



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:46 PM UTC

PDB ID : 3FHA / pdb_00003fha
Title : Structure of endo-beta-N-acetylglucosaminidase A
Authors : Yin, J.; Li, L.; Shaw, N.; Li, Y.; Song, J.K.; Zhang, W.; Xia, C.; Zhang, R.;
Joachimiak, A.; Zhang, H.C.; Wang, L.X.; Wang, P.; Liu, Z.J.
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

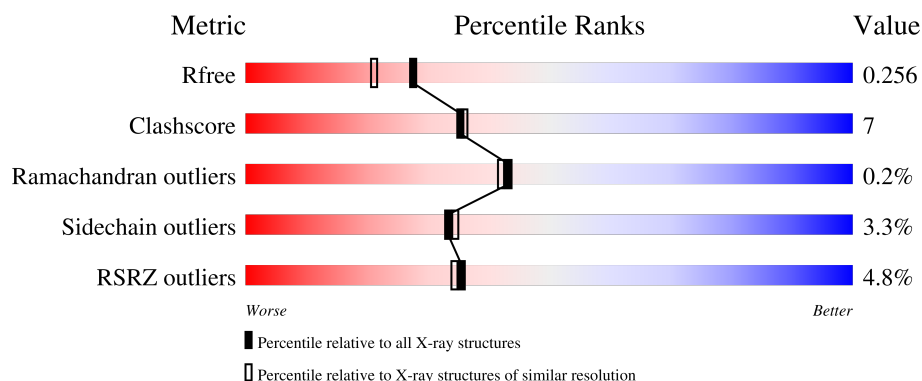
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

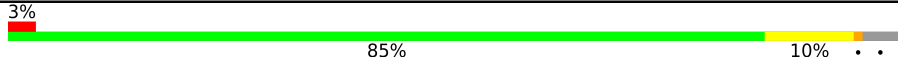
The reported resolution of this entry is 2.00 Å.

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	621	
1	B	621	
1	C	621	
1	D	621	

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

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

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 (CCD ID: CA) (formula: Ca).

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

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

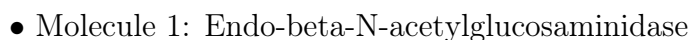
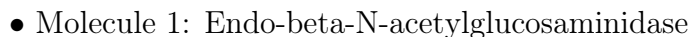
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

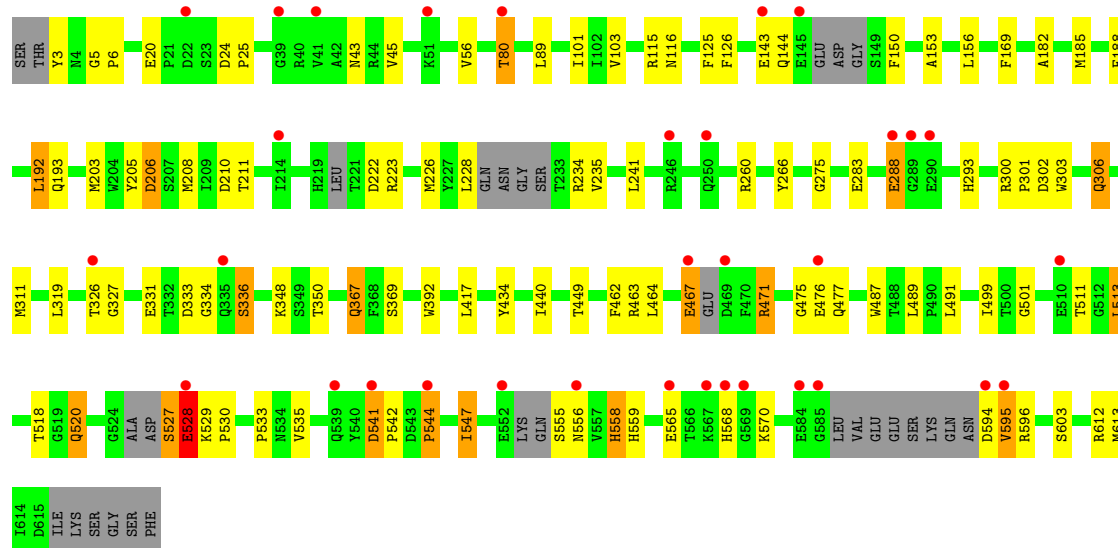
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

