



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:31 pm GMT

PDB ID : 1EEF
Title : HEAT-LABILE ENTEROTOXIN B-PENTAMER COMPLEXED WITH
BOUND LIGAND PEPG
Authors : Merritt, E.A.; Hol, W.G.J.
Deposited on : 2000-01-31
Resolution : 1.80 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

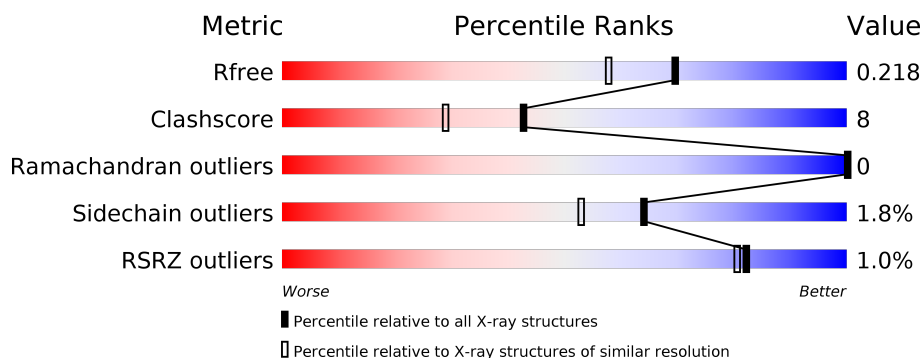
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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






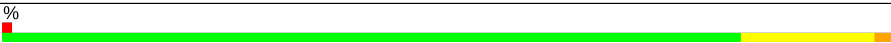
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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	D	103	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>•</div> </div> </div>
1	E	103	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>•</div> </div> </div>
1	F	103	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>•</div> </div> </div>
1	G	103	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>22%</div> <div>•</div> </div> </div>
1	H	103	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>••</div> </div> </div>
1	L	103	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	M	103	 84% 16%
1	N	103	 2% 83% 17%
1	O	103	 % 85% 14%
1	P	103	 % 83% 15%

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
3	I06	G	108	-	-	-	X
3	I06	H	110	-	-	-	X
3	I06	O	115	-	-	-	X

2 Entry composition

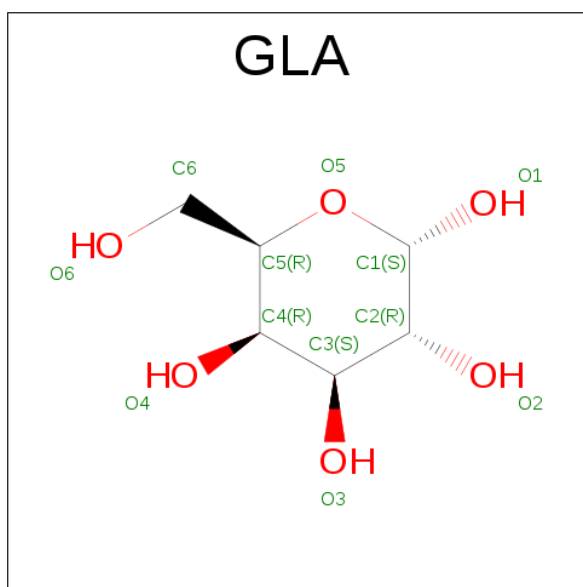
There are 4 unique types of molecules in this entry. The entry contains 9523 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (HEAT-LABILE ENTEROTOXIN B CHAIN).

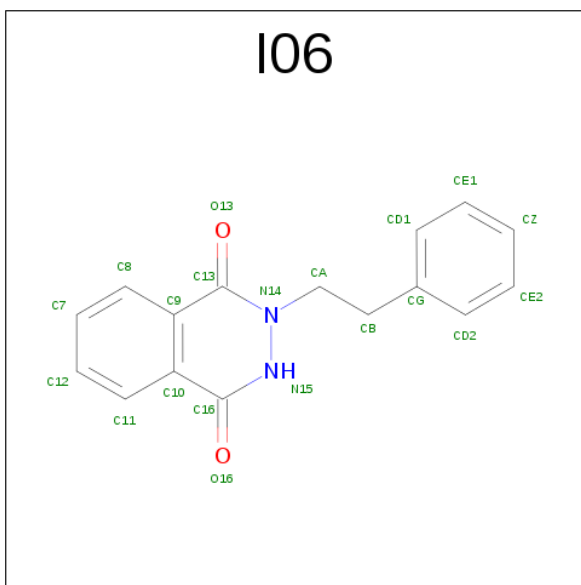
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	E	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	F	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	G	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	H	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	L	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	M	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	N	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	O	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	P	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			

