



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:04 am GMT

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

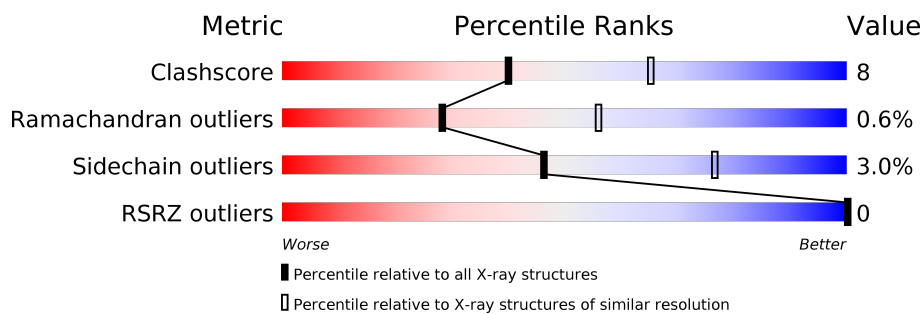
1 Overall quality at a glance

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	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	 77% 21% ..
1	B	301	 81% 17% .
1	D	301	 81% 18% .
1	E	301	 82% 16% ..
1	F	301	 70% 27% ..
1	G	301	 79% 20% .

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	B2P	A	401	-	-	X	X
2	B2P	D	401	-	-	X	-
2	B2P	E	401	-	-	X	X
2	B2P	F	401	-	-	X	X
2	B2P	G	401	-	-	X	X
3	GOL	B	402	-	-	-	X
3	GOL	F	402	-	-	-	X

2 Entry composition

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.

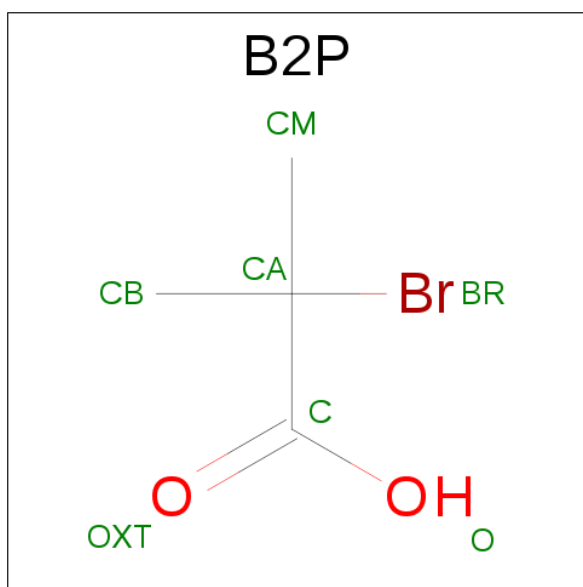
- Molecule 1 is a protein called DL-2-haloacid dehalogenase.

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

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: $C_4H_7BrO_2$).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

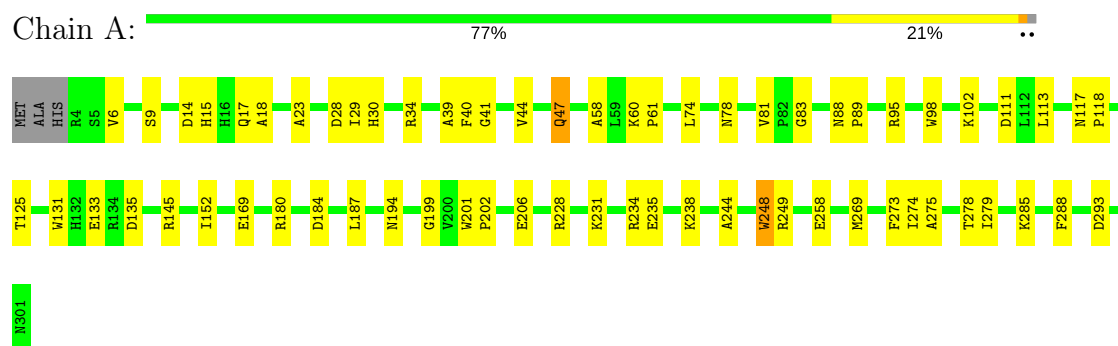
- Molecule 4 is water.