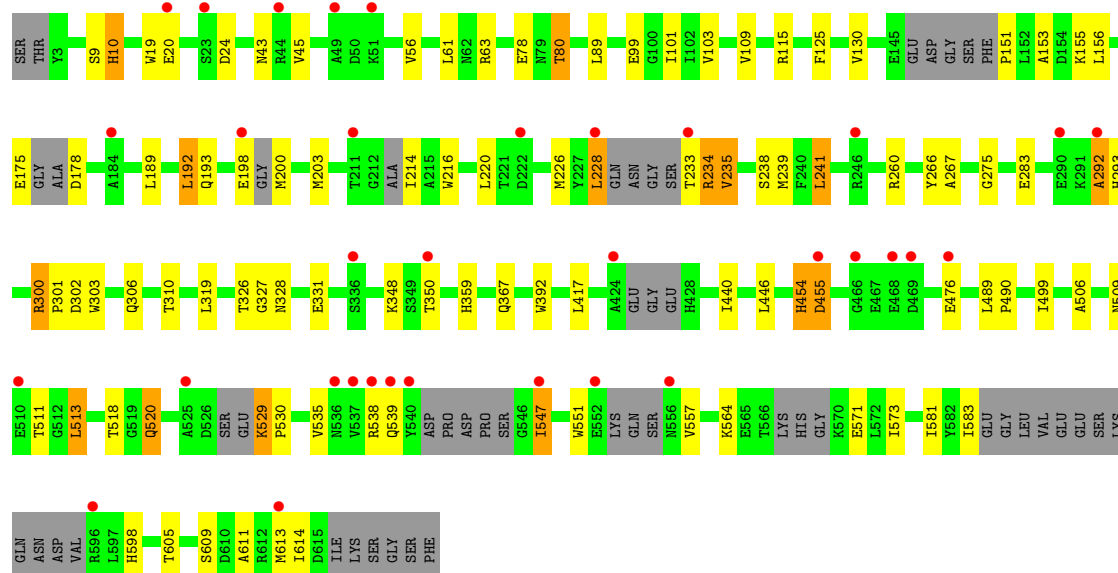
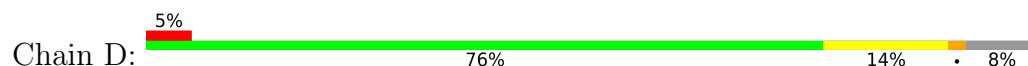
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	598	Total	O	0	0
			598	598		
6	B	602	Total	O	0	0
			602	602		
6	C	499	Total	O	0	0
			499	499		
6	D	472	Total	O	0	0
			472	472		

