W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 01:00 am GMT

PDB ID	:	4KTP
Title	:	Crystal structure of 2-O-alpha-glucosylglycerol phosphorylase in complex with glucose
Authors	:	Touhara, K.K.; Nihira, T.; Kitaoka, M.; Nakai, H.; Fushinobu, S.
Deposited on	:	2013-05-21
Resolution	:	1.90 Å(reported)

The following versions of software and data (see references (i)) 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 1.90 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.
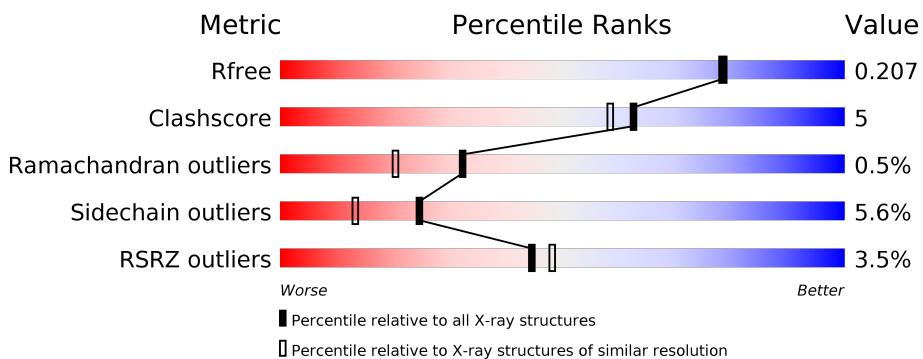
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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 <=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	769	3% 86% 10% · ·
1	B	769	4% 84% 12% · ··
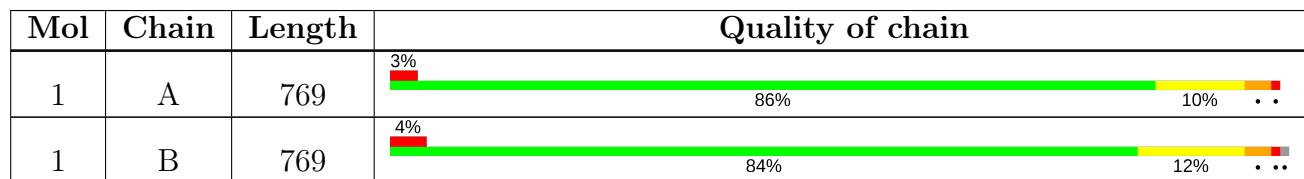
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1PE	A	802	-	-	-	X
4	PG4	B	802	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 13120 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 Glycoside hydrolase family 65 central catalytic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	767	Total 6143	C 3881	N 1048	O 1192	S 22	0	0	0
1	B	761	Total 6086	C 3846	N 1034	O 1184	S 22	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	PRO	SER	ENGINEERED MUTATION	UNP D6XZ22
A	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
A	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
A	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	226	PRO	SER	ENGINEERED MUTATION	UNP D6XZ22
B	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
B	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
B	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	769	HIS	-	EXPRESSION TAG	UNP D6XZ22

- Molecule 2 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: $C_6H_{12}O_6$).