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

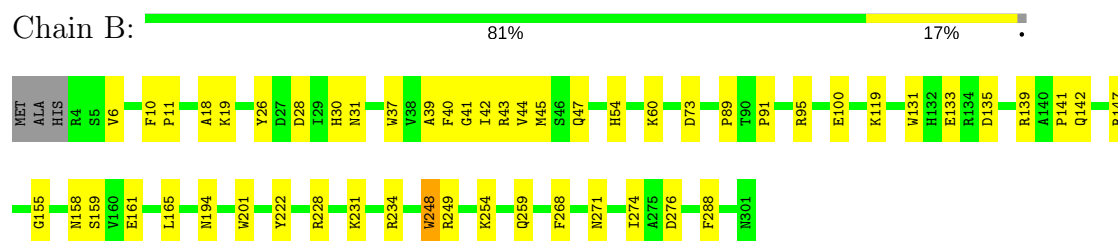
3 Residue-property plots

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.

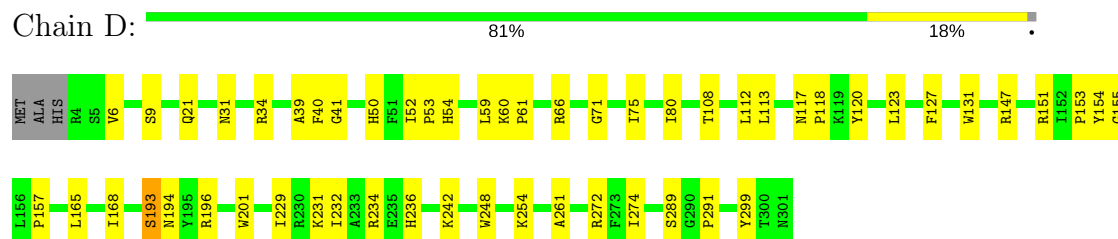
• Molecule 1: DL-2-haloacid dehalogenase



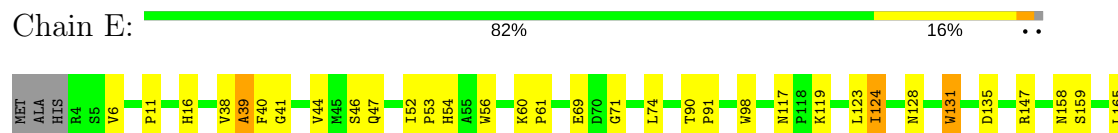
• Molecule 1: DL-2-haloacid dehalogenase



• Molecule 1: DL-2-haloacid dehalogenase



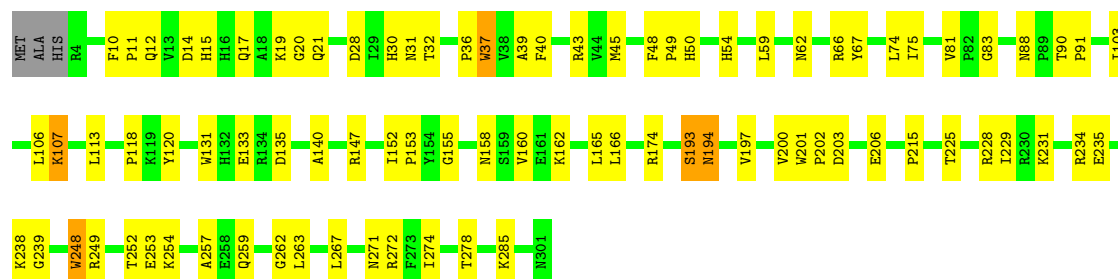
• Molecule 1: DL-2-haloacid dehalogenase