- Molecule 1: Endo-beta-N-acetylglucosaminidase





• Molecule 1: Endo-beta-N-acetylglucosaminidase



4 Data and refinement statistics

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 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 67.8 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (3.39%)	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)	0.38 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, CA, 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	0.67	8/4899 (0.2%)	0.81	4/6677 (0.1%)
1	B	0.66	10/4797 (0.2%)	0.78	1/6531 (0.0%)
1	C	0.72	9/4864 (0.2%)	0.86	10/6626 (0.2%)
1	D	0.69	9/4711 (0.2%)	0.80	12/6413 (0.2%)
All	All	0.69	36/19271 (0.2%)	0.82	27/26247 (0.1%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	455	ASP	C-N	-9.76	1.20	1.33
1	D	193	GLN	C-N	-9.06	1.21	1.34
1	D	454	HIS	C-N	-8.82	1.22	1.33
1	D	10	HIS	C-N	8.41	1.46	1.33
1	C	193	GLN	C-N	-8.07	1.22	1.33
1	B	10	HIS	C-N	7.80	1.44	1.33
1	D	292	ALA	CA-CB	-7.65	1.38	1.52
1	C	210	ASP	C-N	-7.58	1.23	1.34
1	C	334	GLY	C-O	-7.18	1.16	1.24
1	A	10	HIS	C-O	-7.01	1.15	1.23
1	A	194	GLU	C-O	-6.73	1.16	1.24
1	B	194	GLU	C-O	-6.64	1.16	1.24
1	D	9	SER	C-N	-6.37	1.25	1.33
1	B	572	LEU	C-O	-6.32	1.16	1.24
1	B	214	ILE	C-O	-6.22	1.17	1.23
1	B	195	GLN	C-O	-6.02	1.16	1.24
1	A	467	GLU	C-O	-5.94	1.16	1.23
1	A	551	TRP	C-O	-5.83	1.16	1.24
1	A	571	GLU	C-O	-5.69	1.17	1.24
1	B	49	ALA	CA-CB	-5.69	1.43	1.53
1	D	571	GLU	C-O	-5.67	1.17	1.24
1	C	541	ASP	C-O	-5.58	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	306	GLN	C-O	-5.56	1.17	1.24
1	A	148	GLY	C-O	-5.44	1.16	1.24
1	D	216	TRP	C-O	-5.42	1.17	1.23
1	C	570	LYS	C-O	-5.40	1.16	1.23
1	A	9	SER	C-O	-5.37	1.16	1.23
1	D	292	ALA	C-O	-5.30	1.19	1.24
1	B	213	ALA	CA-CB	-5.28	1.44	1.53
1	C	558	HIS	C-O	-5.26	1.18	1.24
1	C	535	VAL	CA-CB	-5.08	1.48	1.54
1	A	552	GLU	CB-CG	-5.08	1.37	1.52
1	C	544	PRO	C-O	-5.04	1.18	1.24
1	B	196	LYS	C-O	-5.04	1.17	1.23
1	B	614	ILE	C-O	-5.03	1.19	1.24
1	B	213	ALA	C-O	-5.02	1.17	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	529	LYS	N-CA-C	-8.47	99.40	110.07
1	D	454	HIS	O-C-N	6.84	131.12	122.22
1	D	506	ALA	CA-C-N	6.48	132.72	122.74
1	D	506	ALA	C-N-CA	6.48	132.72	122.74
1	A	543	ASP	CA-C-N	6.45	126.37	119.28
1	A	543	ASP	C-N-CA	6.45	126.37	119.28
1	C	210	ASP	CA-C-N	6.17	129.69	120.31
1	C	210	ASP	C-N-CA	6.17	129.69	120.31
1	C	528	GLU	N-CA-CB	6.07	118.55	110.29
1	C	288	GLU	N-CA-C	5.93	123.43	110.80
1	D	455	ASP	O-C-N	-5.78	115.80	121.87
1	C	306	GLN	N-CA-C	5.75	118.50	111.82
1	D	520	GLN	N-CA-C	5.67	117.72	108.76
1	D	20	GLU	CB-CA-C	5.56	117.55	110.16
1	C	528	GLU	CA-CB-CG	5.42	124.95	114.10
1	D	234	ARG	N-CA-C	5.41	117.61	109.23
1	A	147	ASP	N-CA-CB	-5.34	101.46	110.49
1	C	126	PHE	CA-C-N	5.25	123.44	119.66
1	C	126	PHE	C-N-CA	5.25	123.44	119.66
1	D	506	ALA	O-C-N	-5.24	117.08	123.10
1	C	568	HIS	N-CA-C	5.20	119.58	112.88
1	A	206	ASP	N-CA-C	5.12	117.89	108.58
1	D	292	ALA	N-CA-C	5.09	116.05	108.31
1	B	214	ILE	CB-CA-C	5.07	116.71	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	547	ILE	N-CA-C	5.05	116.87	108.99
1	D	24	ASP	CA-C-N	5.02	124.68	119.56
1	D	24	ASP	C-N-CA	5.02	124.68	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4755	0	4351	41	0
1	B	4660	0	4269	69	0
1	C	4722	0	4323	76	0
1	D	4577	0	4204	78	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	14	0
6	C	499	0	0	10	0
6	D	472	0	0	6	0
All	All	20919	0	17179	264	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 (264) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:56:VAL:HG21	1:D:203:MET:HE1	1.49	0.93
1:B:595:VAL:CG2	6:B:740:HOH:O	2.22	0.87
1:C:56:VAL:HG11	1:C:203:MET:HE1	1.57	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:A:56:VAL:HG21	1:A:203:MET:HE1	1.55	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:D:292:ALA:HB1	1:D:293:HIS:C	2.05	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:B:56:VAL:HG11	1:B:203:MET:HE1	1.65	0.78
