



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:23 pm BST

PDB ID : 3R25  
Title : Crystal structure of enolase superfamily member from Vibrionales bacterium complexed with Mg and Glycerol in the active site  
Authors : Fedorov, A.A.; Fedorov, E.V.; Wichelecki, D.; Gerlt, J.A.; Almo, S.C.  
Deposited on : 2011-03-13  
Resolution : 1.60 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](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

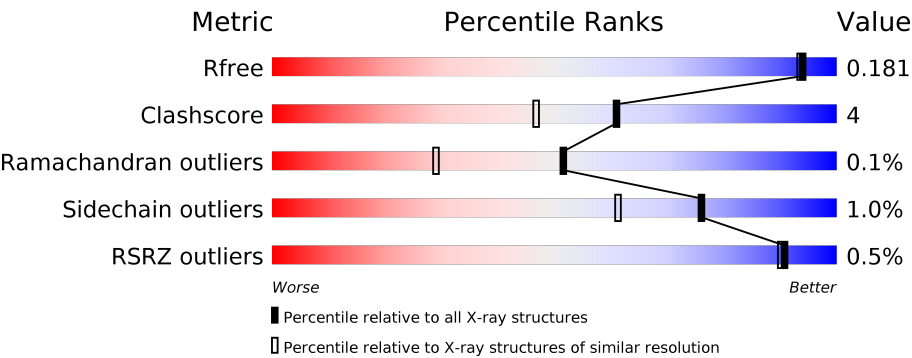
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	401	<div><div></div><div>87%10%•</div></div>
1	B	401	<div><div>%</div><div>89%11%</div></div>
1	C	401	<div><div></div><div>89%8%•</div></div>
1	D	401	<div><div></div><div>89%11%</div></div>
1	E	401	<div><div>%</div><div>87%11%•</div></div>
1	F	401	<div><div></div><div>87%12%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	401	<div><div></div><div>87%</div><div>12%</div><div>.</div></div>
1	H	401	<div>%<div><div></div><div>87%</div><div>10%</div><div>..</div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27265 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 mandelate racemase / muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	3	0
			3146	1999	548	582	17			
1	B	399	Total	C	N	O	S	0	1	0
			3193	2032	554	590	17			
1	C	390	Total	C	N	O	S	0	1	0
			3129	1990	545	577	17			
1	D	399	Total	C	N	O	S	0	1	0
			3193	2032	554	590	17			
1	E	395	Total	C	N	O	S	0	3	0
			3190	2028	556	589	17			
1	F	399	Total	C	N	O	S	0	0	0
			3182	2026	550	589	17			
1	G	395	Total	C	N	O	S	0	4	0
			3194	2030	554	593	17			
1	H	395	Total	C	N	O	S	0	0	0
			3153	2008	546	582	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	EXPRESSION TAG	UNP A5KUH4
A	3	LEU	-	EXPRESSION TAG	UNP A5KUH4
B	2	SER	-	EXPRESSION TAG	UNP A5KUH4
B	3	LEU	-	EXPRESSION TAG	UNP A5KUH4
C	2	SER	-	EXPRESSION TAG	UNP A5KUH4
C	3	LEU	-	EXPRESSION TAG	UNP A5KUH4
D	2	SER	-	EXPRESSION TAG	UNP A5KUH4
D	3	LEU	-	EXPRESSION TAG	UNP A5KUH4
E	2	SER	-	EXPRESSION TAG	UNP A5KUH4
E	3	LEU	-	EXPRESSION TAG	UNP A5KUH4
F	2	SER	-	EXPRESSION TAG	UNP A5KUH4
F	3	LEU	-	EXPRESSION TAG	UNP A5KUH4
G	2	SER	-	EXPRESSION TAG	UNP A5KUH4

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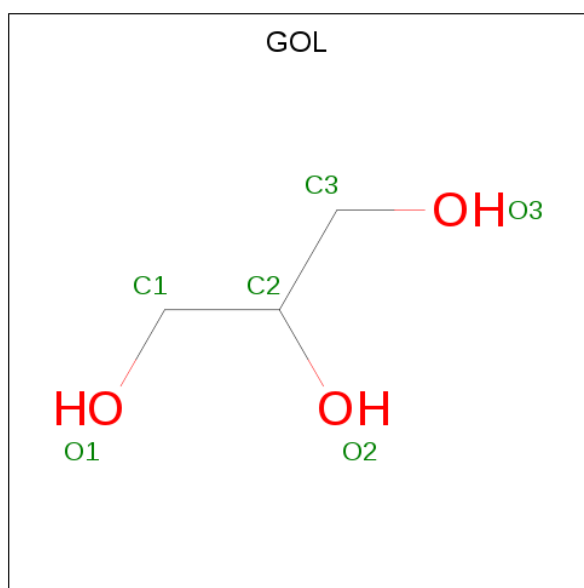
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Chain	Residue	Modelled	Actual	Comment	Reference
G	3	LEU	-	EXPRESSION TAG	UNP A5KUH4
H	2	SER	-	EXPRESSION TAG	UNP A5KUH4
H	3	LEU	-	EXPRESSION TAG	UNP A5KUH4

