Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2021 – 06:44 PM EDT

PDB ID	:	3FHA
Title	:	Structure of endo-beta-N-acetylglucosaminidase A
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Deposited on	:	2008-12-09
Resolution	:	2.00 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 (i) symbol.

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

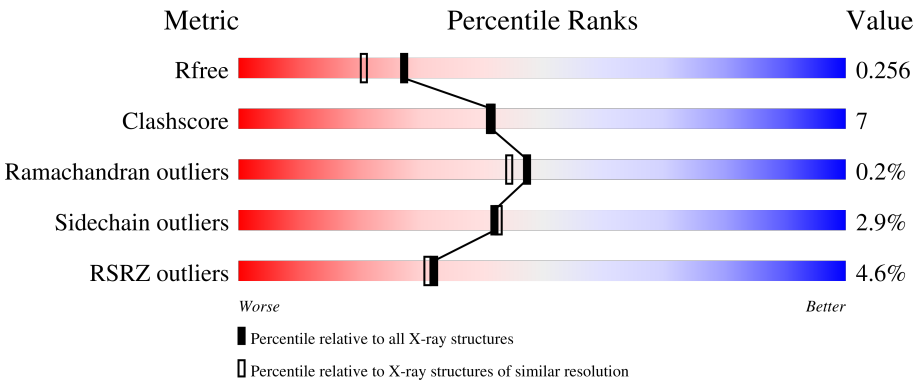
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of 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	621	3% 86% 9% • •
1	B	621	3% 82% 10% • 6%
1	C	621	5% 80% 13% • 5%
1	D	621	6% 77% 13% • 8%

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
4	GOL	B	700[B]	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20919 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 Endo-beta-N-acetylglucosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	598	4755	3014	796	934	11	0	0	0
1	B	583	4660	2955	781	913	11	0	0	0
1	C	592	4722	2994	793	924	11	0	1	0
1	D	572	4577	2910	766	890	11	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	ASP	GLY	engineered mutation	UNP Q9ZB22
A	518	THR	ILE	engineered mutation	UNP Q9ZB22
A	583	ILE	LEU	engineered mutation	UNP Q9ZB22
B	455	ASP	GLY	engineered mutation	UNP Q9ZB22
B	518	THR	ILE	engineered mutation	UNP Q9ZB22
B	583	ILE	LEU	engineered mutation	UNP Q9ZB22
C	455	ASP	GLY	engineered mutation	UNP Q9ZB22
C	518	THR	ILE	engineered mutation	UNP Q9ZB22
C	583	ILE	LEU	engineered mutation	UNP Q9ZB22
D	455	ASP	GLY	engineered mutation	UNP Q9ZB22
D	518	THR	ILE	engineered mutation	UNP Q9ZB22
D	583	ILE	LEU	engineered mutation	UNP Q9ZB22

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

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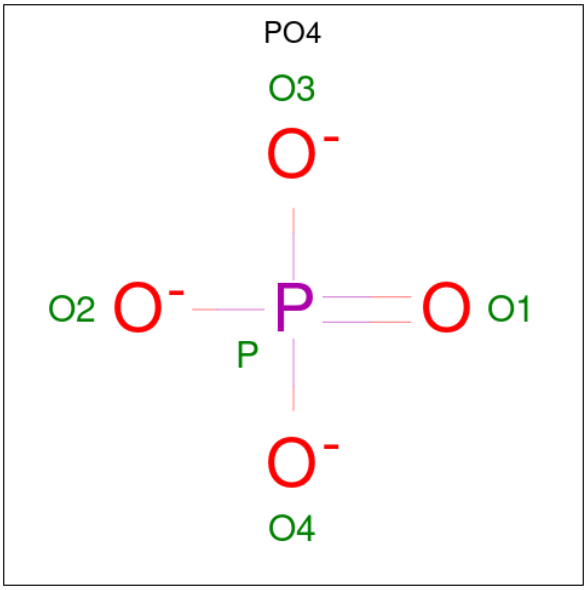
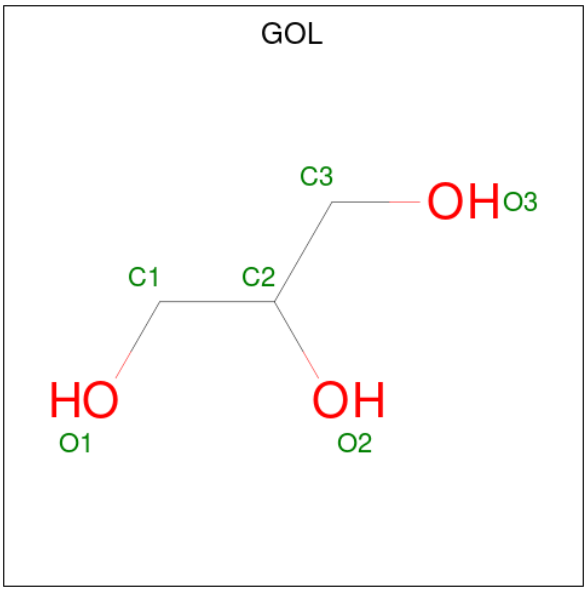
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	12	6	6	0	1
			Total	C	O		
4	D	1	12	6	6	0	1

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	B	1	1	1	0	0

- Molecule 6 is water.

