

Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 06:20 PM JST

PDB ID	:	8ZMU
Title	:	GLUTAMATE DEHYDROGENASE (W89F-MUTANT) FROM THERMO-
		COCCUS PROFUNDUS IN THE UNLIGANDED STATE
Authors	:	Wakabayashi, T.; Matsui, Y.; Masayoshi, M.
Deposited on	:	2024-05-23
Resolution	:	2.03 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	:	2.36.2
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)	:	2.36.2

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 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	٨	410	.% •	
	A	419	91%	7% ••
			% ■	
1	В	419	91%	8% •
			% ■	
1	С	419	90%	9% •
			4%	
1	D	419	90%	9% •
			% •	
1	Ε	419	91%	7% •
			17%	
1	F	419	79% 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
3	ACY	А	512	-	-	Х	-
4	GOL	С	513	-	-	Х	-
4	GOL	С	517	-	-	Х	-



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2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20653 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	1 A	415	Total	С	Ν	0	S	0	1	0
		410	3262	2082	558	608	14	0	L	0
1	р	416	Total	С	Ν	0	S	0	0	0
	D	410	3259	2080	556	609	14	0	0	0
1	1 C	415	Total	С	Ν	0	S	0	0	0
		410	3254	2077	555	608	14		0	0
1	П	415	Total	С	Ν	0	S	0	0	0
	D	410	3243	2068	554	607	14	0	0	0
1	F	416	Total	С	Ν	0	S	0	1	0
		410	3273	2089	560	610	14	0	L	0
1	1 F	398	Total	С	Ν	0	S	0	0	0
			3106	1982	527	583	14	0	0	

• Molecule 1 is a protein called Glutamate dehydrogenase.

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	PHE	TRP	engineered mutation	UNP 074024
В	89	PHE	TRP	engineered mutation	UNP 074024
С	89	PHE	TRP	engineered mutation	UNP 074024
D	89	PHE	TRP	engineered mutation	UNP 074024
Е	89	PHE	TRP	engineered mutation	UNP 074024
F	89	PHE	TRP	engineered mutation	UNP 074024

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





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	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	Е	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	Ε	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Na 1 1	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	190	Total O 190 190	0	0
6	В	184	Total O 184 184	0	0
6	С	172	Total O 172 172	0	0
6	D	93	Total O 93 93	0	0
6	Ε	221	Total O 221 221	0	0
6	F	88	Total O 88 88	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: Glutamate dehydrogenase



D307 E325 K333 K333 H388 K389 B390 K419

• Molecule 1: Glutamate dehydrogenase



• Molecule 1: Glutamate dehydrogenase





Ref MET 265 VAL 265 VAL 265 VAL 265 LLE 272 CU 273 CU 274 K12 275 CU 286 CU 317 L128 318 L128 319 L108 317 L108 318 L136 317 L108 318 L108 319 L108 322 CU 333 L136 333 L136 333 L136 333 CU 334 L206 335 CU 336 CU 337 L146 338

• Molecule 1: Glutamate dehydrogenase



E371 E371 H388 Y408 K419

• Molecule 1: Glutamate dehydrogenase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	113.36Å 163.25Å 132.60Å	Deperitor
a, b, c, α , β , γ	90.00° 113.91° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	21.80 - 2.03	Depositor
Resolution (A)	21.80 - 2.03	EDS
% Data completeness	99.6 (21.80-2.03)	Depositor
(in resolution range)	99.7(21.80-2.03)	EDS
R _{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.10 (at 2.02 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.172 , 0.199	Depositor
Π, Π_{free}	0.184 , 0.209	DCC
R_{free} test set	14013 reflections (4.95%)	wwPDB-VP
Wilson B-factor $(Å^2)$	26.9	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 46.1	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20653	wwPDB-VP
Average B, all atoms $(Å^2)$	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.24% 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: NA, SO4, GOL, ACY

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	
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.81	0/3337	0.90	0/4519
1	В	0.81	0/3331	0.91	0/4512
1	С	0.85	0/3326	0.91	0/4505
1	D	0.80	0/3314	0.92	0/4490
1	Ε	0.79	0/3345	0.88	0/4530
1	F	0.79	0/3166	0.84	0/4282
All	All	0.81	0/19819	0.89	0/26838

