Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:10 PM BST

PDB ID	:	4BQ2
Title	:	Structural analysis of an exo-beta-agarase
Authors	:	Pluvinage, B.; Hehemann, J.H.; Boraston, A.B.
Deposited on	:	2013-05-29
Resolution	:	1.90 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
https://www.wwpdb.org/validation/2017/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:

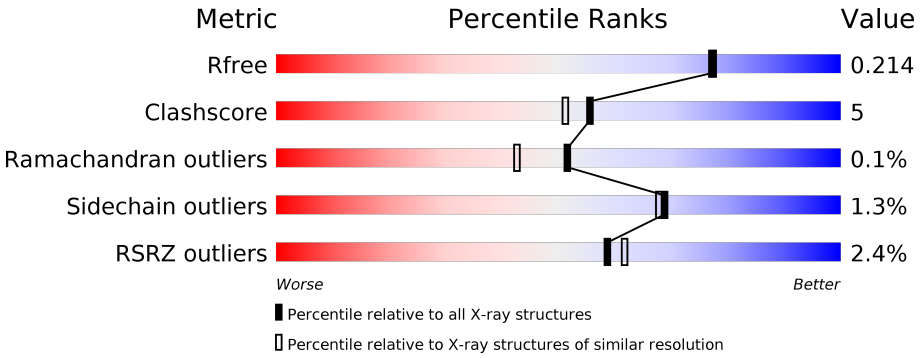
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 respectively. 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	750	89% 10%
1	B	750	89% 11%
1	C	750	3% 91% 8%
1	D	750	4% 83% 13%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	1795	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26607 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.

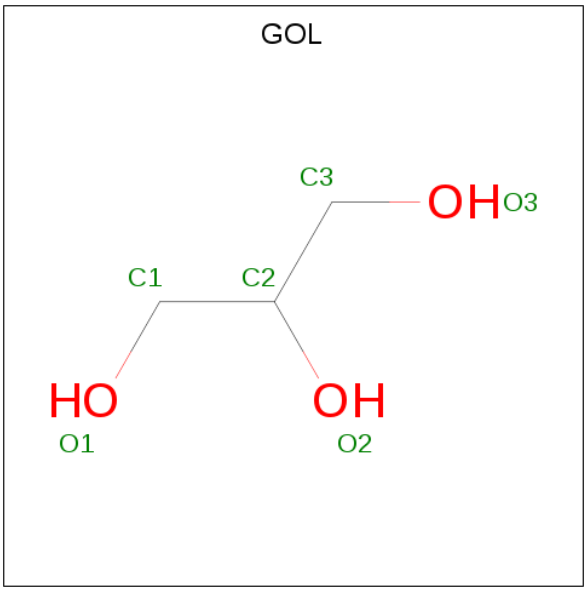
- Molecule 1 is a protein called B-AGARASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	746	Total	C	N	O	S	0	10	0
			6012	3838	1007	1143	24			
1	B	747	Total	C	N	O	S	0	12	0
			6027	3841	1005	1157	24			
1	C	748	Total	C	N	O	S	0	12	0
			6028	3840	1011	1154	23			
1	D	726	Total	C	N	O	S	1	11	0
			5850	3730	981	1116	23			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLY	-	expression tag	UNP Q21HC5
A	45	SER	-	expression tag	UNP Q21HC5
A	46	HIS	-	expression tag	UNP Q21HC5
B	44	GLY	-	expression tag	UNP Q21HC5
B	45	SER	-	expression tag	UNP Q21HC5
B	46	HIS	-	expression tag	UNP Q21HC5
C	44	GLY	-	expression tag	UNP Q21HC5
C	45	SER	-	expression tag	UNP Q21HC5
C	46	HIS	-	expression tag	UNP Q21HC5
D	44	GLY	-	expression tag	UNP Q21HC5
D	45	SER	-	expression tag	UNP Q21HC5
D	46	HIS	-	expression tag	UNP Q21HC5

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is water.

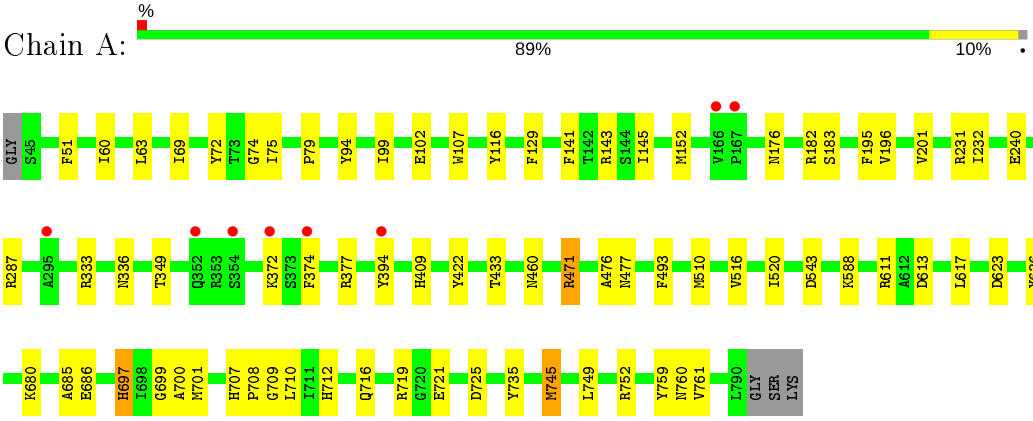
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	645	Total O 645 645	0	0
4	B	655	Total O 655 655	0	0
4	C	651	Total O 651 651	0	0
4	D	603	Total O 603 603	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

