

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 9, 2023 – 06:16 PM EDT

PDB ID	:	4H2H
Title	:	Crystal structure of an enolase (mandalate racemase subgroup, target EFI-
		502101) from Pelagibaca bermudensis htcc2601, with bound mg and l-4-
		hydroxyproline betaine (betonicine)
Authors	:	Vetting, M.W.; Morisco, L.L.; Wasserman, S.R.; Sojitra, S.; Imker, H.J.; Gerlt,
		J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on	:	2012-09-12
Resolution	:	1.70  Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Motria	Whole archive	Similar resolution		
Metric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$		
R <sub>free</sub>	130704	4298 (1.70-1.70)		
Clashscore	141614	4695 (1.70-1.70)		
Ramachandran outliers	138981	4610 (1.70-1.70)		
Sidechain outliers	138945	4610 (1.70-1.70)		
RSRZ outliers	127900	4222 (1.70-1.70)		

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	376	89%	8% ••
1	В	376	4%	8% •
1	С	376	5% 93%	5% •
1	D	376	<mark>6%</mark> 91%	7% •



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Mol	Chain	Length	Quality of chain		
1	Е	376	86%	9%	6%
1	F	376	90%	7%	·
1	G	376	90%	7%	•••
1	Н	376	3% 92%	6%	6.

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	IOD	А	404	-	-	Х	-
5	IOD	А	405	-	-	Х	-
5	IOD	D	409	-	-	Х	-
5	IOD	D	411	-	-	Х	-
5	IOD	Е	409	-	-	Х	-
5	IOD	G	409	-	-	Х	-
5	IOD	G	410	-	-	Х	-
5	IOD	Н	406	-	-	Х	-
5	IOD	Н	408	-	-	Х	-



# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 24627 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	Λ	268	Total	С	Ν	0	$\mathbf{S}$	0	Б	0
1	A	300	2829	1785	498	530	16	0	5	0
1	В	367	Total	С	Ν	0	$\mathbf{S}$	0	Б	0
1	D	307	2828	1783	500	530	15	0	5	0
1	C	267	Total	С	Ν	0	S	0	2	0
1	U	307	2800	1766	494	525	15	0	2	0
1	D 267	367	Total	С	Ν	0	S	0	1	0
1	D	507	2809	1771	494	529	15	0	4	0
1	F	355	Total	С	Ν	0	S	0	1	0
1	Ľ	555	2713	1707	478	512	16	0	4	U
1	F	367	Total	С	Ν	0	S	0	1	0
1	Ľ	507	2792	1762	492	523	15	0	T	0
1	C	367	Total	С	Ν	Ο	$\mathbf{S}$	0	9	0
1	G	507	2800	1768	493	524	15	0	2	0
1	Ц	367	Total	С	Ν	Ο	$\mathbf{S}$	0	9	0
	11	307	2803	1768	496	524	15	0		

• Molecule 1 is a protein called Mandelate racemase/muconate lactonizing enzyme.

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-8	MET	-	expression tag	UNP Q0FPQ4
А	-7	ALA	-	expression tag	UNP Q0FPQ4
А	-6	HIS	-	expression tag	UNP Q0FPQ4
А	-5	HIS	-	expression tag	UNP Q0FPQ4
А	-4	HIS	-	expression tag	UNP Q0FPQ4
А	-3	HIS	-	expression tag	UNP Q0FPQ4
А	-2	HIS	-	expression tag	UNP Q0FPQ4
А	-1	HIS	-	expression tag	UNP Q0FPQ4
А	0	SER	-	expression tag	UNP Q0FPQ4
А	1	LEU	-	expression tag	UNP Q0FPQ4
В	-8	MET	-	expression tag	UNP Q0FPQ4
В	-7	ALA	-	expression tag	UNP Q0FPQ4
В	-6	HIS	-	expression tag	UNP Q0FPQ4



Chain	Residue	Modelled	Actual	Comment	Reference
В	-5	HIS	-	expression tag	UNP Q0FPQ4
В	-4	HIS	-	expression tag	UNP Q0FPQ4
В	-3	HIS	-	expression tag	UNP Q0FPQ4
В	-2	HIS	-	expression tag	UNP Q0FPQ4
В	-1	HIS	-	expression tag	UNP Q0FPQ4
В	0	SER	-	expression tag	UNP Q0FPQ4
В	1	LEU	-	expression tag	UNP Q0FPQ4
С	-8	MET	-	expression tag	UNP Q0FPQ4
С	-7	ALA	-	expression tag	UNP Q0FPQ4
С	-6	HIS	-	expression tag	UNP Q0FPQ4
С	-5	HIS	-	expression tag	UNP Q0FPQ4
С	-4	HIS	-	expression tag	UNP Q0FPQ4
С	-3	HIS	-	expression tag	UNP Q0FPQ4
С	-2	HIS	-	expression tag	UNP Q0FPQ4
С	-1	HIS	-	expression tag	UNP Q0FPQ4
С	0	SER	-	expression tag	UNP Q0FPQ4
С	1	LEU	-	expression tag	UNP Q0FPQ4
D	-8	MET	-	expression tag	UNP Q0FPQ4
D	-7	ALA	-	expression tag	UNP Q0FPQ4
D	-6	HIS	-	expression tag	UNP Q0FPQ4
D	-5	HIS	-	expression tag	UNP Q0FPQ4
D	-4	HIS	-	expression tag	UNP Q0FPQ4
D	-3	HIS	-	expression tag	UNP Q0FPQ4
D	-2	HIS	-	expression tag	UNP Q0FPQ4
D	-1	HIS	-	expression tag	UNP Q0FPQ4
D	0	SER	-	expression tag	UNP Q0FPQ4
D	1	LEU	-	expression tag	UNP Q0FPQ4
Е	-8	MET	-	expression tag	UNP Q0FPQ4
E	-7	ALA	-	expression tag	UNP Q0FPQ4
E	-6	HIS	-	expression tag	UNP Q0FPQ4
E	-5	HIS	-	expression tag	UNP Q0FPQ4
E	-4	HIS	-	expression tag	UNP Q0FPQ4
E	-3	HIS	-	expression tag	UNP Q0FPQ4
E	-2	HIS	-	expression tag	UNP Q0FPQ4
E	-1	HIS	-	expression tag	UNP Q0FPQ4
E	0	SER	-	expression tag	UNP Q0FPQ4
E	1	LEU	-	expression tag	UNP Q0FPQ4
F	-8	MET	-	expression tag	UNP Q0FPQ4
F	-7	ALA	-	expression tag	UNP Q0FPQ4
F	-6	HIS	-	expression tag	UNP Q0FPQ4
F	-5	HIS	-	expression tag	UNP Q0FPQ4
F	-4	HIS	-	expression tag	UNP Q0FPQ4



Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	HIS	-	expression tag	UNP Q0FPQ4
F	-2	HIS	-	expression tag	UNP Q0FPQ4
F	-1	HIS	-	expression tag	UNP Q0FPQ4
F	0	SER	-	expression tag	UNP Q0FPQ4
F	1	LEU	-	expression tag	UNP Q0FPQ4
G	-8	MET	-	expression tag	UNP Q0FPQ4
G	-7	ALA	-	expression tag	UNP Q0FPQ4
G	-6	HIS	-	expression tag	UNP Q0FPQ4
G	-5	HIS	-	expression tag	UNP Q0FPQ4
G	-4	HIS	-	expression tag	UNP Q0FPQ4
G	-3	HIS	-	expression tag	UNP Q0FPQ4
G	-2	HIS	-	expression tag	UNP Q0FPQ4
G	-1	HIS	-	expression tag	UNP Q0FPQ4
G	0	SER	-	expression tag	UNP Q0FPQ4
G	1	LEU	-	expression tag	UNP Q0FPQ4
Н	-8	MET	-	expression tag	UNP Q0FPQ4
Н	-7	ALA	-	expression tag	UNP Q0FPQ4
Н	-6	HIS	-	expression tag	UNP Q0FPQ4
Н	-5	HIS	-	expression tag	UNP Q0FPQ4
Н	-4	HIS	-	expression tag	UNP Q0FPQ4
Н	-3	HIS	-	expression tag	UNP Q0FPQ4
Н	-2	HIS	-	expression tag	UNP Q0FPQ4
Н	-1	HIS	-	expression tag	UNP Q0FPQ4
Н	0	SER	-	expression tag	UNP Q0FPQ4
Н	1	LEU	-	expression tag	UNP Q0FPQ4

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Mg 1 1	0	0
2	В	1	Total Mg 1 1	0	0
2	С	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	Е	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Н	1	Total Mg 1 1	0	0

• Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Ni 1 1	0	0
3	В	1	Total Ni 1 1	0	0

• Molecule 4 is (2S,4R)-4-hydroxy-1,1-dimethylpyrrolidinium-2-carboxylate (three-letter code: 0XW) (formula:  $C_7H_{13}NO_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total         C         N         O           11         7         1         3	0	0
4	В	1	Total         C         N         O           11         7         1         3	0	0
4	С	1	Total         C         N         O           11         7         1         3	0	0
4	D	1	Total         C         N         O           11         7         1         3	0	0
4	Е	1	Total         C         N         O           11         7         1         3	0	0
4	F	1	Total         C         N         O           11         7         1         3	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 11 & 7 & 1 & 3 \end{array}$	0	0
4	Н	1	Total         C         N         O           11         7         1         3	0	0

• Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	8	Total I 8 8	0	0
5	В	6	Total I 6 6	0	0
5	С	10	Total I 10 10	0	0
5	D	8	Total I 8 8	0	0
5	Ε	7	Total I 7 7	0	0
5	F	8	Total I 8 8	0	0
5	G	8	Total I 8 8	0	0
5	Н	6	Total I 6 6	0	0

• Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
6	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	275	Total O 275 275	0	0
7	В	293	Total         O           294         294	0	1
7	С	272	Total O 273 273	0	1
7	D	251	Total O 251 251	0	0
7	Е	250	Total O 251 251	0	1
7	F	266	Total O 266 266	0	0
7	G	227	Total O 228 228	0	1
7	Н	232	Total O 232 232	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: Mandelate racemase/muconate lactonizing enzyme



• Molecule 1: Mandelate racemase/muconate lactonizing enzyme



• Molecule 1: Mandelate racemase/muconate lactonizing enzyme







## 



• Molecule 1: Mandelate racemase/muconate lactonizing enzyme



• Molecule 1: Mandelate racemase/muconate lactonizing enzyme



#### R276 R279 D280 P281 F281 F281 R280 R285 R386 P362 R367

• Molecule 1: Mandelate racemase/muconate lactonizing enzyme



• Molecule 1: Mandelate racemase/muconate lactonizing enzyme





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	91.03Å 152.82Å 113.03Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $105.20^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	25.68 - 1.70	Depositor
	25.68 - 1.70	EDS
% Data completeness	99.9 (25.68-1.70)	Depositor
(in resolution range)	99.9(25.68-1.70)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$< I/\sigma(I) > 1$	$2.11 (at 1.70 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
B B.	0.159 , $0.192$	Depositor
II, II, <i>free</i>	0.159 , $0.193$	DCC
$R_{free}$ test set	16437 reflections $(5.04\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	18.0	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.39, 56.2	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	24627	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 68.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0650e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: IOD, NI, MPD, 0XW, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bond lengths		Bond angles		
MIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.36	0/2894	0.56	0/3936	
1	В	0.37	0/2893	0.56	1/3936~(0.0%)	
1	С	0.35	0/2865	0.55	0/3899	
1	D	0.35	0/2879	0.54	0/3918	
1	Е	0.34	0/2772	0.55	0/3770	
1	F	0.35	0/2857	0.54	0/3888	
1	G	0.34	0/2865	0.53	0/3899	
1	Н	0.32	0/2868	0.51	0/3902	
All	All	0.35	0/22893	0.54	1/31148~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	212	ASP	CB-CG-OD1	5.27	123.04	118.30

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	2829	0	2785	29	0
1	В	2828	0	2782	27	0



