



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:14 PM 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

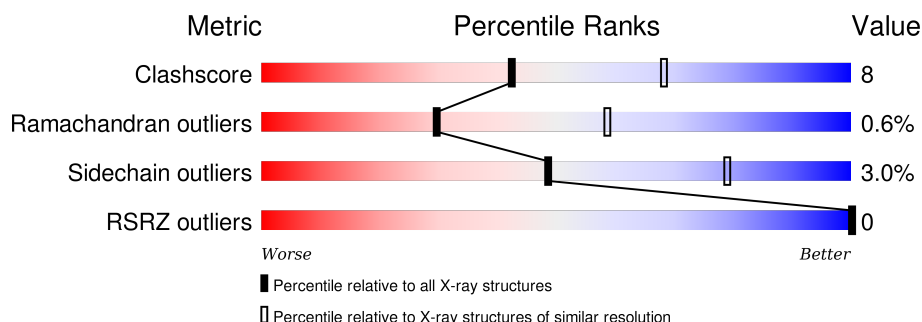
1 Overall quality at a glance

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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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.

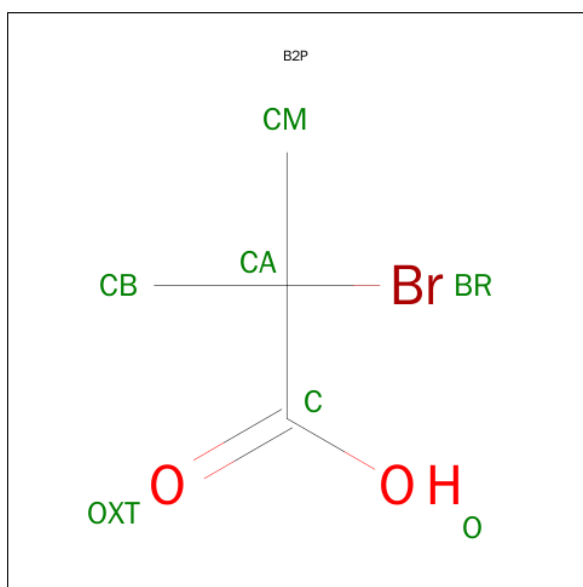
- Molecule 1 is a protein called DL-2-haloacid dehalogenase.

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 7	Br 1	C 4	O 2	0	0
2	B	1	Total 7	Br 1	C 4	O 2	0	0
2	D	1	Total 7	Br 1	C 4	O 2	0	0
2	E	1	Total 7	Br 1	C 4	O 2	0	0
2	F	1	Total 7	Br 1	C 4	O 2	0	0
2	G	1	Total 7	Br 1	C 4	O 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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		

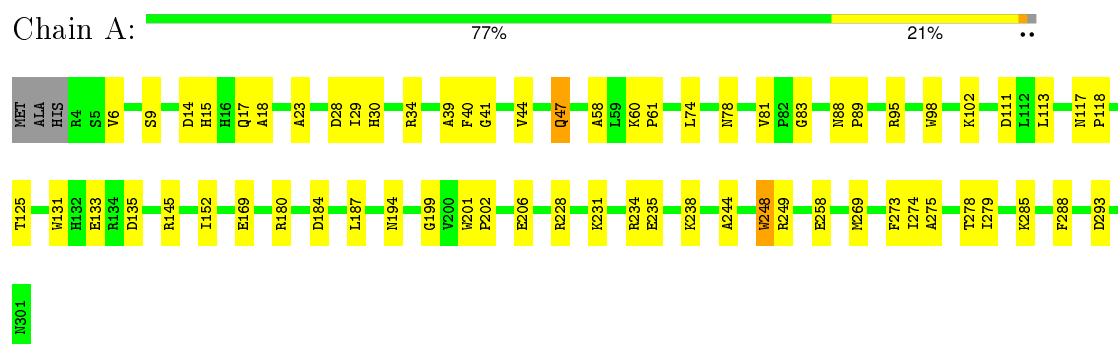
- Molecule 4 is water.

