



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 11:18 AM EST

PDB ID : 3WJ8  
Title : Crystal Structure of DL-2-haloacid dehalogenase mutant with 2-bromo-2-methylpropionate  
Authors : Siwek, A.; Omi, R.; Hirotsu, K.; Jitsumori, K.; Esaki, N.; Kurihara, T.; Paneth, P.  
Deposited on : 2013-10-07  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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

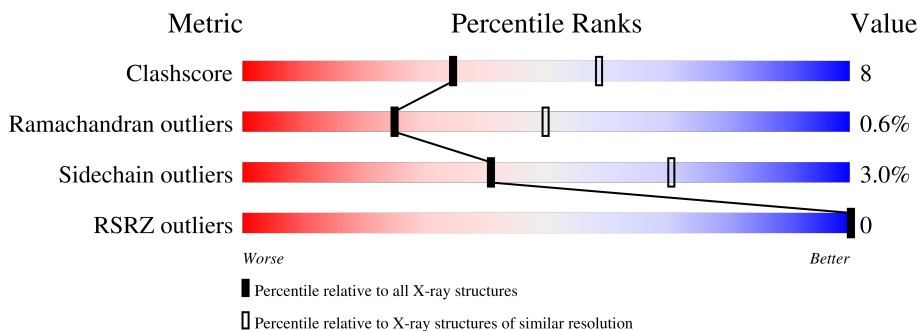
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	301	
1	B	301	
1	D	301	
1	E	301	
1	F	301	
1	G	301	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	B2P	A	401	-	X	X	-
2	B2P	D	401	-	-	X	-
2	B2P	E	401	-	-	X	-
2	B2P	F	401	-	-	X	-
2	B2P	G	401	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15037 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.

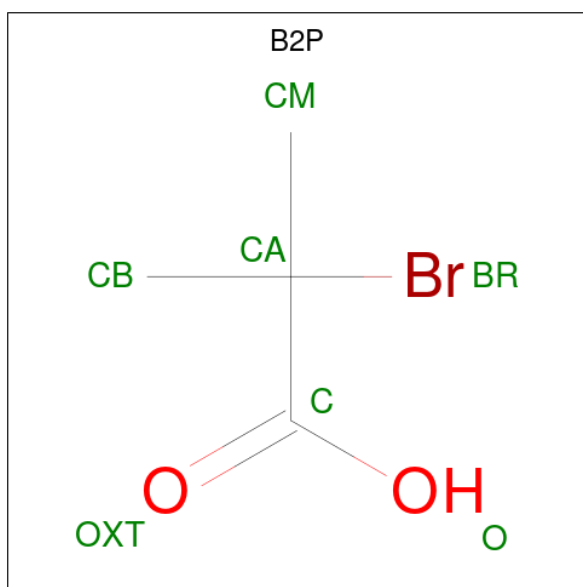
- Molecule 1 is a protein called DL-2-haloacid dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	Total 2386	C 1523	N 426	O 432	S 5	0	1	0
1	B	298	Total 2392	C 1527	N 427	O 433	S 5	0	2	0
1	D	298	Total 2378	C 1518	N 424	O 431	S 5	0	0	0
1	E	298	Total 2393	C 1527	N 427	O 434	S 5	0	2	0
1	F	298	Total 2398	C 1530	N 430	O 433	S 5	0	2	0
1	G	298	Total 2401	C 1532	N 430	O 434	S 5	0	3	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	HIS	ASP	engineered mutation	UNP A6BM74
A	194	ASN	ASP	engineered mutation	UNP A6BM74
B	54	HIS	ASP	engineered mutation	UNP A6BM74
B	194	ASN	ASP	engineered mutation	UNP A6BM74
D	54	HIS	ASP	engineered mutation	UNP A6BM74
D	194	ASN	ASP	engineered mutation	UNP A6BM74
E	54	HIS	ASP	engineered mutation	UNP A6BM74
E	194	ASN	ASP	engineered mutation	UNP A6BM74
F	54	HIS	ASP	engineered mutation	UNP A6BM74
F	194	ASN	ASP	engineered mutation	UNP A6BM74
G	54	HIS	ASP	engineered mutation	UNP A6BM74
G	194	ASN	ASP	engineered mutation	UNP A6BM74

- Molecule 2 is 2-bromo-2-methylpropanoic acid (three-letter code: B2P) (formula: C<sub>4</sub>H<sub>7</sub>BrO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	O		
2	A	1	7	1	4	2	0	0
2	B	1	7	1	4	2	0	0
2	D	1	7	1	4	2	0	0
2	E	1	7	1	4	2	0	0
2	F	1	7	1	4	2	0	0
2	G	1	7	1	4	2	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	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

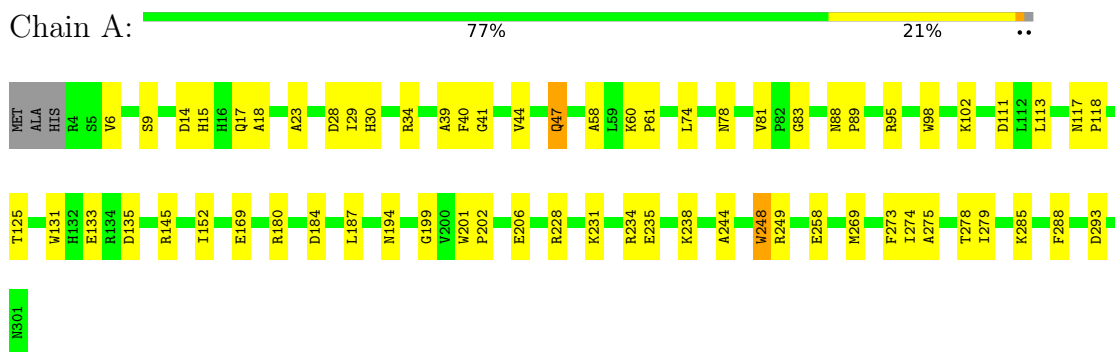
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	97	Total O 97 97	0	0
4	B	101	Total O 101 101	0	0
4	D	99	Total O 99 99	0	0
4	E	114	Total O 114 114	0	0
4	F	102	Total O 102 102	0	0
4	G	98	Total O 98 98	0	0