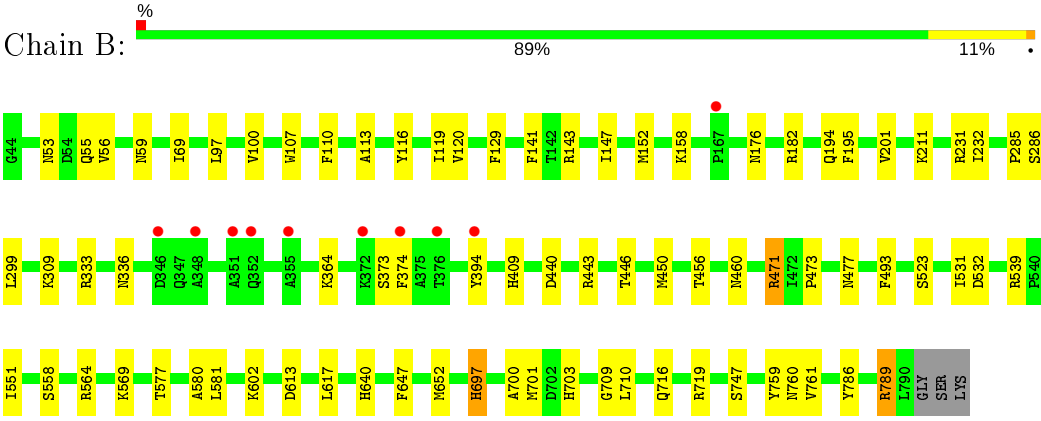
- Molecule 1: B-AGARASE

Chain A:



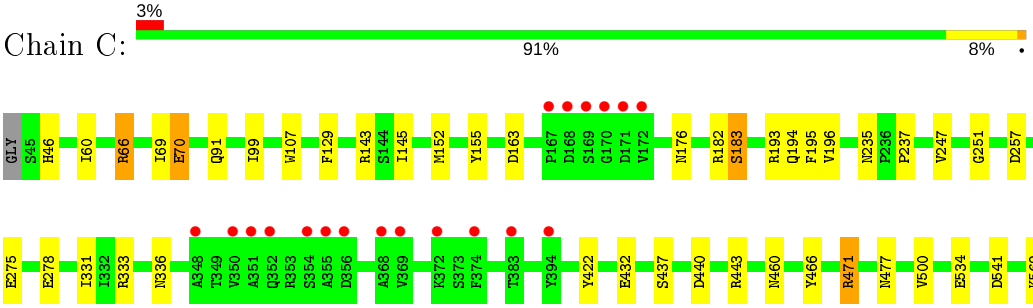
- Molecule 1: B-AGARASE

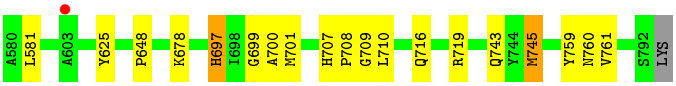
Chain B:



- Molecule 1: B-AGARASE

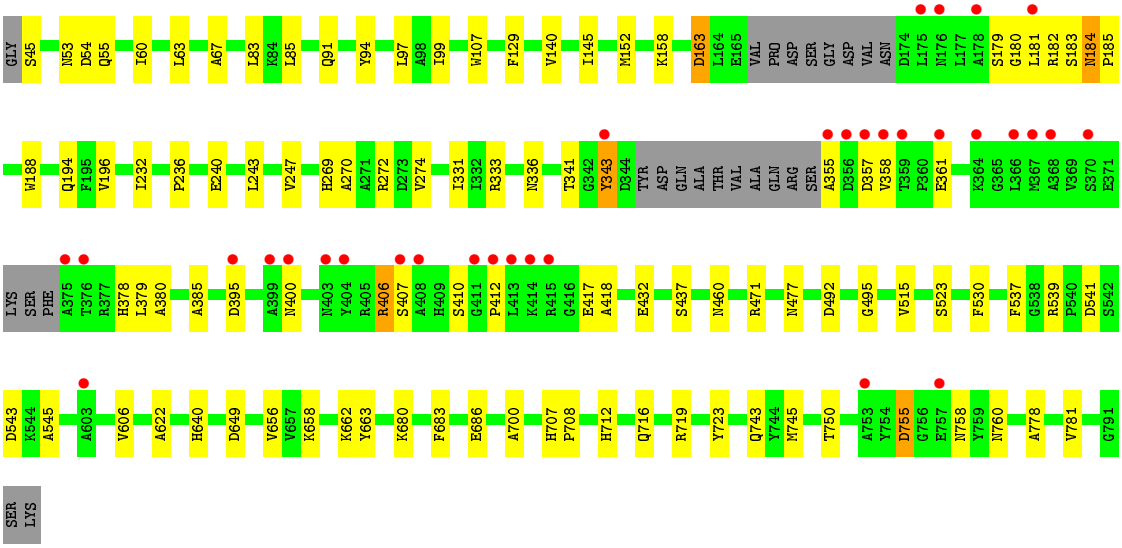
Chain C:





- Molecule 1: B-AGARASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	166.67Å 166.67Å 114.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.28 – 1.90 39.28 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.28-1.90) 99.7 (39.28-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.170 , 0.215 0.170 , 0.214	Depositor DCC
R_{free} test set	12312 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26607	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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 53.49 % 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 4.1852e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, CA

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	0.62	0/6187	0.74	3/8409 (0.0%)
1	B	0.63	0/6202	0.74	3/8430 (0.0%)
1	C	0.64	0/6202	0.74	4/8431 (0.0%)
1	D	0.63	1/6017 (0.0%)	0.72	3/8173 (0.0%)
All	All	0.63	1/24608 (0.0%)	0.73	13/33443 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	658	LYS	CE-NZ	-11.95	1.19	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	471	ARG	NE-CZ-NH2	-12.94	113.83	120.30
1	A	471	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	B	471	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	C	471	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	B	471	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	D	471	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	C	471	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	B	287	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	C	163	ASP	CB-CG-OD1	6.10	123.79	118.30
1	D	471	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	257	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	725	ASP	CB-CG-OD1	5.42	123.18	118.30
1	D	163	ASP	CB-CG-OD1	5.06	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