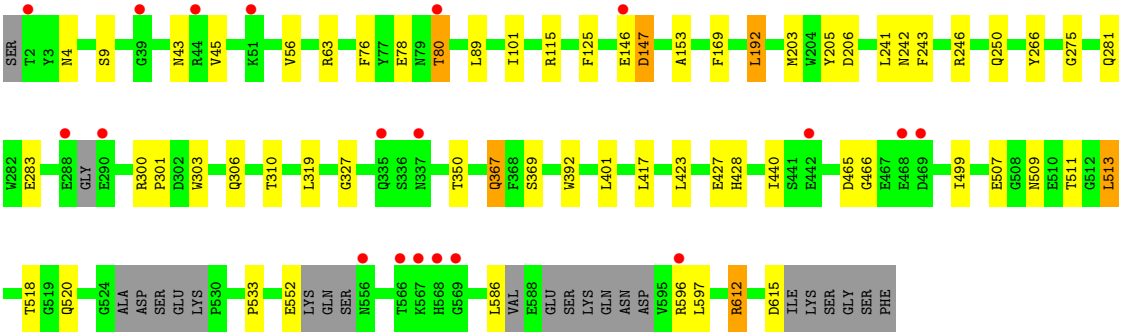
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	598	598	598	0	0
			Total	O		
6	B	602	602	602	0	0
			Total	O		
6	C	499	499	499	0	0
			Total	O		
6	D	472	472	472	0	0

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.

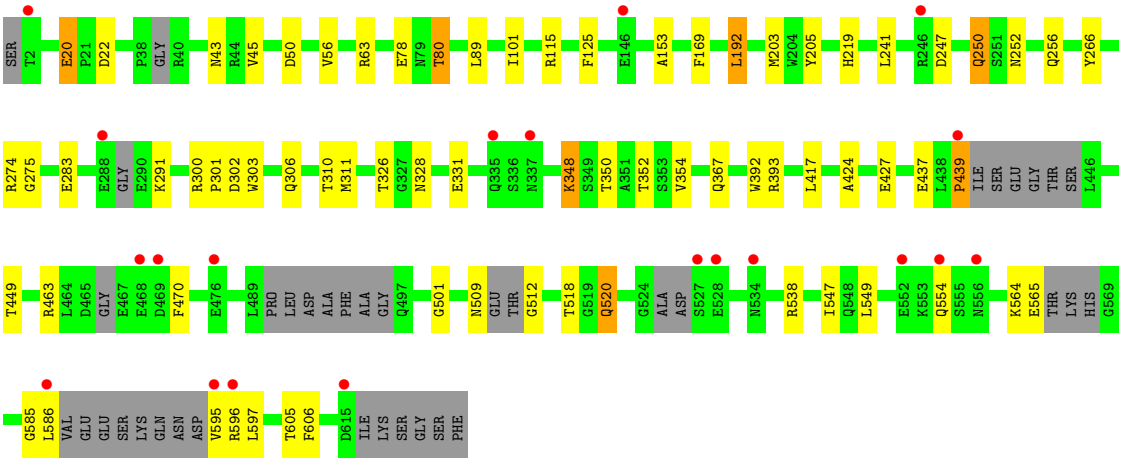
• Molecule 1: Endo-beta-N-acetylglucosaminidase

Chain A:



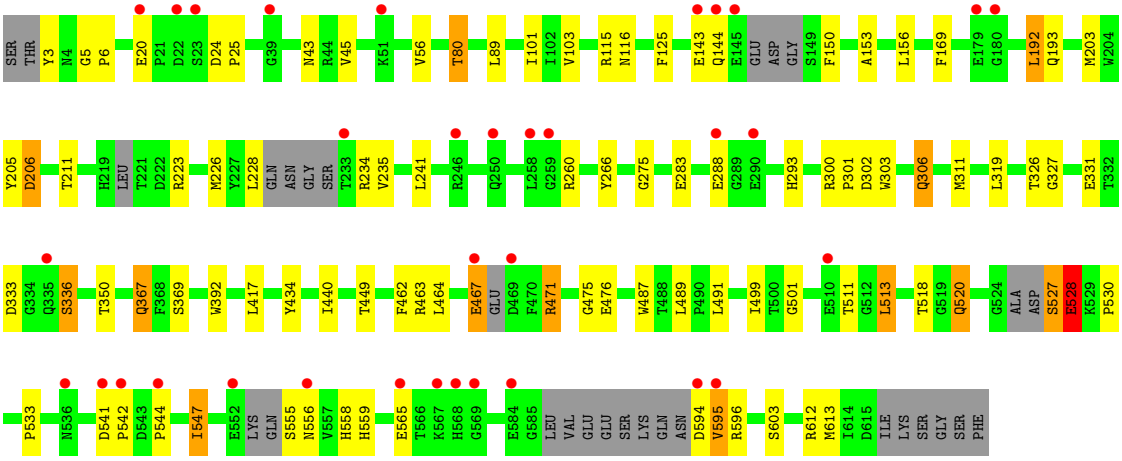
• Molecule 1: Endo-beta-N-acetylglucosaminidase

Chain B:



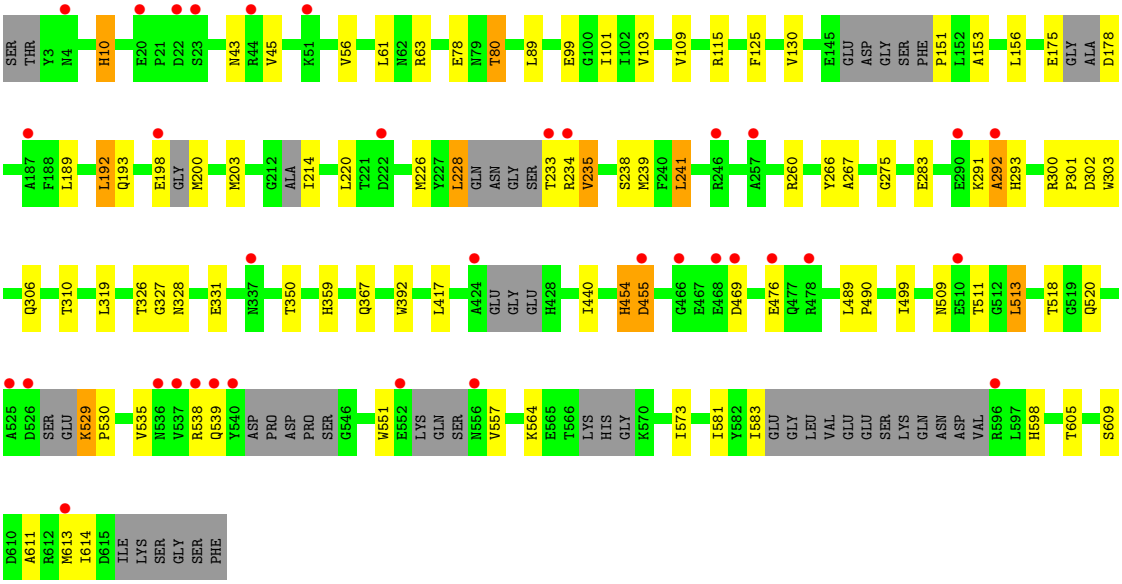
• Molecule 1: Endo-beta-N-acetylglucosaminidase

Chain C:



- Molecule 1: Endo-beta-N-acetylglucosaminidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	79.89Å 78.97Å 117.27Å 84.23° 80.77° 64.01°	Depositor
Resolution (Å)	20.00 – 2.00 19.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 67.9 (19.92-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.85 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.203 , 0.251 0.213 , 0.256	Depositor DCC
R_{free} test set	5824 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20919	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CA, PO4, GOL

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	0.56	2/4899 (0.0%)	0.58	1/6677 (0.0%)
1	B	0.53	0/4797	0.56	1/6531 (0.0%)
1	C	0.59	2/4864 (0.0%)	0.62	1/6626 (0.0%)
1	D	0.54	4/4711 (0.1%)	0.57	3/6413 (0.0%)
All	All	0.56	8/19271 (0.0%)	0.59	6/26247 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	552	GLU	CB-CG	-7.86	1.37	1.52
1	D	292	ALA	CA-CB	-6.68	1.38	1.52
1	D	455	ASP	C-N	-5.87	1.20	1.34
1	C	306	GLN	CB-CG	-5.55	1.37	1.52
1	D	193	GLN	C-N	-5.47	1.21	1.34
1	D	10	HIS	C-N	5.30	1.46	1.34
1	C	193	GLN	C-N	-5.09	1.22	1.34
1	A	9	SER	CB-OG	-5.01	1.35	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	20	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	D	454	HIS	O-C-N	5.26	131.12	122.70
1	C	528	GLU	CA-CB-CG	5.25	124.95	113.40
1	D	469	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	455	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	147	ASP	N-CA-CB	-5.08	101.46	110.60

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	4755	0	4351	40	0
1	B	4660	0	4269	66	0
1	C	4722	0	4322	71	0
1	D	4577	0	4202	75	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0
4	B	12	0	16	7	0
4	D	12	0	16	3	0
5	B	1	0	0	0	0
6	A	598	0	0	2	0
6	B	602	0	0	13	0
6	C	499	0	0	10	0
6	D	472	0	0	6	0
All	All	20919	0	17176	252	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 7.