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	3262	0	3271	11	0
1	В	3259	0	3260	20	0
1	С	3254	0	3258	26	0
1	D	3243	0	3240	18	0
1	Е	3273	0	3281	14	0
1	F	3106	0	3100	42	0
2	А	50	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	35	0	0	0	0
2	С	45	0	0	0	0
2	D	30	0	0	1	0
2	Е	35	0	0	0	0
2	F	20	0	0	0	0
3	А	8	0	6	2	0
3	В	8	0	6	1	0
3	С	12	0	9	0	0
3	Ε	4	0	3	0	0
4	А	6	0	8	1	0
4	В	12	0	16	2	0
4	С	30	0	40	14	0
4	Ε	12	0	16	0	0
5	В	1	0	0	0	0
6	А	190	0	0	1	0
6	В	184	0	0	0	0
6	С	172	0	0	1	0
6	D	93	0	0	0	0
6	Е	221	0	0	2	0
6	F	88	0	0	0	0
All	All	20653	0	19514	127	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (127) 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	distance (Å)	overlap (Å)
1:F:262:LYS:HE3	1:F:262:LYS:HA	1.48	0.95
1:F:218:GLN:HB3	1:F:294:PRO:HA	1.52	0.92
3:A:512:ACY:H1	1:F:36:ARG:HD2	1.52	0.92
1:B:193:GLN:HE22	1:B:234:GLN:HE22	1.19	0.91
1:B:303:GLU:HG3	1:B:325:GLU:HB2	1.54	0.90
1:E:193:GLN:HE22	1:E:234:GLN:HE22	1.25	0.84
4:B:510:GOL:H32	1:D:122:ARG:HE	1.45	0.82
1:F:262:LYS:O	1:F:266:GLU:HG2	1.81	0.81
1:C:272:ASP:H	1:C:278:ASN:HD21	1.28	0.80
1:F:262:LYS:HE3	1:F:262:LYS:CA	2.15	0.76
4:C:513:GOL:H12	1:F:122:ARG:HE	1.51	0.75
1:C:169:PRO:HA	4:C:517:GOL:H11	1.69	0.74
1:F:303:GLU:HG3	1:F:325:GLU:HB2	1.68	0.73