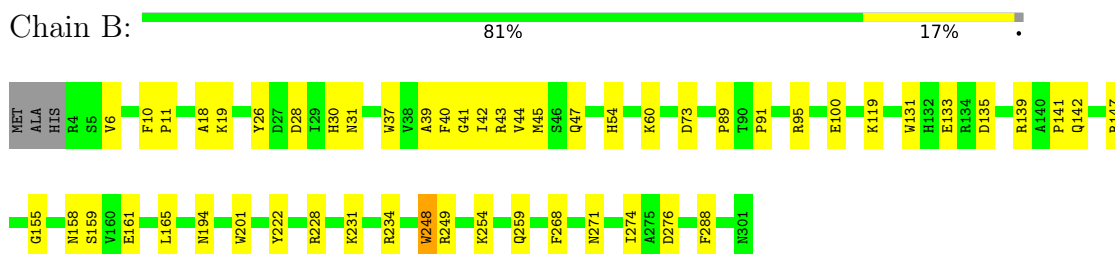
### 3 Residue-property plots

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.

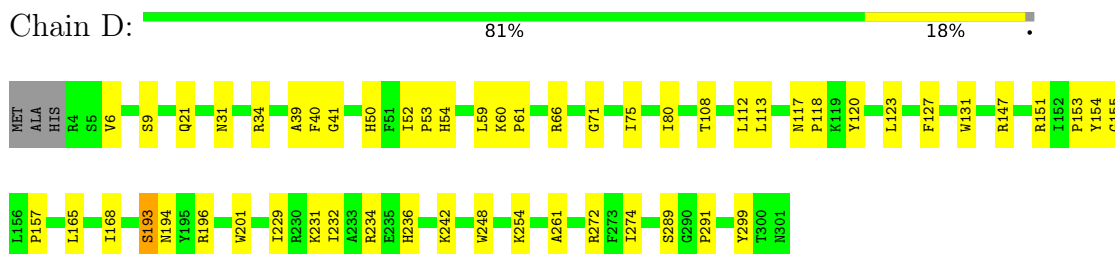
- Molecule 1: DL-2-haloacid dehalogenase



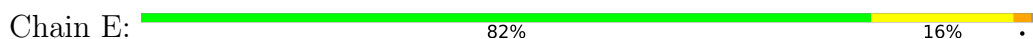
- Molecule 1: DL-2-haloacid dehalogenase

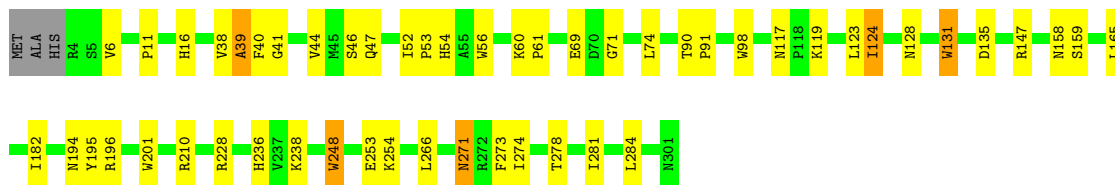


- Molecule 1: DL-2-haloacid dehalogenase



- Molecule 1: DL-2-haloacid dehalogenase

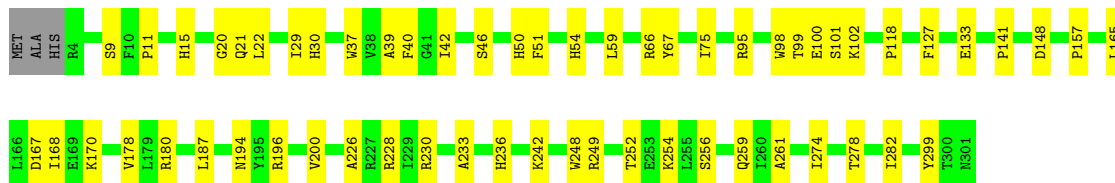
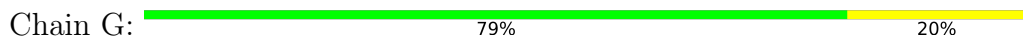




• Molecule 1: DL-2-haloacid dehalogenase



• Molecule 1: DL-2-haloacid dehalogenase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.31Å 186.31Å 114.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 48.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.70) 99.5 (48.67-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.73 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.187 , 0.269 0.198 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtrriage
Anisotropy	0.711	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , -4.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.378 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15037	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7032e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, B2P

