Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:19 PM GMT

PDB ID	:	1A8I
Title	:	SPIROHYDANTOIN INHIBITOR OF GLYCOGEN PHOSPHORYLASE
Authors	:	Gregoriou, M.; Noble, M.E.M.; Watson, K.A.; Garman, E.F.; Krulle, T.M.; De La Fuente, C.; Fleet, G.W.J.; Oikonomakos, N.G.; Johnson, L.N.
Deposited on	:	1998-03-25
Resolution	:	1.78 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

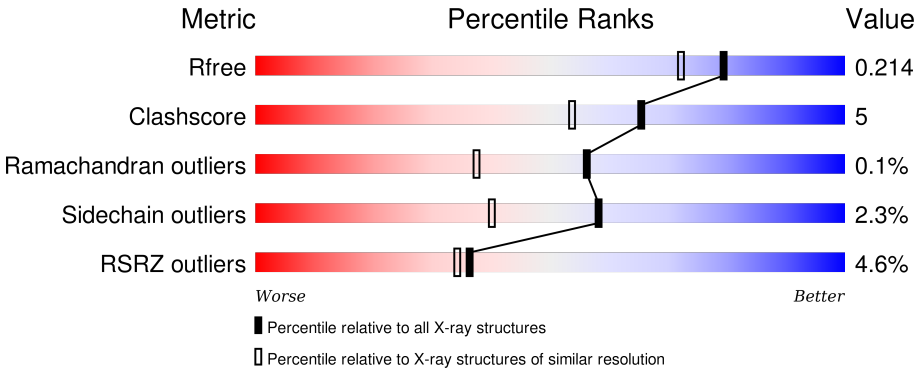
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.78 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}	91344	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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	842	4% 79% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7454 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.

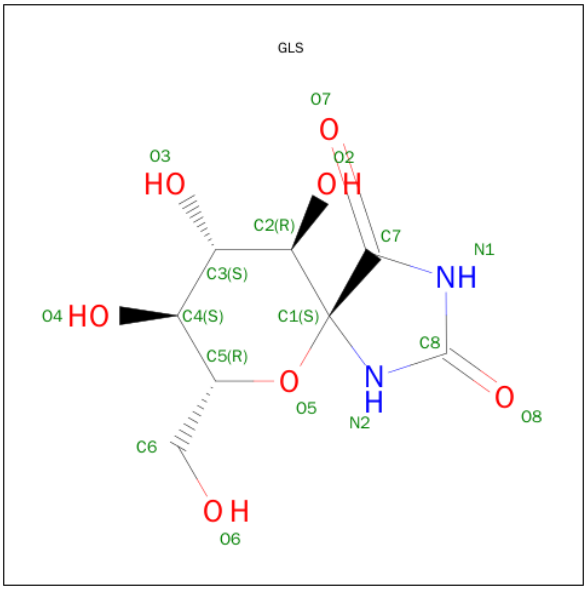
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	813	6642	4232	1173	1207	1	29	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	SEE REMARK 999	UNP P00489
A	680	LLP	LYS	MODIFIED RESIDUE	UNP P00489

- Molecule 2 is SUGAR (BETA-D-GLUCOPYRANOSE SPIROHYDANTOIN) (three-letter code: GLS) (formula: $C_8H_{12}N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	17	8	2	7	0	0

- Molecule 3 is water.