	Chain	Non H	$\mathbf{H}(\mathbf{modol})$	H(addad)	Clashos	Symm Clashes
	Cliain	2800		11(audeu) 9751		Symm-Clashes
1		2800	0	2731	18	0
	D F	2809	0	2108	20	0
		2713	0	2072	20	0
1	F C	2192	0	2740	20	0
1	- G - U	2000	0	2750	29	0
1		2000	0	2138	20	0
	A B	1	0	0	0	0
$\frac{2}{2}$	D C	1	0	0	0	0
$\frac{2}{2}$		1	0	0	0	0
$\frac{2}{2}$	E E	1	0	0	0	0
$\frac{2}{2}$	E F	1	0	0	0	0
2	r C	1	0	0	0	0
	- G - Ц	1	0	0	0	0
		1	0	0	0	0
2	A P	1	0	0	0	0
		1	0	13	0	0
4	R	11	0	13	0	0
4	D C	11	0	13	0	0
4		11	0	13	0	0
4	E E	11	0	13	0	0
4	E F	11	0	13	0	0
4	C I	11	0	13	1	0
4	н Н	11	0	13	2	0
5	Δ	8	0	0	6	0
5	B	6	0	0	2	0
5	C	10	0	0	2	0
5	D	8	0	0	8	0
5	E	7	0	0	6	0
5	F	8	0	0	2	0
5	G	8	0	0	6	0
5	H	6	0	0	7	0
6	С	8	0	14	0	0
6	D	8	0	14	0	0
6	Е	8	0	14	2	0
7	А	275	0	0	5	0
7	В	294	0	0	5	0
7	С	273	0	0	7	0
7	D	251	0	0	5	0
7	Е	251	0	0	8	0
7	F	266	0	0	2	0
7	G	228	0	0	7	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Н	232	0	0	3	0
All	All	24627	0	22154	188	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 (188) 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)	
5:E:406:IOD:I	7:E:693:HOH:O	2.33	1.16	
5:A:407:IOD:I	7:A:663:HOH:O	2.39	1.08	
5:D:406:IOD:I	7:D:638:HOH:O	2.44	1.06	
5:G:404:IOD:I	7:G:614:HOH:O	2.49	1.00	
5:C:405:IOD:I	7:C:709[B]:HOH:O	2.52	0.95	
5:B:408:IOD:I	7:B:787[B]:HOH:O	2.55	0.93	
5:F:403:IOD:I	7:F:667:HOH:O	2.59	0.91	
5:H:404:IOD:I	7:H:645:HOH:O	2.59	0.89	
1:F:21:ARG:HG2	1:F:139:VAL:HB	1.55	0.87	
1:A:254:ALA:HB3	1:A:281[B]:PHE:HZ	1.38	0.87	
1:B:254:ALA:HB3	1:B:281[A]:PHE:HZ	1.41	0.85	
1:D:138:GLY:HA3	5:D:409:IOD:I	2.49	0.83	
1:A:254:ALA:HB3	1:A:281[B]:PHE:CZ	2.16	0.79	
1:C:254:ALA:HB3	1:C:281[B]:PHE:HZ	1.48	0.77	
1:G:254:ALA:HB3	1:G:281[A]:PHE:HZ	1.49	0.77	
1:D:254:ALA:HB3	1:D:281[A]:PHE:HZ	1.48	0.76	
1:G:153:GLN:HG3	1:G:186:THR:HG21	1.68	0.76	
1:C:254:ALA:HB3	1:C:281[B]:PHE:CZ	2.21	0.76	
1:B:254:ALA:HB3	1:B:281[A]:PHE:CZ	2.19	0.76	
1:F:254:ALA:HB3	1:F:281[A]:PHE:HZ	1.51	0.76	
1:E:1:LEU:HD22	1:E:114:ARG:HD3	1.68	0.76	
1:G:254:ALA:HB3	1:G:281[A]:PHE:CZ	2.22	0.75	
1:D:254:ALA:HB3	1:D:281[A]:PHE:CZ	2.21	0.74	
1:E:254:ALA:HB3	1:E:281:PHE:CZ	2.24	0.73	
1:H:254:ALA:HB3	1:H:281[B]:PHE:CZ	2.24	0.73	
1:E:254:ALA:HB3	1:E:281:PHE:HZ	1.52	0.72	
1:A:147:ARG:NH2	1:A:151:GLU:OE2	2.22	0.72	
1:F:254:ALA:HB3	1:F:281[A]:PHE:CZ	2.24	0.72	
1:H:254:ALA:HB3	1:H:281[B]:PHE:HZ	1.55	0.71	
7:A:602:HOH:O	5:E:410:IOD:I	2.80	0.69	
1:D:1:LEU:HD22	1:D:114:ARG:HD3	1.75	0.69	
1:C:254:ALA:O	7:C:518:HOH:O	2.12	0.68	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:D:21:ARG:N	5:D:409:IOD:I	2.92	0.68	
1:A:313:PRO:O	7:A:720:HOH:O	2.11	0.67	
1:A:328:GLU:HG3	1:A:359:ARG:HH22	1.60	0.67	
1:D:17:ASN:N	5:D:410:IOD:I	2.97	0.66	
7:E:591:HOH:O	5:H:408:IOD:I	2.84	0.65	
7:B:609:HOH:O	5:D:405:IOD:I	2.86	0.63	
1:G:317:GLU:OE1	7:G:717:HOH:O	2.15	0.63	
1:E:254:ALA:O	7:E:528:HOH:O	2.15	0.63	
1:D:222:ASN:ND2	7:D:650:HOH:O	2.32	0.63	
1:B:1:LEU:HD22	1:B:114:ARG:HD3	1.79	0.63	
1:E:181:GLU:OE2	1:E:184:ARG:NH1	2.33	0.61	
5:A:404:IOD:I	7:C:549:HOH:O	2.86	0.61	
7:E:691:HOH:O	1:H:286:ASN:HB2	2.01	0.61	
1:E:222:ASN:ND2	7:E:691:HOH:O	2.17	0.60	
1:F:254:ALA:O	7:F:545:HOH:O	2.16	0.60	
1:H:140:MET:HB2	5:H:406:IOD:I	2.72	0.60	
1:E:139:VAL:HG23	5:E:408:IOD:I	2.71	0.59	
1:A:255:ALA:HB3	1:D:255:ALA:HB3	1.85	0.59	
1:C:121:GLU:OE2	1:G:114:ARG:NH2	2.36	0.58	
1:H:184:ARG:NH2	7:H:722:HOH:O	2.36	0.58	
1:G:88:ARG:NH1	5:G:408:IOD:I	3.07	0.57	
1:A:144:GLU:OE2	1:A:147:ARG:NH1	2.27	0.57	
1:E:73:SER:O	7:E:705:HOH:O	2.18	0.56	
7:D:650:HOH:O	1:G:286:ASN:HB2	2.06	0.56	
1:B:328:GLU:OE1	1:B:359:ARG:NH2	2.37	0.56	
1:F:255:ALA:HB2	1:H:251:ILE:HG22	1.88	0.56	
1:A:246:SER:HB2	5:A:405:IOD:I	2.76	0.55	
1:A:177:ARG:HG2	1:A:213:ILE:HD11	1.87	0.55	
1:F:140:MET:HB2	5:F:410:IOD:I	2.77	0.55	
1:A:1:LEU:HD22	1:A:114:ARG:HD3	1.89	0.55	
1:E:113:LYS:HE2	5:E:409:IOD:I	2.76	0.55	
1:C:1:LEU:HD22	1:C:114:ARG:HD3	1.88	0.55	
1:H:141:GLU:CG	5:H:406:IOD:I	3.24	0.55	
1:D:141:GLU:OE1	1:D:143:ASP:N	2.39	0.54	
1:H:141:GLU:HG3	5:H:406:IOD:I	2.78	0.54	
1:D:20:TYR:HA	5:D:409:IOD:I	2.78	0.54	
1:E:113:LYS:NZ	5:E:409:IOD:I	3.08	0.53	
1:C:75:LEU:HD23	1:C:88:ARG:HG2	1.90	0.53	
1:B:255:ALA:HB3	1:E:255:ALA:HB3	1.91	0.53	
1:F:75:LEU:HD23	1:F:88:ARG:HG2	1.91	0.53	
1:A:114:ARG:NH2	1:D:121:GLU:OE2	2.38	0.53	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:328:GLU:OE1	1:B:359:ARG:NH1	2.42	0.52
1:G:183:VAL:O	1:G:186:THR:HB	2.10	0.52
1:D:151:GLU:OE1	1:D:152:LYS:NZ	2.42	0.51
1:C:3:ILE:HG21	1:C:6:ILE:HD11	1.92	0.51
1:G:154:ARG:NH2	7:G:629:HOH:O	2.25	0.51
1:B:255:ALA:HB2	1:E:251:ILE:HG22	1.93	0.51
1:H:141:GLU:HG2	5:H:406:IOD:I	2.81	0.50
1:B:30:LEU:HD13	1:B:295:TRP:NE1	2.27	0.50
1:C:255:ALA:HB3	1:G:255:ALA:HB3	1.93	0.49
1:B:75:LEU:HD23	1:B:88:ARG:HG2	1.93	0.49
1:E:4:ALA:HB2	1:E:40:GLU:HG2	1.94	0.49
1:F:135:TYR:HE2	1:F:137:LEU:HD23	1.78	0.48
1:A:121:GLU:OE2	1:D:114:ARG:NH2	2.46	0.48
1:D:113:LYS:NZ	5:D:411:IOD:I	3.15	0.48
1:A:185:GLY:N	5:A:404:IOD:I	3.11	0.48
1:G:186:THR:HG22	1:G:188[A]:ILE:H	1.78	0.48
1:B:177:ARG:HG2	1:B:213:ILE:HD11	1.95	0.48
1:B:276:ARG:NH1	1:E:280:ASP:OD2	2.39	0.48
1:G:254:ALA:HA	7:G:722:HOH:O	2.14	0.47
7:D:641:HOH:O	5:G:409:IOD:I	2.91	0.47
1:H:75:LEU:HD23	1:H:88:ARG:HG2	1.95	0.47
1:E:344:ARG:NH1	7:E:712:HOH:O	2.47	0.47
1:F:255:ALA:HB3	1:H:255:ALA:CB	2.45	0.47
1:C:359:ARG:NE	7:C:692:HOH:O	2.35	0.47
1:E:224:PHE:CE1	6:E:403:MPD:H13	2.50	0.47
1:G:254:ALA:O	7:G:506:HOH:O	2.21	0.47
1:F:20:TYR:OH	1:F:163:LYS:HE2	2.15	0.46
1:F:254:ALA:HB1	1:F:287:LEU:HD11	1.97	0.46
1:C:11:HIS:NE2	1:C:328:GLU:OE1	2.45	0.46
1:G:186:THR:HG22	1:G:188[B]:ILE:H	1.78	0.46
1:B:233:LEU:HD21	1:D:232:PRO:HA	1.95	0.46
1:E:113:LYS:CE	5:E:409:IOD:I	3.33	0.46
1:H:177:ARG:HG2	1:H:213:ILE:HD11	1.97	0.46
1:A:247[A]:LEU:HB2	5:A:405:IOD:I	2.85	0.46
1:A:255:ALA:HB3	1:D:255:ALA:CB	2.44	0.46
1:H:273:GLN:O	1:H:276:ARG:HG2	2.15	0.46
1:A:233:LEU:HD21	1:E:232:PRO:HA	1.98	0.46
1:F:30:LEU:HD13	1:F:295:TRP:CE2	2.51	0.46
1:C:255:ALA:HB3	1:G:255:ALA:CB	2.46	0.45
1:D:113:LYS:HE2	5:D:411:IOD:I	2.87	0.45
1:G:75:LEU:HD23	1:G:88:ARG:HG2	1.97	0.45