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		

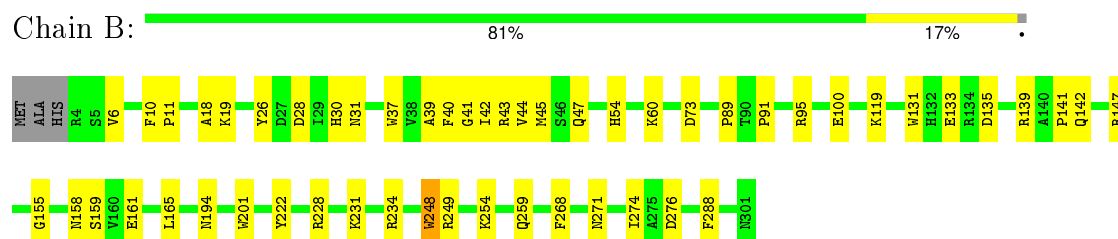
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

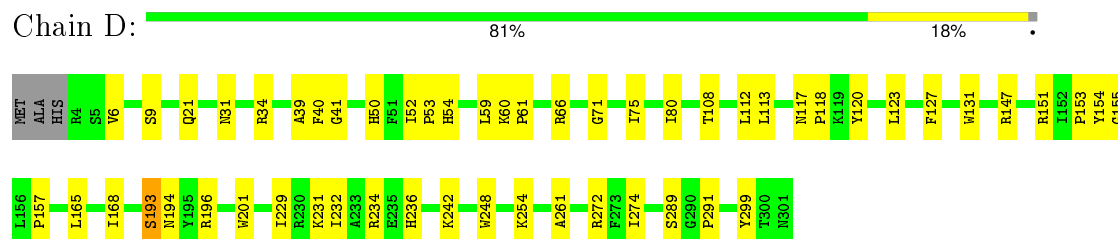
- Molecule 1: DL-2-haloacid dehalogenase



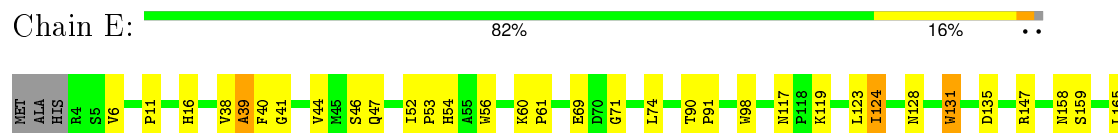
- Molecule 1: DL-2-haloacid dehalogenase

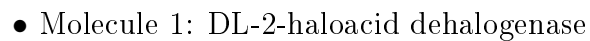


- Molecule 1: DL-2-haloacid dehalogenase



- Molecule 1: DL-2-haloacid dehalogenase





K238	L106	ME1
G239	L107	ALA
W248	K107	HIS
R249	L113	R4
T252	P118	F10
E253	K119	Q12
K254	Y120	V13
A257	W131	D14
E258	H132	H15
Q259	E133	H16
	R134	Q17
G262	D135	A18
L263	A140	K19
		G20
L267	R147	Q21
N271	I152	D28
R272	P153	I29
F273	Y154	E30
I274	G155	N31
		T32
T278	N158	P36
K285	S159	K37
N301	V160	V38
	F161	A39
	K162	P40
	L165	R43
	L166	V44
	R174	N45
	S193	F48
	N194	P49
	V197	E50
	V200	H54
	W201	L59
	P202	N62
	D203	R66
	E206	V67
	P215	L74
	T225	I75
	R228	V81
I229	I229	P82
R230	R230	G83
K231	K231	N88
	R234	P89
	E235	T90
		P91
		T102

- Molecule 1: DL-2-haloacid dehalogenase

Li66	Li67	Li68	Li69	K170	Li78	Li79	R180	Li187	M194	Y195	R196	V200	A226	R227	R228	L229	R230	A233	E236	K242	W248	R249	T252	E253	K254	S256	Q259	A261	L274	T278	L282	Y299	T300	N301					
Met	ALA	HIS	R4	S9	F10	P11	H15	Q20	Q21	L22	I29	H30	W37	R38	A39	F40	G41	I42	S46	H50	F51	H54	L59	R66	Y67	I75	R95	W98	T99	E100	S101	K102	P118	F127	E133	P141	D148	P157	L165