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	2/2449 (0.1%)	0.79	0/3326
1	B	0.69	3/2458 (0.1%)	0.78	1/3338 (0.0%)
1	D	0.68	3/2438 (0.1%)	0.74	0/3312
1	E	0.69	5/2459 (0.2%)	0.76	0/3339
1	F	0.68	3/2464 (0.1%)	0.78	0/3345
1	G	0.69	3/2470 (0.1%)	0.77	0/3353
All	All	0.69	19/14738 (0.1%)	0.77	1/20013 (0.0%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	248	TRP	CD2-CE2	6.43	1.49	1.41
1	A	248	TRP	CD2-CE2	5.94	1.48	1.41
1	B	248	TRP	CD2-CE2	5.77	1.48	1.41
1	E	56	TRP	CD2-CE2	5.72	1.48	1.41
1	G	248	TRP	CD2-CE2	5.66	1.48	1.41
1	D	131	TRP	CD2-CE2	5.54	1.48	1.41
1	A	201	TRP	CD2-CE2	5.51	1.48	1.41
1	E	98	TRP	CD2-CE2	5.51	1.48	1.41
1	G	37	TRP	CD2-CE2	5.45	1.47	1.41
1	E	248	TRP	CD2-CE2	5.44	1.47	1.41
1	E	201	TRP	CD2-CE2	5.41	1.47	1.41
1	F	201	TRP	CD2-CE2	5.31	1.47	1.41
1	D	201	TRP	CD2-CE2	5.30	1.47	1.41
1	E	131	TRP	CD2-CE2	5.25	1.47	1.41
1	G	98	TRP	CD2-CE2	5.17	1.47	1.41
1	F	248	TRP	CD2-CE2	5.13	1.47	1.41
1	B	37	TRP	CD2-CE2	5.09	1.47	1.41
1	B	201	TRP	CD2-CE2	5.05	1.47	1.41
1	F	37	TRP	CD2-CE2	5.04	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	ASP	CB-CG-OD1	6.23	123.91	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	2386	0	2379	42	0
1	B	2392	0	2387	36	0
1	D	2378	0	2368	39	0
1	E	2393	0	2390	34	0
1	F	2398	0	2398	60	0
1	G	2401	0	2403	38	0
2	A	7	0	6	8	0
2	B	7	0	6	3	0
2	D	7	0	6	8	0
2	E	7	0	6	8	0
2	F	7	0	6	8	0
2	G	7	0	6	5	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	2	0
3	G	6	0	8	0	0
4	A	97	0	0	1	0
4	B	101	0	0	6	0
4	D	99	0	0	5	0
4	E	114	0	0	1	0
4	F	102	0	0	5	0
4	G	98	0	0	4	0
All	All	15037	0	14409	239	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 8.