Atom 1 Atom 2		Interatomic	Clash		
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)		
1:A:257:SER:HA	7:A:694:HOH:O	2.16	0.45		
1:C:140:MET:HB2	5:C:412:IOD:I	2.87	0.45		
1:B:254:ALA:O	7:B:528:HOH:O	2.21	0.45		
1:A:140[A]:MET:HE3	1:A:144:GLU:HG3	1.97	0.45		
1:C:257:SER:HA	7:C:623:HOH:O	2.15	0.45		
1:D:181:GLU:HG2	7:D:722:HOH:O	2.16	0.45		
1:B:187:GLY:HA2	5:B:404:IOD:I	2.87	0.45		
1:D:75:LEU:HD23	1:D:88:ARG:HG2	1.98	0.45		
1:E:177:ARG:HG2	1:E:213:ILE:HD11	1.99	0.45		
1:G:152:LYS:HA	1:G:152:LYS:HD3	1.81	0.45		
1:G:140:MET:HB2	5:G:410:IOD:I	2.88	0.44		
1:A:255:ALA:CB	1:D:255:ALA:HB3	2.47	0.44		
6:E:403:MPD:H12	6:E:403:MPD:H4	1.74	0.44		
1:A:251:ILE:HG22	1:D:255:ALA:HB2	1.99	0.44		
1:B:314[A]:ARG:NH1	7:B:751:HOH:O	2.51	0.44		
1:A:39:ALA:HB2	1:A:110:LEU:HD21	1.99	0.44		
1:E:233:LEU:HD21	1:H:232:PRO:HA	2.00	0.44		
1:F:279:ARG:HG3	1:F:311:VAL:HG22	2.00	0.44		
1:B:255:ALA:HB3	1:E:255:ALA:CB	2.48	0.43		
1:F:135:TYR:CD2	1:F:152:LYS:HG3	2.53	0.43		
1:E:135:TYR:CD2	1:E:152:LYS:HG3	2.53	0.43		
1:G:265:LYS:NZ	4:G:402:0XW:H13	2.34	0.43		
1:B:30:LEU:HD13	1:B:295:TRP:CE2	2.53	0.43		
1:E:75:LEU:HD23	1:E:88:ARG:HG2	2.01	0.43		
1:G:141:GLU:HG3	5:G:410:IOD:I	2.89	0.43		
1:H:181:GLU:HG2	7:H:653:HOH:O	2.18	0.43		
1:B:254:ALA:HB1	1:B:287:LEU:HD11	2.01	0.43		
1:B:35:VAL:HG11	1:B:103:LEU:HD23	2.00	0.43		
1:D:254:ALA:HB1	1:D:287:LEU:HD11	2.01	0.43		
1:G:185:GLY:N	5:G:409:IOD:I	3.20	0.43		
1:A:255:ALA:HB2	1:D:251:ILE:HG22	2.01	0.43		
1:A:279:ARG:HG3	1:A:311:VAL:HG22	2.01	0.42		
1:G:257:SER:HA	7:G:722:HOH:O	2.17	0.42		
1:G:336:VAL:HG22	7:G:723:HOH:O	2.19	0.42		
1:B:135:TYR:CD2	1:B:152:LYS:HG3	2.54	0.42		
1:E:254:ALA:HB1	1:E:287:LEU:HD11	2.00	0.42		
1:H:298:ASP:OD2	1:H:329:HIS:HB3	2.19	0.42		
1:D:255:ALA:HA	1:D:285:ARG:NH2	2.33	0.42		
1:F:114:ARG:NH2	1:H:121:GLU:OE2	2.47	0.42		
1:F:254:ALA:HB1	1:F:287:LEU:CD1	2.50	0.42		
1:B:251:ILE:HG22	1:E:255:ALA:HB2	2.01	0.42		