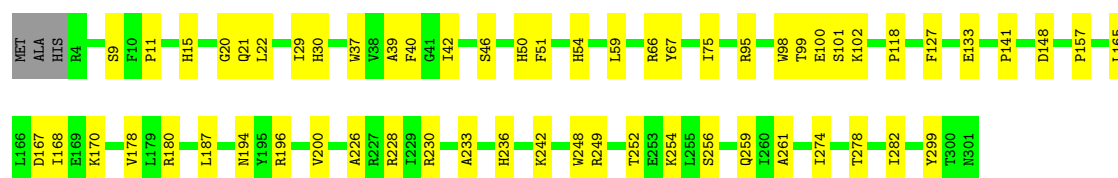
• Molecule 1: DL-2-haloacid dehalogenase

Chain F: 70% 27% ..



• Molecule 1: DL-2-haloacid dehalogenase

Chain G: 79% 20% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	5.73 (at 2.69Å)	Xtriage
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.	DCC
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , -4.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.378 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15037	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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:HD22	1:F:194:ASN:H	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:54:HIS:HE1	1:F:254:LYS:HD3	1.64	0.63
1:F:31:ASN:OD1	1:F:155:GLY:HA2	1.98	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:274:ILE:CG1	2:A:401:B2P:H5	2.34	0.54
1:A:40:PHE:HB3	2:A:401:B2P:BR	2.61	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:124:ILE:HG21	1:E:271:ASN:HA	1.98	0.46
1:E:54:HIS:CE1	1:E:254:LYS:HZ3	2.30	0.46
1:B:147:ARG:HD3	4:B:538:HOH:O	2.16	0.46
1:F:166:LEU:HD12	1:F:166:LEU:C	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:112:LEU:HD23	1:D:299:TYR:CZ	2.53	0.43
1:D:80:ILE:HG13	1:D:291:PRO:HB3	2.00	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:180:ARG:HD2	1:A:184:ASP:OD2	2.19	0.42
1:A:60:LYS:HB3	1:A:61:PRO:HD3	2.00	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:259:GLN:O	1:F:262:GLY:N	2.52	0.42
1:F:45:MET:SD	1:F:267:LEU:HD23	2.59	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:106:LEU:HD12	1:F:106:LEU:O	2.19	0.42
1:F:49:PRO:HB2	1:F:50:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:ASN:O	1:F:91:PRO:HD2	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:119:LYS:HE2	1:B:119:LYS:HB3	1.89	0.41
1:B:39:ALA:HA	2:B:401:B2P:OXT	2.20	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

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	297/301 (99%)	280 (94%)	17 (6%)	0	100	100
1	B	298/301 (99%)	274 (92%)	22 (7%)	2 (1%)	25	53
1	D	296/301 (98%)	277 (94%)	19 (6%)	0	100	100
1	E	298/301 (99%)	277 (93%)	19 (6%)	2 (1%)	25	53
1	F	298/301 (99%)	280 (94%)	17 (6%)	1 (0%)	44	73
1	G	299/301 (99%)	278 (93%)	16 (5%)	5 (2%)	11	27
All	All	1786/1806 (99%)	1666 (93%)	110 (6%)	10 (1%)	28	56

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

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%)	54	83
1	B	250/251 (100%)	244 (98%)	6 (2%)	54	83
1	D	248/251 (99%)	241 (97%)	7 (3%)	49	79
1	E	251/251 (100%)	240 (96%)	11 (4%)	33	63
1	F	251/251 (100%)	242 (96%)	9 (4%)	40	70
1	G	252/251 (100%)	245 (97%)	7 (3%)	49	79
All	All	1501/1506 (100%)	1455 (97%)	46 (3%)	46	75

