



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 03:10 am BST

PDB ID : 3QQM  
Title : Crystal structure of a Putative amino-acid aminotransferase (NP\_104211.1)  
from *Mesorhizobium loti* at 2.30 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2011-02-15  
Resolution : 2.30 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

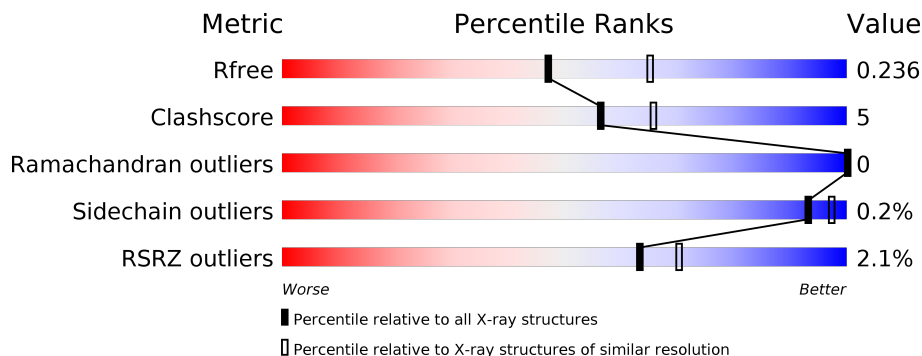
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	A	221	 4% 87% 10% .
1	B	221	 2% 84% 10% 6%
1	C	221	 2% 84% 11% 5%
1	D	221	 2% 86% 10% 5%
1	E	221	 86% 8% 6%
1	F	221	 4% 89% 8% .

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Mol	Chain	Length	Quality of chain
1	G	221	<p>2% 86% 11%</p>
1	H	221	<p>89% 5% 6%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	234	-	-	X	-
2	IOD	B	242	-	-	X	-
2	IOD	C	233	-	-	X	-
2	IOD	F	237	-	-	X	-
3	CL	E	256	-	-	X	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 14246 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.

- Molecule 1 is a protein called Mlr3007 protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S	Se			
1	A	215	1704	1066	309	323	1	3	2	0	4	0
1	B	207	1618	1015	290	307	1	3	2	0	2	0
1	C	209	1631	1019	293	313	1	3	2	0	1	0
1	D	211	1657	1034	297	320	1	3	2	0	2	0
1	E	207	1620	1014	290	310	1	3	2	0	0	0
1	F	215	1667	1043	296	322	1	3	2	0	1	0
1	G	215	1695	1063	307	319	1	3	2	0	4	0
1	H	207	1627	1017	296	308	1	3	2	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP Q98H69
B	0	GLY	-	EXPRESSION TAG	UNP Q98H69
C	0	GLY	-	EXPRESSION TAG	UNP Q98H69
D	0	GLY	-	EXPRESSION TAG	UNP Q98H69
E	0	GLY	-	EXPRESSION TAG	UNP Q98H69
F	0	GLY	-	EXPRESSION TAG	UNP Q98H69
G	0	GLY	-	EXPRESSION TAG	UNP Q98H69
H	0	GLY	-	EXPRESSION TAG	UNP Q98H69

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	3	Total I 4 4	0	1
2	D	3	Total I 4 4	0	1
2	E	2	Total I 3 3	0	1
2	H	4	Total I 5 5	0	1
2	B	4	Total I 4 4	0	0
2	C	4	Total I 5 5	0	1
2	A	3	Total I 4 4	0	1
2	F	3	Total I 4 4	0	1

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	3	Total Cl 3 3	0	0
3	G	1	Total Cl 1 1	0	0
3	A	5	Total Cl 5 5	0	0
3	D	2	Total Cl 2 2	0	0
3	E	3	Total Cl 3 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

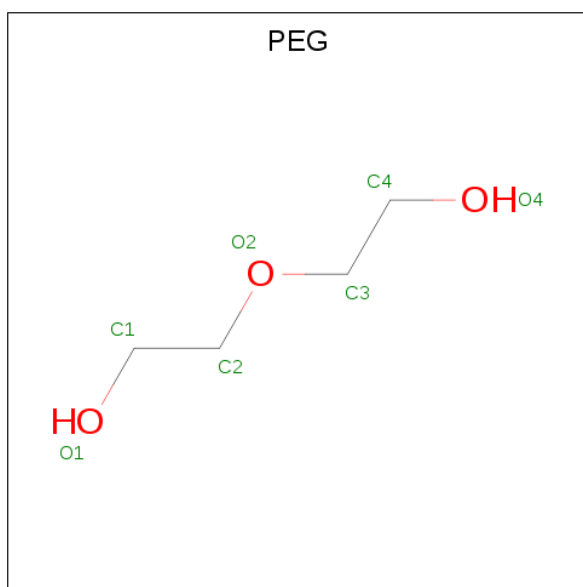
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		