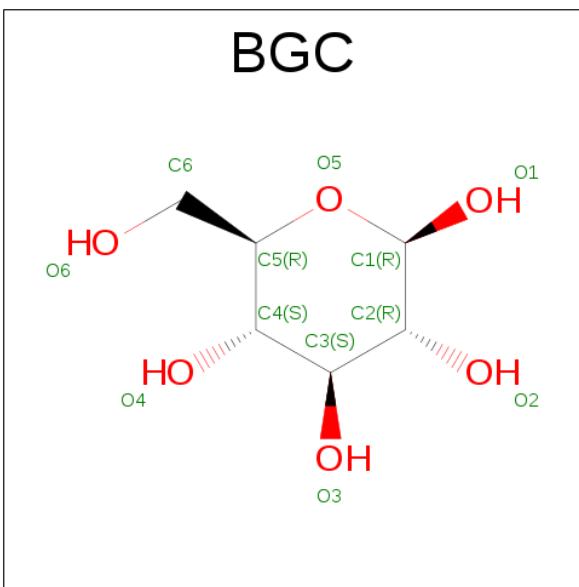
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 12	C 6	O 6	0	0
2	B	1	Total 12	C 6	O 6	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).
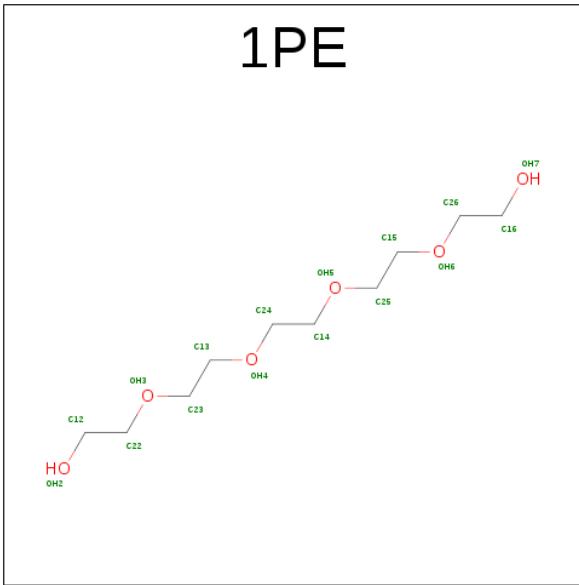
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 16	C 10	O 6	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

PG4
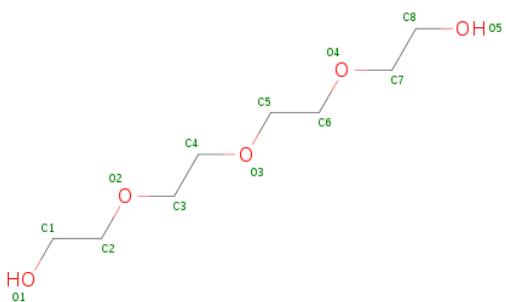
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 13	C 8	O 5	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Ca 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	424	Total 424	O 424	0	0
6	B	412	Total 412	O 412	0	0

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: Glycoside hydrolase family 65 central catalytic
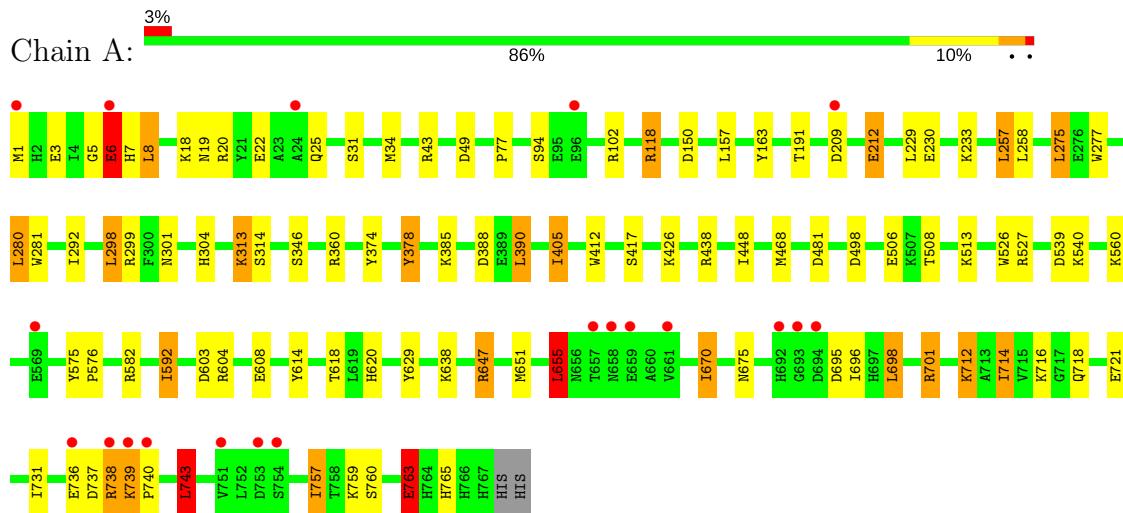
- Molecule 1: Glycoside hydrolase family 65 central catalytic
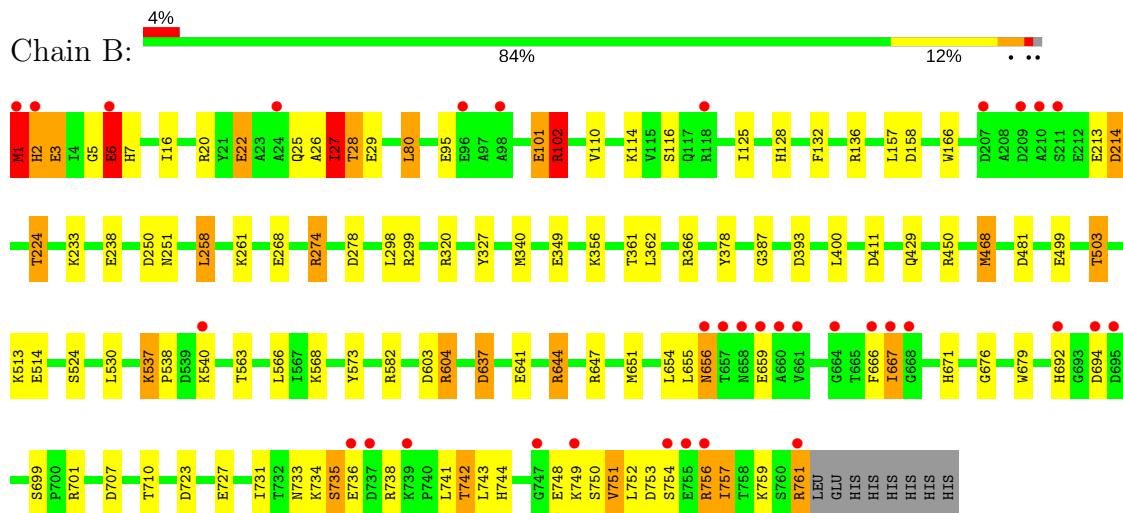
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	206.08Å 76.96Å 145.77Å 90.00° 128.39° 90.00°	Depositor
Resolution (Å)	19.94 – 1.90	Depositor
	19.94 – 1.90	EDS
% Data completeness	99.0 (19.94-1.90)	Depositor
(in resolution range)	99.2 (19.94-1.90)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.40 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.170 , 0.206	Depositor
	0.171 , 0.207	DCC
R_{free} test set	7038 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 56.2	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13120	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, BGC, PG4, 1PE

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	1.26	11/6291 (0.2%)	1.23	43/8532 (0.5%)
1	B	1.27	7/6230 (0.1%)	1.25	41/8449 (0.5%)
All	All	1.27	18/12521 (0.1%)	1.24	84/16981 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	GLU	CD-OE1	7.68	1.34	1.25
1	A	608	GLU	CD-OE2	6.54	1.32	1.25
1	B	524	SER	CB-OG	-6.40	1.33	1.42
1	A	378	TYR	CE1-CZ	6.28	1.46	1.38
1	B	641	GLU	CD-OE2	6.20	1.32	1.25
1	A	412	TRP	CD2-CE2	6.03	1.48	1.41
1	A	526	TRP	CD2-CE2	5.90	1.48	1.41
1	A	374	TYR	CE1-CZ	5.68	1.46	1.38
1	B	251	ASN	N-CA	5.67	1.57	1.46
1	A	614	TYR	CE1-CZ	5.47	1.45	1.38
1	A	760	SER	CB-OG	-5.47	1.35	1.42
1	A	277	TRP	CG-CD1	5.37	1.44	1.36
1	A	281	TRP	CD2-CE2	5.26	1.47	1.41
1	B	679	TRP	CD2-CE2	5.22	1.47	1.41
1	A	498	ASP	CB-CG	5.22	1.62	1.51