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	6012	0	5718	59	0
1	B	6027	0	5702	52	0
1	C	6028	0	5721	49	0
1	D	5850	0	5528	73	0
2	A	36	0	48	4	0
2	B	48	0	64	5	0
2	C	30	0	40	7	1
2	D	18	0	24	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	645	0	0	4	1
4	B	655	0	0	6	0
4	C	651	0	0	11	0
4	D	603	0	0	9	0
All	All	26607	0	22845	238	1

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 (238) 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:786:TYR:O	1:B:789:ARG:O	1.73	1.05
1:C:440:ASP:OD1	1:C:443[A]:ARG:NH2	1.90	1.03
1:A:752:ARG:HH12	2:A:1793:GOL:H31	1.23	1.03
1:A:623:ASP:HB3	4:A:2539:HOH:O	1.57	1.03
1:A:721:GLU:HG3	4:A:2610:HOH:O	1.60	0.99
1:D:179:SER:OG	1:D:184:ASN:ND2	1.96	0.97
1:D:716:GLN:HE22	1:D:719:ARG:HH11	1.12	0.97
1:D:341:THR:OG1	1:D:417:GLU:OE1	1.88	0.91
1:C:716:GLN:HE22	1:C:719:ARG:HH11	1.18	0.91
1:A:697:HIS:HE1	1:A:710:LEU:H	1.20	0.89
1:A:716:GLN:HE22	1:A:719:ARG:HH11	1.20	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240[B]:GLU:CD	1:D:240[B]:GLU:H	1.76	0.87
1:D:53[B]:ASN:HD22	1:D:55:GLN:H	1.20	0.86
1:B:716:GLN:HE22	1:B:719:ARG:HH11	1.21	0.85
1:B:697:HIS:HE1	1:B:710:LEU:H	1.22	0.83
1:C:66:ARG:HD3	2:C:1795:GOL:O2	1.80	0.82
1:B:176:ASN:ND2	1:B:182:ARG:HE	1.78	0.81
1:D:361[B]:GLU:HG3	1:D:407:SER:OG	1.81	0.80
1:B:333:ARG:HH21	1:B:336:ASN:HD21	1.28	0.80
1:C:697:HIS:HE1	1:C:710:LEU:H	1.29	0.79
1:A:752:ARG:NH1	2:A:1793:GOL:H31	1.98	0.78
1:D:63:LEU:HD23	1:D:94:TYR:HD1	1.47	0.78
1:B:577:THR:HG23	1:B:580:ALA:H	1.50	0.76
1:B:700:ALA:H	1:B:760:ASN:HD22	1.32	0.76
1:A:75:ILE:HG23	1:A:152:MET:HG2	1.68	0.75
1:C:333:ARG:HH21	1:C:336:ASN:HD21	1.34	0.75
1:A:700:ALA:H	1:A:760:ASN:HD22	1.35	0.75
1:D:333:ARG:HH21	1:D:336:ASN:HD21	1.33	0.74
1:D:63:LEU:HD23	1:D:94:TYR:CD1	2.24	0.73
1:C:569:LYS:HD3	4:C:2520:HOH:O	1.89	0.72
1:D:355:ALA:HB1	1:D:357:ASP:HB2	1.71	0.72
1:A:176:ASN:ND2	1:A:182:ARG:HE	1.89	0.71
1:B:539:ARG:HH12	2:B:1795:GOL:H31	1.56	0.70
1:C:46:HIS:CE1	1:C:107:TRP:HE1	2.09	0.70
1:C:145[A]:ILE:HD11	1:C:701:MET:HE1	1.74	0.70
1:A:333:ARG:HH21	1:A:336:ASN:HD21	1.40	0.70
1:B:287:ARG:NH1	4:B:2279:HOH:O	2.24	0.68
1:B:440:ASP:OD1	1:B:443:ARG:NH2	2.27	0.68
1:D:683:PHE:O	1:D:686[B]:GLU:HG3	1.95	0.67
1:C:697:HIS:CE1	1:C:710:LEU:H	2.13	0.67
1:A:697:HIS:CE1	1:A:710:LEU:H	2.09	0.67
1:A:476:ALA:HB2	1:A:520[A]:ILE:HD11	1.75	0.66
1:B:59:ASN:ND2	2:B:1797:GOL:O1	2.28	0.65
1:A:433:THR:HG21	4:C:2490:HOH:O	1.95	0.65
1:B:697:HIS:CE1	1:B:710:LEU:H	2.08	0.65
1:C:700:ALA:H	1:C:760:ASN:HD22	1.44	0.65
1:C:176:ASN:ND2	1:C:182:ARG:HE	1.96	0.64
1:D:680:LYS:HG2	4:D:2545:HOH:O	1.97	0.64
1:C:145[A]:ILE:HD11	1:C:701:MET:CE	2.28	0.63
1:C:235:ASN:O	4:C:2211:HOH:O	2.16	0.63
1:B:640:HIS:HD2	4:B:2474:HOH:O	1.81	0.63
1:A:145[A]:ILE:HD13	1:A:196:VAL:HG23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ASN:HB3	1:B:55:GLN:H	1.65	0.61
1:D:412:PRO:HB3	4:D:2177:HOH:O	2.00	0.61
1:A:145[A]:ILE:HD11	1:A:701[A]:MET:SD	2.41	0.60
1:C:237:PRO:HA	2:C:1797:GOL:H11	1.83	0.60
1:D:145[A]:ILE:HD13	1:D:196:VAL:HG23	1.83	0.60
1:C:577[A]:THR:HG22	1:C:579:ALA:H	1.66	0.59
1:D:361[B]:GLU:OE1	1:D:361[B]:GLU:N	2.36	0.59
1:D:640:HIS:HD2	4:D:2436:HOH:O	1.83	0.59
1:C:331:ILE:HG13	1:C:743:GLN:HE21	1.68	0.59
1:D:240[B]:GLU:CD	1:D:240[B]:GLU:N	2.54	0.58
1:A:63[A]:LEU:HD12	1:A:94:TYR:CE1	2.38	0.58
1:A:102:GLU:CD	1:A:102:GLU:H	2.04	0.58
1:C:145[A]:ILE:HD13	1:C:196:VAL:HG23	1.86	0.57
1:C:145[A]:ILE:CD1	1:C:701:MET:HE1	2.34	0.57
1:C:145[B]:ILE:HD12	1:C:194:GLN:O	2.05	0.57
1:C:471:ARG:HD3	4:C:2442:HOH:O	2.05	0.57
1:C:569:LYS:HD2	4:C:2521:HOH:O	2.03	0.57
1:D:53[B]:ASN:ND2	1:D:55:GLN:H	1.96	0.57
1:C:716:GLN:NE2	1:C:719:ARG:HH11	1.97	0.56