- Molecule 2 is SUGAR (D-GALACTOSE) (three-letter code: GLA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			12	6	6		
2	E	1	Total	C	O	0	0
			12	6	6		
2	F	1	Total	C	O	0	0
			12	6	6		
2	G	1	Total	C	O	0	0
			12	6	6		
2	H	1	Total	C	O	0	0
			12	6	6		
2	L	1	Total	C	O	0	0
			12	6	6		
2	M	1	Total	C	O	0	0
			12	6	6		
2	N	1	Total	C	O	0	0
			12	6	6		
2	O	1	Total	C	O	0	0
			12	6	6		
2	P	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 2-PHENETHYL-2,3-DIHYDRO-PHTHALAZINE-1,4-DIONE (three-letter code: I06) (formula: C₁₆H₁₄N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			20	16	2	2		
3	H	1	Total	C	N	O	0	0
			20	16	2	2		
3	O	1	Total	C	N	O	0	0
			20	16	2	2		
3	P	1	Total	C	N	O	0	0
			20	16	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	102	Total	O	0	0
			102	102		
4	E	105	Total	O	0	0
			105	105		
4	F	107	Total	O	0	0
			107	107		
4	G	124	Total	O	0	0
			124	124		
4	H	119	Total	O	0	0
			119	119		
4	L	85	Total	O	0	0
			85	85		
4	M	111	Total	O	0	0
			111	111		
4	N	97	Total	O	0	0
			97	97		

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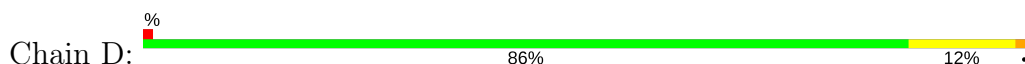
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	107	Total 107	O 107	0	0
4	P	126	Total 126	O 126	0	0

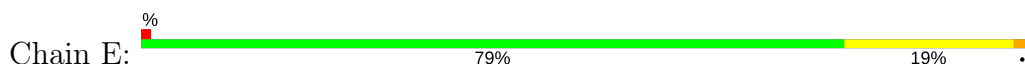
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

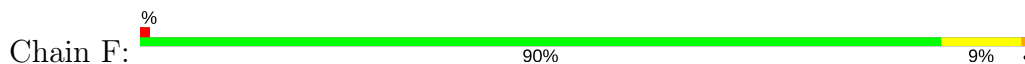
- Molecule 1: PROTEIN (HEAT-LABILE ENTEROTOXIN B CHAIN)



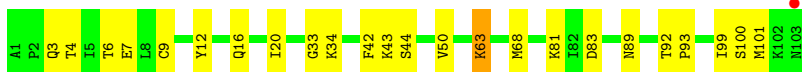
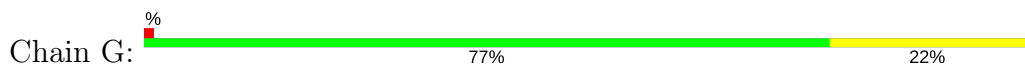
- Molecule 1: PROTEIN (HEAT-LABILE ENTEROTOXIN B CHAIN)



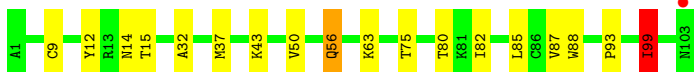
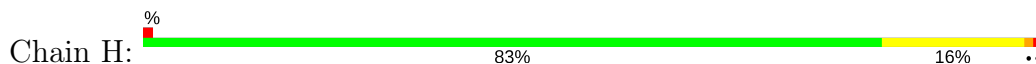
- Molecule 1: PROTEIN (HEAT-LABILE ENTEROTOXIN B CHAIN)



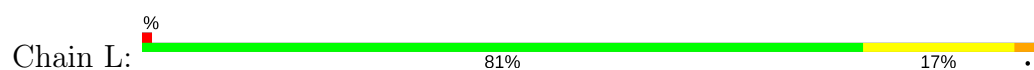
- Molecule 1: PROTEIN (HEAT-LABILE ENTEROTOXIN B CHAIN)



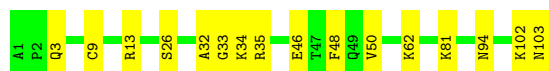
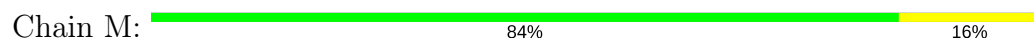
- Molecule 1: PROTEIN (HEAT-LABILE ENTEROTOXIN B CHAIN)



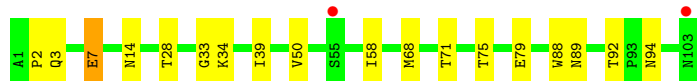
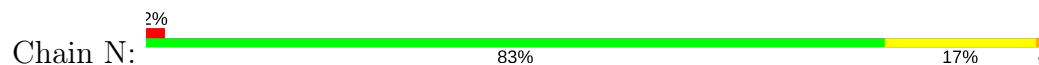
- Molecule 1: PROTEIN (HEAT-LABILE ENTEROTOXIN B CHAIN)



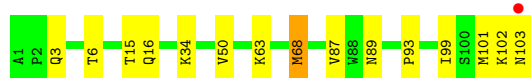
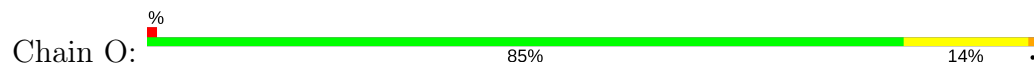
- Molecule 1: PROTEIN (HEAT-LABILE ENTEROTOXIN B CHAIN)



