

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

Feb 25, 2024 – 05:26 AM EST

PDB ID	:	5CH7
Title	:	Crystal structure of the perchlorate reductase PcrAB - Phe164 gate switch
		intermediate - from Azospira suillum PS
Authors	:	Tsai, CL.; Tainer, J.A.
Deposited on	:	2015-07-10
Resolution	:	2.20  Å(reported)

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

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

The 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
$\mathrm{EDS}$	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 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 2.20 Å.

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



Motria	Whole archive	Similar resolution				
wietric	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$				
$R_{free}$	130704	4898 (2.20-2.20)				
Clashscore	141614	5594(2.20-2.20)				
Ramachandran outliers	138981	5503 (2.20-2.20)				
Sidechain outliers	138945	5504 (2.20-2.20)				
RSRZ outliers	127900	4800 (2.20-2.20)				

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	899	% • •	9%
			3%	570 •
1	С	899	85%	14% ••
1	Ε	899	87%	11% •
2	В	333	% 92%	7% •
2	D	333	8%	19% ••



Mol	Chain	Length	Quality of chain		
2	F	333	87%	11%	·



## 2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 31660 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		Α	toms			ZeroOcc	AltConf	Trace
1	Δ	804	Total	С	Ν	Ο	$\mathbf{S}$	0	2	0
	094	7180	4586	1246	1310	38	0	5		
1	C	801	Total	С	Ν	Ο	S	0	1	0
1		091	7151	4568	1239	1306	38	0		
1	F	802	Total	С	Ν	Ο	S	0	2	0
1		892	7171	4583	1240	1310	38	U	ാ	0

• Molecule 1 is a protein called DMSO reductase family type II enzyme, molybdopterin subunit.

• Molecule 2 is a protein called DMSO reductase family type II enzyme, iron-sulfur subunit.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	В	200	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
2 D	529	2564	1627	447	465	25	0	0		
0	р	207	Total	С	Ν	0	S	0	0	0
	D	321	2547	1616	444	463	24	0		
0	Б	200	Total	С	Ν	0	S	0	2	0
	320	2568	1631	448	465	24	0	2	0	

• Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	TotalFeS844	0	0
3	В	1	TotalFeS844	0	0
3	В	1	TotalFeS844	0	0
3	В	1	TotalFeS844	0	0
3	С	1	Total Fe S 8 4 4	0	0
3	D	1	TotalFeS844	0	0
3	D	1	TotalFeS844	0	0
3	D	1	TotalFeS844	0	0
3	Ε	1	Total Fe S 8 4 4	0	0
3	F	1	Total Fe S 8 4 4	0	0
3	F	1	TotalFeS844	0	0
3	F	1	TotalFeS844	0	0

• Molecule 4 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Mo 1 1	0	0
4	С	1	Total Mo 1 1	0	0
4	Е	1	Total Mo 1 1	0	0

• Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues		Atoms					ZeroOcc	AltConf
5	А	1	Total 47	C 20	N 10	0 13	Р 2	${ m S} { m 2}$	0	0
5	С	1	Total 47	C 20	N 10	O 13	Р 2	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0
5	Е	1	Total 47	C 20	N 10	O 13	Р 2	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 6 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).





Mol	Chain	Residues		Atoms					ZeroOcc	AltConf
6	6 1	1	Total	С	Ν	Ο	Р	$\mathbf{S}$	0	0
0 A	L	47	20	10	13	2	2	0	0	
6	6 C	1	Total	С	Ν	Ο	Р	S	0	0
0			47	20	10	13	2	2		0
6	6 E	1	Total	С	Ν	Ο	Р	S	0	0
0		1	<sup>1</sup> 47	20	10	13	2	2		U

• Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	Ε	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	Ε	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	Е	1	$\begin{array}{ccc} \overline{\text{Total}} & \mathcal{C} & \mathcal{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \overline{\text{Total}} & \mathcal{C} & \mathcal{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \overline{\text{Total}} & \mathrm{C} & \mathrm{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	Total Na 1 1	0	0
8	С	1	Total Na 1 1	0	0
8	Е	1	Total Na 1 1	0	0
8	F	1	Total Na 1 1	0	0



• Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	Total Zn 1 1	0	0
9	С	1	Total Zn 1 1	0	0
9	Ε	1	Total Zn 1 1	0	0

• Molecule 10 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
10	А	1	Total 6	${ m C} { m 3}$	O 3	0	0

• Molecule 11 is SULFITE ION (three-letter code: SO3) (formula:  $O_3S$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
11	Δ	1	Total O S	0	0	
11	Л	1	4 3 1	0	0	
11	Δ	1	Total O S	0	0	
11	Л	1	4 3 1	0	0	
11	С	1	Total O S	0	0	
11	U	1	4 3 1	0	0	
11	С	1	Total O S	0	0	
11	U	1	4 3 1	0	0	
11	F	1	Total O S	0	0	
	L'	1	4 3 1		0	

• Molecule 12 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe $_3S_4$ ).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
12	В	1	Total 7	Fe 3	$\frac{S}{4}$	0	0
12	D	1	Total 7	Fe 3	S 4	0	0
12	F	1	Total 7	Fe 3	$\frac{S}{4}$	0	0

• Molecule 13 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{C} \\ 4 & 2 & 2 \end{array}$	О 2	0	0

• Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	А	531	Total O 531 531	0	0
14	В	273	Total         O           273         273	0	0
14	С	362	Total         O           362         362	0	0
14	D	92	Total         O           92         92	0	0
14	Е	520	Total O 520 520	0	0
14	F	198	Total O 198 198	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: DMSO reductase family type II enzyme, molybdopterin subunit











## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	132.88Å 175.67Å 193.28Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	48.38 - 2.20	Depositor
Resolution (A)	48.38 - 2.20	EDS
% Data completeness	99.9 (48.38-2.20)	Depositor
(in resolution range)	99.9 (48.38-2.20)	EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.33 (at 2.20 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
P. P.	0.178 , $0.233$	Depositor
$n, n_{free}$	0.179 , $0.233$	DCC
$R_{free}$ test set	11303  reflections  (4.95%)	wwPDB-VP
Wilson B-factor $(Å^2)$	29.6	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , $42.1$	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	0.95	EDS
Total number of atoms	31660	wwPDB-VP
Average B, all atoms $(Å^2)$	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.

<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: SO3, MGD, MO, NA, F3S, SF4, GOL, EDO, MD1, ZN, ACT

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

Mal	Chain	Bond lengths		Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.56	0/7399	0.65	2/10039~(0.0%)	
1	С	0.50	0/7364	0.61	1/9993~(0.0%)	
1	Е	0.56	0/7391	0.64	2/10030~(0.0%)	
2	В	0.60	0/2632	0.67	1/3567~(0.0%)	
2	D	0.43	0/2615	0.59	0/3546	
2	F	0.55	0/2642	0.65	0/3580	
All	All	0.54	0/30043	0.63	6/40755~(0.0%)	

There are no bond length outliers.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	830	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	Е	830	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	А	830	ARG	NE-CZ-NH1	5.89	123.25	120.30
2	В	117	ASP	CB-CG-OD1	5.62	123.36	118.30
1	Е	830	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	С	830	ARG	NE-CZ-NH2	-5.15	117.73	120.30

All (6) bond angle outliers are listed below:

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	7180	0	7003	61	0
1	С	7151	0	6964	80	0
1	Е	7171	0	6984	73	0
2	В	2564	0	2534	14	0
2	D	2547	0	2513	45	0
2	F	2568	0	2546	27	0
3	А	8	0	0	0	0
3	В	24	0	0	0	0
3	С	8	0	0	0	0
3	D	24	0	0	1	0
3	Е	8	0	0	0	0
3	F	24	0	0	1	0
4	А	1	0	0	0	0
4	С	1	0	0	0	0
4	Ε	1	0	0	0	0
5	А	47	0	21	2	0
5	С	47	0	20	2	0
5	Ε	47	0	20	0	0
6	А	47	0	22	1	0
6	С	47	0	22	1	0
6	Ε	47	0	22	1	0
7	А	16	0	24	1	0
7	В	12	0	18	1	0
7	С	8	0	12	0	0
7	D	8	0	12	0	0
7	Е	12	0	18	2	0
7	F	8	0	12	0	0
8	А	1	0	0	0	0
8	С	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	А	1	0	0	0	0
9	С	1	0	0	0	0
9	Е	1	0	0	0	0
10	А	6	0	8	1	0
11	А	8	0	0	0	0
11	С	8	0	0	0	0
11	Е	4	0	0	0	0
12	В	7	0	0	0	0
12	D	7	0	0	0	0
12	F	7	0	0	0	0
13	С	4	0	3	0	0
14	А	531	0	0	5	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	В	273	0	0	1	0
14	С	362	0	0	7	0
14	D	92	0	0	1	0
14	Е	520	0	0	12	0
14	F	198	0	0	2	0
All	All	31660	0	28778	291	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 5.