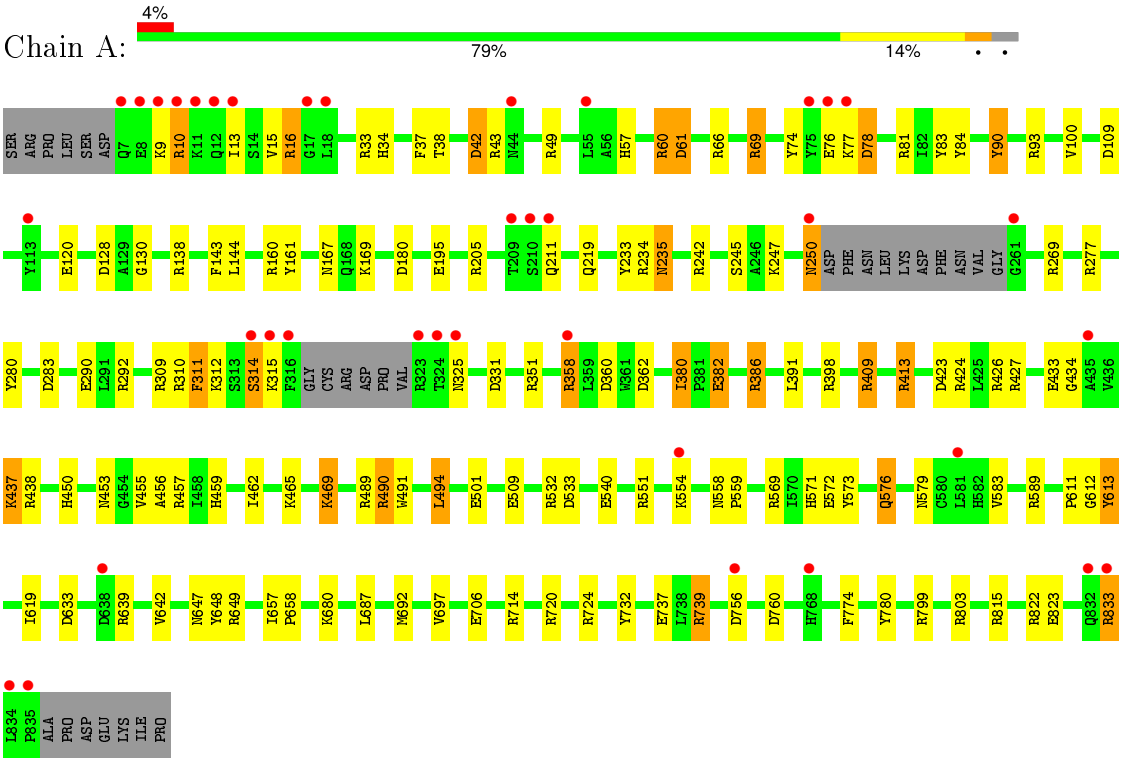
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	795	Total	O	0	0
			795	795		

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: GLYCOGEN PHOSPHORYLASE B

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	127.47Å 127.47Å 115.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 1.78 19.86 – 1.78	Depositor EDS
% Data completeness (in resolution range)	86.4 (19.90-1.78) 86.4 (19.86-1.78)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 1.78Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.229 0.170 , 0.214	Depositor DCC
R_{free} test set	3967 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 78975 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7454	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GLS, LLP

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	0.81	2/6764 (0.0%)	1.62	128/9147 (1.4%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	612	GLY	N-CA	5.67	1.54	1.46
1	A	815	ARG	NE-CZ	5.00	1.39	1.33