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:122:ARG:HH21	4:C:513:GOL:H11	1.56	0.71
1:B:303:GLU:H	1:B:303:GLU:CD	1.97	0.68
1:B:303:GLU:HG3	1:B:325:GLU:CB	2.25	0.67
1:C:171:PHE:CD1	4:C:517:GOL:H32	2.29	0.67
1:C:171:PHE:HB2	4:C:517:GOL:H12	1.77	0.66
1:D:193:GLN:HE22	1:D:234:GLN:HE22	1.43	0.65
1:C:245:SER:HA	4:C:514:GOL:H32	1.78	0.65
1:A:243:SER:HB3	1:A:284:LEU:HD13	1.78	0.65
1:F:256:ASP:O	1:F:260:VAL:HG23	1.98	0.63
1:F:258:ASP:O	1:F:262:LYS:HG2	1.98	0.63
1:C:171:PHE:H	4:C:517:GOL:H12	1.64	0.62
1:F:301:ILE:HA	1:F:305:ASN:HD21	1.64	0.62
1:F:230:LEU:O	1:F:234:GLN:HB2	2.00	0.61
1:F:262:LYS:HA	1:F:262:LYS:CE	2.27	0.60
1:F:301:ILE:HD13	1:F:309:ILE:HG12	1.83	0.60
1:F:292:LEU:HG	1:F:294:PRO:HD3	1.82	0.60
1:D:74:TRP:NE1	1:D:108:ILE:HD12	2.18	0.58
1:D:218:GLN:HE22	1:D:300:VAL:HG21	1.70	0.57
4:C:513:GOL:H12	1:F:122:ARG:NE	2.20	0.56
1:F:230:LEU:HD22	1:F:234:GLN:OE1	2.05	0.56
1:C:149:ASN:HB2	1:C:150:PRO:CD	2.36	0.56
1:E:196:ILE:HG13	1:E:230:LEU:HB3	1.87	0.56
1:F:70:GLY:O	1:F:142:PRO:HA	2.07	0.55
1:D:177:LYS:HZ1	1:D:358:ASN:HD21	1.55	0.55
1:F:220:TYR:OH	1:F:257:PRO:HB3	2.07	0.55
1:C:176:GLY:HA2	1:C:187:ARG:HD3	1.89	0.54
1:B:362:TYR:OH	1:C:372:LYS:HD3	2.08	0.54
1:E:360:ASN:HA	1:F:360:ASN:HD21	1.74	0.53
1:C:171:PHE:HB2	4:C:517:GOL:C1	2.38	0.53
1:F:278:ASN:HD22	1:F:278:ASN:N	2.06	0.52
1:B:164:MET:HE2	1:B:170:ALA:HB2	1.92	0.52
1:D:177:LYS:NZ	1:D:358:ASN:HD21	2.07	0.52
1:D:244:ASP:HB2	2:D:501:SO4:O3	2.09	0.52
1:B:118:ARG:O	1:B:122:ARG:HG3	2.10	0.51
1:F:285:LEU:HB3	1:F:309:ILE:HD11	1.92	0.51
1:E:16:ARG:HG2	6:E:703:HOH:O	2.10	0.51
1:F:259:GLU:HA	1:F:262:LYS:HG3	1.93	0.51
1:A:217:VAL:O	1:A:242:VAL:HA	2.11	0.51
1:C:149:ASN:HB2	1:C:150:PRO:HD2	1.91	0.50
1:A:271:LYS:HG2	1:A:278:ASN:ND2	2.27	0.49
1:D:209:ASP:OD1	1:D:211:LYS:HB2	2.12	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:F:215:ILE:HB	1:F:291:VAL:HG13	1.93	0.49
3:A:512:ACY:CH3	1:F:36:ARG:HD2	2.34	0.49
1:E:295:ALA:HB2	1:E:317:VAL:HB	1.95	0.49
1:C:325:GLU:H	1:C:325:GLU:CD	2.16	0.48
1:C:171:PHE:H	4:C:517:GOL:H31	1.77	0.48
1:E:193:GLN:HE22	1:E:234:GLN:NE2	2.04	0.48
1:E:33:LYS:HE3	6:E:612:HOH:O	2.13	0.48
1:C:68:THR:O	1:C:140:ASP:HA	2.14	0.48
1:B:164:MET:CE	1:B:170:ALA:HB2	2.44	0.47
1:D:295:ALA:HB2	1:D:317:VAL:HB	1.96	0.47
1:F:17:ALA:HB1	1:F:400:TYR:HB3	1.97	0.47
1:B:73:ARG:HG3	1:B:146:VAL:HB	1.97	0.47
1:F:97:VAL:HG23	1:F:99:LEU:HG	1.96	0.47
1:A:97:VAL:HG23	1:A:99:LEU:HG	1.97	0.47
1:B:307:ASP:HA	1:B:333:LYS:CE	2.45	0.46
1:B:97:VAL:HG23	1:B:99:LEU:HG	1.97	0.46
1:C:122:ARG:HE	4:C:513:GOL:H11	1.80	0.46
1:F:256:ASP:HA	1:F:257:PRO:HD3	1.78	0.46
1:A:272:ASP:H	1:A:278:ASN:HD21	1.62	0.46
1:B:38:VAL:HG22	1:E:38:VAL:HG22	1.98	0.46
1:A:28:LEU:O	1:A:32:LYS:HG3	2.16	0.45
1:F:206:LEU:HD12	1:F:206:LEU:HA	1.77	0.45
1:F:316:GLU:HB3	1:F:321:PRO:HG2	1.98	0.45
1:B:280:THR:OG1	1:B:283:GLU:HG3	2.16	0.45
1:C:379:LYS:HE3	6:C:622:HOH:O	2.16	0.45
1:C:169:PRO:CA	4:C:517:GOL:H11	2.43	0.45
1:C:170:ALA:N	4:C:517:GOL:H31	2.31	0.45
1:A:129[A]:ARG:CZ	1:E:162:THR:HG21	2.46	0.45
1:B:217:VAL:O	1:B:242:VAL:HA	2.17	0.45
1:F:370:ARG:HE	1:F:370:ARG:HB3	1.48	0.45
1:E:149:ASN:HB2	1:E:150:PRO:CD	2.47	0.45
1:F:78:GLU:HB3	1:F:109:ILE:HG12	1.99	0.44
1:C:97:VAL:HG23	1:C:99:LEU:HG	2.00	0.44
1:D:322:VAL:HG11	1:D:337:GLN:NE2	2.32	0.44
1:F:299:GLU:HG3	1:F:323:THR:HG22	2.00	0.44
1:C:217:VAL:O	1:C:242:VAL:HA	2.17	0.44
1:B:5:ASP:HB3	1:B:6:PRO:HD3	2.00	0.44
1:D:372:LYS:HD2	1:F:362:TYR:OH	2.17	0.44
1:F:341:PHE:O	1:F:345:ALA:HB2	2.18	0.43
1:D:217:VAL:O	1:D:242:VAL:HA	2.19	0.43
1:E:23:ILE:HA	1:E:408:TYR:CE2	2.53	0.43