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	2	Total Mg 2 2	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	2	Total Mg 2 2	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0

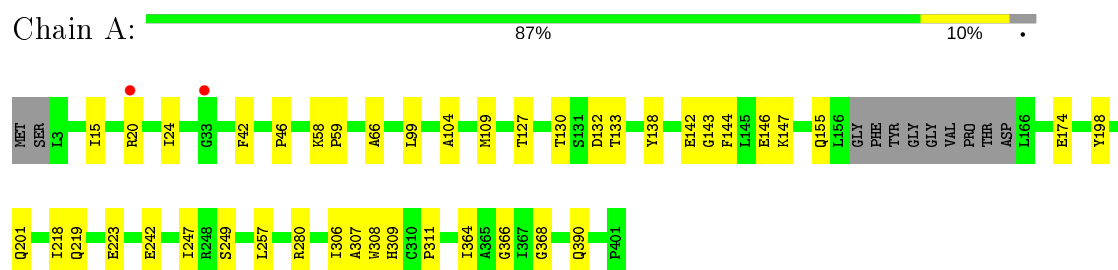
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	207	Total O 207 207	0	0
4	B	265	Total O 265 265	0	0
4	C	216	Total O 216 216	0	0
4	D	247	Total O 247 247	0	0
4	E	218	Total O 218 218	0	0
4	F	224	Total O 224 224	0	0
4	G	220	Total O 220 220	0	0
4	H	230	Total O 230 230	0	0

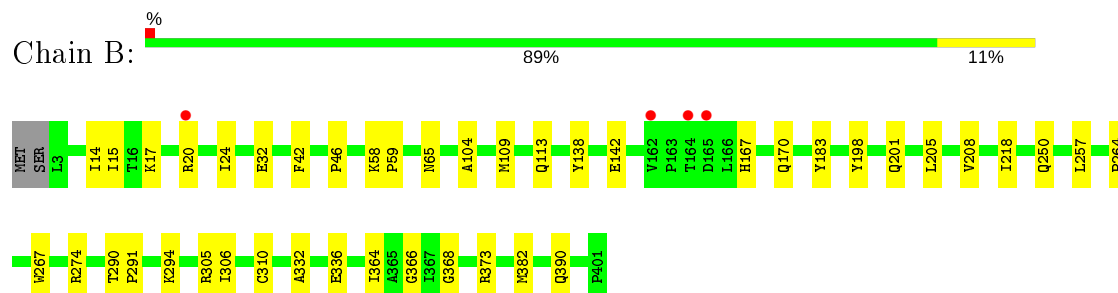
### 3 Residue-property plots [i](#)

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.

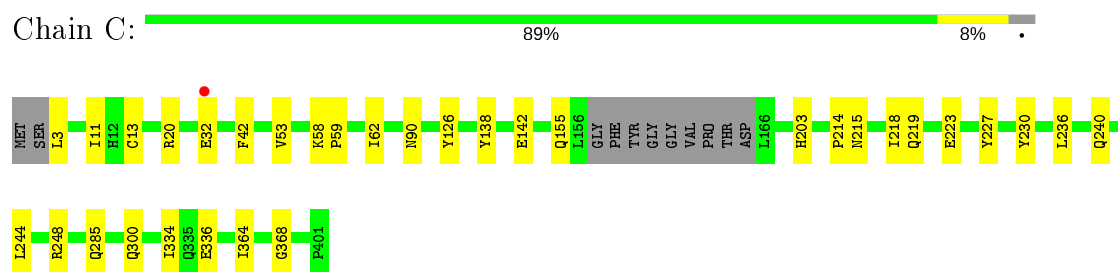
- Molecule 1: mandelate racemase / muconate lactonizing enzyme



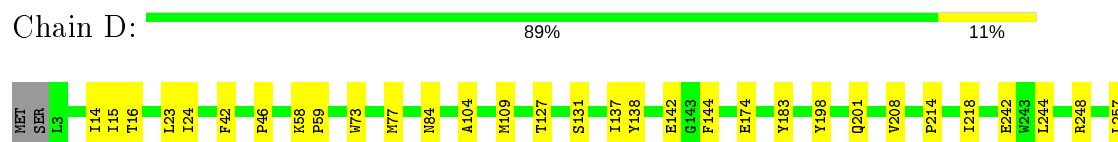
- Molecule 1: mandelate racemase / muconate lactonizing enzyme