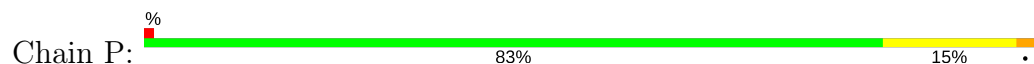
- Molecule 1: PROTEIN (HEAT-LABILE ENTEROTOXIN B CHAIN)



- Molecule 1: PROTEIN (HEAT-LABILE ENTEROTOXIN B CHAIN)



- Molecule 1: PROTEIN (HEAT-LABILE ENTEROTOXIN B CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.54Å 65.02Å 101.93Å 90.00° 115.47° 90.00°	Depositor
Resolution (Å)	22.00 – 1.80 24.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (22.00-1.80) 99.9 (24.66-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.69 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.182 , 0.267 0.180 , 0.218	Depositor DCC
R_{free} test set	4887 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 84.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9523	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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 54.80 % 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 3.4652e-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: GLA, I06

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	D	0.71	2/835 (0.2%)	0.73	1/1124 (0.1%)
1	E	0.59	1/835 (0.1%)	0.76	1/1124 (0.1%)
1	F	0.60	1/835 (0.1%)	0.76	1/1124 (0.1%)
1	G	0.64	1/835 (0.1%)	0.76	1/1124 (0.1%)
1	H	0.58	1/835 (0.1%)	0.79	2/1124 (0.2%)
1	L	0.52	0/835	0.74	1/1124 (0.1%)
1	M	0.56	0/835	0.73	1/1124 (0.1%)
1	N	0.61	1/835 (0.1%)	0.76	1/1124 (0.1%)
1	O	0.69	1/835 (0.1%)	0.78	1/1124 (0.1%)
1	P	0.55	0/835	0.77	1/1124 (0.1%)
All	All	0.61	8/8350 (0.1%)	0.76	11/11240 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	68	MET	CG-SD	12.16	2.12	1.81
1	D	68	MET	CG-SD	-9.46	1.56	1.81
1	G	68	MET	CG-SD	-7.54	1.61	1.81
1	E	68	MET	CG-SD	7.07	1.99	1.81
1	N	68	MET	CG-SD	7.03	1.99	1.81
1	F	68	MET	CG-SD	5.92	1.96	1.81
1	H	37	MET	CG-SD	5.53	1.95	1.81
1	D	68	MET	SD-CE	5.19	2.06	1.77

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	50	VAL	N-CA-C	-6.34	93.87	111.00
1	H	99	ILE	CB-CA-C	-6.27	99.05	111.60
1	H	50	VAL	N-CA-C	-6.12	94.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	50	VAL	N-CA-C	-6.08	94.58	111.00
1	G	50	VAL	N-CA-C	-5.85	95.19	111.00
1	O	50	VAL	N-CA-C	-5.83	95.25	111.00
1	F	50	VAL	N-CA-C	-5.81	95.32	111.00
1	M	50	VAL	N-CA-C	-5.66	95.73	111.00
1	N	50	VAL	N-CA-C	-5.57	95.95	111.00
1	L	50	VAL	N-CA-C	-5.46	96.24	111.00
1	D	50	VAL	N-CA-C	-5.34	96.57	111.00