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:254:ALA:HA	7:B:785:HOH:O	2.18	0.42	
1:G:135:TYR:CE2	1:G:152:LYS:HE3	2.55	0.42	
1:H:185:GLY:N	5:H:408:IOD:I	3.16	0.42	
1:H:265:LYS:NZ	4:H:402:0XW:H13	2.35	0.42	
1:F:30:LEU:CD2	1:F:52:VAL:HA	2.49	0.42	
1:A:254:ALA:HB1	1:A:287:LEU:HD11	2.02	0.42	
1:E:265:LYS:NZ	7:E:617:HOH:O	2.40	0.42	
1:F:160:LEU:HG	1:F:188:ILE:HD13	2.01	0.42	
1:B:20:TYR:HB3	1:B:27:VAL:HG13	2.01	0.41	
1:C:255:ALA:HB2	1:G:251:ILE:HG22	2.02	0.41	
1:G:65:LEU:O	1:G:69:GLU:HG3	2.21	0.41	
4:H:402:0XW:O11	4:H:402:0XW:H2	2.20	0.41	
1:F:152:LYS:HA	1:F:152:LYS:HD3	1.87	0.41	
1:G:177:ARG:HG2	1:G:213:ILE:HD11	2.03	0.41	
1:E:144:GLU:OE1	1:E:147:ARG:NH1	2.53	0.41	
1:A:254:ALA:HA	7:A:694:HOH:O	2.20	0.41	
1:B:22:ILE:HG23	1:B:163:LYS:HE3	2.01	0.41	
1:A:30:LEU:HD13	1:A:295:TRP:CE2	2.55	0.41	
1:B:3:ILE:HG23	1:B:37:ILE:HG23	2.02	0.41	
1:F:35:VAL:HG11	1:F:103:LEU:HD23	2.03	0.41	
1:A:21:ARG:H	1:A:21:ARG:HG2	1.58	0.41	
1:C:114:ARG:NH1	7:C:686:HOH:O	2.28	0.41	
1:C:254:ALA:HB1	1:C:287:LEU:HD11	2.02	0.41	
1:D:362:PRO:HA	1:D:363:PRO:HD3	1.92	0.41	
1:H:152:LYS:HA	1:H:152:LYS:HD3	1.97	0.41	
1:C:255:ALA:CB	1:G:255:ALA:HB3	2.51	0.41	
1:D:1:LEU:HD12	1:D:1:LEU:HA	1.88	0.41	
1:G:279:ARG:HG3	1:G:311:VAL:HG22	2.02	0.41	
1:A:138:GLY:O	1:A:140[A]:MET:HG2	2.21	0.40	
1:A:248:ASN:N	5:A:405:IOD:I	3.13	0.40	
1:B:27:VAL:HG21	1:B:30:LEU:HD21	2.02	0.40	
1:B:255:ALA:CB	1:E:255:ALA:HB3	2.50	0.40	
1:C:254:ALA:HA	7:C:623:HOH:O	2.21	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	Percei	ntiles
1	А	371/376~(99%)	367~(99%)	4 (1%)	0	100	100
1	В	370/376~(98%)	365~(99%)	5(1%)	0	100	100
1	С	367/376~(98%)	362~(99%)	5 (1%)	0	100	100
1	D	369/376~(98%)	364~(99%)	5(1%)	0	100	100
1	Е	355/376~(94%)	351~(99%)	4 (1%)	0	100	100
1	F	366/376~(97%)	360~(98%)	6~(2%)	0	100	100
1	G	367/376~(98%)	362~(99%)	5 (1%)	0	100	100
1	Н	367/376~(98%)	363~(99%)	4 (1%)	0	100	100
All	All	2932/3008~(98%)	2894 (99%)	38 (1%)	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	292/294~(99%)	289~(99%)	3~(1%)	76 67		
1	В	291/294~(99%)	290 (100%)	1 (0%)	92 89		
1	С	288/294~(98%)	286~(99%)	2(1%)	84 77		
1	D	290/294~(99%)	289 (100%)	1 (0%)	92 89		
1	Ε	281/294~(96%)	278~(99%)	3~(1%)	73 63		
1	F	287/294~(98%)	283 (99%)	4 (1%)	67 53		



Mol	Chain	Analysed	Rotameric	Outliers	Percentil		
1	G	288/294~(98%)	284~(99%)	4 (1%)	67	53	
1	Н	288/294~(98%)	288 (100%)	0	100	100	
All	All	2305/2352~(98%)	2287~(99%)	18 (1%)	81	74	