A 4 a m 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:F:176:GLY:HA2	1:F:187:ARG:HD3	2.01	0.43
1:C:143:ALA:HB1	1:C:144:PRO:HD2	2.01	0.43
1:D:297:ILE:HG13	1:D:300:VAL:CG1	2.49	0.43
1:D:295:ALA:HA	1:D:318:ALA:HB2	2.00	0.43
4:A:513:GOL:H31	6:A:767:HOH:O	2.19	0.43
1:F:73:ARG:O	1:F:107:GLY:HA2	2.18	0.42
1:D:271:LYS:HG2	1:D:272:ASP:OD2	2.19	0.42
1:C:171:PHE:H	4:C:517:GOL:C3	2.32	0.42
1:F:304:LYS:HE3	1:F:304:LYS:HB3	1.44	0.42
3:B:508:ACY:H1	1:E:36:ARG:HD3	2.01	0.42
1:B:69:LYS:HD2	1:B:141:ILE:HB	2.02	0.42
1:C:303:GLU:OE1	1:C:304:LYS:HE2	2.20	0.42
1:C:272:ASP:H	1:C:278:ASN:ND2	2.06	0.41
1:B:307:ASP:HA	1:B:333:LYS:HE3	2.02	0.41
1:E:129[A]:ARG:HG2	1:E:163:ILE:HD11	2.02	0.41
1:F:73:ARG:HG2	1:F:145:ASP:OD1	2.20	0.41
1:A:292:LEU:HB2	1:A:311:ALA:HB2	2.03	0.41
1:C:70:GLY:O	1:C:142:PRO:HA	2.21	0.41
1:A:62:ASN:O	1:A:102:GLY:HA3	2.21	0.41
1:B:208:ILE:HA	4:B:511:GOL:H12	2.03	0.41
1:F:62:ASN:O	1:F:102:GLY:HA3	2.21	0.41
1:F:218:GLN:NE2	1:F:285:LEU:HD21	2.36	0.41
1:F:280:THR:HG22	1:F:283:GLU:OE1	2.20	0.41
1:A:418:LYS:H	1:A:418:LYS:HG2	1.73	0.41
1:D:215:ILE:HA	1:D:291:VAL:O	2.20	0.41
1:D:116:SER:O	1:D:120:GLN:HG3	2.21	0.41
1:F:213:LYS:HD3	1:F:213:LYS:HA	1.93	0.41
1:D:97:VAL:HG23	1:D:99:LEU:HG	2.03	0.41
1:A:73:ARG:O	1:A:107:GLY:HA2	2.20	0.40
1:E:28:LEU:HD13	1:E:32:LYS:HD3	2.03	0.40
1:B:193:GLN:HE22	1:B:234:GLN:NE2	2.01	0.40
1:B:149:ASN:HB2	1:B:150:PRO:HD2	2.02	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	414/419~(99%)	399~(96%)	15 (4%)	0	100 100
1	В	414/419~(99%)	404 (98%)	10 (2%)	0	100 100
1	С	413/419~(99%)	402 (97%)	11 (3%)	0	100 100
1	D	413/419~(99%)	399~(97%)	14 (3%)	0	100 100
1	Е	415/419 (99%)	403 (97%)	12 (3%)	0	100 100
1	F	386/419~(92%)	358~(93%)	28 (7%)	0	100 100
All	All	2455/2514~(98%)	2365 (96%)	90 (4%)	0	100 100

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

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	Rotameric Outliers	
1	А	339/342~(99%)	320 (94%)	19 (6%)	21 16
1	В	338/342~(99%)	331 (98%)	7(2%)	53 55
1	С	338/342~(99%)	323~(96%)	15 (4%)	28 24
1	D	336/342~(98%)	324 (96%)	12 (4%)	35 32
1	Е	340/342~(99%)	325~(96%)	15 (4%)	28 24
1	F	321/342 (94%)	297~(92%)	24 (8%)	13 8
All	All	2012/2052~(98%)	1920 (95%)	92 (5%)	27 22

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	12	LYS
1	А	28	LEU
1	А	45	GLU



Mol	Chain	Res	Type
1	А	53	VAL
1	А	97	VAL
1	А	179	LEU
1	А	206	LEU
1	А	220	TYR
1	А	230	LEU
1	А	265	ARG
1	А	271	LYS
1	А	292	LEU
1	А	297	ILE
1	А	304	LYS
1	А	332	GLU
1	А	359	ILE
1	А	388	HIS
1	А	418	LYS
1	А	419	LYS
1	В	28	LEU
1	В	137	PRO
1	В	164	MET
1	В	206	LEU
1	В	211	LYS
1	В	235	LEU
1	В	388	HIS
1	С	28	LEU
1	С	89	PHE
1	С	97	VAL
1	С	111	ASN
1	С	145	ASP
1	С	164	MET
1	С	206	LEU
1	С	211	LYS
1	С	230	LEU
1	С	303	GLU
1	С	367	GLU
1	С	371	GLU
1	С	388	HIS
1	С	389	LYS
1	С	418	LYS
1	D	12	LYS
1	D	25	GLU
1	D	28	LEU
1	D	52	LYS



Mol	Mol Chain		Type
1	D	97	VAL
1	D	145	ASP
1	D	148	THR
1	D	206	LEU
1	D	211	LYS
1	D	220	TYR
1	D	292	LEU
1	D	388	HIS
1	Е	4	ILE
1	Е	12	LYS
1	Е	16	ARG
1	Е	73	ARG
1	Е	145	ASP
1	Е	164	MET
1	E	230	LEU
1	Е	304	LYS
1	Е	307	ASP
1	Е	310	LYS
1	Е	332	GLU
1	Е	336	LEU
1	Е	371	GLU
1	Е	388	HIS
1	Е	419	LYS
1	F	28	LEU
1	F	145	ASP
1	F	204	LYS
1	F	206	LEU
1	F	210	LEU
1	F	215	ILE
1	F	220	TYR
1	F	245	SER
1	F	262	LYS
1	F	278	ASN
1	F	283	GLU
1	F	287	LEU
1	F	290	ASP
1	F	291	VAL
1	F	297	ILE
1	F	299	GLU
1	F	304	LYS
1	F	307	ASP
1	F	310	LYS