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	D	824	0	841	19	0
1	E	824	0	841	22	0
1	F	824	0	841	7	0
1	G	824	0	841	19	0
1	H	824	0	841	18	0
1	L	824	0	841	16	0
1	M	824	0	841	16	0
1	N	824	0	841	11	0
1	O	824	0	841	14	0
1	P	824	0	841	15	0
2	D	12	0	12	0	0
2	E	12	0	12	0	0
2	F	12	0	12	0	0
2	G	12	0	11	0	0
2	H	12	0	11	0	0
2	L	12	0	12	0	0
2	M	12	0	12	0	0
2	N	12	0	12	0	0
2	O	12	0	11	0	0
2	P	12	0	11	1	0
3	G	20	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	20	0	13	1	0
3	O	20	0	13	0	0
3	P	20	0	13	0	0
4	D	102	0	0	2	0
4	E	105	0	0	5	0
4	F	107	0	0	1	0
4	G	124	0	0	5	0
4	H	119	0	0	6	0
4	L	85	0	0	4	0
4	M	111	0	0	2	0
4	N	97	0	0	1	0
4	O	107	0	0	2	0
4	P	126	0	0	2	0
All	All	9523	0	8578	132	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 (132) 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:68:MET:CE	1:D:68:MET:SD	2.06	1.40
1:O:68:MET:SD	1:O:68:MET:CG	2.12	1.38
1:P:56:GLN:HE21	1:P:56:GLN:H	1.01	0.98
1:G:16:GLN:HE21	1:G:89:ASN:HD22	1.13	0.91
1:D:63:LYS:HE3	4:D:1071:HOH:O	1.68	0.91
1:G:43:LYS:HD3	4:G:1355:HOH:O	1.72	0.89
1:D:16:GLN:HE21	1:D:89:ASN:HD22	1.15	0.88
1:H:56:GLN:HE21	1:H:56:GLN:N	1.71	0.87
1:H:9:CYS:HB3	4:H:1621:HOH:O	1.75	0.86
1:H:56:GLN:H	1:H:56:GLN:NE2	1.73	0.85
1:H:56:GLN:HE21	1:H:56:GLN:H	0.89	0.85
1:P:56:GLN:HE21	1:P:56:GLN:N	1.77	0.82
1:D:102:LYS:HE3	1:E:26:SER:HB3	1.62	0.82
1:F:3:GLN:HE22	1:G:92:THR:HG22	1.46	0.79
1:F:71:THR:O	1:F:75:THR:HG23	1.84	0.77
1:F:3:GLN:HB3	1:G:93:PRO:HG3	1.65	0.77
1:P:43:LYS:HE2	4:P:1365:HOH:O	1.85	0.75
1:G:3:GLN:HG2	1:H:93:PRO:HG3	1.71	0.72
1:D:29:GLU:HB3	1:H:99:ILE:CD1	2.20	0.72
1:H:63:LYS:HB2	4:H:1828:HOH:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:16:GLN:HE21	1:O:89:ASN:HD22	1.39	0.71
1:E:16:GLN:HE21	1:E:89:ASN:HD22	1.39	0.70
1:E:3:GLN:HE22	1:F:92:THR:HG22	1.57	0.69
1:E:9:CYS:HB3	4:E:1902:HOH:O	1.93	0.69
1:O:99:ILE:HG12	1:O:101:MET:HE2	1.75	0.69
1:P:56:GLN:NE2	1:P:56:GLN:H	1.84	0.68
1:P:85:LEU:HD12	1:P:99:ILE:HG22	1.76	0.67
1:L:102:LYS:HD2	4:L:1667:HOH:O	1.93	0.67
1:D:16:GLN:NE2	1:D:89:ASN:HD22	1.92	0.66
1:E:13:ARG:HH11	1:E:13:ARG:CG	2.09	0.66
1:M:81:LYS:HD2	1:M:103:ASN:HD22	1.62	0.65
1:P:85:LEU:CD1	1:P:99:ILE:HG22	2.28	0.64
1:L:16:GLN:HE21	1:L:89:ASN:HD22	1.44	0.64
1:O:6:THR:HG23	4:O:1193:HOH:O	1.98	0.63
1:L:37:MET:SD	4:L:1715:HOH:O	2.56	0.62
1:G:6:THR:HG23	4:G:1297:HOH:O	1.99	0.62
1:M:81:LYS:HD2	1:M:103:ASN:ND2	2.15	0.60
1:E:99:ILE:HG12	1:E:101:MET:HE2	1.84	0.59
1:M:3:GLN:HE21	1:N:92:THR:HG22	1.67	0.59
1:G:6:THR:HG21	4:G:1190:HOH:O	2.02	0.58
1:F:92:THR:HG23	4:F:1501:HOH:O	2.04	0.57
1:H:99:ILE:H	1:H:99:ILE:HD12	1.68	0.57
1:D:102:LYS:HG3	1:E:26:SER:HB3	1.86	0.57
1:L:27:TYR:HD1	1:P:101:MET:HE3	1.70	0.57
1:D:68:MET:CG	1:D:68:MET:CE	2.80	0.57
1:E:16:GLN:NE2	1:E:89:ASN:HD22	2.03	0.56
1:G:9:CYS:HB3	4:G:1490:HOH:O	2.05	0.56
1:L:11:GLU:OE1	1:M:35:ARG:HD2	2.06	0.56
1:G:16:GLN:HE21	1:G:89:ASN:ND2	1.95	0.56
1:O:102:LYS:O	1:O:103:ASN:HB2	2.06	0.55
1:E:21:ASN:HB2	4:E:2041:HOH:O	2.05	0.55
1:G:81:LYS:HE2	4:G:1552:HOH:O	2.06	0.55
1:N:71:THR:O	1:N:75:THR:HG23	2.08	0.54
1:P:4:THR:OG1	1:P:7:GLU:HG3	2.08	0.53
1:L:12:TYR:OH	1:M:35:ARG:HG3	2.09	0.53
1:H:43:LYS:HE2	4:H:1587:HOH:O	2.08	0.53
1:G:99:ILE:HG12	1:G:101:MET:HE2	1.91	0.52
1:E:13:ARG:HH11	1:E:13:ARG:HG2	1.73	0.52
1:O:6:THR:HG21	4:O:1661:HOH:O	2.08	0.52
1:L:102:LYS:HE3	1:M:26:SER:HB3	1.91	0.52
1:L:16:GLN:NE2	1:L:89:ASN:HD22	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:3:GLN:NE2	1:N:92:THR:HG22	2.25	0.51
1:O:63:LYS:HB3	4:P:1482:HOH:O	2.10	0.51
1:P:71:THR:HG21	1:P:99:ILE:HD11	1.92	0.50
1:M:33:GLY:O	1:M:34:LYS:HB2	2.11	0.50
1:O:68:MET:SD	1:O:68:MET:CB	2.95	0.49
1:D:3:GLN:HG2	1:E:93:PRO:HG3	1.94	0.49
1:O:68:MET:CE	1:O:68:MET:CG	2.90	0.49
1:G:20:ILE:HG21	1:G:42:PHE:CE1	2.47	0.49
1:D:63:LYS:HG2	4:H:1327:HOH:O	2.12	0.49