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	12	ASP
1	А	21	ARG
1	А	328	GLU
1	В	21	ARG
1	С	12	ASP
1	С	344	ARG
1	D	104	ASP
1	Е	52	VAL
1	Е	104	ASP
1	Е	160	LEU
1	F	21	ARG
1	F	104	ASP
1	F	276	ARG
1	F	359	ARG
1	G	88	ARG
1	G	104	ASP
1	G	160	LEU
1	G	186	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	273	GLN
1	F	17	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 82 ligands modelled in this entry, 71 are monoatomic - leaving 11 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			Chain Bog		B	Bond lengths			Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
4	0XW	D	402	2	9,11,11	1.98	2 (22%)	8,17,17	2.75	3 (37%)	
4	0XW	В	403	2	9,11,11	1.99	2 (22%)	8,17,17	2.78	3 (37%)	
4	0XW	Н	402	2	9,11,11	1.98	2 (22%)	8,17,17	2.87	3 (37%)	
4	0XW	А	403	2	9,11,11	2.11	2 (22%)	8,17,17	2.38	3 (37%)	
4	0XW	G	402	2	9,11,11	2.04	2 (22%)	8,17,17	2.49	3 (37%)	
4	0XW	С	402	2	9,11,11	2.00	3 (33%)	8,17,17	2.87	3 (37%)	
6	MPD	С	403	-	7,7,7	0.25	0	9,10,10	0.78	1 (11%)	
6	MPD	D	403	-	7,7,7	0.27	0	9,10,10	0.62	0	
4	0XW	F	402	2	9,11,11	2.06	3 (33%)	8,17,17	2.52	<mark>3 (37%)</mark>	
6	MPD	Е	403	-	7,7,7	0.30	0	9,10,10	0.59	0	
4	0XW	E	402	2	9,11,11	1.94	2 (22%)	8,17,17	2.64	3 (37%)	

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	0XW	D	402	2	-	3/4/19/19	0/1/1/1
4	0XW	В	403	2	-	3/4/19/19	0/1/1/1
4	0XW	Н	402	2	-	3/4/19/19	0/1/1/1
4	0XW	А	403	2	-	3/4/19/19	0/1/1/1
4	0XW	G	402	2	-	3/4/19/19	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	0XW	С	402	2	-	3/4/19/19	0/1/1/1
6	MPD	С	403	-	-	2/5/5/5	-
6	MPD	D	403	-	-	3/5/5/5	-
4	0XW	F	402	2	-	4/4/19/19	0/1/1/1
6	MPD	Е	403	-	-	4/5/5/5	-
4	0XW	Е	402	2	-	2/4/19/19	0/1/1/1

All	(18)	bond	length	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	403	0XW	C07-C05	-3.58	1.45	1.52
4	F	402	0XW	C07-C05	-3.43	1.46	1.52
4	А	403	0XW	C07-C08	3.38	1.61	1.53
4	G	402	0XW	C07-C05	-3.37	1.46	1.52
4	F	402	0XW	C07-C08	3.34	1.61	1.53
4	Н	402	0XW	C07-C08	3.34	1.61	1.53
4	С	402	0XW	C07-C08	3.34	1.61	1.53
4	В	403	0XW	C07-C05	-3.33	1.46	1.52
4	G	402	0XW	C07-C08	3.31	1.60	1.53
4	В	403	0XW	C07-C08	3.28	1.60	1.53
4	D	402	0XW	C07-C08	3.27	1.60	1.53
4	Ε	402	0XW	C07-C08	3.26	1.60	1.53
4	С	402	0XW	C07-C05	-3.25	1.46	1.52
4	D	402	0XW	C07-C05	-3.20	1.46	1.52
4	Н	402	0XW	C07-C05	-3.12	1.46	1.52
4	Ε	402	0XW	C07-C05	-3.10	1.46	1.52
4	F	402	0XW	C04-C05	-2.06	1.49	1.53
4	C	402	0XW	C04-C05	-2.05	1.49	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
4	Н	402	0XW	O06-C05-C07	6.29	125.60	110.03
4	С	402	0XW	O06-C05-C07	6.16	125.28	110.03
4	G	402	0XW	O06-C05-C07	6.15	125.24	110.03
4	Е	402	0XW	O06-C05-C07	6.08	125.07	110.03
4	D	402	0XW	O06-C05-C07	6.06	125.02	110.03
4	F	402	0XW	O06-C05-C07	5.81	124.41	110.03
4	В	403	0XW	O06-C05-C07	5.68	124.08	110.03
4	А	403	0XW	O06-C05-C07	5.42	123.43	110.03
4	В	403	0XW	O11-C09-C08	4.53	122.63	111.87



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	С	402	0XW	O11-C09-C08	4.38	122.27	111.87
4	Н	402	0XW	O11-C09-C08	4.34	122.17	111.87
4	D	402	0XW	O11-C09-C08	4.06	121.51	111.87
4	Е	402	0XW	O11-C09-C08	3.27	119.64	111.87
4	А	403	0XW	O11-C09-C08	3.01	119.02	111.87
4	F	402	0XW	O11-C09-C08	2.95	118.88	111.87
4	F	402	0XW	O11-C09-O10	-2.74	117.86	124.09
4	Е	402	0XW	O11-C09-O10	-2.70	117.95	124.09
4	В	403	0XW	O11-C09-O10	-2.65	118.06	124.09
4	С	402	0XW	O11-C09-O10	-2.61	118.16	124.09
4	G	402	0XW	O11-C09-C08	2.49	117.77	111.87
4	D	402	0XW	O11-C09-O10	-2.43	118.58	124.09
4	А	403	0XW	O11-C09-O10	-2.42	118.60	124.09
4	Н	402	0XW	O11-C09-O10	-2.28	118.92	124.09
4	G	402	0XW	O11-C09-O10	-2.16	119.17	124.09
6	C	403	MPD	CM-C2-C1	-2.01	106.39	110.57

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	403	0XW	C07-C08-C09-O10
4	А	403	0XW	C07-C08-C09-O11
4	С	402	0XW	N02-C08-C09-O11
4	F	402	0XW	C07-C08-C09-O10
4	F	402	0XW	C07-C08-C09-O11
4	G	402	0XW	C07-C08-C09-O10
4	G	402	0XW	C07-C08-C09-O11
6	С	403	MPD	C2-C3-C4-O4
6	С	403	MPD	C2-C3-C4-C5
6	D	403	MPD	C1-C2-C3-C4
6	D	403	MPD	O2-C2-C3-C4
6	Ε	403	MPD	C1-C2-C3-C4
6	Е	403	MPD	O2-C2-C3-C4
6	Е	403	MPD	C2-C3-C4-O4
4	С	402	0XW	C07-C08-C09-O10
4	С	402	0XW	C07-C08-C09-O11
4	Е	402	0XW	C07-C08-C09-O10
4	Е	402	0XW	C07-C08-C09-O11
4	В	403	0XW	N02-C08-C09-O11
4	В	403	0XW	C07-C08-C09-O10
4	В	403	0XW	C07-C08-C09-O11