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	ARG	CD-NE-CZ	23.13	155.99	123.60
1	A	81	ARG	CD-NE-CZ	19.51	150.91	123.60
1	A	649	ARG	NE-CZ-NH1	18.30	129.45	120.30
1	A	386	ARG	NE-CZ-NH2	17.73	129.16	120.30
1	A	815	ARG	NE-CZ-NH2	-15.76	112.42	120.30
1	A	457	ARG	NE-CZ-NH2	-15.46	112.57	120.30
1	A	489	ARG	NE-CZ-NH1	15.03	127.81	120.30
1	A	714	ARG	NE-CZ-NH2	-14.96	112.82	120.30
1	A	386	ARG	NE-CZ-NH1	-13.58	113.51	120.30
1	A	438	ARG	NE-CZ-NH1	12.63	126.62	120.30
1	A	93	ARG	NE-CZ-NH2	-11.72	114.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	532	ARG	CD-NE-CZ	10.90	138.86	123.60
1	A	43	ARG	NE-CZ-NH2	10.78	125.69	120.30
1	A	234	ARG	CD-NE-CZ	10.47	138.26	123.60
1	A	81	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	A	803	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	A	714	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	A	292	ARG	NE-CZ-NH1	-9.03	115.79	120.30
1	A	739	ARG	NE-CZ-NH2	8.93	124.76	120.30
1	A	569	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	833	ARG	CD-NE-CZ	8.80	135.93	123.60
1	A	799	ARG	NE-CZ-NH2	8.70	124.65	120.30
1	A	438	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	A	438	ARG	CD-NE-CZ	8.22	135.11	123.60
1	A	33	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	A	310	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	A	81	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	A	457	ARG	NH1-CZ-NH2	7.73	127.91	119.40
1	A	16	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	A	803	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	42	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	69	ARG	CD-NE-CZ	7.46	134.04	123.60
1	A	822	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	456	ALA	N-CA-CB	7.30	120.32	110.10
1	A	84	TYR	CB-CG-CD2	-7.28	116.63	121.00
1	A	398	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	490	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	A	93	ARG	NH1-CZ-NH2	7.14	127.25	119.40
1	A	234	ARG	NE-CZ-NH2	7.11	123.86	120.30
1	A	309	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	774	PHE	CB-CG-CD1	7.00	125.70	120.80
1	A	533	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	649	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	A	161	TYR	CB-CG-CD2	6.85	125.11	121.00
1	A	413	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	A	280	TYR	CB-CG-CD2	-6.81	116.91	121.00
1	A	424	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	639	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	A	360	ASP	CB-CG-OD2	6.75	124.37	118.30
1	A	639	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	A	572	GLU	OE1-CD-OE2	6.65	131.28	123.30
1	A	501	GLU	OE1-CD-OE2	-6.56	115.43	123.30
1	A	756	ASP	CB-CG-OD2	-6.53	112.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	84	TYR	CB-CG-CD1	6.49	124.89	121.00
1	A	490	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	242	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	A	234	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	A	494	LEU	CA-CB-CG	6.40	130.03	115.30
1	A	195	GLU	OE1-CD-OE2	-6.39	115.64	123.30
1	A	233	TYR	CB-CG-CD2	-6.36	117.18	121.00
1	A	269	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A	489	ARG	NH1-CZ-NH2	-6.35	112.42	119.40
1	A	160	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	A	360	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	A	589	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	277	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	413	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	756	ASP	CB-CG-OD1	6.12	123.80	118.30
1	A	380	ILE	N-CA-CB	-6.10	96.76	110.80
1	A	309	ARG	CD-NE-CZ	6.10	132.13	123.60
1	A	205	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	569	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	250	ASN	CA-C-O	6.06	132.82	120.10
1	A	60	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	A	43	ARG	NE-CZ-NH1	-5.97	117.32	120.30
1	A	611	PRO	C-N-CA	-5.94	109.83	122.30
1	A	398	ARG	CD-NE-CZ	5.91	131.88	123.60
1	A	69	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	409	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	687	LEU	O-C-N	5.81	131.99	122.70
1	A	706	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	A	311	PHE	CB-CG-CD1	-5.77	116.76	120.80
1	A	351	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	551	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	724	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	A	633	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	780	TYR	CG-CD2-CE2	5.61	125.79	121.30
1	A	160	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	42	ASP	CB-CA-C	5.58	121.56	110.40
1	A	823	GLU	OE1-CD-OE2	-5.57	116.61	123.30
1	A	331	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	648	TYR	CG-CD1-CE1	-5.49	116.91	121.30
1	A	833	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	283	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	83	TYR	CB-CG-CD1	-5.45	117.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	358	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	A	315	LYS	CA-CB-CG	5.43	125.34	113.40
1	A	774	PHE	CB-CG-CD2	-5.38	117.04	120.80
1	A	78	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	427	ARG	CD-NE-CZ	5.35	131.09	123.60
1	A	74	TYR	CB-CG-CD1	5.34	124.20	121.00
1	A	799	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	A	128	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	573	TYR	CB-CG-CD2	5.30	124.18	121.00
1	A	138	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	815	ARG	NH1-CZ-NH2	5.29	125.22	119.40
1	A	423	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	413	ARG	CD-NE-CZ	5.28	130.99	123.60
1	A	143	PHE	CB-CG-CD1	5.26	124.48	120.80
1	A	613	TYR	CB-CG-CD1	5.23	124.14	121.00
1	A	49	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	277	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	424	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
1	A	501	GLU	CG-CD-OE1	5.19	128.69	118.30
1	A	42	ASP	CA-CB-CG	5.17	124.77	113.40
1	A	649	ARG	NH1-CZ-NH2	-5.16	113.73	119.40
1	A	724	ARG	CD-NE-CZ	-5.14	116.41	123.60
1	A	426	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	540	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	A	573	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	A	551	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	453	ASN	O-C-N	5.07	131.81	123.20
1	A	16	ARG	NH1-CZ-NH2	5.06	124.97	119.40
1	A	37	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	A	61	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	382	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	A	737	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	A	362	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	491	TRP	Mainchain