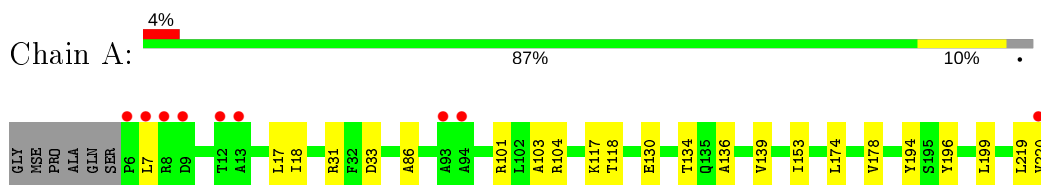
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	105	Total	O	0	0
			105	105		
6	B	96	Total	O	0	0
			96	96		
6	C	112	Total	O	0	0
			112	112		
6	D	111	Total	O	0	0
			111	111		
6	E	106	Total	O	0	0
			106	106		
6	F	61	Total	O	0	0
			61	61		
6	G	73	Total	O	0	0
			73	73		
6	H	109	Total	O	0	0
			109	109		

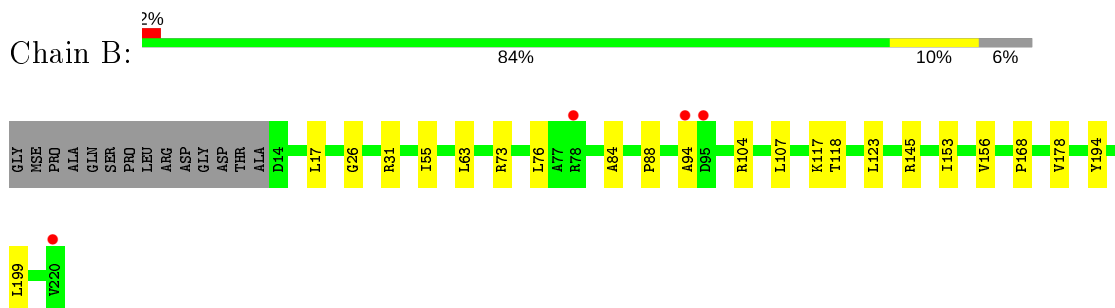
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