1:D:196:VAL:CG1	1:D:707:HIS:CD2	2.88	0.56
1:D:379:LEU:HD11	1:D:385:ALA:HB2	1.85	0.56
2:B:1794:GOL:O3	2:B:1794:GOL:O1	2.21	0.56
1:B:471:ARG:HD3	4:B:2417:HOH:O	2.04	0.56
1:A:75:ILE:CG2	1:A:152:MET:HG2	2.34	0.55
1:B:558:SER:HA	1:B:564:ARG:HG3	1.88	0.55
1:B:374:PHE:CD2	1:B:394[B]:TYR:HB2	2.41	0.55
1:D:158:LYS:NZ	1:D:163:ASP:OD1	2.35	0.55
1:D:432:GLU:HA	1:D:437:SER:OG	2.07	0.55
1:C:471:ARG:CD	4:C:2442:HOH:O	2.55	0.54
1:B:703:HIS:O	2:B:1793:GOL:H31	2.07	0.54
1:D:755:ASP:OD1	1:D:755:ASP:N	2.40	0.54
1:A:72:TYR:CE2	1:A:152:MET:SD	3.01	0.54
1:A:63[A]:LEU:HD12	1:A:94:TYR:HE1	1.72	0.54
1:A:613:ASP:O	1:A:617:LEU:HG	2.08	0.54
1:D:723:TYR:HE1	1:D:781:VAL:HG21	1.73	0.54
1:D:683:PHE:O	1:D:686[A]:GLU:HG2	2.08	0.53
1:D:181:LEU:CD2	1:D:185:PRO:HD3	2.38	0.53
1:D:343:TYR:CD1	1:D:343:TYR:N	2.76	0.53
1:D:145[B]:ILE:HD12	1:D:194:GLN:O	2.07	0.53
1:A:516:VAL:O	1:A:520[A]:ILE:HG12	2.08	0.53
1:D:179:SER:HB3	1:D:243:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:ARG:HH12	2:A:1793:GOL:C3	2.10	0.53
1:D:379:LEU:HD11	1:D:385:ALA:CB	2.39	0.53
1:D:140:VAL:HG21	4:D:2128:HOH:O	2.08	0.53
1:A:374:PHE:O	1:A:377:ARG:HB3	2.09	0.53
1:B:285:PRO:O	1:B:286:SER:HB3	2.09	0.53
1:C:678:LYS:O	4:C:2589:HOH:O	2.18	0.53
1:D:269:HIS:CD2	1:D:272:ARG:NH1	2.77	0.53
1:B:176:ASN:HD22	1:B:182:ARG:HA	1.75	0.52
1:A:476:ALA:CB	1:A:520[A]:ILE:HD11	2.38	0.52
1:D:400:ASN:ND2	4:D:2354:HOH:O	2.42	0.52
1:D:378:HIS:CD2	1:D:380:ALA:HB2	2.44	0.52
1:B:701[A]:MET:HE3	4:B:2606:HOH:O	2.09	0.52
1:D:523:SER:O	1:D:640:HIS:HE1	1.93	0.52
1:D:758:ASN:O	4:D:2564:HOH:O	2.18	0.51
1:A:240[A]:GLU:CD	1:A:240[A]:GLU:H	2.15	0.51
1:B:119:ILE:HG22	1:B:147:ILE:HG21	1.93	0.51
1:D:343:TYR:O	1:D:417:GLU:HB3	2.10	0.51
1:A:708:PRO:HG2	1:A:712:HIS:CD2	2.46	0.50
1:A:72:TYR:CE2	1:A:74:GLY:HA2	2.47	0.50
1:A:143:ARG:HB3	1:A:195:PHE:HB3	1.94	0.49
1:B:364:LYS:HA	2:B:1798:GOL:H12	1.93	0.49
1:B:523:SER:O	1:B:640:HIS:HE1	1.95	0.49
1:A:176:ASN:HD22	1:A:182:ARG:HA	1.78	0.49
1:C:534:GLU:HA	1:C:648:PRO:HD3	1.94	0.49
1:B:97:LEU:HD12	1:B:97:LEU:C	2.33	0.49
1:A:749:LEU:HD13	2:A:1792:GOL:H12	1.95	0.48
1:B:697:HIS:CD2	1:B:761:VAL:HG11	2.48	0.48
1:B:107:TRP:CE2	1:B:232:ILE:HD11	2.48	0.48
1:B:456:THR:O	1:B:473:PRO:HD2	2.12	0.48
1:C:69:ILE:C	1:C:70[A]:GLU:HG2	2.33	0.48
1:C:155:TYR:HA	1:C:193:ARG:O	2.14	0.48
1:A:709:GLY:HA2	1:A:759:TYR:CG	2.49	0.48
1:D:700:ALA:H	1:D:760:ASN:HD22	1.62	0.48
1:B:309:LYS:HD3	4:B:2313:HOH:O	2.14	0.47
1:A:543:ASP:CG	1:A:611:ARG:HH12	2.18	0.47
1:B:110:PHE:HB3	1:B:113:ALA:HB3	1.95	0.47
1:B:716:GLN:HE22	1:B:719:ARG:NH1	2.02	0.47
1:C:460:ASN:OD1	1:C:477:ASN:HB3	2.14	0.47
1:C:60:ILE:HG12	1:C:99:ILE:HG12	1.97	0.47
1:D:649[B]:ASP:OD2	4:D:2525:HOH:O	2.20	0.47
1:C:577[A]:THR:HG22	1:C:579:ALA:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53[B]:ASN:ND2	1:D:55:GLN:HB2	2.30	0.47
1:A:699:GLY:HA3	1:A:708:PRO:O	2.15	0.47
1:D:196:VAL:HG12	1:D:707:HIS:CD2	2.50	0.47
1:D:760:ASN:O	1:D:760:ASN:CG	2.53	0.47
1:D:85:LEU:HD22	1:D:97:LEU:HD23	1.96	0.47
1:D:343:TYR:HD1	1:D:343:TYR:H	1.62	0.46
1:A:72:TYR:HE2	1:A:152:MET:SD	2.38	0.46
1:D:180:GLY:HA2	1:D:412:PRO:HD3	1.97	0.46
2:C:1796:GOL:H12	4:C:2604:HOH:O	2.15	0.46
1:A:60:ILE:HG12	1:A:99:ILE:HG12	1.96	0.46
1:B:759:TYR:HB3	1:B:761:VAL:HG13	1.98	0.46
1:A:588:LYS:HB2	1:A:588:LYS:HE3	1.66	0.46
1:B:460:ASN:OD1	1:B:477:ASN:HB3	2.16	0.46
1:C:176:ASN:HD22	1:C:182:ARG:HA	1.81	0.45
1:D:460:ASN:OD1	1:D:477:ASN:HB3	2.16	0.45
1:A:759:TYR:HB3	1:A:761:VAL:HG13	1.98	0.45
1:D:331:ILE:HG13	1:D:743:GLN:HE21	1.81	0.45
1:A:333:ARG:NH2	1:A:336:ASN:HD21	2.12	0.45
1:C:66:ARG:NH1	2:C:1795:GOL:O3	2.50	0.45
1:D:181:LEU:HD22	1:D:185:PRO:HD3	1.96	0.45