All (252) 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:586:LEU:HD22	1:B:595:VAL:HG21	1.26	1.15
1:D:43:ASN:HD22	1:D:392:TRP:HE1	1.05	1.01
1:B:43:ASN:HD22	1:B:392:TRP:HE1	1.02	1.00
1:B:586:LEU:HD22	1:B:595:VAL:CG2	1.92	1.00
1:C:558:HIS:HD2	1:C:559:HIS:HD1	1.10	0.99
1:D:292:ALA:HB1	1:D:293:HIS:HA	1.44	0.99
1:D:292:ALA:HB1	1:D:293:HIS:CA	1.93	0.98
1:B:595:VAL:HG11	1:B:597:LEU:HD21	1.48	0.96
1:C:43:ASN:HD22	1:C:392:TRP:HE1	1.07	0.96
1:B:586:LEU:CD2	1:B:595:VAL:HG21	1.96	0.95
1:A:43:ASN:HD22	1:A:392:TRP:HE1	1.03	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:ALA:CB	1:D:293:HIS:HA	1.97	0.94
1:B:595:VAL:HG11	1:B:597:LEU:CD2	1.98	0.94
1:B:354:VAL:HG23	1:B:439:PRO:HD2	1.50	0.93
1:B:595:VAL:CG2	6:B:740:HOH:O	2.22	0.87
1:D:598:HIS:CE1	1:D:613:MET:HG2	2.09	0.87
1:D:476:GLU:OE1	1:D:490:PRO:HD2	1.73	0.86
1:B:354:VAL:CG2	1:B:439:PRO:HD2	2.05	0.86
1:C:260:ARG:HD3	6:C:1835:HOH:O	1.76	0.85
1:C:150:PHE:CD1	6:C:1838:HOH:O	2.30	0.84
1:B:595:VAL:HG23	6:B:740:HOH:O	1.78	0.84
1:B:354:VAL:HG23	1:B:439:PRO:CD	2.09	0.83
1:B:565:GLU:HG3	1:B:596:ARG:HB2	1.58	0.83
1:B:115:ARG:O	1:B:350:THR:HG21	1.80	0.82
1:C:56:VAL:HG12	1:C:89:LEU:HB3	1.62	0.81
1:D:56:VAL:HG22	1:D:89:LEU:HB3	1.63	0.80
1:B:310:THR:HB	4:B:700[B]:GOL:H11	1.64	0.80
1:B:311:MET:H	4:B:700[B]:GOL:H31	1.46	0.80
1:B:56:VAL:HG12	1:B:89:LEU:HB3	1.64	0.79
1:C:464:LEU:H	1:C:471[A]:ARG:HH21	1.26	0.79
1:D:228:LEU:HD23	1:D:239:MET:HB2	1.67	0.76
1:D:56:VAL:HG21	1:D:203:MET:HE1	1.66	0.76
1:B:354:VAL:CG2	1:B:439:PRO:CD	2.64	0.76
1:C:144:GLN:HA	6:C:1838:HOH:O	1.84	0.75
1:D:292:ALA:HB1	1:D:293:HIS:C	2.05	0.75
1:D:115:ARG:O	1:D:350:THR:HG21	1.86	0.75
1:B:354:VAL:HG21	1:B:439:PRO:CG	2.18	0.73
1:C:115:ARG:O	1:C:350:THR:HG21	1.89	0.73
1:C:464:LEU:H	1:C:471[A]:ARG:NH2	1.86	0.73
1:D:234:ARG:CD	1:D:260:ARG:HH11	2.02	0.72
1:C:558:HIS:CD2	1:C:559:HIS:HD1	2.02	0.72
1:C:565:GLU:HG3	1:C:596:ARG:CZ	2.21	0.71
1:B:219:HIS:HE1	1:B:247:ASP:O	1.73	0.71
1:B:311:MET:H	4:B:700[B]:GOL:C3	2.03	0.71
1:A:56:VAL:HG21	1:A:203:MET:HE1	1.73	0.70
1:B:595:VAL:CG1	1:B:597:LEU:CD2	2.69	0.70
1:C:511:THR:HG22	1:C:513:LEU:HB2	1.74	0.70
1:A:56:VAL:HG23	1:A:266:TYR:CE1	2.27	0.70
1:A:115:ARG:O	1:A:350:THR:HG21	1.92	0.70
1:C:555:SER:O	1:C:556:ASN:HB2	1.89	0.69
1:C:527:SER:HA	6:C:1698:HOH:O	1.92	0.69
1:B:56:VAL:HG13	1:B:266:TYR:CE1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:VAL:HG23	1:D:266:TYR:CE1	2.29	0.68
1:A:511:THR:HG22	1:A:513:LEU:HB2	1.74	0.68
1:D:310:THR:HB	4:D:701[B]:GOL:H2	1.76	0.68
1:D:581:ILE:HG23	1:D:583:ILE:CD1	2.24	0.68
1:C:555:SER:HB2	6:C:1948:HOH:O	1.95	0.67
1:C:533:PRO:O	1:C:612:ARG:HD2	1.95	0.67
1:D:228:LEU:CD2	1:D:239:MET:HB2	2.25	0.66
1:C:417:LEU:HB3	1:C:518:THR:HG23	1.77	0.65
1:B:449:THR:OG1	1:B:520:GLN:HG2	1.96	0.65
1:B:565:GLU:HG3	1:B:596:ARG:CB	2.27	0.65
1:D:417:LEU:HB3	1:D:518:THR:HG23	1.78	0.65
1:A:56:VAL:HG22	1:A:89:LEU:HB3	1.78	0.65
1:B:512:GLY:N	6:B:850:HOH:O	2.28	0.65
1:C:144:GLN:CA	6:C:1838:HOH:O	2.43	0.65
1:D:10:HIS:HD2	1:D:99:GLU:O	1.79	0.65
1:D:234:ARG:CD	1:D:260:ARG:HD3	2.27	0.65
1:B:564:LYS:HG3	1:B:595:VAL:HG13	1.78	0.65
1:C:56:VAL:HG13	1:C:266:TYR:CE1	2.33	0.63
1:D:440:ILE:HD11	1:D:499:ILE:HG13	1.80	0.63
1:A:310:THR:HB	4:D:701[A]:GOL:H2	1.79	0.63
1:A:63:ARG:NH1	1:A:306:GLN:HG2	2.14	0.62
1:A:76:PHE:CE2	4:D:701[A]:GOL:H12	2.34	0.62
1:B:595:VAL:HG22	6:B:740:HOH:O	1.90	0.62
1:C:326:THR:HG21	1:C:331:GLU:O	2.00	0.62
1:D:476:GLU:OE1	1:D:490:PRO:CD	2.45	0.62
1:A:440:ILE:HD11	1:A:499:ILE:HG13	1.80	0.62
1:D:292:ALA:HB3	1:D:293:HIS:HA	1.83	0.61
1:C:101:ILE:HB	1:C:125:PHE:O	1.99	0.61
1:B:417:LEU:HB3	1:B:518:THR:HG23	1.83	0.60
1:D:234:ARG:HD3	1:D:260:ARG:HH11	1.64	0.60