All (291) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + amo 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:89:ARG:NH1	14:A:1101:HOH:O	1.94	1.01
1:E:226:VAL:HG22	1:E:241:LYS:HB3	1.56	0.87
1:E:308:ASN:HB3	1:E:311:THR:HG22	1.59	0.83
1:A:482:ARG:HB3	1:A:523:MET:HE3	1.65	0.79
1:E:860:ASN:HD22	1:E:878:ALA:H	1.32	0.77
2:B:245:PRO:HB2	2:B:254:PRO:HG2	1.69	0.74
1:C:881:GLN:HE22	1:C:882:ARG:HE	1.35	0.73
1:A:54:GLU:HG2	1:A:585:TYR:OH	1.90	0.72
1:E:695:LYS:NZ	14:E:1102:HOH:O	2.14	0.70
2:D:166:HIS:HB3	2:D:169:LYS:HB2	1.71	0.70
1:A:898:SER:O	1:E:512:ARG:NH1	2.23	0.70
1:C:197:ILE:HB	1:C:225:ILE:HG12	1.74	0.68
1:C:665:ASP:OD2	14:C:1101:HOH:O	2.11	0.68
1:E:358:GLY:O	14:E:1101:HOH:O	2.12	0.68
2:D:245:PRO:HB2	2:D:254:PRO:HG2	1.74	0.68
1:E:195:LYS:HD2	1:E:414:LYS:O	1.94	0.67
2:F:245:PRO:HB2	2:F:254:PRO:HG2	1.76	0.67
1:A:881:GLN:NE2	1:A:882:ARG:HE	1.93	0.67
1:A:62:PRO:HD3	10:A:1010:GOL:H11	1.76	0.66
1:C:512:ARG:NH1	1:E:898:SER:O	2.28	0.66
1:C:860:ASN:HD22	1:C:878:ALA:H	1.41	0.66
1:E:462:LYS:NZ	7:E:1006:EDO:H21	2.11	0.65
1:A:357:GLU:OE2	1:A:380:LYS:HE2	1.96	0.65
1:E:881:GLN:HE22	1:E:882:ARG:HE	1.44	0.65
1:A:860:ASN:HD22	1:A:878:ALA:H	1.44	0.65
1:A:89:ARG:HH11	1:A:89:ARG:HG2	1.61	0.65
2:D:140:CYS:HB3	2:D:252:THR:O	1.97	0.65
1:E:373:ARG:HA	14:E:1101:HOH:O	1.97	0.64



A + a 1		Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance $(\text{\AA})$		
1:E:231:ASP:OD1	1:E:830:ARG:NH2	2.30	0.63	
2:D:227:ASP:OD1	2:D:228:ASP:N	2.31	0.63	
2:D:135:ARG:NH2	2:D:182:TYR:O	2.31	0.63	
2:D:231:SER:HB3	2:D:233:VAL:HG22	1.81	0.63	
1:A:601:MET:HE1	1:A:684:ILE:HG23	1.80	0.62	
2:F:166:HIS:CE1	2:F:168:ASP:HB2	2.34	0.62	
2:D:295:ASP:OD1	2:D:296:VAL:N	2.33	0.62	
1:A:89:ARG:NH2	1:A:586:GLU:OE1	2.32	0.61	
1:C:464:ALA:HB3	1:C:694:PHE:CE1	2.34	0.61	
1:C:54:GLU:HG2	1:C:585:TYR:OH	2.01	0.61	
2:D:240:TYR:OH	2:D:314:ASP:OD2	2.19	0.61	
1:C:791:MET:HG2	1:C:831:VAL:HG12	1.83	0.60	
1:A:881:GLN:HE22	1:A:882:ARG:HE	1.50	0.60	
1:E:359:LYS:HA	14:E:1101:HOH:O	2.00	0.60	
2:F:301:GLN:O	2:F:305:GLU:HG3	2.01	0.60	
1:A:231:ASP:OD1	1:A:830:ARG:NH2	2.35	0.60	
1:A:89:ARG:HH11	1:A:89:ARG:CG	2.15	0.60	
2:F:69:LYS:HE3	2:F:74:GLN:HG3	1.84	0.59	
1:C:690:LYS:NZ	14:C:1108:HOH:O	2.35	0.59	
1:C:306:PHE:HZ	1:C:352:LEU:HD13	1.68	0.59	
1:C:693:ARG:HH12	1:C:702:LEU:HG	1.67	0.59	
2:D:238:LYS:NZ	2:D:241:LYS:HE3	2.18	0.59	
1:E:462:LYS:HZ3	7:E:1006:EDO:H21	1.66	0.59	
1:C:480:LYS:NZ	14:C:1110:HOH:O	2.37	0.58	
1:C:366:ASP:HB3	1:C:368:LYS:H	1.67	0.58	
1:E:264:GLU:OE2	1:E:408:ARG:NH2	2.29	0.57	
1:C:226:VAL:HG22	1:C:241:LYS:HB3	1.87	0.56	
2:F:137:CYS:HB3	2:F:197:CYS:HB3	1.85	0.56	
1:E:227:SER:HB2	1:E:239:VAL:HG11	1.87	0.56	
1:C:683:THR:HG23	1:C:686:MET:H	1.70	0.56	
1:C:685:GLN:NE2	1:C:689:GLU:OE2	2.38	0.56	
2:D:73:LEU:HD21	2:D:148:ALA:HB2	1.87	0.56	
2:B:140:CYS:HB3	2:B:252:THR:O	2.06	0.56	
1:E:860:ASN:HB3	1:E:877:PRO:HA	1.88	0.56	
2:F:166:HIS:HE1	2:F:168:ASP:HB2	1.70	0.56	
1:A:170:ASP:HB3	1:A:458:ILE:HD13	1.88	0.56	
1:C:683:THR:HG22	1:C:686:MET:HG3	1.87	0.56	
1:E:27:LYS:HE3	1:E:43:PHE:CD2	2.41	0.56	
1:E:259:HIS:CE1	1:E:384:MET:HA	2.41	0.56	
1:A:631:LYS:NZ	1:A:636:GLU:OE1	2.40	0.55	
1:E:644:LYS:NZ	14:E:1116:HOH:O	2.38	0.55	