All (239) 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:D:39:ALA:HB1	2:D:401:B2P:H3	1.29	1.12
1:D:274:ILE:HG12	2:D:401:B2P:H5	1.40	1.02
1:F:39:ALA:HB1	2:F:401:B2P:H3	1.47	0.97
1:B:54:HIS:HE1	1:B:254:LYS:NZ	1.66	0.94
1:D:168:ILE:HD11	1:D:196:ARG:HD2	1.54	0.90
1:D:40:PHE:HB3	2:D:401:B2P:BR	2.26	0.89
1:B:54:HIS:CE1	1:B:254:LYS:NZ	2.42	0.88
1:E:40:PHE:HB3	2:E:401:B2P:BR	2.29	0.87
1:A:14:ASP:HB2	1:A:17:GLN:HG3	1.55	0.86
1:G:39:ALA:HB1	2:G:401:B2P:H3	1.56	0.86
1:A:41:GLY:N	2:A:401:B2P:BR	2.65	0.83
1:A:274:ILE:HG13	2:A:401:B2P:H5	1.60	0.82
1:G:54:HIS:NE2	1:G:254:LYS:NZ	2.28	0.78
1:F:40:PHE:HB3	2:F:401:B2P:BR	2.40	0.77
1:G:15:HIS:HE1	1:G:30:HIS:NE2	1.82	0.77
1:E:41:GLY:N	2:E:401:B2P:BR	2.73	0.77
1:B:54:HIS:CE1	1:B:254:LYS:HZ2	2.02	0.76
1:B:44:VAL:O	1:B:47:GLN:HG2	1.86	0.76
1:B:274:ILE:HG12	2:B:401:B2P:H2	1.67	0.76
1:B:231:LYS:HG3	1:B:234:ARG:NH2	2.01	0.75
1:D:39:ALA:HB1	2:D:401:B2P:CB	2.14	0.75
1:B:91:PRO:O	1:B:95:ARG:HG3	1.88	0.74
1:G:54:HIS:CE1	4:G:543:HOH:O	2.41	0.73
1:F:14:ASP:HB2	1:F:17:GLN:HE21	1.53	0.72
1:E:54:HIS:CE1	1:E:254:LYS:NZ	2.58	0.72
1:B:54:HIS:CE1	1:B:254:LYS:HZ3	2.08	0.71
1:A:202:PRO:O	1:A:206:GLU:HG3	1.92	0.70
1:E:54:HIS:CE1	1:E:254:LYS:HZ2	2.11	0.69
1:F:228:ARG:HD3	4:F:501:HOH:O	1.91	0.69
1:F:194:ASN:H	1:F:194:ASN:HD22	1.40	0.68
1:B:95:ARG:NH1	1:G:66:ARG:HD2	2.10	0.67
1:B:54:HIS:HE1	1:B:254:LYS:HZ3	1.40	0.67
1:F:274:ILE:HG12	2:F:401:B2P:H2	1.77	0.67
1:F:133:GLU:OE2	1:F:249:ARG:HD3	1.95	0.66
1:D:50:HIS:HB3	1:D:54:HIS:CE1	2.30	0.66
1:D:231:LYS:HG3	1:D:234:ARG:NH2	2.12	0.65
1:E:147:ARG:NH1	1:G:95:ARG:HA	2.12	0.64
1:G:228:ARG:HD3	4:G:513:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TRP:CE2	1:A:248:TRP:HB3	2.32	0.63
1:F:31:ASN:OD1	1:F:155:GLY:HA2	1.98	0.63
1:F:54:HIS:HE1	1:F:254:LYS:HD3	1.64	0.63
1:G:40:PHE:HB3	2:G:401:B2P:BR	2.53	0.63
1:D:39:ALA:CB	2:D:401:B2P:H3	2.19	0.62
1:F:12:GLN:OE1	1:F:43:ARG:NE	2.26	0.62
1:D:31:ASN:HD22	1:D:155:GLY:HA2	1.66	0.60
1:A:74:LEU:HD11	3:F:402:GOL:O1	2.00	0.60
1:B:40:PHE:HB3	2:B:401:B2P:BR	2.57	0.60
1:E:165:LEU:HD23	1:E:196:ARG:NH1	2.17	0.60
1:B:228:ARG:HD3	4:B:579:HOH:O	2.02	0.59
1:E:52:ILE:HB	1:E:53:PRO:HD3	1.85	0.59
1:B:41:GLY:O	1:B:45:MET:HB2	2.03	0.58
1:F:225:THR:HG23	1:F:228:ARG:NH2	2.19	0.58
1:E:44:VAL:O	1:E:47:GLN:HG2	2.04	0.58
1:F:140:ALA:HB3	4:F:530:HOH:O	2.03	0.57
1:G:167:ASP:HB3	1:G:170:LYS:HB2	1.85	0.57
1:A:231:LYS:HE3	1:A:235[A]:GLU:OE2	2.05	0.57
1:A:88:ASN:OD1	1:A:89:PRO:HD2	2.05	0.57
1:F:54:HIS:CE1	1:F:254:LYS:NZ	2.73	0.57
1:F:202:PRO:O	1:F:206:GLU:HG3	2.05	0.56
1:F:272:ARG:NH1	4:F:571:HOH:O	2.19	0.56
1:E:39:ALA:HB1	2:E:401:B2P:H3	1.88	0.56
1:G:157:PRO:HG2	1:G:299:TYR:CD1	2.40	0.56
1:D:21:GLN:HB3	4:D:536:HOH:O	2.06	0.56
1:A:15:HIS:HE1	1:A:30:HIS:NE2	2.03	0.56
1:F:21:GLN:NE2	4:F:574:HOH:O	2.40	0.55
1:A:18:ALA:O	1:A:23:ALA:HB2	2.07	0.55
1:B:31:ASN:HD22	1:B:155:GLY:HA2	1.72	0.55
1:E:194:ASN:HD22	1:E:194:ASN:H	1.54	0.55
1:F:274:ILE:CG1	2:F:401:B2P:H2	2.35	0.55
1:E:54:HIS:HE1	1:E:254:LYS:NZ	2.03	0.55
1:F:197:VAL:O	1:F:200:VAL:HG22	2.06	0.55
1:A:231:LYS:HG3	1:A:234:ARG:NH2	2.22	0.54
1:A:40:PHE:HB3	2:A:401:B2P:BR	2.61	0.54
1:A:274:ILE:CG1	2:A:401:B2P:H5	2.34	0.54
1:D:39:ALA:HB2	1:D:120:TYR:CE2	2.42	0.54
1:D:50:HIS:CD2	1:D:254:LYS:HG2	2.43	0.54
1:F:15:HIS:HE1	1:F:30:HIS:NE2	2.06	0.54
1:E:274:ILE:HG12	2:E:401:B2P:H5	1.90	0.53
1:B:133:GLU:OE1	1:B:249:ARG:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD11	1:B:234:ARG:HD3	1.91	0.53
1:A:145:ARG:NH1	4:A:524:HOH:O	2.42	0.53
1:D:151:ARG:HD2	4:D:561:HOH:O	2.09	0.53
1:A:274:ILE:HG13	2:A:401:B2P:CM	2.34	0.53