1:C:463:ARG:CG	1:C:467:GLU:HB3	2.31	0.60
1:D:101:ILE:HB	1:D:125:PHE:O	2.02	0.60
1:D:234:ARG:HD2	1:D:260:ARG:HH11	1.67	0.60
1:A:246:ARG:HE	1:A:281:GLN:HG3	1.67	0.59
1:C:476:GLU:HG3	1:C:489:LEU:HD12	1.85	0.59
1:A:596:ARG:HG2	1:A:615:ASP:OD1	2.03	0.58
1:C:293:HIS:HE1	6:C:1549:HOH:O	1.86	0.58
1:C:544:PRO:HB3	6:C:1854:HOH:O	2.03	0.58
1:A:533:PRO:O	1:A:612:ARG:HD2	2.04	0.58
1:D:80:THR:HG21	6:D:1995:HOH:O	2.03	0.58
1:B:439:PRO:O	1:B:439:PRO:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:PHE:O	1:C:471[A]:ARG:HG2	2.04	0.57
1:D:476:GLU:CD	1:D:490:PRO:HD2	2.25	0.57
1:A:417:LEU:HB3	1:A:518:THR:HG23	1.86	0.57
1:A:153:ALA:HB1	1:A:192:LEU:HD13	1.87	0.57
1:B:56:VAL:HG11	1:B:203:MET:HE1	1.86	0.57
1:B:547:ILE:CD1	1:B:586:LEU:HD12	2.35	0.57
1:B:538:ARG:HG3	1:B:538:ARG:HH11	1.71	0.56
1:C:440:ILE:HD11	1:C:499:ILE:HG13	1.87	0.56
1:B:501:GLY:C	6:B:2099:HOH:O	2.43	0.56
1:C:541:ASP:HB2	1:C:542:PRO:HD3	1.85	0.56
1:C:211:THR:CG2	1:C:223:ARG:HH12	2.18	0.56
1:D:80:THR:O	1:D:80:THR:OG1	2.23	0.56
1:C:565:GLU:HG3	1:C:596:ARG:NH2	2.21	0.56
1:D:233:THR:HG22	6:D:1585:HOH:O	2.05	0.56
1:D:581:ILE:HG23	1:D:583:ILE:HD12	1.88	0.55
1:C:319:LEU:HD21	1:C:327:GLY:HA2	1.88	0.55
1:C:449:THR:OG1	1:C:520:GLN:HG2	2.07	0.54
4:B:700[A]:GOL:H11	1:C:311:MET:HB3	1.89	0.54
1:D:581:ILE:HG23	1:D:583:ILE:HD11	1.88	0.54
1:C:3:TYR:OH	1:C:6:PRO:HD2	2.07	0.54
1:B:219:HIS:CE1	1:B:247:ASP:O	2.58	0.54
1:B:595:VAL:CG1	1:B:597:LEU:HD23	2.38	0.54
1:D:511:THR:HG22	1:D:513:LEU:HB2	1.90	0.54
1:A:101:ILE:HB	1:A:125:PHE:O	2.08	0.53
1:D:511:THR:HG22	1:D:513:LEU:H	1.72	0.53
1:C:56:VAL:HG11	1:C:203:MET:HE1	1.91	0.53
1:B:470:PHE:CD1	6:B:2099:HOH:O	2.61	0.53
1:D:63:ARG:HG3	1:D:306:GLN:HE21	1.74	0.53
1:B:348:LYS:HE3	6:B:1129:HOH:O	2.09	0.52
1:D:581:ILE:CG2	1:D:583:ILE:HD11	2.39	0.52
1:B:424:ALA:HB3	1:B:427:GLU:HG3	1.90	0.52
1:D:153:ALA:HB1	1:D:192:LEU:HD13	1.92	0.52
1:B:509:ASN:C	6:B:936:HOH:O	2.48	0.52
1:A:80:THR:OG1	1:A:80:THR:O	2.28	0.51
1:C:211:THR:HG23	1:C:223:ARG:NH1	2.26	0.51
1:B:354:VAL:CG2	1:B:439:PRO:CG	2.87	0.51
1:D:529:LYS:O	1:D:529:LYS:HG2	2.09	0.51
1:A:43:ASN:ND2	1:A:392:TRP:HE1	1.87	0.51
1:B:101:ILE:HB	1:B:125:PHE:O	2.10	0.51
1:B:354:VAL:HG21	1:B:439:PRO:CD	2.36	0.51
1:B:250:GLN:HG3	6:B:711:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:NH1	6:B:1044:HOH:O	2.44	0.51
1:C:43:ASN:ND2	1:C:45:VAL:HG22	2.26	0.51
1:C:541:ASP:CB	1:C:542:PRO:HD3	2.41	0.51
1:A:43:ASN:ND2	1:A:45:VAL:HG22	2.26	0.51
1:A:428:HIS:CE1	1:A:507:GLU:CG	2.94	0.51
1:B:63:ARG:NH1	1:B:306:GLN:HG2	2.26	0.50
1:C:283:GLU:H	1:C:283:GLU:CD	2.15	0.50
1:C:530:PRO:HG3	1:C:603:SER:HB3	1.92	0.50
1:C:527:SER:O	1:C:528:GLU:O	2.30	0.50
1:D:509:ASN:OD1	1:D:511:THR:HB	2.11	0.50
1:C:153:ALA:HB1	1:C:192:LEU:HD13	1.92	0.50
1:D:538:ARG:HG2	1:D:539:GLN:N	2.27	0.50
1:B:326:THR:HG22	1:B:328:ASN:HB3	1.93	0.50
1:A:206:ASP:CG	1:A:206:ASP:O	2.51	0.49
1:B:310:THR:HB	4:B:700[B]:GOL:C1	2.38	0.49
1:C:463:ARG:HD2	1:C:467:GLU:CB	2.42	0.49
1:A:146:GLU:HG3	6:A:920:HOH:O	2.12	0.49
1:D:326:THR:HG22	1:D:328:ASN:HB3	1.94	0.49
1:B:78:GLU:O	1:B:80:THR:HG23	2.13	0.49
1:B:56:VAL:HG13	1:B:266:TYR:CD1	2.48	0.49
1:D:189:LEU:HB2	1:D:235:VAL:HG23	1.93	0.48
1:D:283:GLU:CD	1:D:283:GLU:H	2.14	0.48
1:A:367:GLN:OE1	1:A:369:SER:OG	2.19	0.48
1:C:511:THR:CG2	1:C:513:LEU:HB2	2.40	0.48
1:D:535:VAL:HG22	1:D:551:TRP:HB3	1.95	0.48
1:C:80:THR:O	1:C:80:THR:OG1	2.31	0.48
1:D:300:ARG:N	1:D:301:PRO:HD3	2.29	0.48
1:C:565:GLU:CG	1:C:596:ARG:NH2	2.77	0.48
1:C:235:VAL:HG23	6:C:2047:HOH:O	2.14	0.48
1:C:275:GLY:HA3	1:C:303:TRP:CD2	2.49	0.48
1:C:333:ASP:O	1:C:336:SER:HB3	2.14	0.47
1:A:428:HIS:CE1	1:A:507:GLU:HG3	2.48	0.47
1:D:178:ASP:N	6:D:2020:HOH:O	2.48	0.47