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

Some 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 ⓘ

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 ⓘ

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	$\# Z > 2$
2	B2P	A	401	-	3,6,6	8.30	1 (33%)	5,9,9	2.93	3 (60%)
3	GOL	A	402	-	5,5,5	0.37	0	5,5,5	0.65	0
2	B2P	B	401	-	3,6,6	7.26	1 (33%)	5,9,9	1.53	1 (20%)
3	GOL	B	402	-	5,5,5	0.38	0	5,5,5	0.55	0
2	B2P	D	401	-	3,6,6	7.85	1 (33%)	5,9,9	1.75	1 (20%)
3	GOL	D	402	-	5,5,5	0.43	0	5,5,5	0.30	0
2	B2P	E	401	-	3,6,6	8.19	1 (33%)	5,9,9	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	E	402	-	5,5,5	0.30	0	5,5,5	0.25	0
2	B2P	F	401	-	3,6,6	7.94	1 (33%)	5,9,9	1.68	1 (20%)
3	GOL	F	402	-	5,5,5	0.53	0	5,5,5	0.60	0
2	B2P	G	401	-	3,6,6	7.95	1 (33%)	5,9,9	1.48	1 (20%)
3	GOL	G	402	-	5,5,5	0.35	0	5,5,5	0.17	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
2	B2P	A	401	-	-	0/0/6/6	0/0/0/0
3	GOL	A	402	-	-	0/4/4/4	0/0/0/0
2	B2P	B	401	-	-	0/0/6/6	0/0/0/0
3	GOL	B	402	-	-	0/4/4/4	0/0/0/0
2	B2P	D	401	-	-	0/0/6/6	0/0/0/0
3	GOL	D	402	-	-	0/4/4/4	0/0/0/0
2	B2P	E	401	-	-	0/0/6/6	0/0/0/0
3	GOL	E	402	-	-	0/4/4/4	0/0/0/0
2	B2P	F	401	-	-	0/0/6/6	0/0/0/0
3	GOL	F	402	-	-	0/4/4/4	0/0/0/0
2	B2P	G	401	-	-	0/0/6/6	0/0/0/0
3	GOL	G	402	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	B2P	BR-CA	-14.34	1.55	1.99
2	E	401	B2P	BR-CA	-14.16	1.56	1.99
2	F	401	B2P	BR-CA	-13.74	1.57	1.99
2	G	401	B2P	BR-CA	-13.74	1.57	1.99
2	D	401	B2P	BR-CA	-13.56	1.57	1.99
2	B	401	B2P	BR-CA	-12.57	1.60	1.99

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	B2P	CB-CA-C	-4.71	97.13	109.41
2	F	401	B2P	CM-CA-C	-3.20	101.07	109.41
2	D	401	B2P	CM-CA-C	-2.58	102.68	109.41
2	A	401	B2P	BR-CA-CM	-2.57	93.13	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	B2P	CB-CA-C	-2.45	103.02	109.41
2	G	401	B2P	CM-CA-C	-2.43	103.08	109.41
2	A	401	B2P	CM-CA-C	3.19	117.71	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	B2P	8	0
2	B	401	B2P	3	0
2	D	401	B2P	8	0
2	E	401	B2P	8	0
2	F	401	B2P	8	0
3	F	402	GOL	2	0
2	G	401	B2P	5	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
2	B2P	G	401	7/7	0.87	0.25	6.98	9,11,11,12	0
2	B2P	A	401	7/7	0.88	0.25	4.33	7,8,9,9	0
3	GOL	B	402	6/6	0.88	0.26	3.07	28,29,30,30	0
2	B2P	E	401	7/7	0.91	0.19	2.82	10,13,13,13	0
2	B2P	F	401	7/7	0.93	0.20	2.29	11,13,15,15	0
3	GOL	F	402	6/6	0.91	0.23	2.17	19,21,22,23	0
3	GOL	E	402	6/6	0.92	0.22	1.78	12,13,13,13	0
2	B2P	B	401	7/7	0.96	0.16	1.18	6,7,8,8	0
3	GOL	G	402	6/6	0.91	0.19	0.76	14,16,16,17	0
3	GOL	D	402	6/6	0.93	0.16	0.64	21,22,22,22	0
2	B2P	D	401	7/7	0.96	0.14	-0.12	8,9,10,11	0
3	GOL	A	402	6/6	0.92	0.16	-	16,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.