1:A:78:ASN:O	1:A:228:ARG:NH2	2.37	0.53
1:G:67:TYR:HB2	1:G:148:ASP:HB3	1.91	0.53
1:E:274:ILE:CG1	2:E:401:B2P:H5	2.39	0.52
1:F:215:PRO:HG3	3:F:402:GOL:H31	1.90	0.52
1:G:178:VAL:HA	4:G:564:HOH:O	2.09	0.52
1:G:256:SER:OG	1:G:259:GLN:HG3	2.08	0.52
1:E:182:ILE:HG21	1:E:195:TYR:CZ	2.44	0.52
1:F:54:HIS:CE1	1:F:254:LYS:HD3	2.45	0.52
1:G:133:GLU:OE2	1:G:249:ARG:NH1	2.43	0.52
1:E:273:PHE:CE2	2:E:401:B2P:H7	2.46	0.51
1:G:39:ALA:CB	2:G:401:B2P:H3	2.33	0.51
1:D:274:ILE:HD11	2:D:401:B2P:H2	1.92	0.51
1:D:71:GLY:HA3	1:D:236:HIS:CD2	2.46	0.51
1:F:152:ILE:HB	1:F:153:PRO:CD	2.41	0.51
1:A:98:TRP:CE3	1:A:102:LYS:HD3	2.45	0.51
1:F:174:ARG:NH2	1:F:203:ASP:HA	2.26	0.51
1:F:194:ASN:H	1:F:194:ASN:ND2	2.06	0.51
1:E:228:ARG:HD3	4:E:578:HOH:O	2.11	0.51
1:G:274:ILE:HG12	2:G:401:B2P:H2	1.92	0.51
1:A:39:ALA:HB1	2:A:401:B2P:H3	1.93	0.50
1:A:117:ASN:HB3	1:A:278:THR:OG1	2.11	0.50
1:G:59:LEU:HD22	1:G:127:PHE:CE1	2.47	0.50
1:D:34:ARG:HD2	1:D:153:PRO:O	2.11	0.50
1:A:81:VAL:O	1:A:83:GLY:N	2.44	0.49
1:D:39:ALA:HB2	1:D:120:TYR:CZ	2.47	0.49
1:B:142:GLN:HG2	4:B:549:HOH:O	2.12	0.49
1:G:194:ASN:HD22	1:G:194:ASN:H	1.58	0.49
1:A:135:ASP:HB3	1:A:238:LYS:HD3	1.93	0.49
1:F:59:LEU:O	1:F:62:ASN:HB2	2.13	0.49
1:D:31:ASN:ND2	1:D:155:GLY:HA2	2.28	0.49
1:F:75:ILE:HG23	1:F:229:ILE:HB	1.94	0.49
1:F:257:ALA:HB1	1:G:11:PRO:HB3	1.95	0.49
1:A:34:ARG:HD2	1:A:152:ILE:HD12	1.94	0.48
1:E:182:ILE:HG21	1:E:195:TYR:CE2	2.48	0.48
1:G:75:ILE:HD11	1:G:233:ALA:HB2	1.94	0.48
1:D:34:ARG:NH2	1:D:157:PRO:HA	2.29	0.48
1:B:10:PHE:CG	1:B:11:PRO:HD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ARG:HA	1:D:272:ARG:HD3	1.62	0.48
1:D:168:ILE:CD1	1:D:196:ARG:HD2	2.37	0.47
1:F:90:THR:O	1:F:91:PRO:C	2.51	0.47
1:A:269:MET:HG3	1:B:268:PHE:CG	2.49	0.47
1:F:36:PRO:HG3	1:F:160:VAL:HG11	1.96	0.47
1:D:52:ILE:HB	1:D:53:PRO:HD3	1.95	0.47
1:D:41:GLY:N	2:D:401:B2P:BR	3.01	0.47
1:F:131:TRP:CE2	1:F:248:TRP:HB3	2.50	0.47
1:G:39:ALA:HB3	1:G:42:ILE:HD12	1.96	0.47
1:B:39:ALA:HB3	1:B:42:ILE:HD12	1.97	0.47
1:D:60:LYS:HB3	1:D:61:PRO:HD3	1.97	0.47
1:E:39:ALA:CB	2:E:401:B2P:H3	2.44	0.47
1:F:135:ASP:HB3	1:F:238:LYS:HE2	1.97	0.46
1:F:118:PRO:HD3	1:F:278:THR:HG23	1.98	0.46
1:G:54:HIS:CD2	1:G:254:LYS:HZ3	2.26	0.46
1:D:54:HIS:HD2	4:D:551:HOH:O	1.97	0.46
1:E:71:GLY:HA3	1:E:236:HIS:CD2	2.51	0.46
1:G:50:HIS:CD2	1:G:254:LYS:HB3	2.50	0.46
1:E:117:ASN:HB3	1:E:278:THR:OG1	2.16	0.46
1:G:278:THR:O	1:G:282:ILE:HG13	2.15	0.46
1:A:111:ASP:OD1	1:A:285:LYS:NZ	2.37	0.46
1:E:54:HIS:CE1	1:E:254:LYS:HZ3	2.30	0.46
1:E:124:ILE:HG21	1:E:271:ASN:HA	1.98	0.46
1:B:147:ARG:HD3	4:B:538:HOH:O	2.16	0.46
1:F:166:LEU:C	1:F:166:LEU:HD12	2.36	0.46
1:B:28:ASP:OD1	1:B:60:LYS:NZ	2.44	0.45
1:E:281:ILE:O	1:E:284:LEU:HB2	2.16	0.45
1:F:28:ASP:O	1:F:32:THR:HB	2.16	0.45
1:B:31:ASN:ND2	1:B:155:GLY:HA2	2.31	0.45
1:F:40:PHE:H	2:F:401:B2P:C	2.29	0.45
1:B:231:LYS:HG3	1:B:234:ARG:HH22	1.78	0.45
1:A:275:ALA:O	1:A:279:ILE:HD12	2.15	0.45
1:B:135:ASP:CG	1:B:139:ARG:HD2	2.37	0.45
1:G:274:ILE:HG12	2:G:401:B2P:H5	1.99	0.45
1:F:48:PHE:CD2	1:F:263:LEU:HD21	2.52	0.45
1:A:58:ALA:O	1:A:244:ALA:HA	2.17	0.44
1:D:59:LEU:HD22	1:D:127:PHE:CE1	2.52	0.44
1:A:89:PRO:HG2	1:A:288:PHE:CZ	2.53	0.44
1:F:234:ARG:HD2	1:G:187:LEU:HD21	1.98	0.44
1:B:131:TRP:CE2	1:B:248:TRP:HB3	2.53	0.44
1:E:147:ARG:HH12	1:G:95:ARG:HA	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:TYR:OH	1:F:239:GLY:HA3	2.17	0.44
1:E:135:ASP:OD2	1:E:238:LYS:HG2	2.18	0.44
1:F:30:HIS:CE1	1:F:162:LYS:HG2	2.53	0.44
1:B:228:ARG:HB2	4:B:579:HOH:O	2.17	0.44
1:D:117:ASN:HB2	1:D:118:PRO:HD3	2.00	0.44
1:F:193:SER:OG	2:F:401:B2P:O	2.36	0.44