1:A:612:ARG:HD3	6:A:2019:HOH:O	2.14	0.47
1:C:300:ARG:N	1:C:301:PRO:HD3	2.29	0.47
1:C:594:ASP:O	1:C:595:VAL:HG23	2.15	0.47
1:C:143:GLU:C	6:C:1838:HOH:O	2.53	0.47
1:D:43:ASN:ND2	1:D:45:VAL:HG22	2.30	0.47
1:D:226:MET:O	1:D:235:VAL:HG11	2.15	0.47
1:C:211:THR:CG2	1:C:223:ARG:NH1	2.78	0.47
1:B:153:ALA:HB1	1:B:192:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:547:ILE:HD13	1:C:547:ILE:HA	1.79	0.46
1:A:169:PHE:HZ	1:A:205:TYR:HD1	1.63	0.46
1:D:538:ARG:CG	1:D:539:GLN:N	2.78	0.46
1:C:206:ASP:CG	1:C:206:ASP:O	2.55	0.46
1:D:530:PRO:HG2	1:D:609:SER:HB3	1.98	0.46
1:D:300:ARG:NH1	1:D:302:ASP:OD2	2.50	0.45
1:B:283:GLU:CD	1:B:283:GLU:H	2.19	0.45
1:C:367:GLN:OE1	1:C:369:SER:OG	2.18	0.45
1:A:511:THR:CG2	1:A:513:LEU:HB2	2.42	0.45
1:D:61:LEU:HD13	1:D:109:VAL:HG13	1.99	0.45
1:B:547:ILE:HD11	1:B:586:LEU:HD12	1.98	0.45
1:D:78:GLU:O	1:D:80:THR:HG22	2.17	0.45
1:A:146:GLU:HG3	1:A:146:GLU:H	1.40	0.45
1:B:352:THR:HA	1:B:437:GLU:O	2.17	0.45
1:B:300:ARG:N	1:B:301:PRO:HD3	2.32	0.45
1:B:605:THR:O	1:B:606:PHE:HB2	2.17	0.45
1:D:228:LEU:HD21	1:D:238:SER:C	2.37	0.45
1:C:300:ARG:NH1	1:C:302:ASP:OD2	2.50	0.45
1:D:454:HIS:O	1:D:455:ASP:HB2	2.17	0.45
1:D:605:THR:HG22	1:D:605:THR:O	2.16	0.45
1:D:198:GLU:C	1:D:200:MET:N	2.71	0.45
1:D:214:ILE:N	6:D:2013:HOH:O	2.49	0.45
1:D:476:GLU:HG3	1:D:489:LEU:HD12	1.99	0.45
1:B:326:THR:HG21	1:B:331:GLU:O	2.17	0.44
1:C:56:VAL:HG11	1:C:203:MET:CE	2.47	0.44
1:D:319:LEU:HD21	1:D:327:GLY:HA2	1.99	0.44
1:B:20:GLU:OE2	1:B:22:ASP:HB2	2.17	0.44
1:C:211:THR:HG21	1:C:223:ARG:HH12	1.81	0.44
1:A:319:LEU:HD21	1:A:327:GLY:HA2	2.00	0.43
1:A:300:ARG:N	1:A:301:PRO:HD3	2.33	0.43
1:D:275:GLY:HA3	1:D:303:TRP:CD2	2.53	0.43
1:D:200:MET:N	6:D:814:HOH:O	2.51	0.43
1:B:169:PHE:HZ	1:B:205:TYR:HD1	1.67	0.43
1:B:310:THR:HA	4:B:700[B]:GOL:H31	2.01	0.43
1:B:300:ARG:NH1	1:B:302:ASP:OD2	2.52	0.43
1:D:326:THR:HG21	1:D:331:GLU:O	2.18	0.43
1:A:275:GLY:HA3	1:A:303:TRP:CD2	2.53	0.43
1:A:423:LEU:CD1	1:A:427:GLU:HG2	2.49	0.43
1:D:234:ARG:HD2	1:D:260:ARG:NH1	2.32	0.43
1:C:24:ASP:HA	1:C:25:PRO:HD3	1.89	0.42
1:C:475:GLY:HA3	1:C:487:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ASN:OD1	1:A:511:THR:HB	2.19	0.42
1:D:151:PRO:N	6:D:1020:HOH:O	2.52	0.42
1:B:252:ASN:O	1:B:256:GLN:HG3	2.20	0.42
1:B:463:ARG:N	6:B:2099:HOH:O	2.52	0.42
1:B:554:GLN:HG3	6:B:792:HOH:O	2.19	0.42
1:A:78:GLU:O	1:A:80:THR:HG22	2.20	0.41
1:A:465:ASP:HA	1:A:466:GLY:HA2	1.65	0.41
1:A:586:LEU:CD1	1:A:597:LEU:HD11	2.50	0.41
1:C:228:LEU:O	1:C:235:VAL:N	2.46	0.41
1:A:242:ASN:ND2	1:A:243:PHE:H	2.18	0.41
1:D:10:HIS:CD2	1:D:99:GLU:O	2.66	0.41
1:D:234:ARG:HD3	1:D:260:ARG:HD3	2.00	0.41
1:D:241:LEU:HB2	1:D:267:ALA:HA	2.02	0.41
1:D:564:LYS:HE3	1:D:573:ILE:HG21	2.03	0.41
1:D:598:HIS:HB3	1:D:611:ALA:HB1	2.03	0.41
1:C:434:TYR:O	1:C:501:GLY:HA2	2.20	0.41
1:D:511:THR:CG2	1:D:513:LEU:HB2	2.49	0.41
1:C:116:ASN:HA	1:C:350:THR:HG21	2.03	0.41
1:C:527:SER:O	1:C:528:GLU:C	2.54	0.41
1:D:189:LEU:CB	1:D:235:VAL:HG23	2.50	0.41
1:B:274:ARG:NH2	6:B:760:HOH:O	2.54	0.41
1:C:56:VAL:HG13	1:C:266:TYR:CD1	2.56	0.41
1:D:56:VAL:HG21	1:D:203:MET:CE	2.43	0.41
1:D:175:GLU:HA	1:D:214:ILE:HD12	2.03	0.41
1:C:3:TYR:CZ	1:C:5:GLY:HA3	2.56	0.41
1:A:283:GLU:H	1:A:283:GLU:CD	2.25	0.41
1:C:464:LEU:N	1:C:471[A]:ARG:HH21	2.05	0.41
1:D:61:LEU:HD13	1:D:109:VAL:CG1	2.51	0.41
1:A:586:LEU:HD13	1:A:597:LEU:HD11	2.03	0.40
1:C:20:GLU:HA	1:C:20:GLU:OE1	2.21	0.40
1:C:565:GLU:HG3	1:C:596:ARG:NH1	2.34	0.40
1:D:359:HIS:CD2	1:D:520:GLN:HB3	2.57	0.40
1:B:275:GLY:HA3	1:B:303:TRP:CD2	2.55	0.40
1:A:423:LEU:HD12	1:A:427:GLU:HG2	2.03	0.40
1:B:311:MET:N	4:B:700[B]:GOL:H31	2.25	0.40
1:C:169:PHE:HZ	1:C:205:TYR:HD1	1.69	0.40