1:D:228:LEU:HD23	1:D:239:MET:HB2	1.67	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:43:ASN:HD22	1:C:392:TRP:NE1	1.84	0.71
1:B:311:MET:H	4:B:700[B]:GOL:C3	2.03	0.71
1:B:43:ASN:HD22	1:B:392:TRP:NE1	1.83	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:D:43:ASN:HD22	1:D:392:TRP:NE1	1.85	0.68
1:B:56:VAL:HG13	1:B:266:TYR:CE1	2.27	0.68
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:A:43:ASN:HD22	1:A:392:TRP:NE1	1.86	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ILE:HD11	1:A:499:ILE:HG13	1.80	0.62
1:D:476:GLU:CD	1:D:490:PRO:HD2	2.25	0.62
1:B:501:GLY:C	6:B:2099:HOH:O	2.43	0.61
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
1:C:462:PHE:O	1:C:471[A]:ARG:HG2	2.04	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: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:509:ASN:C	6:B:936:HOH:O	2.48	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:C:565:GLU:HG3	1:C:596:ARG:NH2	2.21	0.56
1:D:80:THR:O	1:D:80:THR:OG1	2.23	0.56
1:D:233:THR:HG22	6:D:1585:HOH:O	2.05	0.56
1:C:283:GLU:H	1:C:283:GLU:CD	2.15	0.55
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
1:A:206:ASP:CG	1:A:206:ASP:O	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:470:PHE:CD1	6:B:2099:HOH:O	2.61	0.53
1:D:283:GLU:CD	1:D:283:GLU:H	2.14	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:C:143:GLU:C	6:C:1838:HOH:O	2.53	0.52
1:A:80:THR:O	1:A:80:THR:OG1	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: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
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:206:ASP:CG	1:C:206:ASP:O	2.55	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:B:283:GLU:CD	1:B:283:GLU:H	2.19	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:B:310:THR:HB	4:B:700[B]:GOL:C1	2.38	0.49
1:D:228:LEU:HD21	1:D:238:SER:C	2.37	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:198:GLU:C	1:D:200:MET:N	2.71	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:C:596:ARG:HG3	1:C:613:MET:HE2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:222:ASP:O	1:C:226:MET:HE1	2.15	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: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:C:80:THR:O	1:C:80:THR:OG1	2.31	0.46
1:B:153:ALA:HB1	1:B:192:LEU:HD13	1.97	0.46
1:D:529:LYS:O	1:D:529:LYS:HG2	2.09	0.46
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: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:C:367:GLN:OE1	1:C:369:SER:OG	2.18	0.45
1:A:283:GLU:H	1:A:283:GLU:CD	2.25	0.45
1:A:511:THR:CG2	1:A:513:LEU:HB2	2.42	0.45
1:C:527:SER:O	1:C:528:GLU:C	2.54	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:THR:HG21	1:B:331:GLU:O	2.17	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:D:228:LEU:C	1:D:235:VAL:HG13	2.43	0.43
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:B:554:GLN:CD	6:B:792:HOH:O	2.62	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:D:19:TRP:O	1:D:155:LYS:NZ	2.52	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
1:A:509:ASN:OD1	1:A:511:THR:HB	2.19	0.42
1:C:182:ALA:HA	1:C:208:MET:HE3	2.02	0.42
1:D:151:PRO:N	6:D:1020:HOH:O	2.52	0.42
1:D:228:LEU:HD23	1:D:239:MET:HE3	2.00	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:C:527:SER:C	1:C:528:GLU:O	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:185:MET:HE3	1:C:188:PHE:HB3	2.03	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:B:20:GLU:CD	1:B:21:PRO:HD2	2.45	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	587/621 (94%)	571 (97%)	15 (3%)	1 (0%)	43	42
1	B	563/621 (91%)	546 (97%)	16 (3%)	1 (0%)	43	42
1	C	577/621 (93%)	558 (97%)	16 (3%)	3 (0%)	24	21
1	D	548/621 (88%)	530 (97%)	18 (3%)	0	100	100
All	All	2275/2484 (92%)	2205 (97%)	65 (3%)	5 (0%)	43	42