1	A	163	TYR	CG-CD2	5.15	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	TRP	CD2-CE2	5.08	1.47	1.41
1	B	214	ASP	CB-CG	-5.08	1.41	1.51

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	ARG	NE-CZ-NH2	-22.45	109.07	120.30
1	B	274	ARG	NE-CZ-NH1	19.05	129.82	120.30
1	B	644	ARG	NE-CZ-NH2	-17.96	111.32	120.30
1	A	102	ARG	NE-CZ-NH1	15.66	128.13	120.30
1	B	274	ARG	NE-CZ-NH2	-14.30	113.15	120.30
1	B	644	ARG	NE-CZ-NH1	12.09	126.34	120.30
1	A	647	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	A	299	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	A	647	ARG	NE-CZ-NH2	-9.43	115.59	120.30
1	B	299	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	A	670	ILE	CG1-CB-CG2	-9.10	91.38	111.40
1	B	468	MET	CG-SD-CE	8.35	113.56	100.20
1	B	450	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	356	LYS	CD-CE-NZ	-8.03	93.22	111.70
1	B	258	LEU	CB-CG-CD1	7.75	124.18	111.00
1	B	647	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	B	80	LEU	CB-CG-CD1	7.53	123.79	111.00
1	A	390	LEU	CB-CG-CD1	7.22	123.27	111.00
1	B	157	LEU	CB-CG-CD1	-7.14	98.86	111.00
1	A	298	LEU	CB-CG-CD2	7.09	123.05	111.00
1	A	8	LEU	CB-CG-CD1	-7.07	98.99	111.00
1	B	481	ASP	CB-CG-OD1	7.04	124.64	118.30
1	B	250	ASP	C-N-CA	-6.96	104.29	121.70
1	A	604	ARG	CG-CD-NE	-6.91	97.28	111.80
1	A	118	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	102	ARG	CD-NE-CZ	6.85	133.19	123.60
1	A	582	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	B	411	ASP	CB-CG-OD2	6.83	124.45	118.30
1	B	340	MET	CG-SD-CE	6.74	110.99	100.20
1	A	701	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	B	644	ARG	CD-NE-CZ	6.68	132.96	123.60
1	A	763	GLU	N-CA-CB	-6.55	98.81	110.60
1	A	360	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	A	8	LEU	CA-CB-CG	6.46	130.15	115.30
1	A	280	LEU	CB-CG-CD1	6.41	121.90	111.00
1	A	513	LYS	CD-CE-NZ	-6.34	97.12	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	647	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	763	GLU	CA-CB-CG	6.29	127.24	113.40
1	B	603	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	655	LEU	CB-CG-CD1	6.12	121.40	111.00
1	B	274	ARG	CD-NE-CZ	6.05	132.07	123.60
1	A	743	LEU	CB-CG-CD2	-6.03	100.74	111.00
1	A	275	LEU	CB-CG-CD1	5.98	121.17	111.00
1	B	320	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	530	LEU	CB-CG-CD1	-5.95	100.88	111.00