- Molecule 1: mandelate racemase / muconate lactonizing enzyme

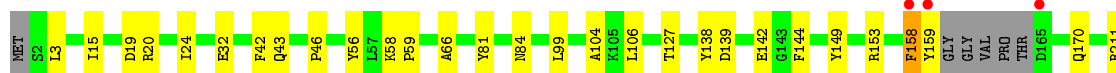
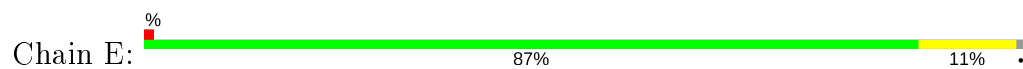


- Molecule 1: mandelate racemase / muconate lactonizing enzyme

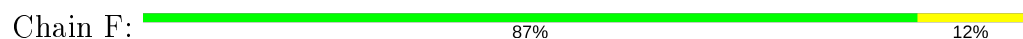




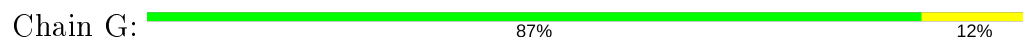
- Molecule 1: mandelate racemase / muconate lactonizing enzyme



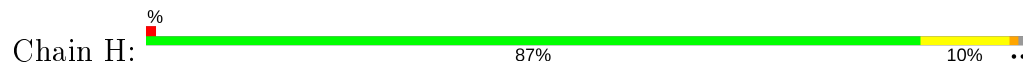
- Molecule 1: mandelate racemase / muconate lactonizing enzyme



- Molecule 1: mandelate racemase / muconate lactonizing enzyme



- Molecule 1: mandelate racemase / muconate lactonizing enzyme





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.99Å 211.52Å 211.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 1.60 39.04 – 1.60	Depositor EDS
% Data completeness (in resolution range)	86.2 (39.04-1.60) 86.2 (39.04-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 1.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.161 , 0.186 0.161 , 0.181	Depositor DCC
$R_{free}$ test set	2000 reflections (0.48%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.248 for -h,-l,-k	Xtriage
Reported twinning fraction	0.262 for -h,-l,-k	Depositor
Outliers	0 of 419783 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	27265	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% 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: GOL, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.35	0/3228	0.51	0/4388
1	B	0.35	0/3279	0.51	0/4460
1	C	0.34	0/3211	0.52	0/4365
1	D	0.34	0/3279	0.50	0/4460
1	E	0.35	0/3274	0.51	0/4450
1	F	0.34	0/3268	0.51	0/4446
1	G	0.35	0/3278	0.51	0/4456
1	H	0.35	0/3237	0.51	0/4400
All	All	0.35	0/26054	0.51	0/35425