There are no symmetry-related clashes.

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	587/621 (94%)	571 (97%)	15 (3%)	1 (0%)	47	44
1	B	563/621 (91%)	546 (97%)	16 (3%)	1 (0%)	47	44
1	C	577/621 (93%)	558 (97%)	16 (3%)	3 (0%)	29	23
1	D	548/621 (88%)	530 (97%)	18 (3%)	0	100	100
All	All	2275/2484 (92%)	2205 (97%)	65 (3%)	5 (0%)	47	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	595	VAL
1	C	288	GLU
1	A	147	ASP
1	B	585	GLY
1	C	206	ASP

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	494/515 (96%)	484 (98%)	10 (2%)	55	58
1	B	486/515 (94%)	473 (97%)	13 (3%)	44	46
1	C	490/515 (95%)	470 (96%)	20 (4%)	30	28
1	D	476/515 (92%)	461 (97%)	15 (3%)	39	38
All	All	1946/2060 (94%)	1888 (97%)	58 (3%)	42	41

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	80	THR
1	A	192	LEU
1	A	241	LEU
1	A	250	GLN
1	A	367	GLN
1	A	401	LEU
1	A	513	LEU
1	A	520	GLN
1	A	612	ARG
1	B	45	VAL
1	B	50	ASP
1	B	80	THR
1	B	192	LEU
1	B	241	LEU
1	B	250	GLN
1	B	291	LYS
1	B	348	LYS
1	B	367	GLN
1	B	393	ARG
1	B	439	PRO
1	B	520	GLN
1	B	549	LEU
1	C	80	THR
1	C	103	VAL
1	C	156	LEU
1	C	192	LEU
1	C	226	MET
1	C	234	ARG
1	C	241	LEU
1	C	306	GLN
1	C	336	SER
1	C	367	GLN
1	C	467	GLU
1	C	471[A]	ARG
1	C	471[B]	ARG
1	C	491	LEU
1	C	513	LEU
1	C	520	GLN
1	C	527	SER
1	C	528	GLU
1	C	547	ILE