1:G:16:GLN:NE2	1:G:89:ASN:HD22	1.96	0.49
1:D:102:LYS:HE3	1:E:26:SER:CB	2.37	0.49
1:D:63:LYS:HE2	1:E:66:GLU:OE1	2.13	0.48
1:O:16:GLN:NE2	1:O:89:ASN:HD22	2.08	0.48
1:P:71:THR:HG21	1:P:99:ILE:CD1	2.43	0.48
1:O:15:THR:HA	1:O:87:VAL:O	2.14	0.47
1:D:4:THR:OG1	1:D:7:GLU:HB2	2.13	0.47
1:L:20:ILE:HG21	1:L:42:PHE:CE1	2.49	0.47
1:E:14:ASN:O	1:E:88:TRP:HA	2.14	0.47
1:L:62:LYS:HB3	4:L:1523:HOH:O	2.14	0.47
1:H:82:ILE:HG21	1:H:85:LEU:CD1	2.46	0.46
1:G:33:GLY:O	1:G:34:LYS:HB2	2.16	0.46
1:D:29:GLU:HB3	1:H:99:ILE:HD11	1.96	0.46
1:L:15:THR:HG22	1:L:88:TRP:CD1	2.50	0.46
1:G:63:LYS:HB3	4:H:1626:HOH:O	2.16	0.45
1:N:58:ILE:HD12	1:O:34:LYS:HE2	1.98	0.45
1:N:89:ASN:HA	1:N:94:ASN:ND2	2.31	0.45
1:E:81:LYS:NZ	4:E:2063:HOH:O	2.48	0.45
1:F:20:ILE:HG21	1:F:42:PHE:CE1	2.51	0.45
1:M:9:CYS:HB3	4:M:1746:HOH:O	2.16	0.45
1:L:32:ALA:HB1	1:P:12:TYR:CZ	2.53	0.44
1:D:63:LYS:HB3	4:E:1570:HOH:O	2.16	0.44
1:N:33:GLY:O	1:N:34:LYS:HB2	2.17	0.44
1:N:28:THR:HB	1:N:39:ILE:HB	1.99	0.44
1:D:63:LYS:HD2	1:E:66:GLU:HG3	2.00	0.44
1:M:102:LYS:HE3	1:M:102:LYS:HB2	1.78	0.44
1:D:30:SER:O	1:D:36:GLU:HA	2.18	0.43
1:L:50:VAL:HG11	1:L:69:LYS:HG3	2.00	0.43
1:H:75:THR:HG23	1:H:80:THR:HB	2.00	0.43
1:E:37:MET:SD	4:E:1696:HOH:O	2.62	0.43
1:M:48:PHE:CD1	1:M:94:ASN:HB2	2.52	0.43
1:P:102:LYS:HE3	1:P:102:LYS:HB2	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:30:SER:O	1:L:36:GLU:HA	2.18	0.43
4:D:1780:HOH:O	1:E:93:PRO:HA	2.18	0.43
1:G:83:ASP:HB3	1:G:100:SER:OG	2.19	0.43
1:H:15:THR:HA	1:H:87:VAL:O	2.19	0.42
1:M:46:GLU:HB3	1:M:48:PHE:CE2	2.54	0.42
1:N:79:GLU:HA	4:N:1730:HOH:O	2.18	0.42
1:O:102:LYS:O	1:O:103:ASN:CB	2.67	0.42
1:N:2:PRO:HB3	1:N:7:GLU:HG3	2.01	0.42
1:P:33:GLY:O	1:P:34:LYS:HB2	2.20	0.42
1:E:89:ASN:HA	1:E:94:ASN:ND2	2.34	0.42
1:F:25:LEU:HD22	1:F:43:LYS:HA	2.02	0.42
1:L:12:TYR:CZ	1:M:32:ALA:HB1	2.54	0.42
1:E:34:LYS:O	1:E:35:ARG:HD3	2.20	0.42
1:L:21:ASN:ND2	1:L:81:LYS:NZ	2.67	0.42
1:M:62:LYS:NZ	4:M:1908:HOH:O	2.48	0.42
1:D:63:LYS:HD3	1:E:66:GLU:OE1	2.20	0.41
3:H:110:I06:O16	4:H:2026:HOH:O	2.21	0.41
1:H:14:ASN:O	1:H:88:TRP:HA	2.21	0.41
1:G:44:SER:O	1:M:13:ARG:HG2	2.20	0.41
4:L:1723:HOH:O	1:P:103:ASN:CB	2.68	0.41
1:N:14:ASN:O	1:N:88:TRP:HA	2.21	0.41
1:N:3:GLN:HE21	1:O:93:PRO:HG3	1.85	0.41
1:H:82:ILE:HG21	1:H:85:LEU:HD13	2.02	0.40
1:H:99:ILE:N	1:H:99:ILE:HD12	2.34	0.40
1:D:32:ALA:HB1	1:H:12:TYR:CZ	2.56	0.40
1:E:48:PHE:CE1	1:E:87:VAL:HG11	2.57	0.40
1:M:48:PHE:HD1	1:M:94:ASN:HB2	1.86	0.40
1:G:12:TYR:CZ	1:H:32:ALA:HB1	2.57	0.40
1:P:88:TRP:CD2	2:P:116:GLA:H4	2.55	0.40
1:G:4:THR:OG1	1:G:7:GLU:HG3	2.21	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	D	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
1	E	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
1	F	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
1	G	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	H	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
1	L	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
1	M	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
1	N	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
1	O	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	P	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
All	All	1010/1030 (98%)	989 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	D	95/95 (100%)	93 (98%)	2 (2%)	59	46
1	E	95/95 (100%)	93 (98%)	2 (2%)	59	46
1	F	95/95 (100%)	94 (99%)	1 (1%)	78	72
1	G	95/95 (100%)	94 (99%)	1 (1%)	78	72
1	H	95/95 (100%)	93 (98%)	2 (2%)	59	46
1	L	95/95 (100%)	92 (97%)	3 (3%)	44	28
1	M	95/95 (100%)	95 (100%)	0	100	100
1	N	95/95 (100%)	94 (99%)	1 (1%)	78	72
1	O	95/95 (100%)	94 (99%)	1 (1%)	78	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	95/95 (100%)	91 (96%)	4 (4%)	34	17
All	All	950/950 (100%)	933 (98%)	17 (2%)	64	53