A + a 1		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
2:D:156:LYS:NZ	2:D:161:GLY:O	2.40	0.55	
1:C:89:ARG:NH1	14:C:1115:HOH:O	2.41	0.54	
1:E:270:HIS:NE2	1:E:349:LEU:HD23	2.22	0.54	
1:C:9:PHE:N	1:C:12:SER:HG	2.05	0.54	
2:D:275:SER:OG	2:D:276:THR:N	2.41	0.54	
1:E:76:LYS:HE3	1:E:766:ARG:O	2.07	0.54	
1:A:683:THR:OG1	1:A:686:MET:HG3	2.08	0.54	
1:C:703:LYS:HB2	1:C:706:VAL:HB	1.90	0.53	
2:D:229:VAL:HG13	2:D:234:TYR:CE1	2.44	0.53	
1:A:373:ARG:NH1	14:A:1102:HOH:O	2.10	0.53	
1:A:144:PRO:HB2	1:A:672:ILE:HD13	1.90	0.53	
2:B:266:ARG:N	2:B:266:ARG:HD2	2.23	0.53	
1:C:335:LEU:HD22	1:C:722:PRO:HG3	1.90	0.53	
1:C:468:GLY:H	1:C:676:ALA:HB2	1.73	0.53	
1:A:871:ARG:HB3	1:A:874:TYR:HB3	1.91	0.52	
2:B:91:ASP:HB3	7:B:407:EDO:H21	1.90	0.52	
1:C:366:ASP:HB3	1:C:368:LYS:N	2.25	0.52	
1:E:40:CYS:SG	1:E:72:ARG:HB3	2.49	0.52	
1:C:40:CYS:SG	1:C:72:ARG:HB3	2.49	0.52	
1:A:112:GLU:OE1	14:A:1105:HOH:O	2.19	0.52	
1:E:289:PHE:HB2	1:E:291:ARG:NH1	2.25	0.52	
1:E:462:LYS:HB3	1:E:594:SER:HB3	1.92	0.52	
1:C:512:ARG:HG3	1:E:899:PHE:HB3	1.92	0.52	
2:D:322:ARG:HH11	2:D:322:ARG:HG3	1.75	0.52	
2:F:141:THR:HG23	2:F:255:ASN:OD1	2.10	0.52	
1:C:207:THR:HA	5:C:1003:MGD:N20	2.25	0.51	
1:C:304:PHE:O	1:C:317:PRO:HD2	2.10	0.51	
1:E:76:LYS:HD2	1:E:769:VAL:HG23	1.91	0.51	
2:B:136:MET:HG3	2:B:137:CYS:O	2.10	0.51	
2:B:15:VAL:HB	2:B:222:HIS:HB2	1.92	0.51	
2:D:181:PRO:HB2	2:D:250:PHE:CD2	2.46	0.51	
1:A:752:ASP:HB3	1:A:885[A]:ARG:NH2	2.26	0.51	
1:C:347:ILE:HG12	1:C:718:LYS:O	2.10	0.51	
2:D:180:CYS:SG	2:D:185:PRO:HD3	2.51	0.51	
2:F:75[B]:LYS:HG2	14:F:501:HOH:O	2.10	0.51	
1:E:380:LYS:O	1:E:384:MET:HG2	2.10	0.50	
1:E:764:HIS:HE2	6:E:1004:MD1:H15	1.59	0.50	
1:C:89:ARG:HH21	1:C:609:MET:HB2	1.75	0.50	
2:B:145:CYS:SG	2:B:146:LEU:N	2.85	0.50	
1:C:217:GLU:HG3	2:D:20:LYS:HE3	1.93	0.50	
1:A:658:MET:HE2	1:A:661:LYS:HD2	1.95	0.49	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:37:THR:HB	1:A:595:GLU:OE1	2.12	0.49	
1:C:693:ARG:NH1	1:C:702:LEU:HG	2.28	0.49	
1:C:366:ASP:N	1:C:367:GLY:HA2	2.28	0.49	
2:D:137:CYS:HB3	2:D:197:CYS:SG	2.53	0.49	
1:E:270:HIS:CD2	1:E:349:LEU:HD23	2.48	0.49	
1:E:892:ILE:HG12	14:E:1220:HOH:O	2.13	0.49	
1:A:283:ARG:HB3	1:A:285:ASP:OD1	2.13	0.49	
1:E:234:SER:OG	2:F:119:ASP:OD2	2.31	0.48	
1:E:280:TYR:O	1:E:374:PRO:HA	2.12	0.48	
1:E:313:LYS:CG	1:E:314:PRO:HD2	2.42	0.48	
1:C:364:LEU:HD21	1:C:370:VAL:HG11	1.95	0.48	
1:E:860:ASN:CB	1:E:877:PRO:HA	2.44	0.48	
1:C:81:HIS:HE2	2:D:33:LYS:HE3	1.79	0.48	
1:C:787:PRO:HD2	1:C:842:ASP:HB3	1.95	0.48	
1:C:700:SER:HB2	1:C:708:TYR:CE1	2.49	0.48	
1:A:227:SER:HB2	1:A:239:VAL:HG11	1.96	0.48	
1:A:237:ILE:HG13	7:A:1012:EDO:H11	1.96	0.48	
1:C:638:PHE:CZ	1:C:647:ARG:HD2	2.49	0.48	
1:C:678:GLN:HG3	1:C:696:SER:OG	2.14	0.48	
2:F:12:LEU:HD22	2:F:162:ILE:HD11	1.95	0.48	
1:C:306:PHE:CZ	1:C:352:LEU:HD13	2.48	0.47	
2:D:242:VAL:HA	2:D:296:VAL:HG13	1.96	0.47	
1:A:152:ARG:HD2	1:A:472:LEU:O	2.15	0.47	
1:C:173:THR:O	1:C:177:GLN:HG3	2.14	0.47	
1:E:144:PRO:HB2	1:E:672:ILE:HD13	1.96	0.47	
2:D:282:LEU:N	14:D:505:HOH:O	2.39	0.47	
1:E:797:LYS:HB3	1:E:798:PRO:HD3	1.96	0.47	
1:E:32:HIS:NE2	1:E:585:TYR:OH	2.46	0.47	
1:C:261:ILE:HG12	1:C:411:ALA:HB2	1.96	0.47	
1:A:84:MET:O	1:A:89:ARG:HD2	2.15	0.47	
2:F:201:PHE:CG	2:F:202:PRO:HD3	2.49	0.47	
2:B:69:LYS:HE3	2:B:69:LYS:HB2	1.74	0.46	
2:D:322:ARG:HG3	2:D:322:ARG:NH1	2.28	0.46	
2:B:138:ASN:HB3	2:B:254:PRO:HB3	1.98	0.46	
2:D:170:CYS:O	2:D:171:LYS:HG3	2.15	0.46	
2:D:157:ARG:NE	2:D:160:ASP:OD2	2.46	0.46	
2:D:238:LYS:HZ1	2:D:241:LYS:HE3	1.79	0.46	
1:E:464:ALA:HB3	1:E:694:PHE:CE1	2.50	0.46	
1:A:272:LEU:HD22	1:A:278:LEU:HD12	1.96	0.46	
2:F:145:CYS:SG	2:F:146:LEU:N	2.88	0.46	
1:C:344:LYS:HB3	1:C:344:LYS:HE2	1.63	0.46	



A + a 1		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:E:458:ILE:HD11	1:E:461:TRP:CD1	2.51	0.46	
1:E:609:MET:HE2	1:E:610:TRP:NE1	2.31	0.46	
1:A:416:SER:O	1:A:452:GLY:HA2	2.15	0.46	
1:E:37:THR:HG21	1:E:208:ARG:NH1	2.31	0.46	
1:E:555:TRP:CE2	1:E:561:ILE:HD13	2.51	0.46	
1:C:860:ASN:HB3	1:C:877:PRO:HA	1.97	0.46	
2:D:155:TYR:HE1	2:D:157:ARG:HG2	1.81	0.46	
1:E:307:TRP:CZ3	1:E:314:PRO:HD3	2.52	0.45	
1:E:374:PRO:HD3	14:E:1101:HOH:O	2.16	0.45	
1:C:37:THR:HB	1:C:595:GLU:OE1	2.17	0.45	
1:C:269:ALA:O	1:C:273:LYS:HG3	2.16	0.45	
1:C:836:CYS:HB2	14:C:1229:HOH:O	2.16	0.45	
1:A:881:GLN:HE22	1:A:882:ARG:NE	2.13	0.45	
1:E:483:PHE:CD2	1:E:872:PRO:HG3	2.51	0.45	
2:F:255:ASN:ND2	14:F:507:HOH:O	2.41	0.45	
2:F:305:GLU:HA	2:F:308:MET:HB2	1.98	0.45	
1:A:431:ASP:OD1	1:A:432:VAL:N	2.48	0.45	
1:A:631:LYS:HZ3	1:A:636:GLU:CD	2.20	0.45	
1:C:623:ALA:HA	1:C:652:LEU:HD23	1.98	0.45	
2:D:200:CYS:SG	2:D:203:ARG:HD3	2.56	0.45	
1:A:155:HIS:CD2	1:A:475:PRO:HD2	2.52	0.45	
2:D:136:MET:HG3	2:D:137:CYS:O	2.17	0.45	
1:C:661:LYS:HB3	1:C:661:LYS:HE3	1.60	0.45	
1:C:719:LYS:NZ	14:C:1127:HOH:O	2.49	0.45	
2:F:324:SER:O	2:F:328:MET:HG2	2.17	0.45	
1:A:76:LYS:H	1:A:76:LYS:HD3	1.82	0.44	
1:C:175:GLN:OE1	1:C:183:GLY:HA2	2.17	0.44	
1:E:152:ARG:HD2	1:E:472:LEU:O	2.17	0.44	
1:C:227:SER:HB2	1:C:239:VAL:HG11	1.98	0.44	
1:E:607:LYS:HB2	1:E:607:LYS:HE2	1.68	0.44	
2:B:204:ILE:HD11	2:B:210:PRO:HD3	1.99	0.44	
1:C:75:ASN:HB3	2:D:24:CYS:O	2.18	0.44	
1:A:638:PHE:CZ	1:A:647:ARG:HD2	2.52	0.44	
5:C:1003:MGD:H2'	5:C:1003:MGD:H8	1.70	0.44	
1:A:601:MET:HG3	1:A:602:THR:N	2.29	0.44	
1:C:809:ALA:HA	1:C:887:ASN:O	2.18	0.44	
2:D:158:GLU:H	2:D:158:GLU:HG2	1.53	0.44	
2:D:244:LEU:O	2:D:258:TYR:N	2.35	0.44	
2:F:140:CYS:HB3	2:F:252:THR:O	2.17	0.44	
1:A:317:PRO:O	14:A:1106:HOH:O	2.21	0.44	
2:D:47:ARG:HB2	3:D:405:SF4:S4	2.58	0.44	



