816
Н	-3	GLY	-	expression tag	UNP P00816
Н	-2	SER	-	expression tag	UNP P00816
Н	-1	HIS	-	expression tag	UNP P00816
Н	0	MET	-	expression tag	UNP P00816
Ι	-3	GLY	-	expression tag	UNP P00816
Ι	-2	SER	-	expression tag	UNP P00816
Ι	-1	HIS	-	expression tag	UNP P00816
Ι	0	MET	-	expression tag	UNP P00816
J	-3	GLY	-	expression tag	UNP P00816
J	-2	SER	-	expression tag	UNP P00816
J	-1	HIS	-	expression tag	UNP P00816
J	0	MET	-	expression tag	UNP P00816

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Ι	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	J	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	62	Total O 62 62	0	0
3	В	60	Total O 60 60	0	0
3	С	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0
3	D	63	Total O 63 63	0	0
3	Е	69	Total O 69 69	0	0
3	F	56	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 56 & 56 \end{array}$	0	0
3	G	59	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 59 & 59 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Н	62	$\begin{array}{cc} \text{Total} & \text{O} \\ 62 & 62 \end{array}$	0	0
3	Ι	55	$\begin{array}{cc} \text{Total} & \text{O} \\ 55 & 55 \end{array}$	0	0
3	J	63	Total O 63 63	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. 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. 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: Cyanate hydratase



• Molecule 1: Cyanate hydratase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	78.40Å 80.90Å 82.30Å	Deperitor
a, b, c, α , β , γ	70.00° 72.00° 65.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	57.13 - 1.90	Depositor
Resolution (A)	75.88 - 1.44	EDS
% Data completeness	100.0 (57.13-1.90)	Depositor
(in resolution range)	69.8(75.88-1.44)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.46 (at 1.44 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
D D.	0.172 , 0.200	Depositor
Π, Π_{free}	0.171 , 0.199	DCC
R_{free} test set	1986 reflections (0.71%)	wwPDB-VP
Wilson B-factor $(Å^2)$	14.2	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 36.0	EDS
L-test for twinning ²	$< L > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12721	wwPDB-VP
Average B, all atoms $(Å^2)$	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.56% 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

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		
MIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.41	0/1232	0.65	1/1664~(0.1%)	
1	В	0.40	0/1225	0.67	0/1654	
1	С	0.40	0/1242	0.67	1/1676~(0.1%)	
1	D	0.41	0/1225	0.68	1/1654~(0.1%)	
1	Е	0.42	0/1233	0.66	0/1665	
1	F	0.41	0/1225	0.66	1/1654~(0.1%)	
1	G	0.44	0/1234	0.69	1/1665~(0.1%)	
1	Н	0.40	0/1225	0.65	0/1654	
1	Ι	0.39	0/1225	0.64	1/1654~(0.1%)	
1	J	0.42	0/1225	0.66	0/1654	
All	All	0.41	0/12291	0.66	6/16594~(0.0%)	

There are no bond length outliers.

All ((6)	bond	angle	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	G	153	THR	C-N-CA	-6.37	105.77	121.70
1	А	128	LEU	CA-CB-CG	6.09	129.31	115.30
1	D	128	LEU	CA-CB-CG	5.97	129.04	115.30
1	F	128	LEU	CA-CB-CG	5.90	128.88	115.30
1	Ι	153	THR	C-N-CA	-5.28	108.50	121.70
1	С	94	MET	CA-CB-CG	5.02	121.84	113.30

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	1210	0	1257	9	0
1	В	1208	0	1252	15	0
1	С	1215	0	1264	19	0
1	D	1208	0	1252	10	0
1	Е	1211	0	1259	16	0
1	F	1208	0	1252	10	0
1	G	1209	0	1249	18	0
1	Н	1208	0	1252	14	0
1	Ι	1208	0	1252	13	0
1	J	1208	0	1252	9	0
2	А	5	0	0	1	0
2	D	5	0	0	2	0
2	Н	5	0	0	1	0
2	Ι	5	0	0	1	0
2	J	5	0	0	0	0
3	А	62	0	0	1	0
3	В	60	0	0	0	0
3	С	54	0	0	1	0
3	D	63	0	0	1	0
3	Е	69	0	0	0	0
3	F	56	0	0	0	0
3	G	59	0	0	1	0
3	Н	62	0	0	1	0
3	Ι	55	0	0	0	0
3	J	63	0	0	0	0
All	All	12721	0	12541	99	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 4.