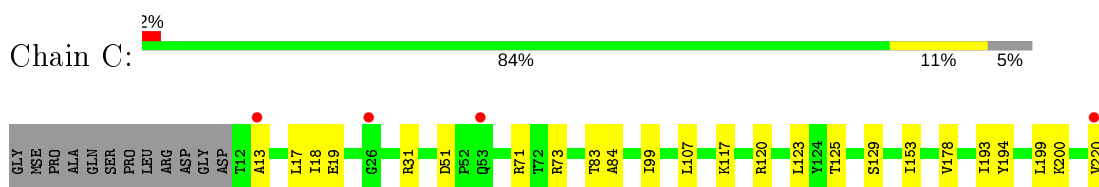
- Molecule 1: Mr3007 protein



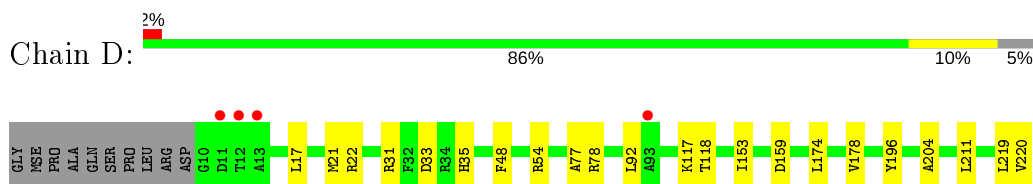
- Molecule 1: Mr3007 protein



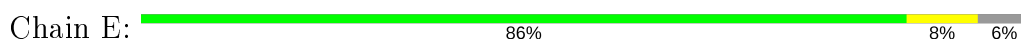
- Molecule 1: Mr3007 protein



- Molecule 1: Mr3007 protein

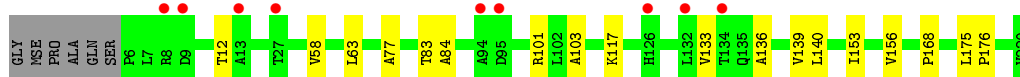
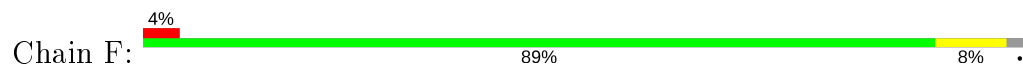


- Molecule 1: Mr3007 protein

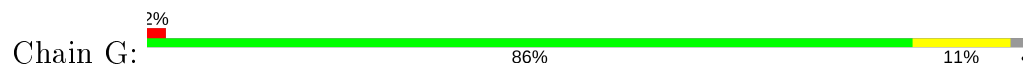




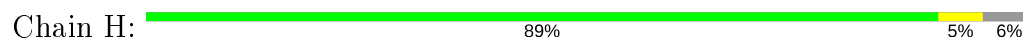
- Molecule 1: Mlr3007 protein



- Molecule 1: Mlr3007 protein



- Molecule 1: Mlr3007 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.18Å 215.57Å 81.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.68 – 2.30 29.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.68-2.30) 99.7 (29.69-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.193 , 0.241 0.190 , 0.236	Depositor DCC
$R_{free}$ test set	4592 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtrriage
Anisotropy	0.231	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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, PEG, EDO, LLP, CL

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.70	0/1716	0.71	0/2318
1	B	0.63	0/1624	0.72	0/2197
1	C	0.68	0/1633	0.75	0/2208
1	D	0.68	0/1662	0.71	0/2247
1	E	0.68	0/1619	0.74	0/2189
1	F	0.63	0/1670	0.68	0/2260
1	G	0.60	0/1708	0.68	0/2309
1	H	0.69	0/1629	0.72	0/2202
All	All	0.66	0/13261	0.71	0/17930

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	A	1704	0	1698	18	0
1	B	1618	0	1591	21	0
1	C	1631	0	1602	22	0
1	D	1657	0	1628	16	0
1	E	1620	0	1597	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1667	0	1630	16	0
1	G	1695	0	1686	26	0
1	H	1627	0	1611	10	0
2	A	4	0	0	2	0
2	B	4	0	0	3	0
2	C	5	0	0	3	0
2	D	4	0	0	1	0
2	E	3	0	0	1	0
2	F	4	0	0	2	0
2	G	4	0	0	1	0
2	H	5	0	0	2	0
3	A	5	0	0	1	0
3	D	2	0	0	1	0
3	E	3	0	0	2	0
3	G	1	0	0	1	0
3	H	3	0	0	0	0
4	A	32	0	48	0	0
4	B	24	0	36	0	0
4	C	28	0	42	0	0
4	D	48	0	72	4	0
4	E	36	0	54	4	0
4	F	8	0	12	0	0
4	G	12	0	18	1	0
4	H	12	0	18	0	0
5	B	7	0	10	1	0
6	A	105	0	0	1	0
6	B	96	0	0	2	0
6	C	112	0	0	4	0
6	D	111	0	0	0	0
6	E	106	0	0	1	0
6	F	61	0	0	1	0
6	G	73	0	0	0	0
6	H	109	0	0	1	0
All	All	14246	0	13353	134	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.

The worst 5 of 134 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:234:IOD:I	6:A:1082:HOH:O	2.41	1.07
1:G:54[B]:ARG:HH11	1:G:54[B]:ARG:HG3	1.20	1.06
1:F:153:ILE:HD12	2:F:237:IOD:I	2.35	0.95
1:G:54[B]:ARG:HH11	1:G:54[B]:ARG:CG	1.83	0.91
1:G:101:ARG:HG2	1:G:136:ALA:HB2	1.53	0.91