 $Continued \ from \ previous \ page...$

Mol	Chain	Res	Type
1	F	328	ASP
1	F	333	LYS
1	F	370	ARG
1	F	382	TRP
1	F	388	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	281	ASN
1	А	386	ASN
1	В	120	GLN
1	В	234	GLN
1	В	267	HIS
1	В	308	ASN
1	В	386	ASN
1	В	392	ASN
1	С	19	GLN
1	С	111	ASN
1	С	222	ASN
1	С	267	HIS
1	С	278	ASN
1	С	308	ASN
1	С	386	ASN
1	D	218	GLN
1	D	234	GLN
1	D	281	ASN
1	D	358	ASN
1	D	386	ASN
1	Е	120	GLN
1	Е	234	GLN
1	Е	308	ASN
1	Е	386	ASN
1	F	120	GLN
1	F	222	ASN
1	F	278	ASN
1	F	308	ASN
1	F	360	ASN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 62 ligands modelled in this entry, 1 is monoatomic - leaving 61 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Type	Chain	Dog	Link	B	ond leng	gths	Bond angles		
	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	SO4	С	505	-	4,4,4	0.38	0	$6,\!6,\!6$	0.13	0
4	GOL	С	513	-	5,5,5	0.26	0	$5,\!5,\!5$	0.85	0
2	SO4	F	501	-	4,4,4	0.43	0	$6,\!6,\!6$	0.17	0
4	GOL	А	513	-	5,5,5	0.16	0	$5,\!5,\!5$	0.42	0
2	SO4	В	503	-	4,4,4	0.30	0	6,6,6	0.28	0
2	SO4	D	505	-	4,4,4	0.48	0	$6,\!6,\!6$	0.05	0
4	GOL	Е	510	-	5,5,5	0.19	0	$5,\!5,\!5$	0.43	0
2	SO4	С	506	-	4,4,4	0.48	0	$6,\!6,\!6$	0.06	0
2	SO4	Е	503	-	4,4,4	0.48	0	$6,\!6,\!6$	0.04	0
3	ACY	С	511	-	3,3,3	0.79	0	3,3,3	1.12	0
3	ACY	А	511	-	3,3,3	1.06	0	3,3,3	1.00	0
2	SO4	С	503	-	4,4,4	0.44	0	$6,\!6,\!6$	0.41	0
2	SO4	А	506	-	4,4,4	0.37	0	$6,\!6,\!6$	0.26	0
3	ACY	А	512	-	3,3,3	1.04	0	3,3,3	1.24	0
4	GOL	С	514	-	5,5,5	0.16	0	$5,\!5,\!5$	0.55	0
2	SO4	С	502	-	4,4,4	0.54	0	6,6,6	0.29	0
2	SO4	F	502	-	4,4,4	0.32	0	$6,\!6,\!6$	0.17	0