All (99) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:C:36:THR:HG22	1:C:38:LEU:H	1.49	0.78	
1:F:96:ARG:O	1:F:100:MET:HG3	1.94	0.67	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:59:ARG:HH11	1:B:59:ARG:HG3	1.59	0.67	
1:D:35:GLY:O	3:D:301:HOH:O	2.12	0.67	
1:C:33:ALA:O	1:C:36:THR:HB	1.96	0.65	
1:G:36:THR:HG21	1:G:43:VAL:HG21	1.79	0.65	
1:C:101[B]:LEU:HG	1:H:84:ILE:HD11	1.79	0.63	
1:C:1:MET:N	3:C:201:HOH:O	2.09	0.63	
1:C:36:THR:HG21	1:C:43:VAL:HG21	1.81	0.62	
1:G:36:THR:HG22	1:G:38:LEU:H	1.64	0.61	
1:G:33:ALA:O	1:G:36:THR:HB	1.99	0.61	
2:A:201:SO4:O2	1:J:87:ARG:NH1	2.28	0.61	
3:H:356:HOH:O	1:I:2:ILE:HG22	2.02	0.58	
3:A:345:HOH:O	1:J:154:LYS:HB2	2.03	0.58	
1:E:116:PHE:CE2	1:G:132:LYS:HG3	2.40	0.57	
1:E:87:ARG:NH1	2:H:201:SO4:O2	2.34	0.56	
1:I:152:PRO:HG2	1:I:154:LYS:HE3	1.86	0.55	
1:B:32:ILE:HG21	1:B:47:LEU:HD11	1.88	0.55	
1:A:132:LYS:HG3	1:D:116:PHE:CE2	2.41	0.55	
1:E:55:ALA:O	1:E:59:ARG:HG3	2.06	0.55	
1:I:55:ALA:HB1	1:I:59:ARG:HH12	1.70	0.55	
1:E:101[B]:LEU:HG	1:G:84:ILE:HD11	1.89	0.55	
1:E:97:PHE:HB3	1:G:101:LEU:HD21	1.91	0.53	
1:E:20:LEU:HG	1:E:24:LYS:HE3	1.90	0.53	
1:G:154:LYS:NZ	1:H:125:ASN:OD1	2.43	0.52	
1:H:129:ASP:OD2	1:H:131:LYS:HE3	2.10	0.51	
1:F:34:ASP:O	1:F:64:LYS:NZ	2.43	0.51	
1:B:21:SER:O	1:B:25:LYS:HG3	2.11	0.51	
1:C:36:THR:CG2	1:C:38:LEU:H	2.23	0.51	
1:F:32:ILE:HG21	1:F:47:LEU:HD11	1.93	0.50	
1:D:129:ASP:OD2	1:D:131:LYS:HD2	2.12	0.50	
1:E:29:PHE:CE2	1:G:110:ALA:HB1	2.46	0.50	
1:B:59:ARG:HG3	1:B:59:ARG:NH1	2.25	0.50	
1:E:132:LYS:HG3	1:G:116:PHE:CE2	2.47	0.50	
3:G:201:HOH:O	1:H:154:LYS:HB2	2.10	0.49	
1:C:74:LEU:HA	1:C:77:MET:HG3	1.96	0.48	
1:I:110:ALA:HB1	1:J:29:PHE:CE2	2.48	0.48	
1:H:88:ILE:HD12	1:H:98:TYR:CZ	2.49	0.48	
1:H:34:ASP:O	1:H:64:LYS:NZ	2.47	0.47	
1:B:152:PRO:HG2	1:B:154:LYS:HE3	1.97	0.47	
1:B:28:SER:OG	1:B:31:GLU:HG3	2.14	0.47	
1:A:101:LEU:HG	1:D:84:ILE:HD11	1.97	0.46	
1:I:132:LYS:HE2	1:I:140:GLU:CD	2.36	0.46	