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	63	LYS
1	D	103	ASN
1	E	13	ARG
1	E	35	ARG
1	F	3	GLN
1	G	63	LYS
1	H	56	GLN
1	H	99	ILE
1	L	59	ASP
1	L	62	LYS
1	L	81	LYS
1	N	7	GLU
1	O	3	GLN
1	P	3	GLN
1	P	11	GLU
1	P	56	GLN
1	P	85	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	16	GLN
1	D	21	ASN
1	D	94	ASN
1	E	3	GLN
1	E	16	GLN
1	E	94	ASN
1	E	103	ASN
1	F	3	GLN
1	F	94	ASN
1	G	3	GLN
1	G	16	GLN
1	H	3	GLN
1	H	56	GLN
1	H	94	ASN

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Mol	Chain	Res	Type
1	L	16	GLN
1	L	21	ASN
1	L	94	ASN
1	M	3	GLN
1	M	16	GLN
1	M	94	ASN
1	M	103	ASN
1	N	3	GLN
1	N	94	ASN
1	O	16	GLN
1	P	3	GLN
1	P	56	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 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	GLA	D	104	-	12,12,12	0.75	0	17,17,17	1.28	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLA	E	105	-	12,12,12	1.47	1 (8%)	17,17,17	0.99	1 (5%)
2	GLA	F	106	-	12,12,12	1.44	1 (8%)	17,17,17	1.40	2 (11%)
2	GLA	G	107	3	12,12,12	0.93	0	17,17,17	0.91	0
3	I06	G	108	2	19,22,22	3.68	8 (42%)	20,30,30	2.93	8 (40%)
2	GLA	H	109	3	12,12,12	0.98	1 (8%)	17,17,17	1.81	5 (29%)
3	I06	H	110	2	19,22,22	3.65	7 (36%)	20,30,30	2.92	8 (40%)
2	GLA	L	111	-	12,12,12	1.17	1 (8%)	17,17,17	1.04	2 (11%)
2	GLA	M	112	-	12,12,12	1.00	0	17,17,17	1.51	2 (11%)
2	GLA	N	113	-	12,12,12	1.05	1 (8%)	17,17,17	1.55	4 (23%)
2	GLA	O	114	3	12,12,12	1.37	1 (8%)	17,17,17	1.84	5 (29%)
3	I06	O	115	2	19,22,22	3.71	9 (47%)	20,30,30	2.90	8 (40%)
2	GLA	P	116	3	12,12,12	1.23	1 (8%)	17,17,17	1.70	4 (23%)
3	I06	P	117	2	19,22,22	3.52	7 (36%)	20,30,30	2.90	8 (40%)