Mal	Turne	Chain	Dec	T in le	B	Bond lengths		Bond angles		
WIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	ACY	В	508	-	3, 3, 3	0.78	0	$3,\!3,\!3$	1.62	1 (33%)
2	SO4	А	507	-	4,4,4	0.30	0	6,6,6	0.25	0
2	SO4	В	506	-	4,4,4	0.28	0	6,6,6	0.33	0
2	SO4	Е	502	-	4,4,4	0.56	0	6,6,6	0.17	0
2	SO4	С	507	-	4,4,4	0.29	0	6,6,6	0.15	0
3	ACY	Е	508	-	3,3,3	1.33	0	3,3,3	0.74	0
2	SO4	В	505	-	4,4,4	0.47	0	6,6,6	0.16	0
3	ACY	В	509	-	3,3,3	1.18	0	3,3,3	0.69	0
2	SO4	А	503	-	4,4,4	0.34	0	6,6,6	0.20	0
2	SO4	В	501	-	4,4,4	0.28	0	6,6,6	0.28	0
2	SO4	С	501	-	4,4,4	0.39	0	6,6,6	0.44	0
2	SO4	С	509	-	4,4,4	0.28	0	6,6,6	0.23	0
2	SO4	С	504	-	4,4,4	0.20	0	6,6,6	0.12	0
2	SO4	D	506	-	4,4,4	0.40	0	6,6,6	0.20	0
2	SO4	Е	504	-	4,4,4	0.32	0	6,6,6	0.19	0
2	SO4	В	507	-	4,4,4	0.49	0	6,6,6	0.05	0
2	SO4	Е	501	-	4,4,4	0.36	0	6,6,6	0.23	0
2	SO4	D	504	-	4,4,4	0.34	0	6,6,6	0.19	0
2	SO4	Е	505	-	4,4,4	0.41	0	6,6,6	0.25	0
4	GOL	Е	509	-	5,5,5	0.18	0	$5,\!5,\!5$	0.41	0
2	SO4	В	504	5	4,4,4	0.21	0	6,6,6	0.12	0
3	ACY	С	510	-	3,3,3	1.40	0	3,3,3	0.60	0
4	GOL	В	510	-	$5,\!5,\!5$	0.09	0	$5,\!5,\!5$	0.54	0
2	SO4	D	501	-	4,4,4	0.38	0	6,6,6	0.22	0
4	GOL	С	517	-	$5,\!5,\!5$	0.32	0	$5,\!5,\!5$	1.02	0
2	SO4	D	502	-	4,4,4	0.36	0	6,6,6	0.18	0
2	SO4	А	502	-	4,4,4	0.32	0	6,6,6	0.10	0
2	SO4	F	503	-	4,4,4	0.32	0	6,6,6	0.16	0
2	SO4	А	509	-	4,4,4	0.35	0	6,6,6	0.21	0
2	SO4	А	501	-	4,4,4	0.33	0	6,6,6	0.59	0
2	SO4	А	505	-	4,4,4	0.21	0	6,6,6	0.47	0
4	GOL	С	515	-	$5,\!5,\!5$	0.11	0	$5,\!5,\!5$	0.39	0
2	SO4	В	502	-	4,4,4	0.51	0	$6,\!6,\!6$	0.30	0
2	SO4	С	508	-	4,4,4	0.23	0	6,6,6	0.35	0
2	SO4	D	503	-	4,4,4	0.22	0	$6,\!6,\!6$	0.40	0
2	SO4	Е	507	-	4,4,4	0.38	0	6,6,6	0.49	0
2	SO4	А	504	-	4,4,4	0.11	0	6,6,6	0.21	0
2	SO4	А	508	-	4,4,4	0.39	0	$6,\!6,\!6$	0.22	0
2	SO4	Е	506	-	4,4,4	0.35	0	6,6,6	0.34	0
4	GOL	В	511	-	$5,\!5,\!5$	0.25	0	$5,\!5,\!5$	0.62	0
2	SO4	F	504	-	4,4,4	0.35	0	6,6,6	0.27	0
3	ACY	С	512	-	3,3,3	1.23	0	3,3,3	1.12	0
2	SO4	A	510	-	4,4,4	0.27	0	6,6,6	0.18	0



Mol	Tuno	Chain	Dog	Tink	Bond lengths			Bond angles		
	Type		res 1		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	GOL	С	516	-	5,5,5	0.19	0	$5,\!5,\!5$	0.46	0

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
4	GOL	С	514	-	-	2/4/4/4	-
4	GOL	С	515	-	-	3/4/4/4	-
4	GOL	Е	509	-	-	0/4/4/4	-
4	GOL	С	513	-	-	2/4/4/4	-
4	GOL	С	517	-	-	2/4/4/4	-
4	GOL	А	513	-	-	2/4/4/4	-
4	GOL	В	510	-	-	2/4/4/4	-
4	GOL	В	511	-	-	2/4/4/4	-
4	GOL	Е	510	-	-	2/4/4/4	-
4	GOL	С	516	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	508	ACY	O-C-CH3	-2.28	113.46	122.33

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	511	GOL	O1-C1-C2-C3
4	С	515	GOL	O1-C1-C2-C3
4	С	517	GOL	O1-C1-C2-C3
4	А	513	GOL	C1-C2-C3-O3
4	В	510	GOL	O1-C1-C2-C3
4	С	513	GOL	C1-C2-C3-O3
4	С	514	GOL	O1-C1-C2-C3
4	Е	510	GOL	O1-C1-C2-C3
4	В	511	GOL	O1-C1-C2-O2
4	С	515	GOL	O1-C1-C2-O2



Mol	Chain	Res	Type	Atoms
4	С	517	GOL	O1-C1-C2-O2
4	Е	510	GOL	O1-C1-C2-O2
4	А	513	GOL	O2-C2-C3-O3
4	С	514	GOL	O1-C1-C2-O2
4	С	513	GOL	O2-C2-C3-O3
4	В	510	GOL	O1-C1-C2-O2
4	С	515	GOL	C1-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	513	GOL	4	0
4	А	513	GOL	1	0
3	А	512	ACY	2	0
4	С	514	GOL	1	0
3	В	508	ACY	1	0
4	В	510	GOL	1	0
2	D	501	SO4	1	0
4	С	517	GOL	9	0
4	В	511	GOL	1	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)