	h i c	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:156[B]:PHE:CG	1:D:127:LYS:HG2	2.50	0.46	
1:C:29:PHE:CE2	1:H:110:ALA:HB1	2.50	0.46	
1:I:132:LYS:HG3	1:J:116:PHE:CE2	2.51	0.46	
1:F:88:ILE:HD12	1:F:98:TYR:CZ	2.51	0.46	
1:G:60:LEU:HD11	1:G:64:LYS:HE3	1.98	0.45	
1:H:87:ARG:NH1	2:I:201:SO4:O1	2.49	0.45	
1:I:88:ILE:HD12	1:I:98:TYR:CZ	2.51	0.45	
1:J:88:ILE:HD12	1:J:98:TYR:CZ	2.52	0.45	
1:C:126:PHE:CZ	1:H:100:MET:HG2	2.52	0.45	
1:J:131:LYS:HB3	1:J:131:LYS:HE3	1.66	0.45	
1:E:149:LYS:HD2	1:G:135:ASP:OD2	2.17	0.45	
1:C:44:THR:O	1:C:48:LEU:HG	2.16	0.45	
1:A:28:SER:OG	1:A:31:GLU:HG3	2.17	0.44	
1:A:132:LYS:HD3	1:A:140:GLU:HG2	1.98	0.44	
1:B:78:ILE:HD12	1:D:113:HIS:HB3	1.99	0.44	
1:C:48:LEU:HD22	1:G:6:ILE:HD13	1.99	0.44	
1:C:110:ALA:HB1	1:H:29:PHE:CE2	2.52	0.44	
1:B:87:ARG:NH1	2:D:201:SO4:O3	2.50	0.44	
1:A:29:PHE:CE2	1:D:110:ALA:HB1	2.52	0.44	
1:I:29:PHE:CE2	1:J:110:ALA:HB1	2.52	0.44	
1:I:2:ILE:HD13	1:I:2:ILE:HG21	1.79	0.44	
1:G:57:ALA:O	1:G:61:VAL:HG13	2.18	0.44	
1:B:155:PRO:HA	1:D:42:PHE:CE1	2.53	0.44	
1:A:32:ILE:HG21	1:A:47:LEU:HD11	2.00	0.43	
1:C:36:THR:HG21	1:C:43:VAL:CG2	2.46	0.43	
1:F:92:PRO:O	1:F:96:ARG:HG2	2.19	0.43	
1:B:29:PHE:CE2	1:F:110:ALA:HB1	2.53	0.43	
1:I:109:LYS:HB2	1:J:94:MET:HG2	2.00	0.43	
1:E:101[A]:LEU:HD21	1:G:97:PHE:HB3	2.00	0.43	
1:G:60:LEU:O	1:G:64:LYS:HG3	2.18	0.43	
1:A:110:ALA:HB1	1:D:29:PHE:CE2	2.54	0.43	
1:E:127:LYS:HG3	1:E:147:ASP:HB3	2.00	0.43	
1:C:84:ILE:HD11	1:H:101:LEU:HG	2.01	0.43	
1:C:114:GLU:HA	1:I:2:ILE:HG13	2.01	0.43	
1:B:110:ALA:HB1	1:F:29:PHE:CE2	2.54	0.43	
1:E:110:ALA:HB1	1:G:29:PHE:CE2	2.54	0.42	
1:B:135:ASP:OD2	1:F:149:LYS:HD2	2.19	0.42	
2:D:201:SO4:O1	1:E:87:ARG:NH1	2.47	0.42	
1:B:128:LEU:HA	1:B:145:THR:O	2.20	0.42	
1:F:28:SER:OG	1:F:31:GLU:HG2	2.19	0.42	
1:G:96:ARG:O	1:G:100:MET:HG3	2.19	0.42	