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	Percentiles	
1	A	216/221 (98%)	212 (98%)	4 (2%)	0	100	100
1	B	206/221 (93%)	200 (97%)	6 (3%)	0	100	100
1	C	207/221 (94%)	202 (98%)	5 (2%)	0	100	100
1	D	210/221 (95%)	205 (98%)	5 (2%)	0	100	100
1	E	204/221 (92%)	200 (98%)	4 (2%)	0	100	100
1	F	213/221 (96%)	207 (97%)	6 (3%)	0	100	100
1	G	216/221 (98%)	212 (98%)	4 (2%)	0	100	100
1	H	205/221 (93%)	200 (98%)	5 (2%)	0	100	100
All	All	1677/1768 (95%)	1638 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/172 (100%)	171 (99%)	1 (1%)	86	94
1	B	160/172 (93%)	160 (100%)	0	100	100
1	C	162/172 (94%)	162 (100%)	0	100	100
1	D	166/172 (96%)	165 (99%)	1 (1%)	86	94
1	E	162/172 (94%)	161 (99%)	1 (1%)	86	94
1	F	165/172 (96%)	165 (100%)	0	100	100
1	G	170/172 (99%)	170 (100%)	0	100	100
1	H	163/172 (95%)	163 (100%)	0	100	100
All	All	1320/1376 (96%)	1317 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	LEU
1	D	174	LEU
1	E	156	VAL

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

Mol	Chain	Res	Type
1	D	24	GLN
1	D	126	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the



expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	F	117	1	23,24,25	1.68	4 (17%)	25,32,34	1.52	5 (20%)
1	LLP	D	117	1	23,24,25	1.77	6 (26%)	25,32,34	1.32	3 (12%)
1	LLP	G	117	1	23,24,25	1.84	6 (26%)	25,32,34	1.37	3 (12%)
1	LLP	A	117	1	23,24,25	1.70	5 (21%)	25,32,34	1.61	5 (20%)
1	LLP	E	117	1	23,24,25	1.64	5 (21%)	25,32,34	1.58	4 (16%)
1	LLP	C	117	1	23,24,25	1.80	4 (17%)	25,32,34	1.50	3 (12%)
1	LLP	H	117	1	23,24,25	1.67	4 (17%)	25,32,34	1.37	3 (12%)
1	LLP	B	117	1	23,24,25	1.68	5 (21%)	25,32,34	1.49	2 (8%)

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
1	LLP	F	117	1	-	2/16/17/19	0/1/1/1
1	LLP	D	117	1	-	2/16/17/19	0/1/1/1
1	LLP	G	117	1	-	2/16/17/19	0/1/1/1
1	LLP	A	117	1	-	2/16/17/19	0/1/1/1
1	LLP	E	117	1	-	2/16/17/19	0/1/1/1
1	LLP	C	117	1	-	2/16/17/19	0/1/1/1
1	LLP	H	117	1	-	2/16/17/19	0/1/1/1
1	LLP	B	117	1	-	2/16/17/19	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	LLP	O3-C3	-5.30	1.24	1.37
1	H	117	LLP	O3-C3	-4.96	1.25	1.37
1	E	117	LLP	O3-C3	-4.93	1.25	1.37
1	B	117	LLP	O3-C3	-4.89	1.25	1.37
1	F	117	LLP	O3-C3	-4.85	1.25	1.37

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	117	LLP	OP4-C5'-C5	4.79	118.48	109.35
1	A	117	LLP	OP4-C5'-C5	4.64	118.19	109.35
1	C	117	LLP	OP4-C5'-C5	4.47	117.87	109.35
1	B	117	LLP	OP4-C5'-C5	4.43	117.79	109.35
1	F	117	LLP	OP4-C5'-C5	4.05	117.07	109.35