5.2 Too-close contacts (i)

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	6642	0	6595	66	0
2	A	17	0	12	0	0
3	A	795	0	0	20	3
All	All	7454	0	6607	66	3

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 (66) 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:A:490:ARG:HA	1:A:494:LEU:HG	1.50	0.92
1:A:100:VAL:HG21	1:A:494:LEU:HD22	1.64	0.79
1:A:60:ARG:HD2	3:A:1103:HOH:O	1.82	0.78
1:A:211:GLN:HB3	1:A:358:ARG:HH22	1.49	0.77
1:A:290:GLU:HG3	1:A:391:LEU:HD11	1.75	0.69
1:A:455:VAL:H	1:A:459:HIS:HD2	1.44	0.65
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.79	0.65
1:A:9:LYS:HG3	1:A:13:ILE:HD11	1.78	0.64
1:A:450:HIS:HD2	3:A:1339:HOH:O	1.80	0.63
1:A:386:ARG:NH1	3:A:1439:HOH:O	2.32	0.61
1:A:211:GLN:HB3	1:A:358:ARG:NH2	2.15	0.61
1:A:692:MET:HE3	1:A:697:VAL:HG22	1.83	0.61
1:A:60:ARG:HD3	3:A:1428:HOH:O	2.00	0.60
1:A:311:PHE:CE2	1:A:325:ASN:HB2	2.36	0.60
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.85	0.60
1:A:100:VAL:HG21	1:A:494:LEU:CD2	2.33	0.58
1:A:583:VAL:HG11	1:A:642:VAL:HG21	1.85	0.56
1:A:235:ASN:H	1:A:235:ASN:HD22	1.52	0.56
1:A:450:HIS:HE1	3:A:1328:HOH:O	1.90	0.55
1:A:211:GLN:HE21	1:A:358:ARG:NH2	2.05	0.54
1:A:433:GLU:HG3	1:A:434:GLY:H	1.75	0.52
1:A:311:PHE:HE2	1:A:325:ASN:HB2	1.74	0.52
1:A:211:GLN:CB	1:A:358:ARG:HH22	2.22	0.51
1:A:380:ILE:HG23	1:A:382:GLU:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:NH2	3:A:1090:HOH:O	2.45	0.50
1:A:69:ARG:NH2	3:A:1182:HOH:O	2.44	0.50
1:A:78:ASP:OD1	1:A:314:SER:HB2	2.12	0.49
1:A:619:ILE:HD13	3:A:1196:HOH:O	2.13	0.48
1:A:16:ARG:HD3	3:A:1694:HOH:O	2.13	0.48
1:A:583:VAL:CG1	1:A:642:VAL:HG21	2.44	0.48
1:A:10:ARG:HB3	3:A:1694:HOH:O	2.14	0.48
1:A:554:LYS:HG3	3:A:1130:HOH:O	2.14	0.48
1:A:312:LYS:NZ	3:A:1096:HOH:O	2.47	0.48
1:A:167:ASN:HD22	1:A:647:ASN:HD21	1.61	0.47
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.49	0.46
1:A:10:ARG:NH1	3:A:1050:HOH:O	2.39	0.46
1:A:167:ASN:ND2	1:A:647:ASN:HD21	2.13	0.46
1:A:380:ILE:CG2	1:A:382:GLU:CD	2.84	0.46
1:A:760:ASP:HB2	3:A:1735:HOH:O	2.16	0.46
1:A:15:VAL:HA	1:A:509:GLU:OE2	2.16	0.45