1:E:124:ILE:CG2	1:E:271:ASN:HA	2.48	0.44
1:F:39:ALA:CB	2:F:401:B2P:H3	2.33	0.44
1:D:66:ARG:HD2	4:D:563:HOH:O	2.18	0.44
1:G:99:THR:O	1:G:102:LYS:N	2.49	0.44
1:B:194:ASN:HD22	1:B:194:ASN:H	1.66	0.43
1:D:274:ILE:CD1	2:D:401:B2P:H2	2.47	0.43
1:E:131:TRP:CE2	1:E:248:TRP:HB3	2.53	0.43
1:G:99:THR:C	1:G:101:SER:N	2.71	0.43
1:A:28:ASP:OD1	1:A:60:LYS:NZ	2.45	0.43
1:D:80:ILE:HG13	1:D:291:PRO:HB3	2.00	0.43
1:D:112:LEU:HD23	1:D:299:TYR:CZ	2.53	0.43
1:E:90:THR:HB	1:E:91:PRO:HD3	2.00	0.43
1:B:18:ALA:HB3	4:B:572:HOH:O	2.18	0.43
1:A:133:GLU:OE1	1:A:249:ARG:HD3	2.19	0.43
4:B:574:HOH:O	1:G:236:HIS:HE1	2.00	0.43
1:G:118:PRO:HD3	1:G:278:THR:HG23	2.01	0.43
1:D:113:LEU:HD13	1:D:194:ASN:ND2	2.34	0.43
1:A:113:LEU:HD22	1:A:194:ASN:CG	2.39	0.43
1:A:39:ALA:HB1	2:A:401:B2P:CB	2.49	0.43
1:D:261:ALA:O	1:E:266:LEU:HD21	2.18	0.43
1:A:44:VAL:O	1:A:47:GLN:HG2	2.18	0.42
1:D:229:ILE:HA	1:D:232:ILE:HD12	2.01	0.42
1:A:60:LYS:HB3	1:A:61:PRO:HD3	2.00	0.42
1:A:180:ARG:HD2	1:A:184:ASP:OD2	2.19	0.42
1:F:54:HIS:HE1	1:F:254:LYS:CD	2.31	0.42
1:A:273:PHE:CD2	2:A:401:B2P:H7	2.54	0.42
1:D:31:ASN:HB3	1:D:154:TYR:CE2	2.54	0.42
1:F:10:PHE:CD1	1:F:11:PRO:HD2	2.53	0.42
1:D:59:LEU:CD2	1:D:123:LEU:HG	2.49	0.42
1:F:45:MET:SD	1:F:267:LEU:HD23	2.59	0.42
1:F:259:GLN:O	1:F:262:GLY:N	2.52	0.42
1:A:34:ARG:CD	1:A:152:ILE:HD12	2.49	0.42
1:D:75:ILE:HG23	1:D:229:ILE:HB	2.00	0.42
1:F:49:PRO:HB2	1:F:50:HIS:CD2	2.54	0.42
1:F:88:ASN:O	1:F:91:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:LEU:HD12	1:F:106:LEU:O	2.19	0.42
1:G:29:ILE:O	1:G:30:HIS:C	2.56	0.42
1:F:147:ARG:HD3	4:F:551:HOH:O	2.20	0.42
1:G:51:PHE:HB3	4:G:565:HOH:O	2.19	0.42
1:A:117:ASN:HB2	1:A:118:PRO:HD3	2.01	0.42
1:D:193:SER:N	4:D:556:HOH:O	2.52	0.42
1:E:38:VAL:O	1:E:39:ALA:C	2.58	0.42
1:F:10:PHE:CG	1:F:11:PRO:HD2	2.54	0.42
1:F:36:PRO:HD2	1:F:37:TRP:HE3	1.84	0.42
1:G:168:ILE:HD11	1:G:196:ARG:HD2	2.00	0.42
1:F:39:ALA:HB2	1:F:120:TYR:CE2	2.55	0.42
1:E:69:GLU:OE1	1:E:119:LYS:HE3	2.20	0.42
1:F:107:LYS:HG2	1:F:285:LYS:HE3	2.02	0.42
1:F:113:LEU:HD13	1:F:194:ASN:HB3	2.01	0.41
1:B:222:TYR:OH	1:B:276:ASP:O	2.32	0.41
1:B:89:PRO:HG2	1:B:288:PHE:CE1	2.56	0.41
1:F:231:LYS:O	1:F:235[A]:GLU:HG3	2.20	0.41
1:F:103:ILE:HG22	1:F:107:LYS:HD2	2.02	0.41
1:F:274:ILE:HG12	2:F:401:B2P:CB	2.48	0.41
1:A:95:ARG:HG2	1:D:147:ARG:HG3	2.02	0.41
1:E:274:ILE:HG12	2:E:401:B2P:CM	2.50	0.41
1:G:99:THR:O	1:G:101:SER:N	2.53	0.41
1:A:125:THR:HG21	1:A:234:ARG:HA	2.01	0.41
1:A:199:GLY:O	1:A:202:PRO:HD3	2.20	0.41
1:B:39:ALA:HA	2:B:401:B2P:OXT	2.20	0.41
1:B:119:LYS:HB3	1:B:119:LYS:HE2	1.89	0.41
1:F:81:VAL:O	1:F:83:GLY:N	2.54	0.41
1:A:258:GLU:OE2	1:B:259:GLN:HG2	2.21	0.41
1:E:74:LEU:HD12	1:E:74:LEU:HA	1.76	0.40
1:G:226:ALA:O	1:G:230:ARG:HG3	2.21	0.40
1:B:158:ASN:O	1:B:159:SER:OG	2.26	0.40
1:E:60:LYS:HB3	1:E:61:PRO:HD3	2.03	0.40
1:G:15:HIS:CE1	1:G:30:HIS:NE2	2.74	0.40
1:B:26:TYR:OH	1:B:43:ARG:HA	2.21	0.40
1:F:66:ARG:HD2	1:F:147:ARG:NH2	2.36	0.40
1:G:22:LEU:HD21	1:G:46:SER:HB3	2.04	0.40
1:F:74:LEU:HD23	1:F:74:LEU:HA	1.94	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	Percentiles	
1	A	297/301 (99%)	280 (94%)	17 (6%)	0	100	100
1	B	298/301 (99%)	274 (92%)	22 (7%)	2 (1%)	22	46
1	D	296/301 (98%)	277 (94%)	19 (6%)	0	100	100
1	E	298/301 (99%)	277 (93%)	19 (6%)	2 (1%)	22	46
1	F	298/301 (99%)	280 (94%)	17 (6%)	1 (0%)	41	66
1	G	299/301 (99%)	278 (93%)	16 (5%)	5 (2%)	9	23
All	All	1786/1806 (99%)	1666 (93%)	110 (6%)	10 (1%)	25	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	100	GLU
1	B	141	PRO
1	E	11	PRO
1	E	39	ALA
1	G	141	PRO
1	B	30	HIS
1	F	20	GLY
1	G	261	ALA
1	G	20	GLY
1	G	200	VAL