1	A	118	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	714	ILE	CG1-CB-CG2	-5.78	98.69	111.40
1	B	102	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	B	268	GLU	OE1-CD-OE2	5.70	130.14	123.30
1	A	280	LEU	CB-CG-CD2	5.69	120.67	111.00
1	B	299	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	B	157	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	A	481	ASP	CB-CG-OD1	5.58	123.33	118.30
1	B	582	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	498	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	527	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	393	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	157	LEU	CB-CG-CD2	-5.41	101.81	111.00
1	A	280	LEU	CA-CB-CG	5.41	127.73	115.30
1	B	744	HIS	N-CA-C	-5.38	96.46	111.00
1	B	268	GLU	CG-CD-OE1	-5.37	107.56	118.30
1	A	43	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	346	SER	CB-CA-C	-5.35	99.94	110.10
1	A	539	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	513	LYS	CD-CE-NZ	-5.35	99.40	111.70
1	A	191	THR	OG1-CB-CG2	5.34	122.28	110.00
1	B	261	LYS	CD-CE-NZ	-5.34	99.42	111.70
1	A	405	ILE	CG1-CB-CG2	-5.32	99.69	111.40
1	B	298	LEU	CB-CG-CD2	-5.32	101.95	111.00
1	A	150	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	698	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	603	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	388	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	257	LEU	CB-CG-CD2	5.21	119.85	111.00
1	B	278	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	102	ARG	CG-CD-NE	5.19	122.70	111.80
1	B	701	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	B	366	ARG	NE-CZ-NH2	-5.18	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	LEU	CA-CB-CG	5.16	127.16	115.30
1	B	656	ASN	N-CA-C	5.12	124.81	111.00
1	A	49	ASP	CB-CG-OD2	5.09	122.89	118.30
1	B	481	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	707	ASP	CB-CG-OD2	5.06	122.86	118.30
1	B	537	LYS	CB-CG-CD	-5.04	98.48	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	MET	Peptide

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	6143	0	5889	56	0
1	B	6086	0	5844	73	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	16	0	22	0	0
4	B	13	0	18	1	0
5	B	2	0	0	0	0
6	A	424	0	0	5	0
6	B	412	0	0	8	0
All	All	13120	0	11797	120	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 5.