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	3146	0	3054	23	0
1	B	3193	0	3099	32	0
1	C	3129	0	3044	21	0
1	D	3193	0	3099	29	0
1	E	3190	0	3094	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3182	0	3087	36	0
1	G	3194	0	3090	34	0
1	H	3153	0	3059	32	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0
4	A	207	0	0	3	0
4	B	265	0	0	6	0
4	C	216	0	0	3	0
4	D	247	0	0	9	0
4	E	218	0	0	4	0
4	F	224	0	0	9	0
4	G	220	0	0	4	0
4	H	230	0	0	5	0
All	All	27265	0	24690	225	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 (225) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:GLN:HG2	4:C:1841:HOH:O	1.64	0.95
1:F:384:ARG:HH11	1:F:384:ARG:HG2	1.32	0.93
1:A:130:THR:HG23	1:A:155:GLN:HB2	1.61	0.81
1:E:138:TYR:O	1:E:142:GLU:HG2	1.79	0.80
1:E:364:ILE:HD11	1:E:368:GLY:HA2	1.67	0.76
1:D:15:ILE:HD13	1:D:46:PRO:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:138:TYR:O	1:H:142:GLU:HG2	1.89	0.73
1:C:138:TYR:O	1:C:142:GLU:HG2	1.89	0.72
1:B:218:ILE:HD11	1:B:250:GLN:NE2	2.04	0.71
1:B:138:TYR:O	1:B:142:GLU:HG2	1.90	0.71
4:B:636:HOH:O	1:D:218:ILE:HD12	1.90	0.71
1:F:138:TYR:O	1:F:142:GLU:HG2	1.91	0.70
1:E:159:TYR:HA	1:E:211:ARG:NH1	2.07	0.69
1:E:15:ILE:HD13	1:E:46:PRO:HB2	1.75	0.69
1:G:19[B]:ASP:OD1	1:G:341:ASN:ND2	2.26	0.69
1:F:167:HIS:HE1	4:H:1857:HOH:O	1.76	0.69
1:H:305:ARG:HH11	1:H:305:ARG:HG3	1.58	0.67
1:F:242:GLU:HG3	4:F:1821:HOH:O	1.95	0.65
1:E:58:LYS:HB3	1:E:59:PRO:HD3	1.79	0.64
1:H:142:GLU:O	1:H:146:GLU:HG3	1.98	0.64
1:F:192:LYS:O	1:F:196:GLU:HG3	1.97	0.64
1:A:138:TYR:O	1:A:142:GLU:HG2	1.96	0.64
1:G:19[B]:ASP:OD2	1:G:341:ASN:OD1	2.16	0.64
4:D:422:HOH:O	1:E:218:ILE:HD12	1.98	0.63
1:C:218:ILE:HD13	4:C:1839:HOH:O	1.97	0.63
1:D:138:TYR:O	1:D:142:GLU:HG2	1.98	0.63
1:F:384:ARG:HH11	1:F:384:ARG:CG	2.10	0.63
1:G:16:THR:HG22	1:G:18:PRO:HD3	1.82	0.62
1:D:259:GLU:HB3	4:D:454:HOH:O	1.98	0.62
1:E:66:ALA:HB1	1:E:99:LEU:HD22	1.82	0.62
1:A:143:GLY:O	1:A:147:LYS:HG3	2.01	0.61
1:E:343:ASN:O	1:E:347:VAL:HG23	2.00	0.61
1:B:294:LYS:HE2	1:C:300:GLN:HE22	1.65	0.61
1:A:142:GLU:O	1:A:146:GLU:HG3	2.01	0.61
1:F:305:ARG:HD3	4:F:1858:HOH:O	2.01	0.60
1:F:385:PRO:HB2	1:F:387:GLU:HG3	1.83	0.60
1:E:159:TYR:HA	1:E:211:ARG:CZ	2.32	0.59
1:D:300:GLN:HG3	1:D:331:ASN:CG	2.22	0.59
1:H:58:LYS:HB3	1:H:59:PRO:HD3	1.85	0.59
1:F:167:HIS:CE1	4:H:1857:HOH:O	2.52	0.59
1:G:127:THR:HG21	1:G:144:PHE:CD1	2.37	0.58
1:B:14:ILE:HD13	1:B:373:ARG:HG2	1.84	0.58
1:C:58:LYS:HB3	1:C:59:PRO:HD3	1.86	0.58
1:H:104:ALA:HB3	1:H:366:GLY:HA2	1.85	0.57
1:D:24:ILE:HD11	1:D:46:PRO:HA	1.87	0.57
1:F:174:GLU:HG2	4:F:1912:HOH:O	2.04	0.57
1:A:390:GLN:NE2	4:A:1315:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:THR:HG21	1:A:144:PHE:CD1	2.39	0.56