### 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	249/251 (99%)	243 (98%)	6 (2%)	49	77
1	B	250/251 (100%)	244 (98%)	6 (2%)	49	77
1	D	248/251 (99%)	241 (97%)	7 (3%)	43	73
1	E	251/251 (100%)	240 (96%)	11 (4%)	28	56
1	F	251/251 (100%)	242 (96%)	9 (4%)	35	64
1	G	252/251 (100%)	245 (97%)	7 (3%)	43	73
All	All	1501/1506 (100%)	1455 (97%)	46 (3%)	41	69

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	9	SER
1	A	29	ILE
1	A	47	GLN
1	A	169	GLU
1	A	293	ASP
1	B	6	VAL
1	B	19	LYS
1	B	100	GLU
1	B	161	GLU
1	B	165	LEU
1	B	271	ASN
1	D	6	VAL
1	D	9	SER
1	D	108	THR
1	D	165	LEU
1	D	193	SER
1	D	242	LYS
1	D	289	SER
1	E	6	VAL
1	E	16	HIS
1	E	46	SER
1	E	123	LEU
1	E	124	ILE
1	E	128	ASN
1	E	158	ASN
1	E	159	SER
1	E	210	ARG
1	E	253	GLU
1	E	271	ASN

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Mol	Chain	Res	Type
1	F	19	LYS
1	F	107	LYS
1	F	158	ASN
1	F	165	LEU
1	F	193	SER
1	F	194	ASN
1	F	252	THR
1	F	253	GLU
1	F	271	ASN
1	G	9[A]	SER
1	G	9[B]	SER
1	G	21	GLN
1	G	165	LEU
1	G	180	ARG
1	G	242	LYS
1	G	252	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	17	GLN
1	A	47	GLN
1	A	54	HIS
1	A	132	HIS
1	A	271	ASN
1	B	31	ASN
1	B	54	HIS
1	B	301	ASN
1	D	15	HIS
1	D	31	ASN
1	D	54	HIS
1	D	117	ASN
1	D	142	GLN
1	D	158	ASN
1	D	164	ASN
1	D	194	ASN
1	E	54	HIS
1	E	117	ASN
1	E	128	ASN
1	E	176	GLN
1	F	15	HIS

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Mol	Chain	Res	Type
1	F	17	GLN
1	F	50	HIS
1	F	54	HIS
1	F	158	ASN
1	G	15	HIS
1	G	47	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](#)

12 ligands 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
3	GOL	A	402	-	5,5,5	0.39	0	5,5,5	0.68	0
2	B2P	F	401	-	6,6,6	5.89	1 (16%)	9,9,9	2.30	4 (44%)
3	GOL	B	402	-	5,5,5	0.42	0	5,5,5	0.57	0
2	B2P	D	401	-	6,6,6	5.83	1 (16%)	9,9,9	2.03	3 (33%)
3	GOL	G	402	-	5,5,5	0.40	0	5,5,5	0.17	0
2	B2P	B	401	-	6,6,6	5.39	1 (16%)	9,9,9	2.19	3 (33%)
2	B2P	E	401	-	6,6,6	6.06	1 (16%)	9,9,9	2.28	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	D	402	-	5,5,5	0.47	0	5,5,5	0.30	0
3	GOL	F	402	-	5,5,5	0.55	0	5,5,5	0.62	0
3	GOL	E	402	-	5,5,5	0.33	0	5,5,5	0.27	0
2	B2P	G	401	-	6,6,6	5.92	1 (16%)	9,9,9	2.06	3 (33%)
2	B2P	A	401	-	6,6,6	6.17	1 (16%)	9,9,9	2.86	5 (55%)