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	117	LLP	O-C-CA-CB
1	D	117	LLP	O-C-CA-CB
1	G	117	LLP	O-C-CA-CB
1	A	117	LLP	O-C-CA-CB
1	E	117	LLP	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	117	LLP	1	0
1	D	117	LLP	1	0
1	A	117	LLP	1	0
1	E	117	LLP	1	0
1	C	117	LLP	1	0
1	B	117	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 98 ligands modelled in this entry, 47 are monoatomic - leaving 51 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	265	-	3,3,3	0.49	0	2,2,2	0.15	0
4	EDO	C	304	-	3,3,3	0.54	0	2,2,2	0.05	0
4	EDO	G	262	-	3,3,3	0.60	0	2,2,2	0.28	0
4	EDO	D	282	-	3,3,3	0.47	0	2,2,2	0.29	0
4	EDO	D	296	-	3,3,3	0.46	0	2,2,2	0.27	0
4	EDO	A	270	-	3,3,3	0.43	0	2,2,2	0.15	0
4	EDO	B	299	-	3,3,3	0.57	0	2,2,2	0.32	0
5	PEG	B	261	-	6,6,6	0.72	0	5,5,5	0.26	0
4	EDO	H	274	-	3,3,3	0.56	0	2,2,2	0.32	0
4	EDO	G	300	-	3,3,3	0.48	0	2,2,2	0.27	0
4	EDO	B	294	-	3,3,3	0.43	0	2,2,2	0.32	0
4	EDO	D	264	-	3,3,3	0.37	0	2,2,2	0.52	0
4	EDO	A	303	-	3,3,3	0.55	0	2,2,2	0.14	0
4	EDO	B	285	-	3,3,3	0.67	0	2,2,2	0.06	0
4	EDO	C	302	-	3,3,3	0.48	0	2,2,2	0.28	0
4	EDO	E	266	-	3,3,3	0.40	0	2,2,2	0.57	0
4	EDO	E	268	-	3,3,3	0.63	0	2,2,2	0.13	0
4	EDO	E	267	-	3,3,3	0.54	0	2,2,2	0.21	0
4	EDO	A	275	-	3,3,3	0.46	0	2,2,2	0.24	0
4	EDO	C	295	-	3,3,3	0.66	0	2,2,2	0.04	0
4	EDO	B	280	-	3,3,3	0.26	0	2,2,2	0.51	0
4	EDO	E	283	-	3,3,3	0.44	0	2,2,2	0.27	0
4	EDO	D	287	-	3,3,3	0.44	0	2,2,2	0.11	0
4	EDO	D	263	-	3,3,3	0.34	0	2,2,2	0.04	0
4	EDO	D	289	-	3,3,3	0.47	0	2,2,2	0.11	0
4	EDO	E	276	-	3,3,3	0.47	0	2,2,2	0.04	0
4	EDO	B	292	-	3,3,3	0.57	0	2,2,2	0.20	0
4	EDO	F	301	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	E	288	-	3,3,3	0.43	0	2,2,2	0.41	0
4	EDO	D	284	-	3,3,3	0.40	0	2,2,2	0.46	0
4	EDO	B	293	-	3,3,3	0.63	0	2,2,2	0.31	0
4	EDO	H	311	-	3,3,3	0.74	0	2,2,2	0.14	0
4	EDO	H	281	-	3,3,3	0.53	0	2,2,2	0.16	0
4	EDO	E	273	-	3,3,3	0.38	0	2,2,2	0.38	0
4	EDO	C	269	-	3,3,3	0.46	0	2,2,2	0.31	0
4	EDO	D	277	-	3,3,3	0.59	0	2,2,2	0.20	0
4	EDO	D	291	-	3,3,3	0.38	0	2,2,2	0.31	0
4	EDO	C	307	-	3,3,3	0.73	0	2,2,2	0.01	0
4	EDO	G	308	-	3,3,3	0.48	0	2,2,2	0.19	0
4	EDO	D	271	-	3,3,3	0.52	0	2,2,2	0.37	0
4	EDO	A	279	-	3,3,3	0.34	0	2,2,2	0.30	0
4	EDO	E	298	-	3,3,3	0.31	0	2,2,2	0.49	0
4	EDO	D	310	-	3,3,3	0.61	0	2,2,2	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	306	-	3,3,3	0.53	0	2,2,2	0.13	0
4	EDO	C	278	-	3,3,3	0.71	0	2,2,2	0.04	0
4	EDO	A	272	-	3,3,3	0.58	0	2,2,2	0.13	0
4	EDO	C	286	-	3,3,3	0.60	0	2,2,2	0.13	0
4	EDO	F	297	-	3,3,3	0.16	0	2,2,2	0.80	0
4	EDO	E	305	-	3,3,3	0.39	0	2,2,2	0.27	0