All (120) 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:B:101:GLU:HG3	6:B:1204:HOH:O	1.51	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:ILE:HD13	1:A:743:LEU:HD21	1.39	1.04
1:B:25:GLN:O	1:B:29:GLU:HG2	1.61	1.00
1:A:757:ILE:HD11	1:A:759:LYS:HE2	1.42	0.99
1:B:710:THR:HG22	1:B:723:ASP:OD2	1.65	0.97
1:B:756:ARG:HH11	1:B:756:ARG:HG3	1.32	0.94
1:A:468:MET:SD	1:B:468:MET:CE	2.59	0.90
1:A:468:MET:SD	1:B:468:MET:HE2	2.13	0.88
1:B:761:ARG:HB3	1:B:761:ARG:NH2	1.93	0.83
1:A:731:ILE:CD1	1:A:743:LEU:HD21	2.08	0.83
1:B:26:ALA:O	1:B:27:ILE:HG23	1.78	0.83
1:B:742:THR:HA	1:B:751:VAL:HA	1.60	0.83
1:A:738:ARG:C	1:A:740:PRO:HD2	1.98	0.82
1:A:19:ASN:O	1:A:20:ARG:HD2	1.83	0.79
1:B:604:ARG:HH11	1:B:604:ARG:HG2	1.46	0.78
1:B:734:LYS:O	1:B:735:SER:OG	2.05	0.75
1:A:738:ARG:HH12	1:A:740:PRO:HG3	1.49	0.75
1:A:718:GLN:HE22	1:A:738:ARG:HB2	1.53	0.73
1:B:5:GLY:O	1:B:6:GLU:C	2.27	0.72
1:A:31:SER:HB3	1:A:670:ILE:HG12	1.71	0.72
1:A:468:MET:CB	1:B:468:MET:HE3	2.21	0.70
1:A:468:MET:HB2	1:B:468:MET:CE	2.23	0.69
1:B:734:LYS:O	1:B:735:SER:CB	2.40	0.69
1:A:738:ARG:HB2	1:A:738:ARG:HH11	1.57	0.69
1:A:468:MET:CB	1:B:468:MET:CE	2.70	0.69
1:A:560:LYS:HG2	6:A:901:HOH:O	1.94	0.67
1:A:468:MET:HB2	1:B:468:MET:HE1	1.76	0.66
1:A:5:GLY:O	1:A:6:GLU:C	2.34	0.65
1:A:468:MET:HB3	1:B:468:MET:HE3	1.77	0.65
1:B:756:ARG:NH1	1:B:756:ARG:HG3	2.06	0.65
1:B:604:ARG:NH1	1:B:604:ARG:HG2	2.13	0.64
1:A:712:LYS:HG3	1:A:721:GLU:HG3	1.80	0.64
1:A:426:LYS:NZ	6:A:1280:HOH:O	2.31	0.63
1:A:468:MET:SD	1:B:468:MET:HE1	2.38	0.63
1:B:741:LEU:HD13	1:B:752:LEU:HD23	1.80	0.62
1:A:1:MET:HA	1:A:292:ILE:HG21	1.80	0.61
1:A:638:LYS:HE3	6:A:1310:HOH:O	2.01	0.59
1:B:102:ARG:HH21	1:B:102:ARG:HG3	1.67	0.59
1:B:710:THR:CG2	1:B:723:ASP:OD2	2.48	0.58
1:B:604:ARG:HH11	1:B:604:ARG:CG	2.15	0.58
1:B:742:THR:HG22	1:B:751:VAL:HG22	1.87	0.57
1:B:761:ARG:HB3	1:B:761:ARG:HH21	1.65	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:ARG:HH12	1:A:740:PRO:CG	2.17	0.56
1:A:714:ILE:HD13	6:A:1170:HOH:O	2.06	0.56
1:A:738:ARG:CB	1:A:738:ARG:HH11	2.19	0.56
1:B:429:GLN:NE2	1:B:692:HIS:O	2.38	0.56
1:B:761:ARG:HB3	1:B:761:ARG:CZ	2.33	0.56
1:B:656:ASN:CG	1:B:656:ASN:O	2.43	0.56
1:A:651:MET:HB3	1:A:655:LEU:HD22	1.87	0.55
1:B:95:GLU:HG3	6:B:1116:HOH:O	2.06	0.55
1:A:738:ARG:NH1	1:A:740:PRO:HG3	2.21	0.54
1:B:27:ILE:HG13	1:B:28:THR:N	2.24	0.54
1:A:22:GLU:HB2	1:A:25:GLN:HG2	1.90	0.53