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	415/419~(99%)	-0.45	4 (0%) 82 82	21, 30, 54, 94	0
1	В	416/419 (99%)	-0.43	4 (0%) 82 82	21, 32, 54, 72	0
1	С	415/419 (99%)	-0.39	4 (0%) 82 82	24, 33, 57, 80	0
1	D	415/419 (99%)	-0.11	18 (4%) 35 34	28, 43, 70, 93	0
1	Е	416/419 (99%)	-0.48	3 (0%) 87 87	23, 31, 53, 78	0
1	F	398/419~(94%)	0.34	70 (17%) 1 1	24, 48, 117, 138	0
All	All	2475/2514 (98%)	-0.26	103 (4%) 36 35	21, 35, 76, 138	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	246	ARG	5.7
1	F	308	ASN	5.7
1	F	266	GLU	5.6
1	F	245	SER	5.4
1	F	265	ARG	5.0
1	F	278	ASN	4.7
1	F	236	GLY	4.7
1	F	325	GLU	4.5
1	F	304	LYS	4.5
1	F	216	ALA	4.5
1	F	298	GLU	4.5
1	F	277	THR	4.4
1	F	212	GLY	4.3
1	F	382	TRP	4.2
1	D	325	GLU	4.2
1	F	297	ILE	4.1
1	F	303	GLU	4.1
1	F	332	GLU	4.0
1	F	279	ILE	3.8



Mol	Chain	Res	Type	RSRZ
1	С	147	TYR	3.6
1	F	269	SER	3.5
1	F	261	LEU	3.5
1	F	280	THR	3.5
1	F	333	LYS	3.4
1	Е	4	ILE	3.4
1	F	310	LYS	3.3
1	В	4	ILE	3.3
1	Е	297	ILE	3.3
1	F	282	GLU	3.2
1	F	218	GLN	3.2
1	D	148	THR	3.2
1	F	338	ILE	3.1
1	А	246	ARG	3.1
1	F	294	PRO	3.0
1	F	210	LEU	3.0
1	F	232	LYS	3.0
1	F	289	VAL	2.9
1	F	247	GLY	2.9
1	F	258	ASP	2.9
1	F	206	LEU	2.9
1	А	419	LYS	2.9
1	В	147	TYR	2.9
1	F	296	ALA	2.9
1	F	203	ALA	2.8
1	F	214	LYS	2.8
1	F	288	GLU	2.8
1	F	299	GLU	2.8
1	F	328	ASP	2.8
1	F	270	VAL	2.8
1	F	291	VAL	2.8
1	Е	19	GLN	2.8
1	D	303	GLU	2.8
1	F	302	THR	2.7
1	F	262	LYS	2.7
1	F	205	ALA	2.7
1	F	248	GLY	2.6
1	F	392	ASN	2.6
1	D	246	ARG	2.6
1	F	147	TYR	2.6
1	F	305	ASN	2.5
1	F	225	TYR	2.4



Mol	Chain	Res	Type	RSRZ
1	F	335	ILE	2.4
1	F	290	ASP	2.4
1	F	215	ILE	2.4
1	F	263	TRP	2.4
1	F	319	ASN	2.3
1	D	242	VAL	2.3
1	D	22	ASP	2.3
1	D	265	ARG	2.3
1	А	265	ARG	2.3
1	F	48	ASP	2.3
1	F	255	LEU	2.2
1	F	312	LYS	2.2
1	D	299	GLU	2.2
1	F	329	ILE	2.2
1	D	245	SER	2.2
1	F	264	LYS	2.2
1	D	268	GLY	2.2
1	D	275	GLY	2.2
1	D	382	TRP	2.2
1	F	285	LEU	2.2
1	D	146	VAL	2.2
1	D	390	ASP	2.1
1	F	307	ASP	2.1
1	А	77	ALA	2.1
1	D	77	ALA	2.1
1	F	259	GLU	2.1
1	В	390	ASP	2.1
1	F	237	MET	2.1
1	В	19	GLN	2.1
1	F	222	ASN	2.1
1	D	292	LEU	2.1
1	D	298	GLU	2.1
1	С	332	GLU	2.0
1	D	392	ASN	2.0
1	С	419	LYS	2.0
1	F	389	LYS	2.0
1	С	77	ALA	2.0
1	F	283	GLU	2.0
1	F	286	GLU	2.0
1	F	334	GLY	2.0
1	F	249	ILE	2.0
1	F	292	LEU	2.0