	At arra 0	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
2:D:278:PRO:HG2	2:D:280:ILE:O	2.17	0.44	
2:F:245:PRO:CB	2:F:254:PRO:HG2	2.45	0.44	
2:B:121:GLY:HA3	2:B:130:PHE:HB3	2.00	0.43	
1:E:37:THR:HB	1:E:595:GLU:OE1	2.18	0.43	
1:C:685:GLN:O	1:C:689:GLU:HG2	2.18	0.43	
2:F:75[A]:LYS:HE3	2:F:178:GLN:NE2	2.33	0.43	
2:D:159:GLN:CD	2:D:159:GLN:H	2.22	0.43	
1:C:302:ASP:HB3	1:C:321:TRP:HB3	2.00	0.43	
1:A:764:HIS:HE2	6:A:1004:MD1:H15	1.67	0.43	
1:E:99[A]:GLU:OE1	14:E:1103:HOH:O	2.21	0.43	
2:F:80:PRO:HD2	2:F:83:ASP:OD2	2.18	0.43	
1:E:683:THR:OG1	1:E:686:MET:HG3	2.18	0.43	
1:C:325:PRO:O	1:C:327:LYS:N	2.52	0.43	
1:C:414:LYS:HA	1:C:415:PRO:HA	1.67	0.43	
1:C:771:SER:HA	1:C:774:LYS:HG3	2.01	0.43	
2:B:154:ILE:HG12	2:B:165:ILE:HG12	2.01	0.43	
1:C:264:GLU:OE1	1:C:408:ARG:NE	2.45	0.43	
1:C:515:ILE:HD13	1:C:522:ASN:HB2	2.01	0.43	
2:D:328:MET:HG3	2:D:329:ILE:O	2.18	0.43	
1:E:91:LYS:HE2	1:E:610:TRP:CZ2	2.54	0.43	
1:A:441:THR:HG21	1:A:453:GLY:HA2	2.01	0.43	
1:A:797:LYS:HB3	1:A:798:PRO:HD3	2.01	0.43	
1:A:207:THR:HA	5:A:1003:MGD:N20	2.34	0.43	
1:E:205:THR:HG23	2:F:22:ILE:HB	2.01	0.43	
1:E:359:LYS:HD2	1:E:371:GLU:OE2	2.18	0.43	
1:A:54:GLU:OE2	1:A:81:HIS:N	2.50	0.42	
1:C:318:LYS:HE2	1:C:346:TYR:O	2.19	0.42	
1:C:666:GLU:HG3	1:C:684:ILE:HG13	2.00	0.42	
1:E:152:ARG:CZ	1:E:475:PRO:HG3	2.48	0.42	
2:F:181:PRO:HG2	2:F:182:TYR:CD2	2.54	0.42	
1:C:283:ARG:HB3	1:C:285:ASP:OD1	2.20	0.42	
1:C:333:GLY:O	1:C:871:ARG:NH1	2.41	0.42	
1:C:464:ALA:HB3	1:C:694:PHE:CZ	2.54	0.42	
1:A:523:MET:HG3	1:A:524:PRO:HA	2.00	0.42	
1:C:670:GLN:HE22	1:C:683:THR:HA	1.84	0.42	
1:C:830:ARG:NH1	14:C:1134:HOH:O	2.51	0.42	
1:E:310:LYS:HD2	1:E:310:LYS:HA	1.78	0.42	
1:A:885[B]:ARG:NH2	14:A:1104:HOH:O	2.17	0.42	
1:C:414:LYS:NZ	1:C:444:THR:O	2.53	0.42	
6:C:1004:MD1:C11	6:C:1004:MD1:H7	2.50	0.42	
1:E:66:ILE:HD11	14:E:1453:HOH:O	2.18	0.42	



Atom 1	Atom 2	Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance $(\text{\AA})$		
1:E:836:CYS:HB2	14:E:1286:HOH:O	2.19	0.42	
2:F:31:CYS:SG	2:F:46:TRP:HB2	2.60	0.42	
1:C:81:HIS:NE2	2:D:33:LYS:HE3	2.35	0.42	
1:E:614:THR:O	1:E:618:ILE:HG13	2.20	0.42	
1:A:210:PRO:HA	2:B:217:VAL:CG1	2.50	0.42	
1:C:190:ASP:OD1	1:C:450:ASN:ND2	2.48	0.42	
2:D:174:GLN:O	2:D:178:GLN:HG3	2.20	0.42	
2:D:333:THR:O	2:D:333:THR:OG1	2.34	0.42	
2:F:47:ARG:HB2	3:F:404:SF4:S4	2.60	0.42	
1:C:519:GLN:HB3	1:C:863:GLY:HA3	2.01	0.42	
1:C:209:ILE:HG22	2:D:217:VAL:HG11	2.01	0.42	
1:A:642:LYS:HD3	1:A:643:PHE:CZ	2.55	0.41	
1:A:39:ALA:HA	1:A:591:ASN:OD1	2.20	0.41	
2:D:190:LEU:HD23	2:D:190:LEU:HA	1.91	0.41	
1:E:259:HIS:ND1	1:E:383:LEU:O	2.50	0.41	
1:A:881:GLN:NE2	1:A:882:ARG:NE	2.65	0.41	
2:B:5:MET:N	14:B:514:HOH:O	2.53	0.41	
1:C:730:PHE:O	1:C:745:PRO:HD3	2.20	0.41	
1:E:197:ILE:HB	1:E:225:ILE:HG12	2.02	0.41	
2:F:265:PRO:HG2	2:F:279:LYS:HE2	2.02	0.41	
1:C:736:THR:O	1:C:739:ASP:HB2	2.20	0.41	
1:E:690:LYS:HE2	14:E:1591:HOH:O	2.20	0.41	
1:A:54:GLU:HG2	1:A:585:TYR:HH	1.84	0.41	
1:A:364:LEU:HD12	1:A:368:LYS:HB3	2.02	0.41	
1:A:613:LYS:HB2	1:A:618:ILE:HG13	2.02	0.41	
2:D:297:LEU:HA	2:D:300:LEU:HD12	2.01	0.41	
1:E:359:LYS:N	14:E:1110:HOH:O	2.34	0.41	
1:E:485:GLN:CD	1:E:877:PRO:HD2	2.41	0.41	
1:E:797:LYS:HB2	1:E:797:LYS:HE3	1.76	0.41	
1:C:236:THR:O	1:C:239:VAL:HG22	2.20	0.41	
1:E:188:THR:HG22	1:E:191:TRP:CZ2	2.55	0.41	
1:C:31:ALA:HB3	1:C:602:THR:HB	2.03	0.41	
1:C:292:GLU:HG2	1:C:299:GLY:HA3	2.02	0.41	
1:C:311:THR:O	1:C:313:LYS:HG3	2.21	0.41	
2:D:280:ILE:HA	2:D:281:PRO:HD3	1.84	0.41	
1:E:399:THR:O	1:E:403:ILE:HG13	2.21	0.41	
2:F:166:HIS:ND1	2:F:169:LYS:HG3	2.35	0.41	
1:E:414:LYS:HA	1:E:415:PRO:HA	1.85	0.41	
1:E:523:MET:HA	1:E:524:PRO:C	2.42	0.41	
1:E:638:PHE:CZ	1:E:647:ARG:HD2	2.56	0.40	
1:A:120:LYS:HA	1:A:120:LYS:HD3	1.90	0.40	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:E:102:GLU:OE1	1:E:104:LYS:HE2	2.21	0.40
1:E:255:MET:HE3	1:E:383:LEU:HD21	2.03	0.40
2:F:140:CYS:O	2:F:143:PRO:HD3	2.20	0.40
1:A:289:PHE:HB2	1:A:291:ARG:NH1	2.37	0.40
1:A:160:HIS:CD2	1:A:523:MET:HG2	2.57	0.40
1:A:734:HIS:HD2	1:A:865:TYR:HB2	1.86	0.40
1:C:147:PHE:CE2	1:C:151:HIS:CE1	3.10	0.40
2:D:25:GLN:NE2	2:D:49:VAL:HB	2.36	0.40
2:D:33:LYS:HA	2:D:33:LYS:HD2	1.76	0.40
2:D:291:LYS:N	2:D:291:LYS:HD2	2.37	0.40
1:A:152:ARG:NE	1:A:656:MET:O	2.54	0.40
1:A:304:PHE:O	1:A:317:PRO:HD2	2.20	0.40
1:A:459:GLY:HA2	5:A:1003:MGD:S13	2.61	0.40
1:A:485:GLN:CD	1:A:877:PRO:HD2	2.42	0.40
1:C:461:TRP:O	1:C:463:PRO:HD3	2.21	0.40
1:E:39:ALA:HA	1:E:591:ASN:OD1	2.22	0.40
2:F:327:MET:HE2	2:F:327:MET:HB3	1.84	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	$\mathbf{ntiles}$
1	А	895/899~(100%)	860 (96%)	33 (4%)	2(0%)	47	55
1	С	890/899~(99%)	838 (94%)	49 (6%)	3~(0%)	41	46
1	Ε	893/899~(99%)	850 (95%)	41 (5%)	2~(0%)	47	55
2	В	327/333~(98%)	317~(97%)	9(3%)	1 (0%)	41	46
2	D	325/333~(98%)	303~(93%)	21 (6%)	1 (0%)	41	46
2	F	328/333~(98%)	313~(95%)	15 (5%)	0	100	100
All	All	3658/3696~(99%)	3481 (95%)	168 (5%)	9~(0%)	47	55