Mol	Chain	Res	Type	Atoms
4	D	402	0XW	C07-C08-C09-O11
4	Η	402	0XW	C07-C08-C09-O10
4	Н	402	0XW	C07-C08-C09-O11
4	D	402	0XW	C07-C08-C09-O10
6	Ε	403	MPD	C2-C3-C4-C5
6	D	403	MPD	CM-C2-C3-C4
4	А	403	0XW	N02-C08-C09-O11
4	D	402	0XW	N02-C08-C09-O11
4	F	402	0XW	N02-C08-C09-O11
4	Н	402	0XW	N02-C08-C09-O11
4	F	402	0XW	N02-C08-C09-O10
4	G	402	0XW	N02-C08-C09-O11

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There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Н	402	0XW	2	0
4	G	402	0XW	1	0
6	Е	403	MPD	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)

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 $>$	# <b>RSRZ</b> >2	2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	368/376~(97%)	-0.15	15 (4%) 37	41	9,17,39,78	0
1	В	367/376~(97%)	-0.15	14 (3%) 40	45	9, 17, 42, 73	0
1	С	367/376~(97%)	-0.17	17 (4%) 32	36	10, 19, 39, 74	0
1	D	367/376~(97%)	-0.11	21 (5%) 23	26	9, 19, 41, 68	0
1	Е	355/376~(94%)	-0.18	9 (2%) 57	61	10, 20, 39, 47	0
1	F	367/376~(97%)	-0.10	18 (4%) 29	33	9, 19, 44, 86	0
1	G	367/376~(97%)	0.06	16 (4%) 34	38	12, 25, 46, 72	0
1	Н	367/376~(97%)	-0.03	12 (3%) 46	51	11, 23, 44, 73	0
All	All	2925/3008~(97%)	-0.10	122 (4%) 36	40	9, 20, 42, 86	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	28	TRP	9.5
1	D	28	TRP	9.1
1	С	28	TRP	8.6
1	В	28	TRP	7.7
1	С	18	GLY	7.0
1	F	18	GLY	6.7
1	С	17	ASN	6.4
1	D	18	GLY	6.3
1	А	28	TRP	6.0
1	F	17	ASN	5.8
1	G	28	TRP	5.8
1	F	25	GLY	5.8
1	F	19	PRO	5.5
1	D	17	ASN	5.5
1	В	23	ALA	5.4
1	Н	28	TRP	5.4



Mol	Chain	Res	Type	RSRZ
1	С	27	VAL	5.1
1	В	22	ILE	5.1
1	Е	15	VAL	4.9
1	D	23	ALA	4.9
1	D	19	PRO	4.8
1	В	27	VAL	4.7
1	В	18	GLY	4.7
1	F	23	ALA	4.6
1	Ε	16	VAL	4.5
1	С	15	VAL	4.4
1	D	15	VAL	4.4
1	А	23	ALA	4.4
1	F	29	SER	4.4
1	D	27	VAL	4.3
1	A	17	ASN	4.2
1	С	19	PRO	4.1
1	А	27	VAL	4.1
1	С	254	ALA	4.1
1	F	15	VAL	4.0
1	А	22	ILE	3.9
1	F	26	ASP	3.9
1	В	15	VAL	3.8
1	Н	254	ALA	3.8
1	D	327	ALA	3.8
1	В	24	SER	3.7
1	В	25	GLY	3.7
1	В	17	ASN	3.6
1	А	24	SER	3.6
1	D	14	PRO	3.6
1	В	19	PRO	3.6
1	G	42	GLY	3.6
1	F	21	ARG	3.6
1	А	26	ASP	3.5
1	А	20	TYR	3.4
1	В	20	TYR	3.4
1	А	19	PRO	3.3
1	D	16	VAL	3.3
1	G	105	ILE	3.3
1	С	26	ASP	3.3
1	В	26	ASP	3.3
1	A	0	SER	3.2
1	D	25	GLY	3.2



Mol	Chain	Res	Type	RSRZ	
1	F	254	ALA	3.2	
1	G	23	ALA	3.2	
1	Н	19	PRO	3.1	
1	С	25	GLY	3.1	
1	G	328	GLU	3.1	
1	Н	105	ILE	3.1	
1	F	14	PRO	3.1	
1	G	17	ASN	3.1	
1	А	21	ARG	3.1	
1	А	15	VAL	3.0	
1	D	29	SER	3.0	
1	Е	254	ALA	2.9	
1	D	26	ASP	2.9	
1	F	27	VAL	2.9	
1	D	20	TYR	2.9	
1	D	255	ALA	2.8	
1	G	18	GLY	2.8	
1	Н	358	GLU	2.8	
1	G	358	GLU	2.7	
1	С	21	ARG	2.7	
1	В	254	ALA	2.7	
1	F	16	VAL	2.7	
1	G	354	THR	2.7	
1	Н	154	ARG	2.7	
1	Е	14	PRO	2.7	
1	С	23	ALA	2.6	
1	G	254	ALA	2.6	
1	А	18	GLY	2.6	
1	А	254	ALA	2.6	
1	Н	18	GLY	2.5	
1	D	1	LEU	2.5	
1	E	30	LEU	2.5	
1	E	105	ILE	2.5	
1	D	22	ILE	2.5	
1	E	166	ALA	2.4	
1	С	41	ASP	2.4	
1	С	24	SER	2.4	
1	F	24	SER	2.4	
1	Н	327	ALA	2.4	
1	Н	17	ASN	2.4	
1	G	185	GLY	2.4	
1	D	344	ARG	2.4	



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Mol	Chain	Res	Type	RSRZ
1	F	22	ILE	2.3
1	G	327	ALA	2.3
1	Н	35	VAL	2.3
1	G	41	ASP	2.3
1	В	21	ARG	2.3
1	Е	56	TYR	2.2
1	G	40	GLU	2.2
1	С	255	ALA	2.2
1	С	1	LEU	2.2
1	D	256	THR	2.2
1	D	24	SER	2.1
1	А	25	GLY	2.1
1	С	40	GLU	2.1
1	D	21	ARG	2.1
1	С	29	SER	2.1
1	F	362	PRO	2.1
1	Н	41	ASP	2.1
1	Е	53	GLY	2.0
1	Н	344	ARG	2.0
1	G	107	VAL	2.0
1	G	216	VAL	2.0
1	F	256	THR	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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
5	IOD	С	411	1/1	0.72	0.12	62,62,62,62	1