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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
2	SO4	D	505	5/5	0.73	0.31	72,74,81,99	0
4	GOL	В	511	6/6	0.78	0.33	62,81,83,90	0
4	GOL	С	515	6/6	0.82	0.20	54,63,69,78	0
2	SO4	С	509	5/5	0.85	0.34	92,97,100,102	0
4	GOL	С	514	6/6	0.86	0.24	51,70,83,83	0
2	SO4	С	506	5/5	0.86	0.26	69,73,84,97	0
4	GOL	А	513	6/6	0.87	0.14	41,45,67,67	0
3	ACY	В	509	4/4	0.88	0.20	52,63,66,70	0
3	ACY	С	511	4/4	0.88	0.17	49,56,57,59	0
2	SO4	А	501	5/5	0.88	0.15	62,67,77,90	0
4	GOL	С	516	6/6	0.88	0.28	42,63,74,78	0
4	GOL	Е	510	6/6	0.88	0.13	54,61,67,70	0
4	GOL	В	510	6/6	0.89	0.23	54,54,56,68	0
2	SO4	Е	503	5/5	0.89	0.29	63,79,82,86	0
2	SO4	В	503	5/5	0.90	0.26	58,75,76,93	0
4	GOL	Е	509	6/6	0.90	0.17	58,73,84,86	0
2	SO4	А	510	5/5	0.90	0.28	44,69,86,110	0
2	SO4	А	505	5/5	0.91	0.24	45,58,96,96	0
4	GOL	С	513	6/6	0.91	0.18	50,56,58,75	0
2	SO4	F	504	5/5	0.91	0.26	63,78,83,93	0
2	SO4	С	507	5/5	0.91	0.29	71,88,100,120	0
2	SO4	В	504	5/5	0.91	0.33	77,82,85,95	0
4	GOL	С	517	6/6	0.91	0.17	45,52,54,61	0
2	SO4	С	505	5/5	0.91	0.33	82,88,96,103	0
2	SO4	D	506	5/5	0.91	0.24	69,82,104,109	0
2	SO4	Е	507	5/5	0.92	0.18	63,65,66,69	0
3	ACY	С	512	4/4	0.92	0.17	57,59,61,65	0



Conti	Continued from previous page									
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9		
2	SO4	А	504	5/5	0.93	0.13	53,71,76,87	0		
2	SO4	D	502	5/5	0.93	0.29	86,90,97,105	0		
2	SO4	D	504	5/5	0.93	0.24	75,76,98,102	0		
2	SO4	Е	506	5/5	0.95	0.15	50,68,76,78	0		
2	SO4	В	506	5/5	0.95	0.18	54,69,76,77	0		
2	SO4	F	501	5/5	0.95	0.21	68,68,77,91	0		
2	SO4	Е	504	5/5	0.95	0.18	68,71,77,98	0		
3	ACY	В	508	4/4	0.95	0.10	33,35,37,40	0		
2	SO4	Е	505	5/5	0.95	0.23	70,78,89,93	0		
2	SO4	F	502	5/5	0.96	0.31	71,92,101,106	0		
2	SO4	F	503	5/5	0.96	0.23	54,68,87,97	0		
2	SO4	D	503	5/5	0.96	0.24	54,55,77,81	0		
3	ACY	А	511	4/4	0.96	0.09	49,57,63,69	0		
3	ACY	А	512	4/4	0.96	0.14	35,36,38,42	0		
2	SO4	А	509	5/5	0.96	0.24	68,73,82,85	0		
2	SO4	В	507	5/5	0.96	0.26	78,89,97,97	0		
3	ACY	С	510	4/4	0.96	0.09	42,42,44,46	0		
2	SO4	С	501	5/5	0.96	0.20	49,57,65,69	0		
2	SO4	А	508	5/5	0.96	0.26	63,78,79,91	0		
2	SO4	D	501	5/5	0.97	0.17	66,74,82,95	0		
3	ACY	Е	508	4/4	0.97	0.08	34,35,36,38	0		
2	SO4	В	505	5/5	0.97	0.20	65,66,71,77	0		
2	SO4	А	507	5/5	0.97	0.22	66,69,84,90	0		
2	SO4	С	504	5/5	0.98	0.20	57,59,71,74	0		
2	SO4	А	503	5/5	0.98	0.17	60,66,76,90	0		
2	SO4	Е	501	5/5	0.98	0.19	42,55,66,80	0		
2	SO4	А	506	5/5	0.98	0.19	53,54,59,62	0		
2	SO4	В	501	5/5	0.98	0.15	47,52,63,71	0		
2	SO4	С	508	5/5	0.98	0.06	43,45,55,58	0		
5	NA	В	512	1/1	0.98	0.06	39,39,39,39	0		
2	SO4	А	502	5/5	0.99	0.18	42,54,55,55	0		
2	SO4	Е	502	5/5	0.99	0.12	48,51,59,66	0		
2	SO4	В	502	5/5	0.99	0.07	41,49,56,56	0		
2	SO4	С	502	5/5	0.99	0.13	42,44,52,52	0		
2	SO4	С	503	5/5	0.99	0.12	46,52,58,69	0		

 α ntia J fa .

Other polymers (i) 6.5

There are no such residues in this entry.