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Mol	Chain	Res	Type
1	C	613	MET
1	D	80	THR
1	D	103	VAL
1	D	130	VAL
1	D	156	LEU
1	D	192	LEU
1	D	220	LEU
1	D	228	LEU
1	D	235	VAL
1	D	241	LEU
1	D	291	LYS
1	D	367	GLN
1	D	513	LEU
1	D	529	LYS
1	D	557	VAL
1	D	614	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	HIS
1	B	219	HIS
1	B	250	GLN
1	B	539	GLN
1	C	43	ASN
1	C	195	GLN
1	C	548	GLN
1	C	558	HIS
1	D	10	HIS
1	D	482	ASN
1	D	520	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
3	PO4	A	707	-	4,4,4	0.86	0	6,6,6	0.48	0
4	GOL	B	700[A]	-	5,5,5	0.33	0	5,5,5	0.30	0
4	GOL	D	701[A]	-	5,5,5	0.27	0	5,5,5	0.31	0
4	GOL	B	700[B]	-	5,5,5	0.41	0	5,5,5	0.41	0
4	GOL	D	701[B]	-	5,5,5	0.32	0	5,5,5	0.29	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
4	GOL	D	701[A]	-	-	4/4/4/4	-
4	GOL	B	700[B]	-	-	2/4/4/4	-
4	GOL	D	701[B]	-	-	4/4/4/4	-
4	GOL	B	700[A]	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	700[A]	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	700[B]	GOL	O1-C1-C2-C3
4	D	701[A]	GOL	O1-C1-C2-O2
4	D	701[A]	GOL	O1-C1-C2-C3
4	D	701[B]	GOL	O1-C1-C2-O2
4	D	701[B]	GOL	O1-C1-C2-C3
4	D	701[B]	GOL	C1-C2-C3-O3
4	D	701[B]	GOL	O2-C2-C3-O3
4	D	701[A]	GOL	C1-C2-C3-O3
4	B	700[A]	GOL	O2-C2-C3-O3
4	B	700[B]	GOL	O1-C1-C2-O2
4	B	700[A]	GOL	O1-C1-C2-C3
4	D	701[A]	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	700[A]	GOL	1	0
4	D	701[A]	GOL	2	0
4	B	700[B]	GOL	6	0
4	D	701[B]	GOL	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	598/621 (96%)	0.01	19 (3%)	47	46	10, 19, 32, 42	0
1	B	583/621 (93%)	0.06	20 (3%)	45	44	10, 19, 32, 41	0
1	C	592/621 (95%)	0.16	34 (5%)	23	23	10, 21, 35, 55	0
1	D	572/621 (92%)	0.22	35 (6%)	21	20	10, 22, 35, 47	0
All	All	2345/2484 (94%)	0.11	108 (4%)	32	31	10, 20, 34, 55	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	466	GLY	7.1
1	C	510	GLU	5.5
1	C	288	GLU	5.3
1	C	250	GLN	5.1
1	C	569	GLY	5.1
1	C	565	GLU	5.1
1	B	335	GLN	4.9
1	D	510	GLU	4.9
1	D	246	ARG	4.8
1	B	2	THR	4.8
1	A	335	GLN	4.7
1	B	596	ARG	4.7
1	C	594	ASP	4.6
1	C	246	ARG	4.6
1	A	568	HIS	4.6
1	D	613	MET	4.5
1	A	556	ASN	4.5
1	D	556	ASN	4.3
1	D	552	GLU	4.3
1	C	544	PRO	4.2
1	A	468	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	567	LYS	4.2
1	D	596	ARG	4.1
1	C	51	LYS	4.1
1	B	586	LEU	4.0
1	C	568	HIS	4.0
1	D	198	GLU	4.0
1	D	222	ASP	3.9
1	C	595	VAL	3.9
1	A	2	THR	3.9
1	D	539	GLN	3.9
1	D	468	GLU	3.9
1	D	23	SER	3.9
1	A	288	GLU	3.8
1	A	569	GLY	3.7
1	A	596	ARG	3.6
1	B	468	GLU	3.6
1	D	233	THR	3.6
1	B	288	GLU	3.5
1	D	51	LYS	3.5
1	C	467	GLU	3.5
1	C	584	GLU	3.4
1	A	337	ASN	3.4
1	B	528	GLU	3.4
1	B	556	ASN	3.3
1	B	146	GLU	3.3
1	B	476	GLU	3.3
1	A	44	ARG	3.3
1	B	615	ASP	3.3
1	C	145	GLU	3.2
1	B	246	ARG	3.2
1	B	595	VAL	3.1
1	C	39	GLY	3.1
1	B	337	ASN	3.1
1	A	567	LYS	3.1
1	C	259	GLY	3.0
1	D	476	GLU	3.0
1	D	455	ASP	3.0
1	D	234	ARG	3.0
1	D	424	ALA	3.0
1	D	22	ASP	2.9
1	C	552	GLU	2.9
1	C	22	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	20	GLU	2.9
1	C	556	ASN	2.8
1	D	525	ALA	2.8
1	C	258	LEU	2.8
1	D	257	ALA	2.7
1	C	469	ASP	2.7
1	A	146	GLU	2.7
1	C	233	THR	2.7
1	D	44	ARG	2.7
1	D	337	ASN	2.6
1	D	290	GLU	2.6
1	C	144	GLN	2.6
1	C	290	GLU	2.6
1	D	536	ASN	2.5
1	C	23	SER	2.5
1	A	469	ASP	2.5
1	C	536	ASN	2.5
1	A	51	LYS	2.5
1	C	335	GLN	2.4
1	C	143	GLU	2.4
1	D	469	ASP	2.4
1	D	478	ARG	2.4
1	B	552	GLU	2.3
1	B	534	ASN	2.3
1	C	541	ASP	2.3
1	C	180	GLY	2.3
1	B	469	ASP	2.2
1	C	20	GLU	2.2
1	B	554	GLN	2.2
1	B	439	PRO	2.2
1	D	4	ASN	2.2
1	D	537	VAL	2.2
1	D	540	TYR	2.1
1	D	187	ALA	2.1
1	A	290	GLU	2.1
1	C	542	PRO	2.1
1	A	80	THR	2.1
1	D	292	ALA	2.1
1	D	538	ARG	2.1
1	A	39	GLY	2.1
1	D	526	ASP	2.0
1	B	527	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	442	GLU	2.0
1	C	179	GLU	2.0
1	A	566	THR	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, 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	B-factors(Å^2)	Q<0.9
3	PO4	A	707	5/5	0.85	0.18	47,57,58,58	0
5	MG	B	706	1/1	0.85	0.26	43,43,43,43	0
4	GOL	D	701[B]	6/6	0.86	0.36	13,13,15,15	6
4	GOL	D	701[A]	6/6	0.86	0.36	12,13,13,15	6
4	GOL	B	700[B]	6/6	0.89	0.38	8,9,10,10	6
4	GOL	B	700[A]	6/6	0.89	0.38	8,9,10,11	6
2	CA	A	705	1/1	0.98	0.05	29,29,29,29	0
2	CA	D	703	1/1	0.98	0.05	32,32,32,32	0
2	CA	C	702	1/1	0.99	0.07	31,31,31,31	0
2	CA	B	704	1/1	1.00	0.03	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.