4	EDO	D	290	-	3,3,3	0.63	0	2,2,2	0.25	0
4	EDO	A	309	-	3,3,3	0.44	0	2,2,2	0.33	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	EDO	A	265	-	-	1/1/1/1	-
4	EDO	C	304	-	-	0/1/1/1	-
4	EDO	G	262	-	-	1/1/1/1	-
4	EDO	D	282	-	-	1/1/1/1	-
4	EDO	D	296	-	-	1/1/1/1	-
4	EDO	A	270	-	-	1/1/1/1	-
4	EDO	B	299	-	-	0/1/1/1	-
5	PEG	B	261	-	-	2/4/4/4	-
4	EDO	H	274	-	-	1/1/1/1	-
4	EDO	G	300	-	-	1/1/1/1	-
4	EDO	B	294	-	-	1/1/1/1	-
4	EDO	D	264	-	-	0/1/1/1	-
4	EDO	A	303	-	-	0/1/1/1	-
4	EDO	B	285	-	-	0/1/1/1	-
4	EDO	C	302	-	-	0/1/1/1	-
4	EDO	E	266	-	-	0/1/1/1	-
4	EDO	E	268	-	-	0/1/1/1	-
4	EDO	E	267	-	-	1/1/1/1	-
4	EDO	A	275	-	-	1/1/1/1	-
4	EDO	C	295	-	-	0/1/1/1	-
4	EDO	B	280	-	-	1/1/1/1	-
4	EDO	E	283	-	-	1/1/1/1	-
4	EDO	D	287	-	-	0/1/1/1	-
4	EDO	D	263	-	-	1/1/1/1	-
4	EDO	D	289	-	-	0/1/1/1	-
4	EDO	E	276	-	-	0/1/1/1	-
4	EDO	B	292	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	F	301	-	-	1/1/1/1	-
4	EDO	E	288	-	-	1/1/1/1	-
4	EDO	D	284	-	-	1/1/1/1	-
4	EDO	B	293	-	-	0/1/1/1	-
4	EDO	H	311	-	-	1/1/1/1	-
4	EDO	H	281	-	-	1/1/1/1	-
4	EDO	E	273	-	-	1/1/1/1	-
4	EDO	C	269	-	-	0/1/1/1	-
4	EDO	D	277	-	-	0/1/1/1	-
4	EDO	D	291	-	-	1/1/1/1	-
4	EDO	C	307	-	-	1/1/1/1	-
4	EDO	G	308	-	-	1/1/1/1	-
4	EDO	D	271	-	-	0/1/1/1	-
4	EDO	A	279	-	-	1/1/1/1	-
4	EDO	E	298	-	-	1/1/1/1	-
4	EDO	D	310	-	-	1/1/1/1	-
4	EDO	A	306	-	-	0/1/1/1	-
4	EDO	C	278	-	-	0/1/1/1	-
4	EDO	A	272	-	-	1/1/1/1	-
4	EDO	C	286	-	-	0/1/1/1	-
4	EDO	F	297	-	-	1/1/1/1	-
4	EDO	E	305	-	-	0/1/1/1	-
4	EDO	D	290	-	-	1/1/1/1	-
4	EDO	A	309	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	292	EDO	O1-C1-C2-O2
5	B	261	PEG	O2-C3-C4-O4
4	D	296	EDO	O1-C1-C2-O2
4	A	272	EDO	O1-C1-C2-O2
4	D	290	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	261	PEG	1	0
4	G	300	EDO	1	0
4	E	268	EDO	1	0
4	D	287	EDO	2	0
4	D	263	EDO	1	0
4	E	276	EDO	2	0
4	E	273	EDO	1	0
4	D	291	EDO	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	212/221 (95%)	-0.08	9 (4%) 36 43	12, 20, 32, 50	0
1	B	204/221 (92%)	-0.09	4 (1%) 65 71	15, 22, 32, 37	0
1	C	206/221 (93%)	-0.15	4 (1%) 66 73	14, 21, 29, 34	0
1	D	208/221 (94%)	-0.22	4 (1%) 66 73	13, 19, 29, 36	0
1	E	204/221 (92%)	-0.33	0 100 100	13, 20, 28, 32	0
1	F	212/221 (95%)	0.15	9 (4%) 36 43	17, 27, 42, 50	0
1	G	212/221 (95%)	0.09	4 (1%) 66 73	18, 28, 39, 52	0
1	H	204/221 (92%)	-0.13	1 (0%) 91 94	13, 22, 30, 34	0
All	All	1662/1768 (94%)	-0.09	35 (2%) 63 70	12, 22, 35, 52	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	220	VAL	6.3
1	A	13	ALA	5.0
1	D	12	THR	4.7
1	F	94	ALA	4.5
1	A	7	LEU	4.4