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
6	MPD	D	403	8/8	0.72	0.17	43,48,49,50	0
5	IOD	Н	407	1/1	0.74	0.13	73,73,73,73	1
5	IOD	D	410	1/1	0.77	0.28	91,91,91,91	1
5	IOD	Н	406	1/1	0.81	0.14	64,64,64,64	1
6	MPD	Е	403	8/8	0.83	0.13	32,45,48,50	0
5	IOD	С	413	1/1	0.84	0.17	79,79,79,79	1
6	MPD	С	403	8/8	0.86	0.15	32,35,39,40	0
4	0XW	G	402	11/11	0.87	0.15	23,36,41,42	0
4	0XW	Е	402	11/11	0.88	0.12	39,40,45,49	0
5	IOD	А	410	1/1	0.88	0.10	69,69,69,69	1
5	IOD	G	410	1/1	0.90	0.15	66,66,66,66	1
4	0XW	F	402	11/11	0.90	0.11	29,35,40,40	0
4	0XW	С	402	11/11	0.90	0.14	23,38,45,47	0
5	IOD	С	412	1/1	0.90	0.21	$65,\!65,\!65,\!65$	1
4	0XW	Н	402	11/11	0.90	0.13	27,39,45,48	0
5	IOD	А	408	1/1	0.90	0.07	52,52,52,52	1
5	IOD	Е	407	1/1	0.91	0.07	50,50,50,50	1
4	0XW	В	403	11/11	0.92	0.10	24,28,31,32	0
5	IOD	D	409	1/1	0.92	0.11	77,77,77,77	1
4	0XW	D	402	11/11	0.93	0.14	24,38,43,45	0
5	IOD	G	406	1/1	0.93	0.10	64,64,64,64	1
5	IOD	G	408	1/1	0.93	0.17	76,76,76,76	1
5	IOD	A	409	1/1	0.93	0.10	$57,\!57,\!57,\!57$	1
5	IOD	Н	405	1/1	0.93	0.05	$35,\!35,\!35,\!35$	1
5	IOD	D	408	1/1	0.94	0.10	49,49,49,49	1
5	IOD	В	409	1/1	0.94	0.15	83,83,83,83	1
4	0XW	А	403	11/11	0.94	0.10	$25,\!29,\!31,\!32$	0
5	IOD	В	404	1/1	0.94	0.04	46,46,46,46	1
5	IOD	В	407	1/1	0.94	0.05	$53,\!53,\!53,\!53$	1
5	IOD	D	404	1/1	0.94	0.04	46,46,46,46	1
5	IOD	G	409	1/1	0.94	0.04	52,52,52,52	1
5	IOD	F	410	1/1	0.95	0.20	49,49,49,49	1
5	IOD	G	405	1/1	0.95	0.04	34,34,34,34	1
5	IOD	С	404	1/1	0.95	0.05	34,34,34,34	1
5	IOD	E	410	1/1	0.96	0.04	47,47,47,47	1
5	IOD	F	404	1/1	0.96	0.05	$35,\!35,\!35,\!35$	1
5	IOD	F	405	1/1	0.96	0.04	41,41,41,41	1
5	IOD	A	404	1/1	0.96	0.07	44,44,44,44	1
5	IOD	E	409	1/1	0.96	0.05	40,40,40,40	1
5	IOD	F	406	1/1	0.97	0.04	31,31,31,31	1
2	MG	E	401	1/1	0.97	0.05	18,18,18,18	0
5	IOD	C	408	1/1	$0.9\overline{7}$	0.05	40,40,40,40	1



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9	
5	IOD	D	405	1/1	0.97	0.03	41,41,41,41	1	
5	IOD	G	407	1/1	0.97	0.13	47,47,47,47	1	
5	IOD	Е	404	1/1	0.97	0.03	45,45,45,45	1	
5	IOD	Е	406	1/1	0.97	0.07	29,29,29,29	1	
5	IOD	А	405	1/1	0.98	0.04	30,30,30,30	1	
5	IOD	С	409	1/1	0.98	0.04	23,23,23,23	1	
5	IOD	Е	408	1/1	0.98	0.15	$65,\!65,\!65,\!65$	1	
5	IOD	С	410	1/1	0.98	0.03	34,34,34,34	1	
5	IOD	Н	408	1/1	0.98	0.03	45,45,45,45	1	
5	IOD	А	406	1/1	0.98	0.04	23,23,23,23	1	
2	MG	F	401	1/1	0.98	0.03	15,15,15,15	0	
5	IOD	С	406	1/1	0.98	0.03	29,29,29,29	1	
5	IOD	F	403	1/1	0.99	0.03	27,27,27,27	1	
5	IOD	В	405	1/1	0.99	0.03	23,23,23,23	1	
5	IOD	В	406	1/1	0.99	0.03	25,25,25,25	1	
2	MG	В	401	1/1	0.99	0.05	$15,\!15,\!15,\!15$	0	
5	IOD	F	407	1/1	0.99	0.03	27,27,27,27	1	
5	IOD	F	408	1/1	0.99	0.05	$19,\!19,\!19,\!19$	1	
5	IOD	F	409	1/1	0.99	0.03	24,24,24,24	1	
5	IOD	В	408	1/1	0.99	0.04	22,22,22,22	1	
5	IOD	G	403	1/1	0.99	0.03	30,30,30,30	1	
5	IOD	G	404	1/1	0.99	0.03	23,23,23,23	1	
5	IOD	D	406	1/1	0.99	0.05	18,18,18,18	1	
5	IOD	D	407	1/1	0.99	0.04	28,28,28,28	1	
2	MG	G	401	1/1	0.99	0.03	17,17,17,17	0	
5	IOD	А	407	1/1	0.99	0.04	20,20,20,20	1	
5	IOD	С	405	1/1	0.99	0.04	23,23,23,23	1	
5	IOD	D	411	1/1	0.99	0.04	39,39,39,39	1	
5	IOD	Н	403	1/1	0.99	0.03	27,27,27,27	1	
2	MG	Н	401	1/1	0.99	0.03	16,16,16,16	0	
5	IOD	Е	405	1/1	0.99	0.03	29,29,29,29	1	
5	IOD	С	407	1/1	0.99	0.03	23,23,23,23	1	
2	MG	С	401	1/1	0.99	0.04	14,14,14,14	0	
2	MG	D	401	1/1	0.99	0.03	$17,\!17,\!17,\!17$	0	
5	IOD	А	411	1/1	0.99	0.03	31,31,31,31	1	
2	MG	А	401	1/1	0.99	0.04	14,14,14,14	0	
3	NI	В	402	1/1	1.00	0.02	12,12,12,12	1	
5	IOD	Н	404	1/1	1.00	0.03	22,22,22,22	1	
3	NI	А	402	1/1	1.00	0.02	12,12,12,12	1	



## 6.5 Other polymers (i)

There are no such residues in this entry.