Mol	Chain	Res	Type
1	А	458	ILE
1	С	458	ILE
2	D	205	GLU
1	Е	458	ILE
2	В	6	LYS
1	С	463	PRO
1	Е	463	PRO
1	С	47	LYS
1	А	463	PRO

All (9) Ramachandran outliers are listed below:

#### 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	768/768~(100%)	762~(99%)	6 (1%)	81	90
1	$\mathbf{C}$	765/768~(100%)	758~(99%)	7~(1%)	78	88
1	Ε	767/768~(100%)	762~(99%)	5 (1%)	84	91
2	В	278/281~(99%)	278~(100%)	0	100	100
2	D	276/281~(98%)	273~(99%)	3~(1%)	73	85
2	$\mathbf{F}$	279/281~(99%)	278~(100%)	1 (0%)	91	96
All	All	3133/3147~(100%)	3111 (99%)	22 (1%)	84	91

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	458	ILE
1	А	465	PHE
1	А	555	TRP
1	А	601	MET
1	А	637	LYS
1	А	881	GLN
1	С	11	TYR
1	С	276	THR



Mol	Chain	Res	Type
1	С	327	LYS
1	С	458	ILE
1	С	465	PHE
1	С	555	TRP
1	С	881	GLN
2	D	158	GLU
2	D	160	ASP
2	D	197	CYS
1	Ε	137	SER
1	Ε	165	TYR
1	Е	458	ILE
1	Е	465	PHE
1	Е	881	GLN
2	F	137	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	860	ASN
1	А	881	GLN
1	С	860	ASN
1	С	881	GLN
1	Е	860	ASN
1	Е	881	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)

Of 54 ligands modelled in this entry, 10 are monoatomic - leaving 44 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).

Mol	Type	Chain	Dog	Tipk	В	ond leng	gths	Bond angles		
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
7	EDO	А	1012	-	$3,\!3,\!3$	0.51	0	2,2,2	0.24	0
6	MD1	Е	1004	4	$39,\!51,\!51$	3.73	11 (28%)	38,78,78	1.93	13 (34%)
7	EDO	С	1005	-	3,3,3	0.77	0	2,2,2	0.36	0
7	EDO	Е	1006	-	3,3,3	0.89	0	2,2,2	0.43	0
12	F3S	F	401	2	0,9,9	-	-	-		
3	SF4	D	404	2	0,12,12	-	-	-		
7	EDO	Е	1007	-	3,3,3	0.55	0	2,2,2	0.32	0
11	SO3	Е	1008	9	$1,\!3,\!3$	1.21	0	0,3,3	-	-
7	EDO	F	405	-	3, 3, 3	0.62	0	2,2,2	0.36	0
6	MD1	С	1004	4	$39,\!51,\!51$	<mark>3.98</mark>	9 (23%)	38,78,78	1.88	11 (28%)
7	EDO	В	406	-	3,3,3	0.57	0	2,2,2	0.31	0
10	GOL	А	1010	-	$5,\!5,\!5$	0.27	0	5,5,5	0.62	0
3	SF4	В	402	2	0,12,12	-	-	-		
3	SF4	D	403	2	0,12,12	-	-	-		
7	EDO	С	1006	-	3,3,3	0.57	0	2,2,2	0.26	0
7	EDO	Е	1005	-	3,3,3	0.74	0	2,2,2	0.47	0
12	F3S	D	402	2	0,9,9	-	-	-		
13	ACT	С	1008	-	3,3,3	0.76	0	3,3,3	1.06	0
5	MGD	А	1003	4	41,52,52	<mark>5.66</mark>	25 (60%)	40,81,81	<mark>3.00</mark>	14 (35%)
7	EDO	А	1007	-	3,3,3	0.57	0	2,2,2	0.22	0
3	SF4	С	1001	1	0,12,12	-	-	-		
3	SF4	В	404	2	0,12,12	-	-	-		
3	SF4	F	404	2	0,12,12	-	-	-		
3	SF4	D	405	2	0,12,12	-	-	-		
3	SF4	А	1001	1	0,12,12	-	-	-		
3	SF4	F	403	2	$0,\!12,\!12$	-	-	-		
5	MGD	E	1003	4	41,52,52	<mark>5.53</mark>	25 (60%)	40,81,81	2.51	9 (22%)
7	EDO	D	406	-	3, 3, 3	0.50	0	2,2,2	0.37	0
12	F3S	В	401	2	$0,\!9,\!9$	-	-	-		
7	EDO	А	1005	-	3,3,3	0.80	0	2,2,2	0.39	0
3	SF4	Е	1001	1	$0,\!12,\!12$	-	-	-		



Mal	Turne	Chain	Dec	T inl.	В	ond leng	gths	E	Bond ang	gles
	туре	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	SO3	С	1009	-	1,3,3	0.77	0	0,3,3	-	-
7	EDO	В	405	-	3,3,3	0.30	0	2,2,2	0.67	0
7	EDO	D	401	-	3,3,3	0.71	0	2,2,2	0.12	0
11	SO3	А	1013	-	1,3,3	0.88	0	0,3,3	-	-
7	EDO	F	406	-	3,3,3	0.52	0	2,2,2	0.49	0
5	MGD	С	1003	4	41,52,52	<b>5.60</b>	27 (65%)	40,81,81	2.64	13 (32%)
7	EDO	В	407	-	3,3,3	0.76	0	2,2,2	0.23	0
6	MD1	А	1004	4	39,51,51	4.00	11 (28%)	38,78,78	2.03	12 (31%)
7	EDO	А	1006	-	3,3,3	0.54	0	2,2,2	0.31	0
3	SF4	F	402	2	0,12,12	-	-	-		
3	SF4	В	403	2	0,12,12	-	-	-		
11	SO3	А	1011	9	1,3,3	1.05	0	0,3,3	-	-
11	SO3	С	1010	9	$1,\!3,\!3$	0.81	0	0,3,3	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	А	1012	-	-	0/1/1/1	-
6	MD1	Е	1004	4	-	2/18/59/59	0/5/5/5
7	EDO	С	1005	-	-	0/1/1/1	-
7	EDO	Е	1006	-	-	0/1/1/1	-
12	F3S	F	401	2	-	-	0/3/3/3
3	SF4	D	404	2	-	-	0/6/5/5
7	EDO	Е	1007	-	-	0/1/1/1	-
7	EDO	F	405	-	_	0/1/1/1	-
6	MD1	С	1004	4	-	4/18/59/59	0/5/5/5
7	EDO	В	406	-	-	0/1/1/1	-
10	GOL	А	1010	-	-	0/4/4/4	-
3	SF4	В	402	2	-	-	0/6/5/5
3	SF4	D	403	2	-	-	0/6/5/5
7	EDO	С	1006	-	-	0/1/1/1	-
7	EDO	Ε	1005	-	-	0/1/1/1	-
12	F3S	D	402	2	_	_	0/3/3/3
7	EDO	А	1007	-	-	1/1/1/1	-
5	MGD	A	1003	4	-	2/18/66/66	0/6/6/6
3	SF4	С	1001	1	-	-	0/6/5/5
3	SF4	В	404	2	-	-	0/6/5/5
3	SF4	F	404	2	-	-	0/6/5/5