1:A:10:ARG:NH1	1:A:120:GLU:HG3	2.31	0.44
1:A:57:HIS:HE1	3:A:1506:HOH:O	2.00	0.44
1:A:437:LYS:HB3	1:A:437:LYS:HE2	1.83	0.44
1:A:469:LYS:HZ2	1:A:469:LYS:HB3	1.81	0.44
1:A:692:MET:CE	1:A:697:VAL:HG13	2.48	0.43
1:A:10:ARG:NH2	1:A:109:ASP:OD1	2.44	0.43
1:A:219:GLN:HG2	3:A:1106:HOH:O	2.17	0.43
1:A:680:LLP:NZ	1:A:680:LLP:O3	2.47	0.43
1:A:409:ARG:HD3	1:A:409:ARG:HH11	1.63	0.43
1:A:692:MET:HE3	1:A:697:VAL:HG13	2.01	0.43
1:A:433:GLU:HG3	1:A:434:GLY:N	2.34	0.43
1:A:462:ILE:HA	1:A:462:ILE:HD12	1.93	0.42
1:A:10:ARG:HE	1:A:109:ASP:CG	2.23	0.42
1:A:833:ARG:NH2	3:A:1737:HOH:O	2.52	0.42
1:A:211:GLN:CG	1:A:358:ARG:HH22	2.33	0.42
1:A:100:VAL:CG2	1:A:494:LEU:HD22	2.42	0.41
1:A:657:ILE:N	1:A:658:PRO:CD	2.83	0.41
1:A:571:HIS:H	1:A:576:GLN:HE22	1.68	0.41
1:A:90:TYR:CE1	1:A:130:GLY:HA2	2.56	0.41
1:A:720:ARG:NH1	3:A:1174:HOH:O	2.53	0.41
1:A:380:ILE:HG23	1:A:382:GLU:CD	2.41	0.41
1:A:558:ASN:HA	1:A:559:PRO:HD2	1.93	0.40
1:A:413:ARG:HD3	3:A:1342:HOH:O	2.21	0.40
1:A:245:SER:OG	1:A:247:LYS:NZ	2.54	0.40
1:A:10:ARG:HD3	3:A:1050:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:HD2	1:A:66:ARG:HH11	1.64	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1173:HOH:O	3:A:1173:HOH:O[7_556]	1.83	0.37
3:A:1065:HOH:O	3:A:1521:HOH:O[7_556]	1.94	0.26
3:A:1254:HOH:O	3:A:1648:HOH:O[7_555]	2.04	0.16

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	806/842 (96%)	777 (96%)	28 (4%)	1 (0%)	56 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	704/730 (96%)	688 (98%)	16 (2%)	58 40

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	42	ASP
1	A	76	GLU
1	A	77	LYS
1	A	90	TYR
1	A	144	LEU
1	A	169	LYS
1	A	180	ASP
1	A	235	ASN
1	A	250	ASN
1	A	437	LYS
1	A	465	LYS
1	A	469	LYS
1	A	576	GLN
1	A	579	ASN
1	A	613	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	57	HIS
1	A	97	ASN
1	A	106	ASN
1	A	167	ASN
1	A	211	GLN
1	A	235	ASN
1	A	264	GLN
1	A	284	ASN
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	767	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	LLP	A	680	1	23,24,25	3.07	6 (26%)	28,32,34	1.68	9 (32%)