1:B:400:LEU:HD23	1:B:568:LYS:HD3	1.91	0.53
1:A:739:LYS:N	1:A:740:PRO:CD	2.72	0.53
1:B:16:ILE:HD13	1:B:654:LEU:HD21	1.90	0.53
1:B:537:LYS:HB2	1:B:538:PRO:CD	2.39	0.53
1:B:563:THR:HG22	1:B:573:TYR:OH	2.08	0.53
1:A:5:GLY:O	1:A:6:GLU:O	2.27	0.52
1:B:537:LYS:HB2	1:B:538:PRO:HD2	1.90	0.52
1:B:738:ARG:HD3	1:B:754:SER:OG	2.09	0.52
1:B:5:GLY:O	1:B:6:GLU:O	2.27	0.52
1:B:637:ASP:HB3	6:B:903:HOH:O	2.09	0.52
1:B:110:VAL:HG22	1:B:132:PHE:HB3	1.94	0.50
1:B:756:ARG:O	1:B:757:ILE:HG22	2.11	0.50
1:B:667:ILE:O	1:B:667:ILE:CG2	2.59	0.50
1:A:738:ARG:C	1:A:740:PRO:CD	2.77	0.50
1:A:718:GLN:NE2	1:A:738:ARG:HB2	2.26	0.49
1:A:8:LEU:HD23	1:A:18:LYS:HB2	1.93	0.49
1:A:468:MET:CB	1:B:468:MET:HE1	2.41	0.48
1:B:1:MET:HB3	1:B:2:HIS:CG	2.49	0.48
1:B:499:GLU:O	1:B:503:THR:HB	2.13	0.48
1:B:741:LEU:HD12	1:B:741:LEU:N	2.28	0.48
1:B:26:ALA:O	1:B:27:ILE:CG2	2.58	0.48
1:B:6:GLU:OE2	1:B:7:HIS:HD2	1.98	0.47
1:B:158:ASP:OD1	1:B:224:THR:HB	2.15	0.47
1:A:385:LYS:HE2	6:A:1071:HOH:O	2.13	0.47
1:A:212:GLU:HG2	1:A:212:GLU:O	2.15	0.47
1:A:438:ARG:HG2	1:A:508:THR:HG21	1.96	0.46
1:B:327:TYR:OH	1:B:667:ILE:HG13	2.16	0.46
1:B:671:HIS:HB3	6:B:1044:HOH:O	2.14	0.46
1:B:274:ARG:HD3	6:B:1084:HOH:O	2.15	0.46
1:A:405:ILE:HG21	1:A:405:ILE:HD13	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLN:O	1:B:29:GLU:CG	2.50	0.45
1:A:738:ARG:O	1:A:740:PRO:HD2	2.14	0.45
1:A:575:TYR:CG	1:A:576:PRO:HA	2.52	0.45
1:B:604:ARG:HG3	6:B:1140:HOH:O	2.17	0.45
1:A:738:ARG:NH1	1:A:738:ARG:CB	2.81	0.44
1:A:34:MET:HG2	1:A:304:HIS:HE1	1.82	0.44
1:B:6:GLU:HB3	1:B:7:HIS:H	1.64	0.44
1:B:651:MET:HB3	1:B:655:LEU:HD12	1.99	0.43
1:B:676:GLY:HA2	6:B:1097:HOH:O	2.17	0.43
1:B:731:ILE:HB	1:B:757:ILE:HG23	2.00	0.43
1:B:733:ASN:HB2	1:B:752:LEU:HD21	2.00	0.43
1:B:667:ILE:O	1:B:667:ILE:HG22	2.17	0.43
1:A:230:GLU:HB2	1:A:233:LYS:HB3	1.99	0.43
1:B:566:LEU:HD11	1:B:573:TYR:OH	2.19	0.43
1:B:116:SER:HA	1:B:125:ILE:O	2.19	0.43
1:A:592:ILE:HG12	1:A:629:TYR:CE1	2.54	0.42
1:A:738:ARG:NH1	1:A:740:PRO:CG	2.81	0.42
1:A:618:THR:HG22	1:A:620:HIS:H	1.83	0.42
1:B:22:GLU:HG2	1:B:25:GLN:HB2	2.00	0.42
1:A:739:LYS:HD2	1:A:739:LYS:N	2.34	0.42
1:B:114:LYS:HG2	1:B:128:HIS:CD2	2.54	0.42
1:A:313:LYS:HG2	1:A:314:SER:N	2.35	0.42
1:A:301:ASN:O	1:A:675:ASN:HB3	2.20	0.42
1:A:468:MET:HB2	1:B:468:MET:HE3	1.93	0.42
1:B:1:MET:HB3	1:B:2:HIS:CD2	2.55	0.41
1:A:739:LYS:N	1:A:740:PRO:HD2	2.33	0.41
1:B:644:ARG:NH2	6:B:1311:HOH:O	2.52	0.41