5CH7
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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	D	405	2	-	-	0/6/5/5
3	SF4	А	1001	1	-	-	0/6/5/5
5	MGD	Е	1003	4	-	2/18/66/66	0/6/6/6
7	EDO	D	406	-	-	0/1/1/1	-
3	SF4	F	403	2	-	-	0/6/5/5
12	F3S	В	401	2	-	-	0/3/3/3
7	EDO	А	1005	-	-	0/1/1/1	-
3	SF4	Е	1001	1	-	-	0/6/5/5
7	EDO	D	401	-	-	0/1/1/1	-
7	EDO	В	405	-	-	0/1/1/1	-
7	EDO	F	406	-	-	0/1/1/1	-
7	EDO	В	407	-	-	0/1/1/1	-
5	MGD	С	1003	4	-	0/18/66/66	0/6/6/6
6	MD1	А	1004	4	-	4/18/59/59	0/5/5/5
7	EDO	A	1006	-	-	0/1/1/1	-
3	SF4	F	402	2	-	-	0/6/5/5
3	SF4	В	403	2	-	-	0/6/5/5

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
5	А	1003	MGD	C23-C14	-19.14	1.38	1.53
5	Е	1003	MGD	C23-C14	-19.03	1.38	1.53
5	С	1003	MGD	C23-C14	-18.51	1.38	1.53
5	Е	1003	MGD	C16-C21	14.97	1.64	1.38
5	А	1003	MGD	C16-C21	14.72	1.63	1.38
5	С	1003	MGD	C16-C21	14.25	1.62	1.38
6	С	1004	MD1	O4'-C1'	14.18	1.60	1.41
6	А	1004	MD1	O4'-C1'	13.84	1.60	1.41
6	С	1004	MD1	C2'-C1'	-12.84	1.34	1.53
5	А	1003	MGD	O11-C11	12.58	1.60	1.43
6	А	1004	MD1	C2'-C1'	-12.56	1.34	1.53
5	Е	1003	MGD	O11-C11	12.50	1.60	1.43
6	Е	1004	MD1	C2'-C1'	-12.47	1.34	1.53
5	С	1003	MGD	O11-C11	12.34	1.60	1.43
6	Е	1004	MD1	O4'-C1'	11.93	1.57	1.41
6	А	1004	MD1	C7-N8	11.66	1.41	1.27
6	С	1004	MD1	C7-N8	10.98	1.40	1.27
6	Е	1004	MD1	C7-N8	10.52	1.40	1.27
5	С	1003	MGD	C2'-C3'	-10.03	1.25	1.53
5	Е	1003	MGD	C2'-C3'	-9.65	1.26	1.53
5	А	1003	MGD	C2'-C3'	-9.35	1.27	1.53



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
5	Е	1003	MGD	C19-N18	7.19	1.55	1.37
5	С	1003	MGD	O4'-C1'	7.17	1.51	1.41
5	А	1003	MGD	C14-N15	7.14	1.54	1.46
5	А	1003	MGD	C21-N22	7.10	1.43	1.35
5	Е	1003	MGD	O4'-C1'	7.07	1.50	1.41
5	С	1003	MGD	C19-N18	6.94	1.54	1.37
5	А	1003	MGD	O4'-C1'	6.93	1.50	1.41
5	С	1003	MGD	O4'-C4'	-6.90	1.29	1.45
5	А	1003	MGD	O4'-C4'	-6.83	1.29	1.45
5	С	1003	MGD	C21-N22	6.62	1.42	1.35
5	Ε	1003	MGD	O4'-C4'	-6.56	1.30	1.45
5	А	1003	MGD	C19-N20	6.51	1.48	1.33
5	С	1003	MGD	C14-N15	6.47	1.54	1.46
5	А	1003	MGD	C19-N18	6.45	1.53	1.37
5	С	1003	MGD	C19-N20	6.39	1.48	1.33
5	Ε	1003	MGD	C19-N20	6.28	1.48	1.33
5	Ε	1003	MGD	C14-N15	5.36	1.52	1.46
5	С	1003	MGD	C23-N22	5.35	1.54	1.45
5	А	1003	MGD	C3'-C4'	5.29	1.66	1.53
5	С	1003	MGD	C3'-C4'	5.21	1.66	1.53
6	С	1004	MD1	C2-N2	5.20	1.44	1.33
6	Ε	1004	MD1	O4'-C4'	-5.10	1.33	1.45
6	Ε	1004	MD1	C2-N2	5.09	1.44	1.33
6	А	1004	MD1	C2-N2	5.03	1.44	1.33
5	Ε	1003	MGD	C3'-C4'	4.98	1.65	1.53
6	С	1004	MD1	O4'-C4'	-4.91	1.34	1.45
5	Ε	1003	MGD	C23-N22	4.91	1.53	1.45
6	А	1004	MD1	C16-N15	4.61	1.47	1.38
5	А	1003	MGD	C23-N22	4.57	1.52	1.45
6	А	1004	MD1	O4'-C4'	-4.48	1.35	1.45
5	E	1003	MGD	C21-N22	4.48	1.40	1.35
5	A	1003	MGD	C2-N3	4.47	1.44	1.33
6	С	1004	MD1	C16-N15	4.43	1.47	1.38
6	A	1004	MD1	C17-N16	4.42	1.42	1.33
5	С	1003	MGD	C2-N3	4.37	1.43	1.33
5	E	1003	MGD	C2-N3	4.31	1.43	1.33
6	E	1004	MD1	C16-N15	4.16	1.46	1.38
5	A	1003	MGD	O2'-C2'	4.15	1.52	1.43
5	A	1003	MGD	C19-N19	3.92	1.43	1.34
5	C	1003	MGD	C2-N2	3.86	1.43	1.34
5	С	1003	MGD	C17-N18	3.84	1.46	1.38
5	${ m E}$	1003	MGD	C17-N18	3.84	1.46	1.38



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Е	1004	MD1	C17-N16	3.75	1.41	1.33
5	А	1003	MGD	C17-N18	3.75	1.45	1.38
5	С	1003	MGD	O2'-C2'	3.69	1.51	1.43
5	С	1003	MGD	C19-N19	3.67	1.42	1.34
5	С	1003	MGD	O11-C23	-3.55	1.38	1.43
5	Е	1003	MGD	C2-N2	3.45	1.42	1.34
5	А	1003	MGD	C2-N2	3.41	1.42	1.34
5	Е	1003	MGD	C4-N3	3.29	1.45	1.37
6	С	1004	MD1	C17-N16	3.28	1.40	1.33
5	Е	1003	MGD	C19-N19	3.22	1.41	1.34
5	А	1003	MGD	C2'-C1'	3.18	1.58	1.53
5	А	1003	MGD	C6-N1	3.16	1.42	1.37
5	С	1003	MGD	C4-N3	3.05	1.44	1.37
5	Е	1003	MGD	C6-N1	3.01	1.42	1.37
5	С	1003	MGD	C6-N1	3.01	1.42	1.37
5	А	1003	MGD	C4-N3	2.97	1.44	1.37
5	А	1003	MGD	C12-C13	2.90	1.54	1.35
5	Е	1003	MGD	C5-C4	-2.86	1.35	1.43
5	С	1003	MGD	C12-C13	2.82	1.53	1.35
5	Е	1003	MGD	C8-N7	2.79	1.39	1.35
5	Е	1003	MGD	C12-C13	2.78	1.53	1.35
5	С	1003	MGD	C2'-C1'	2.71	1.57	1.53
5	Е	1003	MGD	C2'-C1'	2.60	1.57	1.53
5	А	1003	MGD	C5-C4	-2.60	1.36	1.43
6	А	1004	MD1	C16-C15	-2.56	1.38	1.41
6	Е	1004	MD1	C16-C15	-2.56	1.38	1.41
6	С	1004	MD1	C12-C13	2.53	1.42	1.34
5	С	1003	MGD	C5-C4	-2.50	1.36	1.43
6	А	1004	MD1	C12-C13	2.48	1.42	1.34
5	А	1003	MGD	C10-C11	2.46	1.55	1.52
6	Е	1004	MD1	C5-C6	-2.41	1.37	1.41
5	E	1003	MGD	C5-C6	2.39	1.52	1.47
5	С	1003	MGD	C8-N7	2.35	1.39	1.35
6	С	1004	MD1	O3'-C3'	-2.34	1.37	1.43
5	А	1003	MGD	C8-N7	2.34	1.39	1.35
5	A	1003	MGD	C5-C6	2.31	1.52	1.47
6	A	1004	MD1	C14-C7	2.31	1.56	1.50
5	C	1003	MGD	C21-N20	$2.2\overline{8}$	1.39	1.36
6	E	1004	MD1	O3'-C3'	-2.28	1.37	1.43
6	E	1004	MD1	C12-C13	2.21	1.41	1.34
5	C	1003	MGD	C5-C6	2.20	1.51	1.47

MGD

1003

Е

5

O2'-C2'

Continued on next page...