### 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	LLP	F	117	24/25	0.96	0.17	17,19,20,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	LLP	G	117	24/25	0.96	0.17	17,20,22,23	0
1	LLP	B	117	24/25	0.96	0.17	12,15,19,19	0
1	LLP	A	117	24/25	0.97	0.16	9,13,15,15	0
1	LLP	E	117	24/25	0.97	0.12	12,14,16,16	0
1	LLP	C	117	24/25	0.97	0.15	11,14,16,16	0
1	LLP	H	117	24/25	0.97	0.17	11,14,16,17	0
1	LLP	D	117	24/25	0.97	0.14	9,12,15,15	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	285	4/4	0.57	0.23	47,48,48,49	0
4	EDO	B	292	4/4	0.57	0.21	51,51,51,52	0
4	EDO	C	307	4/4	0.65	0.22	44,45,45,46	0
4	EDO	C	286	4/4	0.67	0.20	46,47,47,48	0
4	EDO	F	301	4/4	0.68	0.30	55,55,55,55	0
4	EDO	C	302	4/4	0.70	0.22	44,44,45,46	0
4	EDO	D	277	4/4	0.72	0.34	28,29,32,33	0
4	EDO	D	296	4/4	0.77	0.28	40,40,41,42	0
4	EDO	C	295	4/4	0.80	0.26	41,41,42,42	0
4	EDO	H	311	4/4	0.80	0.25	16,19,21,23	0
4	EDO	D	310	4/4	0.83	0.18	39,40,40,41	0
4	EDO	A	306	4/4	0.84	0.21	59,60,60,60	0
4	EDO	G	300	4/4	0.84	0.17	43,44,45,45	0
4	EDO	A	303	4/4	0.84	0.19	45,46,46,46	0
4	EDO	A	272	4/4	0.85	0.21	32,33,33,34	0
4	EDO	E	298	4/4	0.85	0.19	31,31,32,34	0
4	EDO	E	273	4/4	0.86	0.24	39,39,39,39	0
5	PEG	B	261	7/7	0.86	0.29	40,40,41,42	0
4	EDO	B	293	4/4	0.86	0.20	42,42,42,43	0
4	EDO	D	282	4/4	0.87	0.17	46,47,47,47	0
4	EDO	C	278	4/4	0.87	0.19	38,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	G	308	4/4	0.87	0.17	35,36,36,36	0
4	EDO	G	262	4/4	0.88	0.16	26,26,27,28	0
3	CL	A	260	1/1	0.88	0.07	55,55,55,55	0
4	EDO	A	275	4/4	0.88	0.16	24,27,28,28	0
4	EDO	A	309	4/4	0.88	0.23	44,45,45,46	0
4	EDO	E	288	4/4	0.90	0.18	33,34,34,34	0
4	EDO	D	291	4/4	0.90	0.23	33,34,34,35	0
4	EDO	C	304	4/4	0.90	0.24	32,33,33,33	0
4	EDO	E	268	4/4	0.90	0.16	29,31,32,33	0
2	IOD	B	246	1/1	0.90	0.07	55,55,55,55	1
4	EDO	D	271	4/4	0.91	0.12	25,25,26,26	0
4	EDO	D	290	4/4	0.91	0.13	35,36,36,37	0
4	EDO	B	280	4/4	0.91	0.16	32,33,33,34	0
3	CL	A	252	1/1	0.92	0.07	52,52,52,52	0
4	EDO	D	284	4/4	0.92	0.20	31,31,31,32	0
4	EDO	B	294	4/4	0.92	0.42	49,50,51,51	0
4	EDO	A	279	4/4	0.92	0.22	33,33,33,34	0
4	EDO	H	274	4/4	0.93	0.12	22,24,25,25	0
4	EDO	E	283	4/4	0.93	0.19	31,32,32,33	0
4	EDO	H	281	4/4	0.93	0.14	29,30,30,31	0
4	EDO	E	305	4/4	0.93	0.19	35,36,37,37	0
4	EDO	E	267	4/4	0.93	0.14	37,38,39,40	0
3	CL	A	248	1/1	0.93	0.11	36,36,36,36	0