1:B:2:HIS:HB2	1:B:3:GLU:H	1.21	0.41
4:B:802:PG4:H12	4:B:802:PG4:H32	1.62	0.41
1:A:6:GLU:HB3	1:A:7:HIS:H	1.34	0.41
1:B:361:THR:HB	1:B:387:GLY:HA3	2.02	0.41
1:B:6:GLU:OE2	1:B:7:HIS:CD2	2.73	0.41
1:A:763:GLU:OE2	1:A:765:HIS:HB2	2.20	0.41
1:A:417:SER:HB3	1:A:448:ILE:HG23	2.02	0.41
1:B:22:GLU:CG	1:B:25:GLN:HB2	2.51	0.41
1:A:670:ILE:HG23	1:A:670:ILE:HD12	1.40	0.40
1:B:742:THR:HG22	1:B:751:VAL:HG13	2.04	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	765/769 (100%)	735 (96%)	28 (4%)	2 (0%)	44	34
1	B	759/769 (99%)	714 (94%)	39 (5%)	6 (1%)	22	11
All	All	1524/1538 (99%)	1449 (95%)	67 (4%)	8 (0%)	32	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	B	6	GLU
1	B	735	SER
1	B	751	VAL
1	B	757	ILE
1	A	737	ASP
1	B	736	GLU
1	B	27	ILE

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	656/658 (100%)	623 (95%)	33 (5%)	28	17
1	B	650/658 (99%)	610 (94%)	40 (6%)	21	10
All	All	1306/1316 (99%)	1233 (94%)	73 (6%)	25	13

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	6	GLU
1	A	77	PRO
1	A	94	SER
1	A	118	ARG
1	A	209	ASP
1	A	212	GLU
1	A	229	LEU
1	A	257	LEU
1	A	258	LEU
1	A	275	LEU
1	A	280	LEU
1	A	298	LEU
1	A	313	LYS
1	A	378	TYR
1	A	390	LEU
1	A	506	GLU
1	A	540	LYS
1	A	592	ILE
1	A	647	ARG
1	A	655	LEU
1	A	695	ASP
1	A	696	ILE
1	A	698	LEU
1	A	701	ARG
1	A	712	LYS
1	A	716	LYS
1	A	736	GLU
1	A	738	ARG
1	A	739	LYS
1	A	743	LEU
1	A	757	ILE
1	A	763	GLU
1	B	1	MET
1	B	2	HIS
1	B	3	GLU
1	B	6	GLU
1	B	20	ARG
1	B	22	GLU
1	B	27	ILE
1	B	28	THR
1	B	80	LEU
1	B	101	GLU

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Mol	Chain	Res	Type
1	B	102	ARG
1	B	136	ARG
1	B	213	GLU
1	B	214	ASP
1	B	224	THR
1	B	233	LYS
1	B	258	LEU
1	B	349	GLU
1	B	362	LEU
1	B	378	TYR
1	B	503	THR
1	B	514	GLU
1	B	540	LYS
1	B	604	ARG
1	B	637	ASP
1	B	659	GLU
1	B	666	PHE
1	B	667	ILE
1	B	694	ASP
1	B	699	SER
1	B	727	GLU
1	B	742	THR
1	B	743	LEU
1	B	748	GLU
1	B	749	LYS
1	B	750	SER
1	B	753	ASP
1	B	756	ARG
1	B	759	LYS
1	B	761	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	7	HIS
1	B	216	GLN
1	B	289	GLN
1	B	656	ASN
1	B	744	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	BGC	A	801	-	12,12,12	0.84	0	17,17,17	1.64	6 (35%)
3	1PE	A	802	-	15,15,15	0.55	0	14,14,14	1.34	2 (14%)
2	BGC	B	801	-	12,12,12	1.30	1 (8%)	17,17,17	1.41	4 (23%)
4	PG4	B	802	-	12,12,12	0.63	0	11,11,11	1.27	1 (9%)

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	BGC	A	801	-	-	0/2/22/22	0/1/1/1