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	GLA	D	104	-	-	0/2/22/22	0/1/1/1
2	GLA	E	105	-	-	0/2/22/22	0/1/1/1
2	GLA	F	106	-	-	0/2/22/22	0/1/1/1
2	GLA	G	107	3	-	0/2/22/22	0/1/1/1
3	I06	G	108	2	-	0/5/5/5	0/3/3/3
2	GLA	H	109	3	-	0/2/22/22	0/1/1/1
3	I06	H	110	2	-	0/5/5/5	0/3/3/3
2	GLA	L	111	-	-	0/2/22/22	0/1/1/1
2	GLA	M	112	-	-	0/2/22/22	0/1/1/1
2	GLA	N	113	-	-	0/2/22/22	0/1/1/1
2	GLA	O	114	3	-	0/2/22/22	0/1/1/1
3	I06	O	115	2	-	0/5/5/5	0/3/3/3
2	GLA	P	116	3	-	0/2/22/22	0/1/1/1
3	I06	P	117	2	-	0/5/5/5	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	115	I06	C8-C9	-8.15	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	115	I06	C10-C9	-7.68	1.40	1.54
3	P	117	I06	C8-C9	-7.64	1.39	1.53
3	H	110	I06	C8-C9	-7.64	1.39	1.53
3	G	108	I06	C10-C9	-7.52	1.40	1.54
3	G	108	I06	C8-C9	-7.46	1.39	1.53
3	G	108	I06	C11-C10	-7.11	1.40	1.53
3	P	117	I06	C11-C10	-7.07	1.40	1.53
3	H	110	I06	C11-C10	-7.07	1.40	1.53
3	H	110	I06	C10-C9	-6.88	1.42	1.54
3	O	115	I06	C11-C10	-6.82	1.41	1.53
3	P	117	I06	C10-C9	-6.71	1.42	1.54
3	H	110	I06	C7-C8	-6.18	1.36	1.53
3	H	110	I06	C12-C11	-6.02	1.37	1.53
3	O	115	I06	C7-C8	-5.67	1.38	1.53
3	G	108	I06	C7-C8	-5.65	1.38	1.53
3	P	117	I06	C7-C8	-5.55	1.38	1.53
3	G	108	I06	C12-C11	-5.49	1.38	1.53
3	P	117	I06	C12-C11	-5.23	1.39	1.53
3	O	115	I06	C12-C11	-5.04	1.39	1.53
2	O	114	GLA	C1-C2	-3.59	1.45	1.52
3	G	108	I06	C13-N14	-3.17	1.31	1.36
3	O	115	I06	C9-C13	-3.04	1.46	1.51
3	O	115	I06	C12-C7	-2.91	1.39	1.51
3	P	117	I06	C12-C7	-2.89	1.39	1.51
3	H	110	I06	C12-C7	-2.87	1.40	1.51
3	G	108	I06	C12-C7	-2.78	1.40	1.51
3	G	108	I06	C9-C13	-2.70	1.46	1.51
3	P	117	I06	C9-C13	-2.57	1.46	1.51
2	N	113	GLA	O4-C4	-2.55	1.37	1.43
2	H	109	GLA	C1-C2	-2.51	1.47	1.52
3	O	115	I06	C13-N14	-2.35	1.32	1.36
3	O	115	I06	C10-C16	-2.35	1.47	1.51
3	H	110	I06	C10-C16	-2.18	1.48	1.51
2	P	116	GLA	C4-C5	2.04	1.57	1.53
2	L	111	GLA	C1-C2	2.34	1.57	1.52
2	F	106	GLA	C1-C2	3.09	1.59	1.52
2	E	105	GLA	C1-C2	3.33	1.59	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	114	GLA	O2-C2-C3	-3.90	101.86	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	109	GLA	C4-C3-C2	-3.89	103.97	110.84
2	M	112	GLA	C6-C5-C4	-3.76	104.19	113.00
2	O	114	GLA	C3-C4-C5	-3.41	104.20	110.22
2	N	113	GLA	O1-C1-O5	-3.39	100.19	110.20
2	P	116	GLA	O2-C2-C3	-3.26	103.27	110.36
2	H	109	GLA	O4-C4-C3	-2.72	104.43	110.36
2	P	116	GLA	C6-C5-C4	-2.64	106.82	113.00
2	D	104	GLA	O2-C2-C3	-2.63	104.64	110.36
2	H	109	GLA	O1-C1-C2	-2.57	102.18	109.42
2	N	113	GLA	O2-C2-C3	-2.48	104.97	110.36
2	F	106	GLA	O6-C6-C5	-2.33	103.51	111.34
2	L	111	GLA	O4-C4-C3	-2.23	105.50	110.36
2	E	105	GLA	C6-C5-C4	-2.18	107.91	113.00
2	O	114	GLA	C6-C5-C4	-2.10	108.09	113.00
2	N	113	GLA	C4-C3-C2	-2.02	107.27	110.84
2	L	111	GLA	O3-C3-C2	-2.01	105.99	110.36
2	H	109	GLA	C1-C2-C3	2.18	114.58	110.65
2	N	113	GLA	C1-C2-C3	2.20	114.63	110.65
2	M	112	GLA	C1-C2-C3	2.21	114.65	110.65
2	P	116	GLA	O5-C5-C4	2.35	114.00	109.66
2	D	104	GLA	C1-C2-C3	2.37	114.94	110.65
2	O	114	GLA	C1-C2-C3	2.62	115.38	110.65
2	H	109	GLA	O5-C1-C2	2.71	114.53	110.04
2	O	114	GLA	O4-C4-C5	2.78	116.30	109.28
2	F	106	GLA	C1-O5-C5	2.99	118.79	113.39
2	P	116	GLA	C1-C2-C3	3.07	116.20	110.65
3	O	115	I06	C8-C9-C13	3.67	118.68	111.41
3	P	117	I06	C8-C9-C13	3.77	118.86	111.41
3	G	108	I06	C8-C9-C13	3.80	118.93	111.41
3	H	110	I06	C12-C11-C10	4.00	118.79	111.79
3	O	115	I06	C7-C12-C11	4.09	119.88	111.42
3	H	110	I06	C8-C9-C13	4.10	119.53	111.41
3	G	108	I06	C7-C12-C11	4.17	120.03	111.42
3	P	117	I06	C7-C12-C11	4.21	120.12	111.42
3	H	110	I06	C11-C10-C16	4.33	119.92	111.13
3	O	115	I06	C11-C10-C16	4.36	119.98	111.13
3	O	115	I06	C12-C11-C10	4.39	119.48	111.79
3	G	108	I06	C7-C8-C9	4.41	119.52	111.79
3	H	110	I06	C7-C8-C9	4.43	119.55	111.79
3	P	117	I06	C11-C10-C16	4.44	120.14	111.13
3	O	115	I06	C12-C7-C8	4.45	120.63	111.42
3	G	108	I06	C11-C10-C16	4.52	120.31	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	108	I06	C12-C7-C8	4.52	120.76	111.42
3	P	117	I06	C12-C7-C8	4.56	120.85	111.42
3	P	117	I06	C7-C8-C9	4.56	119.78	111.79
3	H	110	I06	C12-C7-C8	4.59	120.92	111.42
3	P	117	I06	C12-C11-C10	4.62	119.89	111.79
3	G	108	I06	C12-C11-C10	4.64	119.91	111.79
3	H	110	I06	C7-C12-C11	4.68	121.10	111.42
3	P	117	I06	C11-C10-C9	4.77	119.27	110.84
3	O	115	I06	C7-C8-C9	4.80	120.20	111.79
3	G	108	I06	C11-C10-C9	4.88	119.47	110.84
3	O	115	I06	C11-C10-C9	4.91	119.52	110.84
3	H	110	I06	C8-C9-C10	4.99	119.66	110.84
3	H	110	I06	C11-C10-C9	5.16	119.96	110.84
3	P	117	I06	C8-C9-C10	5.23	120.09	110.84
3	O	115	I06	C8-C9-C10	5.34	120.28	110.84
3	G	108	I06	C8-C9-C10	5.35	120.29	110.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	110	I06	1	0
2	P	116	GLA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	D	103/103 (100%)	-0.35	1 (0%) 82 80	7, 13, 25, 50	0
1	E	103/103 (100%)	-0.42	1 (0%) 82 80	9, 13, 25, 36	0
1	F	103/103 (100%)	-0.38	1 (0%) 82 80	8, 13, 23, 52	0
1	G	103/103 (100%)	-0.40	1 (0%) 82 80	8, 12, 24, 41	0
1	H	103/103 (100%)	-0.39	1 (0%) 82 80	9, 12, 22, 56	0
1	L	103/103 (100%)	-0.10	1 (0%) 82 80	10, 17, 30, 53	0
1	M	103/103 (100%)	-0.26	0 100 100	9, 14, 29, 43	0
1	N	103/103 (100%)	-0.31	2 (1%) 67 63	9, 15, 27, 50	0
1	O	103/103 (100%)	-0.35	1 (0%) 82 80	8, 14, 26, 48	0
1	P	103/103 (100%)	-0.33	1 (0%) 82 80	10, 14, 27, 50	0
All	All	1030/1030 (100%)	-0.33	10 (0%) 82 80	7, 13, 27, 56	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	103	ASN	4.5
1	H	103	ASN	4.2
1	O	103	ASN	3.7
1	L	13	ARG	2.8
1	D	103	ASN	2.7
1	G	103	ASN	2.7
1	N	103	ASN	2.2
1	E	59	ASP	2.2
1	N	55	SER	2.1
1	P	103	ASN	2.1