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
Estimated twinning fraction	0.378 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 61648 reflections (0.003%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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:D:39:ALA:HB1	2:D:401:B2P:CB	2.14	0.75
1:B:231:LYS:HG3	1:B:234:ARG:NH2	2.01	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:F:274:ILE:CG1	2:F:401:B2P:H2	2.35	0.55
1:E:194:ASN:HD22	1:E:194:ASN:H	1.54	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:D:39:ALA:HB2	1:D:120:TYR:CE2	2.42	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: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:G:67:TYR:HB2	1:G:148:ASP:HB3	1.91	0.53
1:A:78:ASN:O	1:A:228:ARG:NH2	2.37	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:256:SER:OG	1:G:259:GLN:HG3	2.08	0.52
1:G:178:VAL:HA	4:G:564:HOH:O	2.09	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:F:152:ILE:HB	1:F:153:PRO:CD	2.41	0.51
1:D:71:GLY:HA3	1:D:236:HIS:CD2	2.46	0.51
1:F:194:ASN:H	1:F:194:ASN:ND2	2.06	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: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:G:194:ASN:HD22	1:G:194:ASN:H	1.58	0.49
1:B:142:GLN:HG2	4:B:549:HOH:O	2.12	0.49
1:F:59:LEU:O	1:F:62:ASN:HB2	2.13	0.49
1:A:135:ASP:HB3	1:A:238:LYS:HD3	1.93	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:E:39:ALA:CB	2:E:401:B2P:H3	2.44	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:F:135:ASP:HB3	1:F:238:LYS:HE2	1.97	0.46
1:G:54:HIS:CD2	1:G:254:LYS:HZ3	2.26	0.46
1:F:118:PRO:HD3	1:F:278:THR:HG23	1.98	0.46
1:D:54:HIS:HD2	4:D:551:HOH:O	1.97	0.46
1:G:50:HIS:CD2	1:G:254:LYS:HB3	2.50	0.46
1:E:71:GLY:HA3	1:E:236:HIS:CD2	2.51	0.46
1:G:278:THR:O	1:G:282:ILE:HG13	2.15	0.46
1:E:117:ASN:HB3	1:E:278:THR:OG1	2.16	0.46
1:E:54:HIS:CE1	1:E:254:LYS:HZ3	2.30	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:F:166:LEU:C	1:F:166:LEU:HD12	2.36	0.46
1:B:147:ARG:HD3	4:B:538:HOH:O	2.16	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:F:40:PHE:H	2:F:401:B2P:C	2.29	0.45
1:B:31:ASN:ND2	1:B:155:GLY:HA2	2.31	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:G:274:ILE:HG12	2:G:401:B2P:H5	1.99	0.45
1:B:135:ASP:CG	1:B:139:ARG:HD2	2.37	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:E:147:ARG:HH12	1:G:95:ARG:HA	1.79	0.44
1:B:131:TRP:CE2	1:B:248:TRP:HB3	2.53	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:F:30:HIS:CE1	1:F:162:LYS:HG2	2.53	0.44
1:E:135:ASP:OD2	1:E:238:LYS:HG2	2.18	0.44
1:F:193:SER:OG	2:F:401:B2P:O	2.36	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:39:ALA:CB	2:F:401:B2P:H3	2.33	0.44
1:E:124:ILE:CG2	1:E:271:ASN:HA	2.48	0.44
1:G:99:THR:O	1:G:102:LYS:N	2.49	0.44
1:D:66:ARG:HD2	4:D:563:HOH:O	2.18	0.44
1:D:274:ILE:CD1	2:D:401:B2P:H2	2.47	0.43
1:G:99:THR:C	1:G:101:SER:N	2.71	0.43
1:E:131:TRP:CE2	1:E:248:TRP:HB3	2.53	0.43
1:B:194:ASN:HD22	1:B:194:ASN:H	1.66	0.43
1:E:90:THR:HB	1:E:91:PRO:HD3	2.00	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: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
1:G:118:PRO:HD3	1:G:278:THR:HG23	2.01	0.43
4:B:574:HOH:O	1:G:236:HIS:HE1	2.00	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:D:229:ILE:HA	1:D:232:ILE:HD12	2.01	0.42
1:A:44:VAL:O	1:A:47:GLN:HG2	2.18	0.42
1:F:54:HIS:HE1	1:F:254:LYS:CD	2.31	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: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:G:29:ILE:O	1:G:30:HIS:C	2.56	0.42
1:A:34:ARG:CD	1:A:152:ILE:HD12	2.49	0.42
1:F:88:ASN:O	1:F:91:PRO:HD2	2.19	0.42
1:D:75:ILE:HG23	1:D:229:ILE:HB	2.00	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:F:49:PRO:HB2	1:F:50:HIS:CD2	2.54	0.42
1:G:51:PHE:HB3	4:G:565:HOH:O	2.19	0.42
1:F:147:ARG:HD3	4:F:551:HOH:O	2.20	0.42
1:E:38:VAL:O	1:E:39:ALA:C	2.58	0.42
1:A:117:ASN:HB2	1:A:118:PRO:HD3	2.01	0.42
1:F:36:PRO:HD2	1:F:37:TRP:HE3	1.84	0.42
1:F:10:PHE:CG	1:F:11:PRO:HD2	2.54	0.42
1:D:193:SER:N	4:D:556:HOH:O	2.52	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:F:107:LYS:HG2	1:F:285:LYS:HE3	2.02	0.42
1:E:69:GLU:OE1	1:E:119:LYS:HE3	2.20	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: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:95:ARG:HG2	1:D:147:ARG:HG3	2.02	0.41
1:B:39:ALA:HA	2:B:401:B2P:OXT	2.20	0.41
1:A:199:GLY:O	1:A:202:PRO:HD3	2.20	0.41
1:A:125:THR:HG21	1:A:234:ARG:HA	2.01	0.41
1:F:81:VAL:O	1:F:83:GLY:N	2.54	0.41
1:B:119:LYS:HE2	1:B:119:LYS:HB3	1.89	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:G:15:HIS:CE1	1:G:30:HIS:NE2	2.74	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:F:66:ARG:HD2	1:F:147:ARG:NH2	2.36	0.40
1:B:26:TYR:OH	1:B:43:ARG:HA	2.21	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%)	26	55
1	D	296/301 (98%)	277 (94%)	19 (6%)	0	100	100
1	E	298/301 (99%)	277 (93%)	19 (6%)	2 (1%)	26	55
1	F	298/301 (99%)	280 (94%)	17 (6%)	1 (0%)	46	75
1	G	299/301 (99%)	278 (93%)	16 (5%)	5 (2%)	11	29
All	All	1786/1806 (99%)	1666 (93%)	110 (6%)	10 (1%)	30	59