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:96:ARG:O	1:C:100:MET:HG3	2.19	0.42
1:H:36:THR:HG22	1:H:60:LEU:HD23	2.02	0.42
1:I:122:SER:HB2	1:I:151:LEU:HD23	2.01	0.41
1:E:18:ILE:HG23	1:E:65:LEU:HD13	2.02	0.41
1:E:88:ILE:HD12	1:E:98:TYR:CZ	2.55	0.41
1:A:18:ILE:HG23	1:A:65:LEU:HD13	2.01	0.41
1:D:44:THR:O	1:D:48:LEU:HG	2.21	0.41
1:C:140:GLU:O	1:H:149:LYS:HD2	2.20	0.41
1:B:5:GLN:HE21	1:B:77:MET:CE	2.34	0.41
1:C:6:ILE:HD13	1:J:48:LEU:HD22	2.02	0.41
1:F:122:SER:HB2	1:F:151:LEU:CD2	2.50	0.40
1:C:18:ILE:HG23	1:C:65:LEU:HD13	2.04	0.40
1:A:81:ARG:HB2	1:I:92:PRO:HD2	2.04	0.40
1:E:25:LYS:HZ3	1:E:25:LYS:HG3	1.71	0.40
1:G:154:LYS:HZ1	1:H:125:ASN:CG	2.25	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	155/160~(97%)	151 (97%)	4 (3%)	0	100	100
1	В	154/160~(96%)	150 (97%)	4 (3%)	0	100	100
1	С	156/160~(98%)	153 (98%)	3 (2%)	0	100	100
1	D	154/160~(96%)	151 (98%)	3 (2%)	0	100	100
1	Е	155/160~(97%)	151 (97%)	4 (3%)	0	100	100
1	F	154/160~(96%)	151 (98%)	3 (2%)	0	100	100
1	G	155/160~(97%)	152 (98%)	3 (2%)	0	100	100
1	Н	154/160~(96%)	151 (98%)	3 (2%)	0	100	100



00.000	e entenada ji ente presenta pagenti								
Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles			
1	Ι	154/160~(96%)	151 (98%)	3~(2%)	0	100 100			
1	J	154/160~(96%)	151 (98%)	3~(2%)	0	100 100			
All	All	1545/1600~(97%)	1512 (98%)	33~(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 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	Perce	ntiles
1	А	129/130~(99%)	128~(99%)	1 (1%)	81	82
1	В	128/130~(98%)	127~(99%)	1 (1%)	81	82
1	С	130/130~(100%)	129 (99%)	1 (1%)	81	82
1	D	128/130~(98%)	127 (99%)	1 (1%)	81	82
1	Ε	129/130~(99%)	128 (99%)	1 (1%)	81	82
1	F	128/130~(98%)	126 (98%)	2(2%)	62	60
1	G	129/130~(99%)	126 (98%)	3(2%)	50	45
1	Н	128/130~(98%)	127 (99%)	1 (1%)	81	82
1	Ι	128/130~(98%)	127~(99%)	1 (1%)	81	82
1	J	128/130~(98%)	127 (99%)	1 (1%)	81	82
All	All	1285/1300 (99%)	1272 (99%)	13 (1%)	76	76

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	136	PRO
1	В	131	LYS
1	С	36	THR
1	D	131	LYS
1	Е	128	LEU
1	F	129	ASP



Continued from previous page...

Mol	Chain	Res	Type
1	F	131	LYS
1	G	36	THR
1	G	128	LEU
1	G	131	LYS
1	Н	66	ASP
1	Ι	129	ASP
1	J	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	9	ASN
1	В	5	GLN
1	F	5	GLN
1	G	5	GLN
1	Н	5	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 Trm		Chain	Dec	Tinle	Bond lengths			Bond angles		
Type	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	SO4	Н	201	-	4,4,4	0.17	0	$6,\!6,\!6$	0.22	0
2	SO4	J	201	-	4,4,4	0.17	0	6,6,6	0.23	0
2	SO4	Ι	201	-	4,4,4	0.21	0	$6,\!6,\!6$	0.19	0
2	SO4	А	201	-	4,4,4	0.18	0	$6,\!6,\!6$	0.14	0
2	SO4	D	201	-	4,4,4	0.16	0	$6,\!6,\!6$	0.17	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Н	201	SO4	1	0
2	Ι	201	SO4	1	0
2	А	201	SO4	1	0
2	D	201	SO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