3	1PE	A	802	-	-	0/13/13/13	0/0/0/0
2	BGC	B	801	-	-	0/2/22/22	0/1/1/1
4	PG4	B	802	-	-	0/10/10/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	BGC	C4-C5	2.72	1.58	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	BGC	C1-C2-C3	-2.96	105.30	110.65
2	A	801	BGC	O4-C4-C3	-2.88	104.10	110.36
3	A	802	1PE	OH3-C22-C12	-2.81	97.16	110.15
3	A	802	1PE	OH3-C23-C13	-2.46	99.12	110.41
2	B	801	BGC	O2-C2-C1	-2.23	105.13	109.75
2	B	801	BGC	C4-C3-C2	-2.20	106.96	110.84
2	A	801	BGC	O5-C5-C4	-2.16	105.68	109.66
2	B	801	BGC	C6-C5-C4	-2.07	108.16	113.00
2	B	801	BGC	C1-O5-C5	-2.03	109.73	113.39
2	A	801	BGC	C4-C3-C2	-2.02	107.27	110.84
2	A	801	BGC	O4-C4-C5	-2.02	104.20	109.28
2	A	801	BGC	C1-O5-C5	-2.00	109.78	113.39
4	B	802	PG4	C5-O3-C4	2.46	123.98	113.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	802	PG4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	767/769 (99%)	-0.28	20 (2%)	56	60	16, 25, 47, 100	0
1	B	761/769 (98%)	-0.22	34 (4%)	34	37	14, 24, 58, 104	0
All	All	1528/1538 (99%)	-0.25	54 (3%)	44	48	14, 25, 54, 104	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	756	ARG	6.4
1	B	661	VAL	5.8
1	B	737	ASP	5.2
1	A	657	THR	5.0
1	B	657	THR	5.0
1	A	209	ASP	5.0
1	A	739	LYS	4.8
1	B	24	ALA	4.5
1	B	664	GLY	4.5
1	B	761	ARG	4.4
1	B	666	PHE	4.3
1	A	754	SER	4.2
1	B	2	HIS	3.9
1	A	738	ARG	3.9
1	A	693	GLY	3.8
1	A	1	MET	3.7
1	A	753	ASP	3.7
1	B	6	GLU	3.7
1	B	210	ALA	3.6
1	B	1	MET	3.6
1	B	692	HIS	3.5
1	B	209	ASP	3.4
1	B	667	ILE	3.2
1	A	659	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	24	ALA	3.1
1	B	658	ASN	3.1
1	A	740	PRO	3.0
1	B	754	SER	3.0
1	B	739	LYS	3.0
1	A	751	VAL	2.9
1	B	659	GLU	2.9
1	B	207	ASP	2.8
1	B	668	GLY	2.8
1	B	98	ALA	2.8
1	A	692	HIS	2.7
1	B	747	GLY	2.6
1	A	736	GLU	2.5
1	B	736	GLU	2.5
1	A	694	ASP	2.4
1	A	661	VAL	2.4
1	B	118	ARG	2.4
1	A	658	ASN	2.3
1	B	694	ASP	2.3
1	B	660	ALA	2.3
1	B	540	LYS	2.3
1	B	96	GLU	2.2
1	A	569	GLU	2.2
1	B	695	ASP	2.1
1	A	6	GLU	2.1
1	B	211	SER	2.0
1	B	749	LYS	2.0
1	A	96	GLU	2.0
1	B	656	ASN	2.0
1	B	755	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
4	PG4	B	802	13/13	0.80	0.14	3.08	31,36,47,53	0
3	1PE	A	802	16/16	0.83	0.18	3.02	35,47,62,64	0
2	BGC	B	801	12/12	0.98	0.05	-0.95	19,20,23,27	0
2	BGC	A	801	12/12	0.98	0.06	-1.17	18,21,23,24	0
5	CA	B	804	1/1	0.95	0.10	-	45,45,45,45	0
5	CA	B	803	1/1	0.99	0.07	-	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.