1:H:306:ILE:HB	1:H:332:ALA:HA	1.87	0.56
1:H:364:ILE:HD11	1:H:368:GLY:HA2	1.87	0.55
1:G:58:LYS:HB3	1:G:59:PRO:HD3	1.89	0.55
1:E:310:CYS:HB2	1:E:336:GLU:HB3	1.87	0.54
1:E:84:ASN:ND2	4:E:476:HOH:O	2.37	0.54
1:F:58:LYS:HB3	1:F:59:PRO:HD3	1.88	0.54
1:E:19:ASP:HB3	4:E:1243:HOH:O	2.09	0.53
1:C:244:LEU:O	1:C:248:ARG:HG2	2.09	0.53
4:A:1840:HOH:O	1:H:218:ILE:HD12	2.08	0.53
1:D:310:CYS:HB2	1:D:336:GLU:HB3	1.91	0.52
1:H:197:LYS:HD3	1:H:198:TYR:CE2	2.44	0.52
1:H:374:GLU:HG3	1:H:375:ALA:N	2.23	0.52
1:B:104:ALA:HB3	1:B:366:GLY:HA2	1.91	0.52
1:D:16:THR:HG22	4:D:1085:HOH:O	2.10	0.52
1:F:66:ALA:HB1	1:F:99:LEU:HD22	1.91	0.52
1:A:127:THR:HG21	1:A:144:PHE:CE1	2.44	0.52
1:H:305:ARG:HG3	1:H:305:ARG:NH1	2.23	0.52
1:H:10:ASP:O	1:H:11:ILE:HG13	2.10	0.52
1:H:42:PHE:CE2	1:H:86:PRO:HB2	2.45	0.52
1:A:219:GLN:O	1:A:223:GLU:HG3	2.09	0.51
1:A:364:ILE:HD11	1:A:368:GLY:HA2	1.90	0.51
1:B:198:TYR:O	1:B:201:GLN:HG3	2.11	0.51
1:E:32:GLU:OE1	1:E:32:GLU:N	2.43	0.51
1:D:244:LEU:O	1:D:248:ARG:HG2	2.10	0.51
1:E:3:LEU:HD11	1:E:106:LEU:HD13	1.93	0.51
1:H:219:GLN:O	1:H:223:GLU:HG3	2.11	0.51
1:D:300:GLN:OE1	1:F:294:LYS:HE2	2.11	0.51
1:G:246:ASN:O	1:G:250:GLN:HG2	2.11	0.50
1:H:374:GLU:HG2	4:H:1121:HOH:O	2.11	0.50
1:B:170:GLN:HG2	1:G:360:TYR:OH	2.12	0.50
1:A:198:TYR:O	1:A:201:GLN:HG3	2.11	0.50
4:D:1534:HOH:O	1:E:219:GLN:HB2	2.11	0.50
1:F:19:ASP:HB3	4:F:1894:HOH:O	2.12	0.49
1:H:244:LEU:O	1:H:248:ARG:HG2	2.11	0.49
1:E:104:ALA:HB3	1:E:366:GLY:HA2	1.94	0.49
1:E:24:ILE:HD11	1:E:46:PRO:HA	1.92	0.49
1:A:104:ALA:HB3	1:A:366:GLY:HA2	1.95	0.49
1:B:290:THR:HB	1:B:291:PRO:HD3	1.93	0.49
1:F:218:ILE:HD12	4:F:1846:HOH:O	2.11	0.49
1:B:167:HIS:CE1	1:G:356:ASN:O	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:CYS:HB2	1:B:336:GLU:HB3	1.93	0.49
1:C:58:LYS:N	1:C:59:PRO:CD	2.76	0.49
1:E:153:ARG:NH2	1:E:159:TYR:OH	2.38	0.49
1:E:219:GLN:HE21	1:E:223:GLU:HG3	1.77	0.49
1:B:32:GLU:O	1:B:32:GLU:HG2	2.12	0.48
1:F:384:ARG:HG2	1:F:384:ARG:NH1	2.12	0.48
1:B:290:THR:HB	1:B:291:PRO:CD	2.43	0.48
1:D:127:THR:HG21	1:D:144:PHE:CD1	2.48	0.48
1:C:13:CYS:HB2	1:C:53:VAL:HG11	1.96	0.48
1:E:43:GLN:O	1:E:46:PRO:HD3	2.13	0.48
1:B:305[A]:ARG:HG3	4:B:885:HOH:O	2.12	0.48
1:D:131:SER:HB3	1:D:137:ILE:HG13	1.95	0.48
1:A:66:ALA:HB1	1:A:99:LEU:HD22	1.96	0.48
1:E:159:TYR:CA	1:E:211:ARG:NH1	2.77	0.48
1:D:109:MET:HG2	1:F:3:LEU:HD22	1.96	0.48
1:H:350:ASN:N	4:H:1069:HOH:O	2.46	0.47
1:C:364:ILE:HD11	1:C:368:GLY:HA2	1.97	0.47
1:G:257:LEU:HD23	1:G:258:GLY:N	2.29	0.47
1:H:13:CYS:HB2	1:H:53:VAL:HG11	1.96	0.47
1:A:24:ILE:HD11	1:A:46:PRO:HA	1.95	0.47
1:B:364:ILE:HD11	1:B:368:GLY:HA2	1.95	0.47
1:D:214:PRO:O	1:D:218:ILE:HG13	2.15	0.47
1:B:167:HIS:HE1	1:G:356:ASN:O	1.98	0.47
1:D:14:ILE:CD1	1:D:373:ARG:HG2	2.45	0.47