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 ⓘ

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%)	482 (98%)	12 (2%)	43	47
1	B	486/515 (94%)	471 (97%)	15 (3%)	35	37
1	C	490/515 (95%)	470 (96%)	20 (4%)	27	26
1	D	476/515 (92%)	458 (96%)	18 (4%)	29	29
All	All	1946/2060 (94%)	1881 (97%)	65 (3%)	33	34

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	80	THR
1	A	103	VAL
1	A	192	LEU
1	A	241	LEU
1	A	250	GLN
1	A	300	ARG
1	A	367	GLN
1	A	401	LEU
1	A	513	LEU
1	A	520	GLN
1	A	549	LEU
1	B	45	VAL
1	B	50	ASP
1	B	80	THR
1	B	103	VAL
1	B	192	LEU

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Mol	Chain	Res	Type
1	B	241	LEU
1	B	250	GLN
1	B	300	ARG
1	B	348	LYS
1	B	367	GLN
1	B	439	PRO
1	B	446	LEU
1	B	513	LEU
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	234	ARG
1	C	241	LEU
1	C	306	GLN
1	C	336	SER
1	C	348	LYS
1	C	367	GLN
1	C	467	GLU
1	C	471[A]	ARG
1	C	471[B]	ARG
1	C	477	GLN
1	C	491	LEU
1	C	513	LEU
1	C	520	GLN
1	C	527	SER
1	C	528	GLU
1	C	547	ILE
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	300	ARG
1	D	348	LYS
1	D	367	GLN