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
1	LLP	A	680	1	-	0/15/17/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	C3-C2	-9.59	1.34	1.40
1	A	680	LLP	P-OP3	-3.66	1.41	1.54
1	A	680	LLP	C4-C3	-3.51	1.36	1.40
1	A	680	LLP	C4-C4'	2.98	1.51	1.46
1	A	680	LLP	C2-N1	4.18	1.43	1.34
1	A	680	LLP	C4'-NZ	7.14	1.48	1.27

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	680	LLP	OP4-C5'-C5	-2.95	104.11	108.99
1	A	680	LLP	C5-C4-C4'	-2.74	117.58	121.52
1	A	680	LLP	C6-N1-C2	-2.45	114.28	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	680	LLP	CG-CD-CE	-2.36	104.34	113.97
1	A	680	LLP	OP4-P-OP1	-2.21	101.51	107.14
1	A	680	LLP	CD-CE-NZ	-2.04	107.63	110.98
1	A	680	LLP	C5'-C5-C6	2.07	123.19	119.28
1	A	680	LLP	C3-C4-C4'	2.61	123.53	120.16
1	A	680	LLP	C2'-C2-C3	3.17	124.86	121.04

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
1	A	680	LLP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	GLS	A	998	-	16,18,18	1.08	1 (6%)	17,28,28	3.34	8 (47%)

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	GLS	A	998	-	-	0/2/40/40	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	998	GLS	C8-N1	-2.86	1.33	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	998	GLS	C7-N1-C8	-7.91	104.18	111.60
2	A	998	GLS	O7-C7-N1	-3.56	121.07	126.22
2	A	998	GLS	C4-C3-C2	-3.13	106.91	111.33
2	A	998	GLS	O3-C3-C2	-3.03	103.59	109.69
2	A	998	GLS	O8-C8-N2	-2.81	122.50	126.72
2	A	998	GLS	C7-C1-N2	-2.52	98.83	101.31
2	A	998	GLS	O8-C8-N1	-2.48	120.98	125.44
2	A	998	GLS	N1-C8-N2	7.83	116.52	107.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	812/842 (96%)	-0.02	37 (4%) 36 34	15, 23, 45, 100	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	THR	15.0
1	A	7	GLN	13.1
1	A	8	GLU	9.9
1	A	12	GLN	9.1
1	A	316	PHE	7.4
1	A	323	ARG	7.3
1	A	9	LYS	7.3
1	A	435	ALA	7.3
1	A	11	LYS	6.5
1	A	325	ASN	5.3
1	A	75	TYR	4.8
1	A	10	ARG	4.8
1	A	44	ASN	4.3
1	A	315	LYS	4.1
1	A	210	SER	4.1
1	A	835	PRO	3.9
1	A	211	GLN	3.8
1	A	834	LEU	3.5
1	A	18	LEU	3.2
1	A	314	SER	3.1
1	A	17	GLY	2.8
1	A	77	LYS	2.7
1	A	113	TYR	2.7
1	A	209	THR	2.6
1	A	55	LEU	2.6
1	A	554	LYS	2.6
1	A	261	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	768	HIS	2.3
1	A	638	ASP	2.3
1	A	250	ASN	2.2
1	A	76	GLU	2.2
1	A	358	ARG	2.1
1	A	832	GLN	2.1
1	A	13	ILE	2.1
1	A	756	ASP	2.1
1	A	833	ARG	2.1
1	A	581	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	LLP	A	680	24/25	0.98	0.06	-	14,17,19,20	0

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, 95^{th} 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
2	GLS	A	998	17/17	0.98	0.06	-1.10	12,15,19,20	0

6.5 Other polymers (i)

There are no such residues in this entry.