1:F:127:THR:HG21	1:F:144:PHE:CD1	2.50	0.46
1:H:390:GLN:NE2	4:H:430:HOH:O	2.47	0.46
1:D:104:ALA:HB3	1:D:366:GLY:HA2	1.97	0.46
1:A:306:ILE:HG21	1:A:308:TRP:CE2	2.50	0.46
1:F:384:ARG:NH1	1:F:384:ARG:CG	2.75	0.46
1:H:238:PRO:HB3	1:H:261:PHE:HE1	1.79	0.46
1:D:306:ILE:HB	1:D:332:ALA:HA	1.97	0.46
1:G:264:PRO:HA	1:G:267:TRP:CE2	2.51	0.46
1:E:159:TYR:C	1:E:211:ARG:HD3	2.35	0.46
1:B:167:HIS:HD2	4:G:948:HOH:O	1.98	0.46
1:C:126:TYR:CZ	1:C:336:GLU:HB2	2.50	0.46
1:D:218:ILE:CG1	4:D:1896:HOH:O	2.64	0.46
1:H:372:ASP:OD2	1:H:374:GLU:HB3	2.15	0.46
1:C:203:HIS:HB3	1:C:230:TYR:HB2	1.98	0.46
1:A:132:ASP:OD1	1:A:133:THR:HG23	2.16	0.46
1:C:20:ARG:HH11	1:C:20:ARG:HA	1.81	0.46
1:F:115:PHE:HB3	1:F:328:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:PRO:O	1:F:218:ILE:HG13	2.16	0.46
1:E:127:THR:HG21	1:E:144:PHE:CD1	2.51	0.45
1:H:214:PRO:O	1:H:218:ILE:HG13	2.16	0.45
1:F:349:PRO:O	1:F:350:ASN:HB2	2.16	0.45
1:G:310:CYS:HB2	1:G:336:GLU:HB3	1.97	0.45
1:A:218:ILE:HG12	1:A:247:ILE:HG13	1.97	0.45
1:B:15:ILE:HD13	1:B:46:PRO:HB2	1.98	0.45
1:A:58:LYS:N	1:A:59:PRO:HD2	2.32	0.45
1:C:126:TYR:HB3	1:C:334:ILE:HD11	1.99	0.45
1:A:280:ARG:HD2	1:A:307:ALA:O	2.17	0.45
1:E:159:TYR:C	1:E:211:ARG:NH1	2.70	0.45
1:E:300:GLN:HE22	1:H:294:LYS:HE2	1.81	0.45
1:D:257:LEU:HD23	1:D:258:GLY:N	2.32	0.45
1:F:364:ILE:HD11	1:F:368:GLY:HA2	1.99	0.45
1:E:274:ARG:HD2	4:E:1781:HOH:O	2.17	0.45
1:F:24:ILE:HD11	1:F:46:PRO:HA	1.98	0.45
1:E:300:GLN:NE2	1:H:294:LYS:HE2	2.31	0.45
1:A:109:MET:HG2	1:G:3:LEU:HD22	2.00	0.44
1:B:390:GLN:NE2	4:B:464:HOH:O	2.48	0.44
1:E:158:PHE:CG	1:E:159:TYR:N	2.85	0.44
1:E:56:TYR:OH	1:F:46:PRO:HD2	2.18	0.44
4:E:1100:HOH:O	1:G:214:PRO:HD2	2.17	0.44
1:D:58:LYS:N	1:D:59:PRO:HD2	2.33	0.44
1:F:23:LEU:HB3	1:F:315:THR:HG22	1.98	0.44
1:G:142:GLU:O	1:G:146:GLU:HG3	2.18	0.44
1:C:219:GLN:HE21	1:C:223:GLU:CD	2.20	0.44
1:D:390:GLN:NE2	4:D:989:HOH:O	2.44	0.44
1:F:248:ARG:HD2	1:F:248:ARG:HA	1.88	0.44
1:H:137:ILE:O	1:H:141:VAL:HG23	2.18	0.44
1:B:109:MET:HG2	1:C:3:LEU:HD22	1.99	0.44
1:F:305:ARG:CD	4:F:1858:HOH:O	2.64	0.44
1:F:311:PRO:HB2	1:F:313:ASP:OD2	2.17	0.44
1:D:84:ASN:ND2	4:D:692:HOH:O	2.39	0.43
1:D:73:TRP:CH2	1:D:77:MET:HG3	2.53	0.43
1:G:211:ARG:HD3	1:G:211:ARG:HA	1.71	0.43
1:B:24:ILE:HD11	1:B:46:PRO:HA	2.00	0.43
1:F:207:ASP:HA	1:F:233:GLU:HB3	1.99	0.43
1:H:214:PRO:HA	1:H:236:LEU:HD21	2.01	0.43
1:G:264:PRO:HA	1:G:267:TRP:CZ2	2.54	0.43
1:G:44:GLN:O	1:G:45:ARG:HD3	2.19	0.43
1:A:15:ILE:HD13	1:A:46:PRO:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASN:HB3	4:B:1056:HOH:O	2.18	0.43
1:B:17:LYS:HD3	1:B:382:MET:CE	2.49	0.43
1:E:297:HIS:CD2	1:H:294:LYS:HG2	2.54	0.43
1:B:274:ARG:HD2	4:B:1784:HOH:O	2.19	0.42
1:B:58:LYS:N	1:B:59:PRO:HD2	2.34	0.42