1:B:56:VAL:HG22	1:B:69:ILE:HD11	1.98	0.45
2:D:1793:GOL:C3	4:D:2267:HOH:O	2.65	0.45
1:B:158:LYS:NZ	1:B:194:GLN:HE22	2.15	0.44
1:D:543:ASP:HB3	1:D:606:VAL:HG21	1.98	0.44
1:D:410:SER:O	1:D:755:ASP:HA	2.18	0.44
1:B:716:GLN:NE2	1:B:719:ARG:HH11	2.00	0.44
1:D:477:ASN:HA	1:D:530:PHE:O	2.17	0.44
1:D:778:ALA:HA	1:D:781:VAL:HG22	1.98	0.44
1:A:716:GLN:NE2	1:A:719:ARG:HH11	2.01	0.44
1:C:709:GLY:HA2	1:C:759:TYR:CG	2.52	0.44
1:D:91[B]:GLN:HG2	4:D:2063:HOH:O	2.17	0.44
1:D:67:ALA:HB1	1:D:83:LEU:HD11	2.00	0.44
1:C:422:TYR:CE1	1:C:745:MET:HG2	2.52	0.44
1:C:697:HIS:CD2	1:C:761:VAL:HG11	2.53	0.44
1:A:107:TRP:CE2	1:A:232:ILE:HD11	2.53	0.44
1:D:270:ALA:O	1:D:274:VAL:HG23	2.18	0.44
1:D:358:VAL:HG21	1:D:515:VAL:HG11	2.00	0.44
1:C:443[A]:ARG:HG2	1:C:466:TYR:CZ	2.53	0.44
1:B:709:GLY:HA2	1:B:759:TYR:CG	2.53	0.43
1:D:537:PHE:HB3	1:D:656:VAL:HG21	1.99	0.43
1:A:409:HIS:HE1	1:A:493:PHE:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:HIS:HE1	1:B:493:PHE:O	2.01	0.43
1:B:120:VAL:HB	1:B:152:MET:HA	2.00	0.43
1:B:141:PHE:HB3	1:B:201:VAL:O	2.18	0.43
1:D:107:TRP:CH2	1:D:232:ILE:HD11	2.54	0.43
1:A:287:ARG:NH1	4:A:2288:HOH:O	2.52	0.43
1:B:143:ARG:HB3	1:B:195:PHE:HB3	2.00	0.43
1:A:422:TYR:CE1	1:A:745:MET:HG2	2.53	0.43
1:A:72:TYR:O	1:A:79:PRO:HA	2.18	0.43
1:C:247:VAL:CG1	1:C:251:GLY:HA2	2.48	0.43
1:C:700:ALA:H	1:C:760:ASN:ND2	2.13	0.43
2:C:1795:GOL:H12	4:C:2029:HOH:O	2.19	0.43
1:B:549:ILE:HB	1:B:550:PRO:HD3	2.01	0.43
1:C:91[B]:GLN:HG2	4:C:2061:HOH:O	2.18	0.43
1:C:500:VAL:HG11	1:C:625:TYR:HB2	2.01	0.42
1:D:196:VAL:HG11	1:D:707:HIS:CD2	2.52	0.42
1:A:141:PHE:HB3	1:A:201:VAL:O	2.19	0.42
1:A:647:PHE:HB3	1:A:652:MET:HB3	2.00	0.42
1:C:66:ARG:HH11	2:C:1795:GOL:C3	2.32	0.42
1:A:471:ARG:HD3	4:A:2430:HOH:O	2.20	0.42
1:C:699:GLY:HA3	1:C:708:PRO:O	2.19	0.42
1:C:269:HIS:CD2	1:C:272:ARG:NH1	2.87	0.42
1:D:716:GLN:NE2	1:D:719:ARG:HH11	1.96	0.42
1:A:349:THR:HG22	1:A:372:LYS:HE2	2.02	0.42
2:C:1795:GOL:C1	4:C:2029:HOH:O	2.67	0.42
1:C:709:GLY:HA2	1:C:759:TYR:CD1	2.54	0.42
1:D:60:ILE:HG12	1:D:99:ILE:HG12	2.02	0.42
1:A:247:VAL:CG1	1:A:251:GLY:HA2	2.50	0.42
1:A:183:SER:HB2	1:A:707:HIS:CD2	2.55	0.42
1:A:116:TYR:HB2	1:A:231:ARG:HG2	2.02	0.42
1:B:551:ILE:CG2	1:B:602:LYS:HB3	2.50	0.42
1:D:417:GLU:HG2	1:D:418:ALA:N	2.35	0.42
1:D:53[B]:ASN:HD22	1:D:54:ASP:N	2.18	0.42
1:D:622:ALA:HB2	1:D:656:VAL:HG22	2.00	0.42
1:D:662:LYS:HE3	1:D:663:TYR:CZ	2.55	0.42
1:A:460:ASN:OD1	1:A:477:ASN:HB3	2.20	0.41
1:D:188:TRP:CD1	1:D:236:PRO:HG2	2.55	0.41
1:D:247:VAL:HG21	1:D:750:THR:HG23	2.03	0.41
1:D:708:PRO:HG2	1:D:712:HIS:CD2	2.55	0.41
1:C:143:ARG:HB3	1:C:195:PHE:HB3	2.01	0.41
1:D:179:SER:O	1:D:412:PRO:HG3	2.20	0.41
1:A:433:THR:O	1:A:433:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:ALA:H	1:B:760:ASN:ND2	2.06	0.41
1:C:183:SER:HB2	1:C:707:HIS:CD2	2.56	0.41
1:A:72:TYR:HE2	1:A:74:GLY:HA2	1.84	0.41
1:B:647:PHE:HB3	1:B:652:MET:HB3	2.01	0.41
1:A:685:ALA:HA	1:A:735:TYR:CZ	2.56	0.41
1:B:116:TYR:HB2	1:B:231:ARG:HG2	2.02	0.41
1:B:446:THR:O	1:B:450:MET:HG2	2.21	0.41
1:B:613:ASP:O	1:B:617:LEU:HG	2.21	0.41
1:D:539:ARG:HB2	1:D:545:ALA:HB1	2.02	0.41
1:C:569:LYS:HB3	1:C:569:LYS:HE3	1.87	0.41
1:D:492:ASP:HB3	1:D:495:GLY:O	2.21	0.41
1:A:510:MET:HE3	1:A:636:TYR:CE2	2.56	0.40
1:B:569:LYS:HB2	1:B:569:LYS:HE3	1.79	0.40
1:D:361[A]:GLU:OE2	1:D:406:ARG:HG2	2.21	0.40
1:A:51:PHE:HB3	1:A:69:ILE:HD12	2.03	0.40
1:C:432:GLU:HA	1:C:437:SER:OG	2.20	0.40
1:A:700:ALA:H	1:A:760:ASN:ND2	2.12	0.40
1:B:100:VAL:HG22	1:B:211:LYS:HG3	2.03	0.40
1:B:531:ILE:O	1:B:532:ASP:HB2	2.21	0.40
1:B:471:ARG:CD	4:B:2417:HOH:O	2.66	0.40
1:C:275:GLU:O	1:C:278:GLU:HG2	2.21	0.40
1:D:179:SER:HB3	1:D:243:LEU:CD1	2.50	0.40