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Mol	Chain	Res	Type
1	D	446	LEU
1	D	513	LEU
1	D	529	LYS
1	D	547	ILE
1	D	557	VAL
1	D	614	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	46	ASN
1	A	64	HIS
1	A	134	GLN
1	A	186	GLN
1	A	242	ASN
1	A	428	HIS
1	A	459	ASN
1	A	482	ASN
1	B	43	ASN
1	B	64	HIS
1	B	134	GLN
1	B	219	HIS
1	B	242	ASN
1	B	250	GLN
1	B	454	HIS
1	B	486	GLN
1	C	4	ASN
1	C	10	HIS
1	C	33	HIS
1	C	43	ASN
1	C	48	ASN
1	C	486	GLN
1	C	548	GLN
1	C	558	HIS
1	D	10	HIS
1	D	43	ASN
1	D	64	HIS
1	D	242	ASN
1	D	250	GLN
1	D	477	GLN
1	D	486	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	GOL	B	700[A]	-	5,5,5	0.33	0	5,5,5	0.31	0
4	GOL	B	700[B]	-	5,5,5	0.41	0	5,5,5	0.44	0
4	GOL	D	701[A]	-	5,5,5	0.28	0	5,5,5	0.35	0
3	PO4	A	707	-	4,4,4	0.91	0	6,6,6	0.51	0
4	GOL	D	701[B]	-	5,5,5	0.33	0	5,5,5	0.31	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[B]	-	-	4/4/4/4	-
4	GOL	B	700[B]	-	-	2/4/4/4	-
4	GOL	D	701[A]	-	-	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
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	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	C1-C2-C3-O3
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	B	700[B]	GOL	6	0
4	D	701[A]	GOL	2	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	598/621 (96%)	0.08	16 (2%) 56 55	10, 19, 32, 42	0
1	B	583/621 (93%)	0.17	29 (4%) 34 33	10, 19, 32, 41	0
1	C	592/621 (95%)	0.31	33 (5%) 30 29	10, 21, 35, 55	1 (0%)
1	D	572/621 (92%)	0.36	34 (5%) 28 27	10, 22, 35, 47	0
All	All	2345/2484 (94%)	0.23	112 (4%) 35 34	10, 20, 34, 55	1 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	556	ASN	6.0
1	B	596	ARG	5.9
1	C	569	GLY	5.3
1	C	565	GLU	4.9
1	D	556	ASN	4.8
1	A	288	GLU	4.6
1	C	288	GLU	4.6
1	C	250	GLN	4.6
1	C	510	GLU	4.5
1	B	595	VAL	4.5
1	A	468	GLU	4.5
1	B	554	GLN	4.4
1	D	552	GLU	4.4
1	B	476	GLU	4.3
1	B	335	GLN	4.2
1	B	556	ASN	4.1
1	B	586	LEU	4.1
1	D	198	GLU	4.1
1	D	613	MET	4.0
1	B	246	ARG	4.0
1	D	525	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	468	GLU	3.9
1	B	288	GLU	3.8
1	B	528	GLU	3.8
1	D	466	GLY	3.7
1	D	539	GLN	3.7
1	D	476	GLU	3.7
1	B	2	THR	3.7
1	D	222	ASP	3.6
1	A	596	ARG	3.5
1	C	467	GLU	3.5
1	C	585	GLY	3.4
1	A	335	GLN	3.4
1	A	44	ARG	3.4
1	D	510	GLU	3.3
1	D	468	GLU	3.3
1	B	146	GLU	3.2
1	C	584	GLU	3.2
1	C	568	HIS	3.2
1	B	615	ASP	3.2
1	B	534	ASN	3.2
1	D	596	ARG	3.2
1	D	540	TYR	3.1
1	D	290	GLU	3.0
1	C	594	ASP	3.0
1	A	2	THR	3.0
1	D	233	THR	3.0
1	D	455	ASP	3.0
1	C	246	ARG	3.0
1	B	555	SER	3.0
1	A	325	SER	2.9
1	C	556	ASN	2.9
1	C	552	GLU	2.9
1	D	246	ARG	2.9
1	B	552	GLU	2.9
1	D	292	ALA	2.9
1	B	426	GLY	2.9
1	D	350	THR	2.8
1	D	51	LYS	2.7
1	C	544	PRO	2.7
1	C	145	GLU	2.7
1	A	568	HIS	2.6
1	C	567	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	80	THR	2.6
1	C	290	GLU	2.5
1	B	147	ASP	2.4
1	C	528	GLU	2.4
1	D	538	ARG	2.4
1	A	290	GLU	2.4
1	B	584	GLU	2.4
1	D	23	SER	2.4
1	C	80	THR	2.4
1	D	49	ALA	2.4
1	C	595	VAL	2.4
1	C	22	ASP	2.3
1	D	469	ASP	2.3
1	C	214	ILE	2.3
1	D	547	ILE	2.3
1	C	143	GLU	2.3
1	C	335	GLN	2.3
1	D	44	ARG	2.3
1	D	424	ALA	2.3
1	D	336	SER	2.2
1	D	211	THR	2.2
1	D	537	VAL	2.2
1	C	469	ASP	2.2
1	C	541	ASP	2.2
1	A	39	GLY	2.2
1	D	20	GLU	2.2
1	B	325	SER	2.2
1	C	326	THR	2.2
1	D	536	ASN	2.2
1	B	231	GLY	2.2
1	B	23	SER	2.2
1	B	488	THR	2.2
1	B	20	GLU	2.2
1	C	39	GLY	2.2
1	C	289	GLY	2.2
1	D	228	LEU	2.2
1	A	23	SER	2.2
1	C	41	VAL	2.1
1	A	466	GLY	2.1
1	D	184	ALA	2.1
1	A	586	LEU	2.1
1	A	326	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	56	VAL	2.1
1	B	531	ALA	2.1
1	C	476	GLU	2.1
1	B	585	GLY	2.1
1	C	539	GLN	2.0
1	B	565	GLU	2.0
1	C	51	LYS	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 oligosaccharides 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
4	GOL	D	701[A]	6/6	0.77	0.20	12,13,13,15	6
4	GOL	D	701[B]	6/6	0.77	0.20	13,13,15,15	6
4	GOL	B	700[A]	6/6	0.79	0.19	8,9,10,11	6
4	GOL	B	700[B]	6/6	0.79	0.19	8,9,10,10	6
3	PO4	A	707	5/5	0.83	0.17	47,57,58,58	0
5	MG	B	706	1/1	0.83	0.25	43,43,43,43	0
2	CA	A	705	1/1	0.96	0.06	29,29,29,29	0
2	CA	D	703	1/1	0.96	0.04	32,32,32,32	0
2	CA	C	702	1/1	0.98	0.08	31,31,31,31	0
2	CA	B	704	1/1	0.99	0.03	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.