1:D:183:TYR:OH	1:D:208:VAL:HA	2.19	0.42
1:D:23:LEU:HB3	1:D:315:THR:HG22	2.01	0.42
1:C:58:LYS:O	1:C:62:ILE:HG12	2.20	0.42
1:G:104:ALA:HB3	1:G:366:GLY:HA2	2.01	0.42
1:D:218:ILE:CD1	4:D:1862:HOH:O	2.66	0.42
1:D:198:TYR:O	1:D:201:GLN:HG3	2.20	0.42
1:E:149:TYR:OH	1:E:354:PRO:HG2	2.20	0.42
1:E:290:THR:HB	1:E:291:PRO:CD	2.50	0.42
1:G:259:GLU:HB3	4:G:422:HOH:O	2.19	0.42
1:G:280:ARG:HD2	1:G:307:ALA:O	2.19	0.42
1:H:309:HIS:CE1	1:H:311:PRO:HG3	2.54	0.42
1:G:19[B]:ASP:CG	1:G:341:ASN:OD1	2.58	0.42
1:B:17:LYS:HD3	1:B:382:MET:HE2	2.02	0.42
1:F:297:HIS:HB3	4:F:1535:HOH:O	2.20	0.42
1:F:310:CYS:HB2	1:F:336:GLU:HB3	2.02	0.42
1:G:73:TRP:CH2	1:G:77:MET:HG3	2.55	0.42
1:A:242:GLU:HG3	4:A:1843:HOH:O	2.20	0.42
1:A:309:HIS:CE1	1:A:311:PRO:HG3	2.55	0.42
1:B:183:TYR:OH	1:B:208:VAL:HA	2.20	0.41
1:D:360:TYR:OH	1:E:170:GLN:HG2	2.20	0.41
1:E:290:THR:HB	1:E:291:PRO:HD3	2.03	0.41
1:E:356:ASN:O	1:G:167:HIS:CE1	2.72	0.41
1:D:242:GLU:HG3	4:D:1816:HOH:O	2.19	0.41
1:G:183:TYR:OH	1:G:208:VAL:HA	2.20	0.41
1:G:205:LEU:HD12	1:G:205:LEU:N	2.34	0.41
1:B:264:PRO:HA	1:B:267:TRP:CE2	2.55	0.41
1:B:113:GLN:HG3	1:C:3:LEU:HD23	2.00	0.41
1:F:167:HIS:CD2	1:H:150:LYS:HE3	2.55	0.41
1:G:15:ILE:HD13	1:G:46:PRO:HB2	2.03	0.41
1:H:256:GLY:HA2	1:H:278:PHE:O	2.21	0.41
1:B:205:LEU:N	1:B:205:LEU:HD12	2.35	0.41
1:B:264:PRO:HA	1:B:267:TRP:CZ2	2.55	0.41
1:B:167:HIS:CD2	4:B:1829:HOH:O	2.73	0.41
1:C:215:ASN:HA	4:F:732:HOH:O	2.21	0.41
1:F:246:ASN:O	1:F:250:GLN:HG2	2.21	0.41
1:G:19[A]:ASP:HB3	4:G:444:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:HIS:HB3	1:G:230:TYR:HB2	2.02	0.41
1:F:280:ARG:HD2	1:F:307:ALA:O	2.21	0.40
1:G:127:THR:HG21	1:G:144:PHE:CE1	2.57	0.40
1:G:385:PRO:HG2	4:G:621:HOH:O	2.21	0.40
1:A:249:SER:O	1:H:250:GLN:HB3	2.20	0.40
1:C:227:TYR:HA	4:C:1772:HOH:O	2.21	0.40
1:G:95:VAL:O	1:G:99:LEU:HG	2.22	0.40
1:F:84:ASN:ND2	4:F:872:HOH:O	2.52	0.40
1:G:164:THR:O	1:G:165:ASP:C	2.59	0.40
1:H:244:LEU:HA	1:H:244:LEU:HD23	1.74	0.40
1:B:306:ILE:HB	1:B:332:ALA:HA	2.03	0.40
1:C:214:PRO:HA	1:C:236:LEU:HD21	2.02	0.40
1:C:90:ASN:HD21	1:C:285:GLN:NE2	2.20	0.40
1:G:300:GLN:HG3	1:G:331:ASN:CG	2.41	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	389/401 (97%)	383 (98%)	6 (2%)	0	100	100
1	B	398/401 (99%)	389 (98%)	9 (2%)	0	100	100
1	C	387/401 (96%)	377 (97%)	10 (3%)	0	100	100
1	D	398/401 (99%)	393 (99%)	5 (1%)	0	100	100
1	E	394/401 (98%)	383 (97%)	9 (2%)	2 (0%)	29	11
1	F	397/401 (99%)	386 (97%)	10 (2%)	1 (0%)	41	21
1	G	395/401 (98%)	385 (98%)	10 (2%)	0	100	100
1	H	391/401 (98%)	381 (97%)	9 (2%)	1 (0%)	41	21
All	All	3149/3208 (98%)	3077 (98%)	68 (2%)	4 (0%)	51	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	158	PHE
1	E	81	TYR
1	H	19	ASP
1	F	81	TYR