All (1) 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)
2:C:1795:GOL:O1	4:A:2023:HOH:O[1_556]	1.86	0.34

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	754/750 (100%)	731 (97%)	23 (3%)	0	100	100
1	B	757/750 (101%)	734 (97%)	23 (3%)	0	100	100
1	C	758/750 (101%)	734 (97%)	24 (3%)	0	100	100
1	D	729/750 (97%)	702 (96%)	25 (3%)	2 (0%)	41	31
All	All	2998/3000 (100%)	2901 (97%)	95 (3%)	2 (0%)	51	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	755	ASP
1	D	184	ASN

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	637/630 (101%)	630 (99%)	7 (1%)	73	73
1	B	639/630 (101%)	631 (99%)	8 (1%)	69	68
1	C	640/630 (102%)	630 (98%)	10 (2%)	62	60
1	D	615/630 (98%)	605 (98%)	10 (2%)	62	60
All	All	2531/2520 (100%)	2496 (99%)	35 (1%)	69	65

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	PHE
1	A	394[A]	TYR
1	A	394[B]	TYR
1	A	680	LYS
1	A	686	GLU
1	A	697	HIS
1	A	745	MET
1	B	129	PHE
1	B	299	LEU

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Mol	Chain	Res	Type
1	B	373	SER
1	B	541	ASP
1	B	581	LEU
1	B	697	HIS
1	B	747	SER
1	B	789	ARG
1	C	66	ARG
1	C	70[A]	GLU
1	C	70[B]	GLU
1	C	129	PHE
1	C	152	MET
1	C	183	SER
1	C	541	ASP
1	C	581	LEU
1	C	697	HIS
1	C	745	MET
1	D	45	SER
1	D	129	PHE
1	D	152	MET
1	D	182	ARG
1	D	183	SER
1	D	343	TYR
1	D	395	ASP
1	D	406	ARG
1	D	541	ASP
1	D	745	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	A	194	GLN
1	A	336	ASN
1	A	409	HIS
1	A	546	GLN
1	A	697	HIS
1	A	716	GLN
1	A	760	ASN
1	B	59	ASN
1	B	176	ASN
1	B	194	GLN
1	B	336	ASN