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%)	57	85
1	B	250/251 (100%)	244 (98%)	6 (2%)	57	85
1	D	248/251 (99%)	241 (97%)	7 (3%)	51	81
1	E	251/251 (100%)	240 (96%)	11 (4%)	35	65
1	F	251/251 (100%)	242 (96%)	9 (4%)	42	73
1	G	252/251 (100%)	245 (97%)	7 (3%)	51	81
All	All	1501/1506 (100%)	1455 (97%)	46 (3%)	48	78

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	7.97	1 (33%)	5,9,9	2.75	3 (60%)
3	GOL	A	402	-	5,5,5	0.36	0	5,5,5	0.67	0
2	B2P	B	401	-	3,6,6	6.97	1 (33%)	5,9,9	1.43	1 (20%)
3	GOL	B	402	-	5,5,5	0.37	0	5,5,5	0.57	0
2	B2P	D	401	-	3,6,6	7.54	1 (33%)	5,9,9	1.64	1 (20%)
3	GOL	D	402	-	5,5,5	0.42	0	5,5,5	0.31	0
2	B2P	E	401	-	3,6,6	7.87	1 (33%)	5,9,9	0.81	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	0.28	0
2	B2P	F	401	-	3,6,6	7.63	1 (33%)	5,9,9	1.58	1 (20%)
3	GOL	F	402	-	5,5,5	0.51	0	5,5,5	0.62	0
2	B2P	G	401	-	3,6,6	7.63	1 (33%)	5,9,9	1.39	1 (20%)
3	GOL	G	402	-	5,5,5	0.34	0	5,5,5	0.22	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	-13.77	1.55	1.99
2	E	401	B2P	BR-CA	-13.61	1.56	1.99
2	F	401	B2P	BR-CA	-13.20	1.57	1.99
2	G	401	B2P	BR-CA	-13.20	1.57	1.99
2	D	401	B2P	BR-CA	-13.03	1.57	1.99
2	B	401	B2P	BR-CA	-12.07	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	-4.46	97.13	109.43
2	F	401	B2P	CM-CA-C	-3.03	101.07	109.43
2	D	401	B2P	CM-CA-C	-2.45	102.68	109.43
2	A	401	B2P	BR-CA-CM	-2.34	93.13	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	B2P	CB-CA-C	-2.33	103.02	109.43
2	G	401	B2P	CM-CA-C	-2.30	103.08	109.43
2	A	401	B2P	CM-CA-C	3.01	117.71	109.43

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 ⓘ

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, 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%)	-0.50	0 100 100	6, 13, 32, 49	0
1	B	298/301 (99%)	-0.50	0 100 100	7, 13, 34, 56	0
1	D	298/301 (99%)	-0.34	0 100 100	7, 15, 38, 57	0
1	E	298/301 (99%)	-0.45	0 100 100	9, 14, 34, 56	0
1	F	298/301 (99%)	-0.46	0 100 100	7, 15, 36, 57	0
1	G	298/301 (99%)	-0.40	0 100 100	7, 15, 38, 57	0
All	All	1788/1806 (99%)	-0.44	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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	6.95	9,11,11,12	0
2	B2P	A	401	7/7	0.88	0.25	4.29	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	2.80	10,13,13,13	0
2	B2P	F	401	7/7	0.93	0.20	2.30	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	0.18	0.72	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	-0.13	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.