### 5.3.2 Protein sidechains ⓘ

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	340/345 (99%)	336 (99%)	4 (1%)	71	54
1	B	344/345 (100%)	341 (99%)	3 (1%)	78	65
1	C	338/345 (98%)	334 (99%)	4 (1%)	71	54
1	D	344/345 (100%)	342 (99%)	2 (1%)	86	77
1	E	344/345 (100%)	341 (99%)	3 (1%)	78	65
1	F	343/345 (99%)	339 (99%)	4 (1%)	71	54
1	G	345/345 (100%)	343 (99%)	2 (1%)	86	77
1	H	339/345 (98%)	335 (99%)	4 (1%)	71	54
All	All	2737/2760 (99%)	2711 (99%)	26 (1%)	76	65

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	42	PHE
1	A	174	GLU
1	A	257	LEU
1	B	20	ARG
1	B	42	PHE
1	B	257	LEU
1	C	11	ILE
1	C	32	GLU
1	C	42	PHE

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Mol	Chain	Res	Type
1	C	155	GLN
1	D	42	PHE
1	D	174	GLU
1	E	20	ARG
1	E	42	PHE
1	E	139	ASP
1	F	168	THR
1	F	257	LEU
1	F	374	GLU
1	F	384	ARG
1	G	42	PHE
1	G	257	LEU
1	H	42	PHE
1	H	257	LEU
1	H	305	ARG
1	H	374	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	GLN
1	B	167	HIS
1	C	90	ASN
1	C	200	ASN
1	C	300	GLN
1	E	170	GLN
1	F	167	HIS
1	G	182	GLN
1	H	171	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	$\# Z  > 2$
3	GOL	B	404	-	5,5,5	0.34	0	5,5,5	0.30	0
3	GOL	D	404	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	F	403	-	5,5,5	0.39	0	5,5,5	0.21	0
3	GOL	E	403	-	5,5,5	0.47	0	5,5,5	0.20	0
3	GOL	G	403	-	5,5,5	0.38	0	5,5,5	0.21	0
3	GOL	A	403	-	5,5,5	0.35	0	5,5,5	0.21	0
3	GOL	C	403	-	5,5,5	0.33	0	5,5,5	0.34	0
3	GOL	H	403	-	5,5,5	0.43	0	5,5,5	0.15	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
3	GOL	B	404	-	-	0/4/4/4	-
3	GOL	D	404	-	-	0/4/4/4	-
3	GOL	F	403	-	-	0/4/4/4	-
3	GOL	E	403	-	-	0/4/4/4	-
3	GOL	G	403	-	-	0/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	C	403	-	-	2/4/4/4	-
3	GOL	H	403	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	403	GOL	O1-C1-C2-C3
3	C	403	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	390/401 (97%)	-0.41	2 (0%) 91 90	20, 26, 39, 49	0
1	B	399/401 (99%)	-0.46	4 (1%) 82 82	19, 24, 34, 63	0
1	C	390/401 (97%)	-0.46	1 (0%) 94 93	19, 25, 36, 46	0
1	D	399/401 (99%)	-0.50	0 100 100	19, 24, 34, 50	0
1	E	395/401 (98%)	-0.45	3 (0%) 86 86	21, 25, 37, 58	0
1	F	399/401 (99%)	-0.44	0 100 100	20, 26, 38, 51	0
1	G	395/401 (98%)	-0.45	2 (0%) 91 90	19, 26, 36, 58	0
1	H	395/401 (98%)	-0.43	3 (0%) 86 86	21, 26, 38, 53	0
All	All	3162/3208 (98%)	-0.45	15 (0%) 91 90	19, 25, 37, 63	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	ASP	5.9
1	B	162	VAL	4.3
1	H	33	GLY	4.0
1	G	165	ASP	4.0
1	G	158	PHE	4.0
1	B	164	THR	3.9
1	E	159	TYR	3.2
1	H	158	PHE	2.8
1	A	33	GLY	2.4
1	E	165	ASP	2.4
1	E	158	PHE	2.3
1	C	32	GLU	2.3
1	B	20	ARG	2.2
1	A	20	ARG	2.1
1	H	374	GLU	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 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
2	MG	D	403	1/1	0.87	0.11	46,46,46,46	0
3	GOL	D	404	6/6	0.92	0.08	24,26,27,28	0
3	GOL	G	403	6/6	0.94	0.12	28,29,31,32	0
2	MG	B	403	1/1	0.95	0.05	39,39,39,39	0
3	GOL	A	403	6/6	0.95	0.08	25,27,28,29	0
3	GOL	H	403	6/6	0.95	0.09	25,27,28,29	0
3	GOL	F	403	6/6	0.96	0.07	25,26,28,28	0
3	GOL	E	403	6/6	0.96	0.05	24,26,28,29	0
3	GOL	B	404	6/6	0.96	0.06	24,24,25,27	0
2	MG	C	402	1/1	0.97	0.08	24,24,24,24	0
2	MG	F	402	1/1	0.97	0.07	23,23,23,23	0
3	GOL	C	403	6/6	0.98	0.05	25,27,28,32	0
2	MG	E	402	1/1	0.98	0.13	25,25,25,25	0
2	MG	B	402	1/1	0.99	0.11	22,22,22,22	0
2	MG	D	402	1/1	0.99	0.07	24,24,24,24	0
2	MG	G	402	1/1	0.99	0.07	27,27,27,27	0
2	MG	A	402	1/1	0.99	0.07	26,26,26,26	0
2	MG	H	402	1/1	1.00	0.08	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.