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Mol	Chain	Res	Type
1	B	409	HIS
1	B	639	ASN
1	B	640	HIS
1	B	697	HIS
1	B	716	GLN
1	B	760	ASN
1	C	125	HIS
1	C	176	ASN
1	C	194	GLN
1	C	336	ASN
1	C	409	HIS
1	C	546	GLN
1	C	697	HIS
1	C	716	GLN
1	C	743	GLN
1	C	760	ASN
1	D	184	ASN
1	D	194	GLN
1	D	336	ASN
1	D	409	HIS
1	D	640	HIS
1	D	716	GLN
1	D	743	GLN
1	D	760	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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	GOL	C	1796	-	5,5,5	0.40	0	5,5,5	0.65	0
2	GOL	D	1794	-	5,5,5	0.48	0	5,5,5	0.69	0
2	GOL	D	1793	-	5,5,5	0.46	0	5,5,5	0.79	0
2	GOL	B	1794	-	5,5,5	0.43	0	5,5,5	1.45	1 (20%)
2	GOL	C	1793	-	5,5,5	0.43	0	5,5,5	0.64	0
2	GOL	A	1792	-	5,5,5	0.86	0	5,5,5	1.03	0
2	GOL	D	1792	-	5,5,5	0.20	0	5,5,5	0.53	0
2	GOL	A	1796	-	5,5,5	0.28	0	5,5,5	0.37	0
2	GOL	B	1793	-	5,5,5	0.74	0	5,5,5	0.52	0
2	GOL	B	1797	-	5,5,5	0.31	0	5,5,5	0.70	0
2	GOL	A	1794	-	5,5,5	0.21	0	5,5,5	0.71	0
2	GOL	C	1794	-	5,5,5	0.37	0	5,5,5	0.60	0
2	GOL	B	1798	-	5,5,5	0.19	0	5,5,5	0.28	0
2	GOL	B	1791	-	5,5,5	0.23	0	5,5,5	1.20	1 (20%)
2	GOL	B	1792	-	5,5,5	0.55	0	5,5,5	0.21	0
2	GOL	B	1795	-	5,5,5	0.39	0	5,5,5	0.33	0
2	GOL	A	1791	-	5,5,5	0.37	0	5,5,5	0.50	0
2	GOL	A	1795	-	5,5,5	0.48	0	5,5,5	0.39	0
2	GOL	A	1793	-	5,5,5	0.61	0	5,5,5	0.74	0
2	GOL	C	1797	-	5,5,5	0.14	0	5,5,5	0.73	0
2	GOL	B	1796	-	5,5,5	0.31	0	5,5,5	0.27	0
2	GOL	C	1795	-	5,5,5	0.34	0	5,5,5	1.03	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	GOL	C	1796	-	-	0/4/4/4	-
2	GOL	D	1794	-	-	4/4/4/4	-
2	GOL	D	1793	-	-	1/4/4/4	-
2	GOL	B	1794	-	-	2/4/4/4	-
2	GOL	C	1793	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	1792	-	-	2/4/4/4	-
2	GOL	D	1792	-	-	4/4/4/4	-
2	GOL	A	1796	-	-	0/4/4/4	-
2	GOL	B	1793	-	-	0/4/4/4	-
2	GOL	B	1797	-	-	2/4/4/4	-
2	GOL	A	1794	-	-	0/4/4/4	-
2	GOL	C	1794	-	-	0/4/4/4	-
2	GOL	B	1798	-	-	2/4/4/4	-
2	GOL	B	1791	-	-	2/4/4/4	-
2	GOL	B	1792	-	-	0/4/4/4	-
2	GOL	B	1795	-	-	2/4/4/4	-
2	GOL	A	1791	-	-	2/4/4/4	-
2	GOL	A	1795	-	-	0/4/4/4	-
2	GOL	A	1793	-	-	2/4/4/4	-
2	GOL	C	1797	-	-	0/4/4/4	-
2	GOL	B	1796	-	-	2/4/4/4	-
2	GOL	C	1795	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1794	GOL	O1-C1-C2	-2.27	99.30	110.20
2	B	1791	GOL	C3-C2-C1	-2.14	103.37	111.70

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1792	GOL	C1-C2-C3-O3
2	D	1792	GOL	O1-C1-C2-C3
2	B	1797	GOL	O1-C1-C2-C3
2	B	1798	GOL	O1-C1-C2-C3
2	B	1791	GOL	C1-C2-C3-O3
2	B	1795	GOL	O1-C1-C2-C3
2	A	1791	GOL	C1-C2-C3-O3
2	A	1791	GOL	O2-C2-C3-O3
2	B	1796	GOL	O1-C1-C2-C3
2	D	1794	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	D	1792	GOL	C1-C2-C3-O3
2	A	1793	GOL	C1-C2-C3-O3
2	C	1795	GOL	O1-C1-C2-C3
2	D	1792	GOL	O1-C1-C2-O2
2	B	1797	GOL	O1-C1-C2-O2
2	B	1798	GOL	O1-C1-C2-O2
2	B	1791	GOL	O2-C2-C3-O3
2	B	1796	GOL	O1-C1-C2-O2
2	C	1795	GOL	O1-C1-C2-O2
2	D	1794	GOL	O2-C2-C3-O3
2	A	1792	GOL	O2-C2-C3-O3
2	B	1795	GOL	O1-C1-C2-O2
2	D	1794	GOL	O1-C1-C2-O2
2	B	1794	GOL	O2-C2-C3-O3
2	A	1793	GOL	O2-C2-C3-O3
2	D	1794	GOL	O1-C1-C2-C3
2	D	1793	GOL	C1-C2-C3-O3
2	B	1794	GOL	C1-C2-C3-O3
2	D	1792	GOL	O2-C2-C3-O3

There are no ring outliers.