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	A	402	-	-	3/4/4/4	-
2	B2P	F	401	-	-	1/5/6/6	-
3	GOL	B	402	-	-	4/4/4/4	-
2	B2P	D	401	-	-	0/5/6/6	-
3	GOL	G	402	-	-	4/4/4/4	-
2	B2P	B	401	-	-	3/5/6/6	-
2	B2P	E	401	-	-	0/5/6/6	-
3	GOL	D	402	-	-	4/4/4/4	-
3	GOL	F	402	-	-	4/4/4/4	-
3	GOL	E	402	-	-	0/4/4/4	-
2	B2P	G	401	-	-	1/5/6/6	-
2	B2P	A	401	-	-	3/5/6/6	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	B2P	BR-CA	-14.94	1.55	1.98
2	E	401	B2P	BR-CA	-14.76	1.56	1.98
2	F	401	B2P	BR-CA	-14.32	1.57	1.98
2	G	401	B2P	BR-CA	-14.32	1.57	1.98
2	D	401	B2P	BR-CA	-14.13	1.57	1.98
2	B	401	B2P	BR-CA	-13.09	1.60	1.98

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	B2P	O-C-CA	4.85	125.54	114.90
2	A	401	B2P	BR-CA-C	4.45	124.94	102.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	B2P	BR-CA-C	4.38	124.56	102.27
2	E	401	B2P	O-C-CA	4.34	124.42	114.90
2	E	401	B2P	BR-CA-C	4.23	123.79	102.27
2	F	401	B2P	BR-CA-C	4.13	123.33	102.27
2	F	401	B2P	O-C-CA	3.84	123.33	114.90
2	D	401	B2P	BR-CA-C	3.76	121.44	102.27
2	B	401	B2P	BR-CA-C	3.67	120.98	102.27
2	B	401	B2P	O-C-CA	3.32	122.19	114.90
2	A	401	B2P	CB-CA-C	-3.09	97.13	111.81
2	B	401	B2P	O-C-OXT	-2.96	114.42	123.82
2	D	401	B2P	O-C-CA	2.75	120.95	114.90
2	A	401	B2P	BR-CA-CM	-2.69	93.13	107.06
2	F	401	B2P	O-C-OXT	-2.57	115.63	123.82
2	D	401	B2P	O-C-OXT	-2.49	115.89	123.82
2	G	401	B2P	O-C-OXT	-2.39	116.20	123.82
2	A	401	B2P	O-C-OXT	-2.32	116.42	123.82
2	G	401	B2P	O-C-CA	2.28	119.91	114.90
2	F	401	B2P	CM-CA-C	-2.26	101.07	111.81
2	E	401	B2P	O-C-OXT	-2.12	117.08	123.82

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	GOL	O1-C1-C2-O2
3	B	402	GOL	O1-C1-C2-C3
3	B	402	GOL	C1-C2-C3-O3
3	D	402	GOL	O1-C1-C2-O2
3	D	402	GOL	O1-C1-C2-C3
3	D	402	GOL	C1-C2-C3-O3
3	G	402	GOL	O1-C1-C2-C3
3	A	402	GOL	O1-C1-C2-O2
3	A	402	GOL	O1-C1-C2-C3
3	F	402	GOL	O1-C1-C2-C3
3	F	402	GOL	C1-C2-C3-O3
3	G	402	GOL	C1-C2-C3-O3
3	B	402	GOL	O2-C2-C3-O3
3	D	402	GOL	O2-C2-C3-O3
3	F	402	GOL	O1-C1-C2-O2
3	G	402	GOL	O1-C1-C2-O2
3	G	402	GOL	O2-C2-C3-O3
2	A	401	B2P	OXT-C-CA-CM

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Mol	Chain	Res	Type	Atoms
2	A	401	B2P	O-C-CA-CM
2	B	401	B2P	OXT-C-CA-CB
2	B	401	B2P	O-C-CA-CB
2	G	401	B2P	O-C-CA-CB
3	F	402	GOL	O2-C2-C3-O3
3	A	402	GOL	C1-C2-C3-O3
2	A	401	B2P	OXT-C-CA-BR
2	B	401	B2P	OXT-C-CA-BR
2	F	401	B2P	OXT-C-CA-CB

There are no ring outliers.

7 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	B2P	8	0
2	D	401	B2P	8	0
2	B	401	B2P	3	0
2	E	401	B2P	8	0
3	F	402	GOL	2	0
2	G	401	B2P	5	0
2	A	401	B2P	8	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	298/301 (99%)	-0.53	0 100 100	6, 13, 32, 49	0
1	B	298/301 (99%)	-0.53	0 100 100	7, 13, 34, 56	0
1	D	298/301 (99%)	-0.37	0 100 100	7, 15, 38, 57	0
1	E	298/301 (99%)	-0.48	0 100 100	9, 14, 34, 56	0
1	F	298/301 (99%)	-0.48	0 100 100	7, 15, 36, 57	0
1	G	298/301 (99%)	-0.43	0 100 100	7, 15, 38, 57	0
All	All	1788/1806 (99%)	-0.47	0 100 100	6, 14, 36, 57	0

There are no RSRZ outliers to report.

### 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<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
2	B2P	G	401	7/7	0.87	0.25	9,11,11,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	B2P	A	401	7/7	0.88	0.25	7,8,9,9	0
3	GOL	B	402	6/6	0.88	0.26	28,29,30,30	0
2	B2P	E	401	7/7	0.91	0.19	10,13,13,13	0
3	GOL	F	402	6/6	0.91	0.23	19,21,22,23	0
3	GOL	G	402	6/6	0.91	0.19	14,16,16,17	0
3	GOL	A	402	6/6	0.92	0.16	16,19,19,19	0
3	GOL	E	402	6/6	0.92	0.22	12,13,13,13	0
3	GOL	D	402	6/6	0.93	0.16	21,22,22,22	0
2	B2P	F	401	7/7	0.93	0.20	11,13,15,15	0
2	B2P	D	401	7/7	0.96	0.14	8,9,10,11	0
2	B2P	B	401	7/7	0.96	0.16	6,7,8,8	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.