4	EDO	F	297	4/4	0.94	0.18	22,22,22,24	0
3	CL	E	251	1/1	0.94	0.12	45,45,45,45	0
4	EDO	E	276	4/4	0.94	0.12	23,23,24,24	0
3	CL	H	253	1/1	0.95	0.09	51,51,51,51	0
4	EDO	A	270	4/4	0.95	0.15	26,27,27,27	0
4	EDO	B	299	4/4	0.95	0.15	31,31,31,31	0
4	EDO	C	269	4/4	0.95	0.13	33,34,34,34	0
3	CL	E	247	1/1	0.95	0.07	48,48,48,48	0
4	EDO	A	265	4/4	0.95	0.14	17,17,17,18	0
2	IOD	C	245	1/1	0.96	0.08	34,34,34,34	1
4	EDO	E	266	4/4	0.96	0.12	24,24,25,25	0
4	EDO	D	264	4/4	0.96	0.08	16,17,18,18	0
2	IOD	H	244	1/1	0.96	0.08	44,44,44,44	1
3	CL	A	250	1/1	0.96	0.09	41,41,41,41	0
2	IOD	G	238	1/1	0.96	0.07	46,46,46,46	1
3	CL	D	257	1/1	0.97	0.09	28,28,28,28	0
4	EDO	D	289	4/4	0.97	0.11	28,28,28,29	0
3	CL	G	255	1/1	0.97	0.09	38,38,38,38	0
4	EDO	D	287	4/4	0.97	0.12	27,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	IOD	G	229[B]	1/1	0.98	0.05	28,28,28,28	1
3	CL	A	258	1/1	0.98	0.05	20,20,20,20	0
2	IOD	D	232	1/1	0.98	0.04	32,32,32,32	1
3	CL	E	256	1/1	0.98	0.07	27,27,27,27	0
2	IOD	F	228[B]	1/1	0.98	0.04	35,35,35,35	1
2	IOD	F	228[A]	1/1	0.98	0.04	44,44,44,44	1
3	CL	H	249	1/1	0.98	0.07	33,33,33,33	0
2	IOD	B	236	1/1	0.98	0.05	42,42,42,42	1
2	IOD	E	231[A]	1/1	0.98	0.05	36,36,36,36	1
2	IOD	G	229[A]	1/1	0.98	0.05	38,38,38,38	1
2	IOD	B	240	1/1	0.98	0.04	30,30,30,30	1
3	CL	H	254	1/1	0.98	0.07	17,17,17,17	0
2	IOD	B	242	1/1	0.98	0.05	30,30,30,30	1
2	IOD	E	231[B]	1/1	0.98	0.05	45,45,45,45	1
2	IOD	D	227[A]	1/1	0.99	0.09	26,26,26,26	1
2	IOD	A	225[A]	1/1	0.99	0.09	27,27,27,27	1
2	IOD	C	226[B]	1/1	0.99	0.04	32,32,32,32	1
2	IOD	A	225[B]	1/1	0.99	0.09	33,33,33,33	1
2	IOD	E	241	1/1	0.99	0.03	27,27,27,27	1
4	EDO	D	263	4/4	0.99	0.11	17,18,19,19	0
2	IOD	D	227[B]	1/1	0.99	0.09	23,23,23,23	1
2	IOD	H	230[A]	1/1	0.99	0.05	32,32,32,32	1
2	IOD	C	226[A]	1/1	0.99	0.04	38,38,38,38	1
2	IOD	C	233	1/1	0.99	0.04	34,34,34,34	1
2	IOD	F	237	1/1	0.99	0.03	44,44,44,44	1
2	IOD	H	243	1/1	0.99	0.04	30,30,30,30	1
2	IOD	H	235	1/1	0.99	0.04	38,38,38,38	1
2	IOD	A	221	1/1	0.99	0.04	28,28,28,28	0
3	CL	D	259	1/1	0.99	0.05	26,26,26,26	0
2	IOD	A	234	1/1	0.99	0.04	35,35,35,35	1
2	IOD	G	224	1/1	0.99	0.03	32,32,32,32	0
2	IOD	H	230[B]	1/1	0.99	0.05	36,36,36,36	1
2	IOD	C	239	1/1	0.99	0.09	27,27,27,27	1
2	IOD	D	222	1/1	1.00	0.02	22,22,22,22	0
2	IOD	F	223	1/1	1.00	0.02	31,31,31,31	0

## 6.5 Other polymers

There are no such residues in this entry.