11 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1796	GOL	1	0
2	D	1793	GOL	1	0
2	B	1794	GOL	1	0
2	A	1792	GOL	1	0
2	B	1793	GOL	1	0
2	B	1797	GOL	1	0
2	B	1798	GOL	1	0
2	B	1795	GOL	1	0
2	A	1793	GOL	3	0
2	C	1797	GOL	1	0
2	C	1795	GOL	5	1

5.7 Other polymers (i)

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	746/750 (99%)	-0.17	8 (1%)	80	82	12, 21, 37, 57	0
1	B	747/750 (99%)	-0.18	11 (1%)	73	76	12, 20, 38, 54	0
1	C	748/750 (99%)	-0.10	20 (2%)	54	57	12, 21, 41, 72	0
1	D	726/750 (96%)	-0.03	33 (4%)	33	36	12, 22, 51, 81	1 (0%)
All	All	2967/3000 (98%)	-0.12	72 (2%)	59	62	12, 21, 41, 81	1 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	354	SER	6.1
1	C	167	PRO	5.2
1	C	169	SER	5.1
1	D	404	TYR	5.0
1	C	172	VAL	5.0
1	D	175	LEU	4.3
1	C	355	ALA	4.2
1	D	178	ALA	4.1
1	D	358	VAL	4.1
1	D	412	PRO	4.0
1	C	168	ASP	4.0
1	C	350	VAL	3.9
1	D	366	LEU	3.8
1	D	355	ALA	3.8
1	D	376	THR	3.8
1	C	348	ALA	3.8
1	D	356	ASP	3.7
1	C	603	ALA	3.7
1	A	394[A]	TYR	3.7
1	B	355	ALA	3.6
1	C	170	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	367	MET	3.5
1	C	369	VAL	3.5
1	C	394	TYR	3.4
1	D	407	SER	3.3
1	D	357	ASP	3.3
1	C	351	ALA	3.1
1	C	352	GLN	3.0
1	C	171	ASP	3.0
1	D	364	LYS	2.8
1	D	399	ALA	2.7
1	D	368	ALA	2.7
1	D	395	ASP	2.7
1	B	394[A]	TYR	2.7
1	D	415	ARG	2.6
1	B	346[A]	ASP	2.6
1	D	400	ASN	2.6
1	B	348	ALA	2.6
1	A	167	PRO	2.5
1	D	757[A]	GLU	2.5
1	B	351	ALA	2.5
1	C	374	PHE	2.5
1	D	408	ALA	2.4
1	D	411	GLY	2.4
1	B	352	GLN	2.4
1	D	343	TYR	2.4
1	A	372	LYS	2.4
1	D	413	LEU	2.4
1	B	374	PHE	2.4
1	D	181	LEU	2.3
1	B	167	PRO	2.3
1	C	368	ALA	2.3
1	D	375	ALA	2.3
1	C	356	ASP	2.3
1	D	403	ASN	2.3
1	A	295	ALA	2.3
1	B	372	LYS	2.3
1	D	414	LYS	2.3
1	B	297	PRO	2.2
1	C	383	THR	2.2
1	A	374	PHE	2.2
1	B	376	THR	2.2
1	D	753	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	176	ASN	2.2
1	A	352	GLN	2.2
1	D	361[A]	GLU	2.2
1	A	166	VAL	2.2
1	D	359	THR	2.1
1	D	370	SER	2.1
1	C	372	LYS	2.1
1	D	603	ALA	2.1
1	A	354	SER	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	GOL	C	1795	6/6	0.78	0.22	39,45,47,53	0
2	GOL	B	1797	6/6	0.83	0.32	50,51,57,65	0
2	GOL	C	1797	6/6	0.87	0.21	49,52,54,54	0
2	GOL	D	1794	6/6	0.87	0.27	40,43,44,47	0
2	GOL	B	1795	6/6	0.88	0.25	36,41,42,45	0
2	GOL	A	1796	6/6	0.89	0.19	48,49,55,60	0
2	GOL	D	1792	6/6	0.90	0.16	39,46,50,52	0
2	GOL	B	1796	6/6	0.90	0.13	44,47,50,50	0
2	GOL	A	1791	6/6	0.90	0.12	35,36,38,41	0
2	GOL	B	1794	6/6	0.91	0.20	38,39,41,47	0
2	GOL	A	1793	6/6	0.92	0.18	23,28,34,40	0
2	GOL	B	1798	6/6	0.92	0.15	47,49,51,53	0
2	GOL	D	1793	6/6	0.93	0.11	27,32,34,38	0
2	GOL	B	1791	6/6	0.93	0.19	26,31,34,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	1794	6/6	0.93	0.15	32,39,43,43	0
2	GOL	C	1794	6/6	0.93	0.15	26,29,30,31	0
2	GOL	C	1793	6/6	0.94	0.13	24,25,26,29	0
2	GOL	C	1796	6/6	0.94	0.13	19,30,33,39	0
2	GOL	B	1793	6/6	0.95	0.11	19,27,28,33	0
2	GOL	A	1792	6/6	0.95	0.11	19,25,28,31	0
2	GOL	B	1792	6/6	0.96	0.16	19,23,24,25	0
2	GOL	A	1795	6/6	0.96	0.20	20,24,27,27	0
3	CA	B	1799	1/1	0.98	0.17	55,55,55,55	0
3	CA	C	1798	1/1	0.99	0.04	22,22,22,22	0
3	CA	D	1795	1/1	1.00	0.03	20,20,20,20	0
3	CA	A	1797	1/1	1.00	0.07	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.