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(Å ²)	Q<0.9
3	I06	G	108	20/20	0.89	0.15	6.27	9,11,14,16	0
3	I06	O	115	20/20	0.90	0.16	4.18	12,15,19,20	0
3	I06	H	110	20/20	0.86	0.15	3.93	13,15,18,18	0
2	GLA	L	111	12/12	0.91	0.14	1.92	19,22,25,30	0
2	GLA	O	114	12/12	0.95	0.09	1.31	11,14,16,17	0
3	I06	P	117	20/20	0.93	0.10	0.96	12,15,18,19	0
2	GLA	N	113	12/12	0.92	0.10	0.75	11,14,18,20	0
2	GLA	D	104	12/12	0.95	0.08	0.66	9,13,18,22	0
2	GLA	E	105	12/12	0.96	0.08	0.34	10,13,17,19	0
2	GLA	F	106	12/12	0.94	0.09	0.15	8,13,18,24	0
2	GLA	G	107	12/12	0.96	0.07	0.05	9,10,12,14	0
2	GLA	H	109	12/12	0.96	0.08	0.03	10,12,13,13	0
2	GLA	P	116	12/12	0.95	0.08	-0.62	10,13,15,15	0
2	GLA	M	112	12/12	0.96	0.07	-1.46	12,13,16,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.