1.43

1.48



2.17

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
6	А	1004	MD1	O3'-C3'	-2.10	1.38	1.43
5	Е	1003	MGD	O11-C23	-2.05	1.40	1.43
5	С	1003	MGD	C10-C11	2.03	1.54	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	А	1003	MGD	O11-C23-N22	-15.12	93.03	108.57
5	С	1003	MGD	O11-C23-N22	-12.58	95.64	108.57
5	Е	1003	MGD	O11-C23-N22	-12.27	95.95	108.57
6	С	1004	MD1	O11-C11-C12	-5.20	101.68	111.05
6	Е	1004	MD1	N3-C2-N1	-4.96	120.61	127.22
6	С	1004	MD1	N3-C2-N1	-4.87	120.72	127.22
6	А	1004	MD1	N3-C2-N1	-4.77	120.86	127.22
5	А	1003	MGD	C19-N20-C21	4.35	121.28	113.43
6	А	1004	MD1	C15-C16-N15	-3.91	115.84	119.12
6	А	1004	MD1	O11-C11-C12	-3.91	104.02	111.05
6	А	1004	MD1	N18-C17-N17	-3.82	119.42	125.42
5	С	1003	MGD	O17-C17-C16	-3.74	118.67	127.24
6	С	1004	MD1	C2-N3-C4	3.73	119.62	115.36
5	Е	1003	MGD	O4'-C1'-C2'	-3.70	101.52	106.93
6	А	1004	MD1	C17-N17-C15	3.63	121.70	115.93
6	Е	1004	MD1	O11-C11-C12	-3.63	104.51	111.05
6	А	1004	MD1	C2-N3-C4	3.62	119.49	115.36
5	А	1003	MGD	N2-C2-N1	3.45	124.07	116.71
5	С	1003	MGD	O4'-C1'-C2'	-3.44	101.90	106.93
5	С	1003	MGD	C19-N20-C21	3.38	119.54	113.43
6	Е	1004	MD1	C2-N3-C4	3.33	119.16	115.36
6	А	1004	MD1	C5-C6-N1	-3.29	118.93	123.43
6	Е	1004	MD1	N18-C17-N17	-3.23	120.35	125.42
5	А	1003	MGD	C2'-C3'-C4'	3.19	108.84	102.64
6	С	1004	MD1	N2-C2-N3	3.10	122.85	117.79
5	А	1003	MGD	C5-C6-N1	3.07	119.38	113.95
5	С	1003	MGD	N2-C2-N1	3.06	123.23	116.71
5	А	1003	MGD	C17-C16-N15	3.03	124.90	116.76
5	Е	1003	MGD	O17-C17-C16	-3.00	120.36	127.24
6	Е	1004	MD1	O4'-C1'-C2'	-2.96	102.59	106.93
5	Е	1003	MGD	N2-C2-N1	2.96	123.02	116.71
6	С	1004	MD1	N18-C17-N17	-2.95	120.79	125.42
6	Е	1004	MD1	C5-C6-N1	-2.93	119.42	123.43
6	Е	1004	MD1	C17-N17-C15	2.88	120.51	115.93
5	А	1003	MGD	O17-C17-C16	-2.88	120.64	127.24



$5 \mathrm{CH7}$

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	С	1003	MGD	C5-C6-N1	2.85	118.98	113.95
5	С	1003	MGD	N1-C2-N3	-2.84	118.00	123.32
5	Е	1003	MGD	C8-N7-C5	2.82	108.36	102.99
6	А	1004	MD1	N16-C17-N18	2.82	121.64	117.25
5	С	1003	MGD	C17-C16-N15	2.82	124.32	116.76
6	С	1004	MD1	O4'-C1'-C2'	-2.75	102.91	106.93
5	А	1003	MGD	N1-C2-N3	-2.68	118.31	123.32
5	А	1003	MGD	C8-N7-C5	2.68	108.09	102.99
6	Е	1004	MD1	PA-O3B-PB	-2.66	123.70	132.83
6	А	1004	MD1	PA-O3B-PB	-2.63	123.81	132.83
6	А	1004	MD1	C2-N1-C6	2.61	120.08	115.93
5	А	1003	MGD	O3'-C3'-C4'	-2.59	103.56	111.05
5	Е	1003	MGD	C5-C6-N1	2.56	118.47	113.95
6	С	1004	MD1	C17-N17-C15	2.51	119.92	115.93
6	Е	1004	MD1	C5'-C4'-C3'	-2.48	105.88	115.18
5	Е	1003	MGD	C19-N20-C21	2.46	117.88	113.43
6	Е	1004	MD1	C2-N1-C6	2.46	119.84	115.93
6	С	1004	MD1	C5-C6-N1	-2.44	120.09	123.43
6	Е	1004	MD1	N2-C2-N3	2.43	121.75	117.79
5	Е	1003	MGD	C17-C16-N15	2.40	123.20	116.76
5	Е	1003	MGD	C19-N18-C17	-2.36	120.80	125.10
5	А	1003	MGD	C16-C17-N18	2.34	119.29	112.31
6	Е	1004	MD1	C15-C16-N15	-2.33	117.17	119.12
5	С	1003	MGD	O6-C6-N1	-2.32	117.90	120.65
6	А	1004	MD1	C4-C5-N7	-2.31	106.99	109.40
6	Е	1004	MD1	O2'-C2'-C3'	-2.28	104.44	111.82
5	С	1003	MGD	C16-C17-N18	2.27	119.08	112.31
5	С	1003	MGD	C19-N18-C17	-2.26	120.97	125.10
6	С	1004	MD1	C2-N1-C6	2.25	119.50	115.93
6	С	1004	MD1	N16-C17-N17	2.23	120.72	117.25
5	С	1003	MGD	O11-C23-C14	2.23	110.45	108.96
6	А	1004	MD1	N2-C2-N3	2.22	121.41	117.79
5	С	1003	MGD	C8-N7-C5	2.21	107.21	102.99
5	А	1003	MGD	N18-C19-N20	-2.21	119.21	123.32
5	А	1003	MGD	N19-C19-N18	2.19	121.37	116.71
5	А	1003	MGD	O11-C23-C14	-2.18	107.51	108.96
6	С	1004	MD1	PA-O3B-PB	-2.05	125.79	132.83

There are no chirality outliers.

All (15) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
5	А	1003	MGD	C5'-O5'-PB-O1B
6	С	1004	MD1	C10-O3A-PB-O1B
5	А	1003	MGD	C5'-O5'-PB-O3B
6	С	1004	MD1	C10-O3A-PB-O3B
6	А	1004	MD1	C10-O3A-PB-O2B
6	С	1004	MD1	C10-O3A-PB-O2B
6	Е	1004	MD1	O4'-C4'-C5'-O5'
6	А	1004	MD1	O4'-C4'-C5'-O5'
6	Е	1004	MD1	C3'-C4'-C5'-O5'
7	А	1007	EDO	O1-C1-C2-O2
6	А	1004	MD1	C10-O3A-PB-O3B
5	Ε	1003	MGD	PA-O3B-PB-O1B
5	Е	1003	MGD	PA-O3B-PB-O2B
6	А	1004	MD1	PA-O3B-PB-O1B
6	С	1004	MD1	O4'-C4'-C5'-O5'

There are no ring outliers.

11	monomers	are	invo	lved	$\mathrm{in}$	14	$\operatorname{short}$	contacts:
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	А	1012	EDO	1	0
6	Е	1004	MD1	1	0
7	Е	1006	EDO	2	0
6	С	1004	MD1	1	0
10	А	1010	GOL	1	0
5	А	1003	MGD	2	0
3	F	404	SF4	1	0
3	D	405	SF4	1	0
5	С	1003	MGD	2	0
7	В	407	EDO	1	0
6	А	1004	MD1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient





equivalents in the CSD to analyse the geometry.

















## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9
1	А	894/899~(99%)	-0.36	10 (1%) 80	79	16, 30, 49, 68	0
1	С	891/899~(99%)	-0.04	29 (3%) 46	44	19, 39, 62, 97	0
1	Ε	892/899~(99%)	-0.34	14 (1%) 72	70	17, 30, 51, 70	0
2	В	329/333~(98%)	-0.62	2 (0%) 89	88	17, 24, 38, 64	0
2	D	327/333~(98%)	0.43	27 (8%) 11	10	25, 54, 71, 89	0
2	F	328/333~(98%)	-0.36	1 (0%) 94	93	18, 32, 50, 66	0
All	All	3661/3696~(99%)	-0.23	83 (2%) 60	58	16, 32, 59, 97	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	11	TYR	5.5
1	А	8	ALA	5.2
1	С	9	PHE	4.7
1	С	164[A]	PHE	4.6
1	Е	164[A]	PHE	4.2
1	С	298	GLY	4.2
1	А	164[A]	PHE	4.1
2	D	7	ALA	3.7
2	D	295	ASP	3.7
2	В	5	MET	3.7
1	С	368	LYS	3.4
1	С	366	ASP	3.2
1	А	7	GLY	3.2
2	D	170	CYS	3.2
2	D	69	LYS	3.1
2	В	6	LYS	3.1
1	А	297	ALA	3.0
1	С	458	ILE	3.0
2	D	250	PHE	2.9



Mol	Chain	Res	Type	RSRZ
2	D	10	ARG	2.9
2	D	171	LYS	2.8
1	Е	298	GLY	2.8
2	D	154	ILE	2.8
2	D	8	PRO	2.7
1	С	207	THR	2.7
1	С	365	LEU	2.7
1	А	328	LYS	2.7
2	D	9	ARG	2.6
1	А	769	VAL	2.6
1	С	363	GLN	2.6
2	D	152	GLU	2.6
1	С	689	GLU	2.6
2	D	65	GLY	2.5
1	С	168	TYR	2.5
1	Е	314	PRO	2.5
1	С	769	VAL	2.5
2	D	145	CYS	2.5
1	А	6	SER	2.4
1	Ε	366	ASP	2.4
2	D	150	PRO	2.4
1	С	770	HIS	2.4
2	D	240	TYR	2.4
2	D	153	ALA	2.4
1	С	139	VAL	2.4
1	С	209	ILE	2.4
1	Е	328	LYS	2.4
2	D	312	ALA	2.4
1	С	309	ALA	2.3
1	Е	365	LEU	2.3
2	D	311	LEU	2.3
1	Е	370	VAL	2.3
1	С	299	GLY	2.3
1	А	168	TYR	2.3
2	D	142	LYS	2.3
2	D	24	CYS	2.3
1	С	768	SER	2.3
2	D	159	GLN	2.3
2	D	76	GLY	2.2
2	D	68	TYR	2.2
1	Е	313	LYS	2.2
2	D	158	GLU	2.2



Mol	Chain	Res	Type	RSRZ
1	С	36	CYS	2.2
1	С	420	CYS	2.2
1	С	297	ALA	2.2
1	С	327	LYS	2.2
1	Е	327	LYS	2.2
1	С	704	GLU	2.2
1	С	313	LYS	2.2
1	С	74	CYS	2.2
1	Е	209	ILE	2.2
2	D	140	CYS	2.1
1	Е	381	SER	2.1
1	А	351	ASP	2.1
2	D	73	LEU	2.1
1	С	35	ASN	2.1
1	С	17	PHE	2.1
1	Е	168	TYR	2.1
2	F	272	GLY	2.1
1	Е	769	VAL	2.0
1	Е	297	ALA	2.0
1	А	327	LYS	2.0
1	С	361	ASN	2.0
2	D	238	LYS	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
11	SO3	Ε	1008	4/4	0.44	0.25	34,38,48,71	0



Mol	Type	Chain	$\frac{13 \text{ page.}}{\text{Res}}$	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
7	EDO	Е	1006	4/4	0.71	0.23	34,35,38,41	0
7	EDO	С	1005	4/4	0.80	0.27	33,36,45,45	0
11	SO3	С	1010	4/4	0.83	0.17	61,62,70,83	0
11	SO3	А	1011	4/4	0.83	0.14	38,39,51,70	0
10	GOL	А	1010	6/6	0.84	0.21	35,42,48,48	0
7	EDO	В	407	4/4	0.85	0.23	34,36,37,42	0
7	EDO	F	406	4/4	0.88	0.23	39,42,43,44	0
7	EDO	Е	1007	4/4	0.89	0.16	28,40,44,49	0
13	ACT	С	1008	4/4	0.89	0.14	31,36,40,44	0
3	SF4	D	403	8/8	0.90	0.06	39,45,57,57	0
7	EDO	А	1005	4/4	0.90	0.20	25,26,31,39	0
11	SO3	С	1009	4/4	0.91	0.29	43,48,50,68	0
7	EDO	В	406	4/4	0.91	0.14	32,34,40,41	0
7	EDO	А	1006	4/4	0.92	0.15	32,34,35,37	0
11	SO3	А	1013	4/4	0.93	0.35	38,42,42,57	0
3	SF4	D	405	8/8	0.94	0.10	34,48,53,54	0
7	EDO	Е	1005	4/4	0.94	0.11	16,20,23,23	0
7	EDO	А	1012	4/4	0.94	0.18	21,22,27,29	0
8	NA	С	1007	1/1	0.95	0.21	26,26,26,26	0
12	F3S	D	402	7/7	0.95	0.05	53,58,64,74	0
7	EDO	А	1007	4/4	0.95	0.11	26,28,29,32	0
7	EDO	С	1006	4/4	0.96	0.08	20,24,25,27	0
7	EDO	D	406	4/4	0.96	0.15	30,36,37,38	0
3	SF4	F	404	8/8	0.96	0.10	26,28,29,29	0
5	MGD	С	1003	47/47	0.96	0.21	21,28,32,33	0
3	SF4	F	402	8/8	0.96	0.07	29,31,35,40	0
9	ZN	Е	1010	1/1	0.97	0.07	33,33,33,33	0
6	MD1	А	1004	47/47	0.97	0.15	19,23,28,30	0
6	MD1	С	1004	47/47	0.97	0.16	20,29,32,35	0
5	MGD	А	1003	47/47	0.97	0.17	13,20,25,28	0
3	SF4	С	1001	8/8	0.97	0.14	34,36,40,42	0
5	MGD	E	1003	47/47	0.97	0.18	16,24,30,31	0
8	NA	А	1008	1/1	0.97	0.17	18,18,18,18	0
7	EDO	D	401	4/4	0.97	0.12	24,24,28,31	0
8	NA	F	407	1/1	0.97	0.09	41,41,41,41	0
7	EDO	F	405	4/4	0.98	0.12	23,23,23,25	0
3	SF4	E	1001	8/8	0.98	0.12	19,22,25,26	0
6	MD1	E	1004	47/47	0.98	0.14	15,22,28,29	0
3	SF4	D	404	8/8	0.98	0.13	45,49,56,57	0
8	NA	Е	1009	1/1	0.98	0.17	14,14,14,14	0
3	SF4	F	403	8/8	0.98	0.13	27,31,37,38	0
9	ZN	С	1011	1/1	0.98	0.07	58, 58, 58, 58	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B$ -factors( $Å^2$ )	Q<0.9
12	F3S	F	401	7/7	0.98	0.04	28,31,33,36	0
3	SF4	В	402	8/8	0.98	0.08	22,24,24,30	0
3	SF4	В	403	8/8	0.99	0.10	19,22,24,28	0
4	MO	А	1002	1/1	0.99	0.08	33,33,33,33	0
7	EDO	В	405	4/4	0.99	0.09	22,22,23,23	0
4	MO	С	1002	1/1	0.99	0.10	38,38,38,38	0
9	ZN	А	1009	1/1	0.99	0.08	34,34,34,34	0
12	F3S	В	401	7/7	0.99	0.04	26,27,28,31	0
4	MO	Е	1002	1/1	0.99	0.11	32,32,32,32	0
3	SF4	В	404	8/8	0.99	0.09	19,21,22,23	0
3	SF4	А	1001	8/8	0.99	0.13	20,22,26,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.















## 6.5 Other polymers (i)

There are no such residues in this entry.

