



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:06 AM UTC

PDB ID : 3GXM / pdb_00003gxm
Title : Crystal structure of acid-beta-glucosidase at pH 4.5, phosphate crystallization condition
Authors : Lieberman, R.L.
Deposited on : 2009-04-02
Resolution : 2.20 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

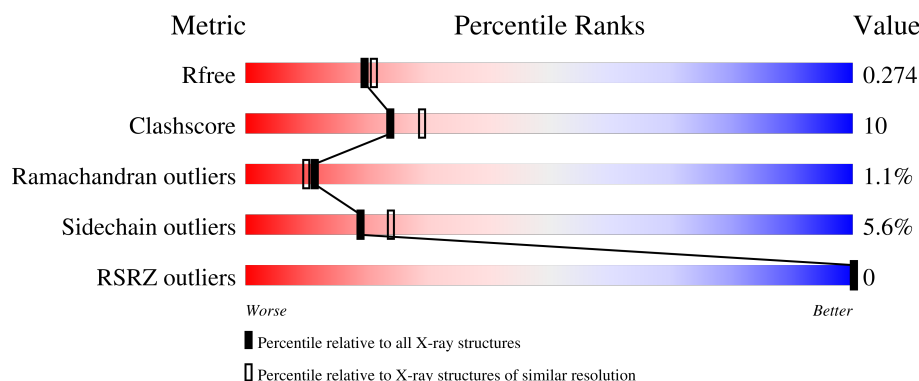
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	497	 78% 19% .
1	B	497	 77% 19% .
1	C	497	 77% 20% ..
1	D	497	 77% 20% ..

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
2	NAG	D	498	X	-	-	-
3	SO4	A	506	-	-	X	-
3	SO4	B	503	-	-	X	-
3	SO4	C	504	-	-	X	-
3	SO4	D	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17060 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 Glucosylceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3930	2532	671	711	16			
1	B	497	Total	C	N	O	S	0	0	0
			3930	2532	671	711	16			
1	C	497	Total	C	N	O	S	0	0	0
			3930	2532	671	711	16			
1	D	497	Total	C	N	O	S	0	0	0
			3930	2532	671	711	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	HIS	ARG	variant	UNP P04062
B	495	HIS	ARG	variant	UNP P04062
C	495	HIS	ARG	variant	UNP P04062
D	495	HIS	ARG	variant	UNP P04062

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

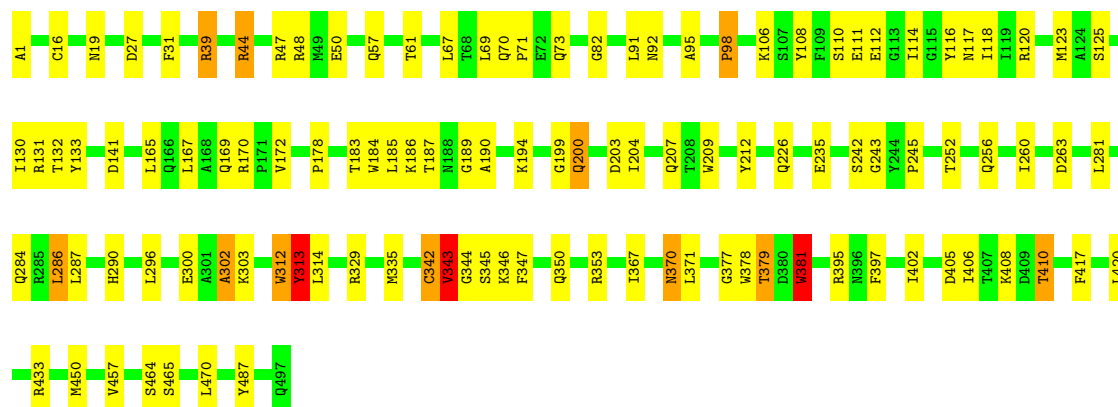
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

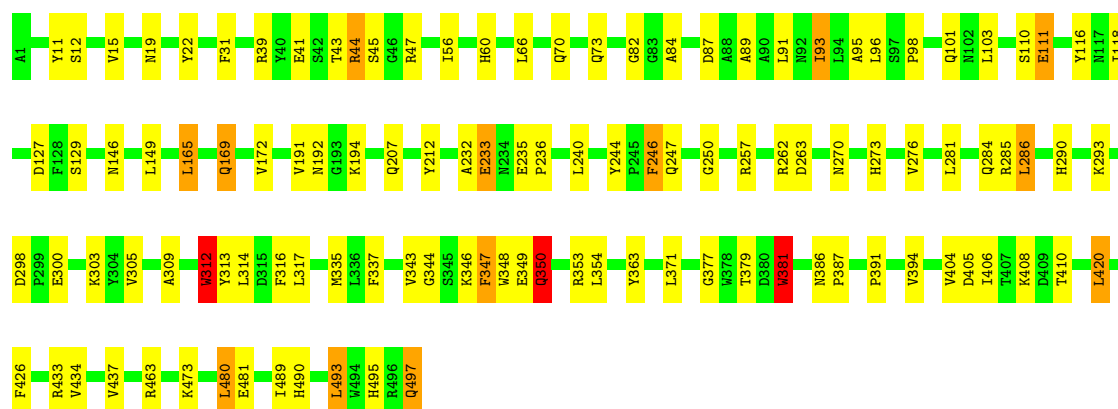
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	288	Total	O	0	0
			288	288		
4	B	272	Total	O	0	0
			272	272		
4	C	290	Total	O	0	0
			290	290		
4	D	294	Total	O	0	0
			294	294		



• Molecule 1: Glucosylceramidase

Chain D: 77% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.50Å 91.78Å 152.75Å 90.00° 111.24° 90.00°	Depositor
Resolution (Å)	34.34 – 2.20 34.34 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.3 (34.34-2.20) 96.1 (34.34-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.276 0.220 , 0.274	Depositor DCC
R_{free} test set	6970 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 12.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.459 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17060	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4

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	0.91	0/4051	1.07	12/5523 (0.2%)
1	B	0.90	0/4051	1.06	16/5523 (0.3%)
1	C	0.96	2/4051 (0.0%)	1.14	15/5523 (0.3%)
1	D	0.91	1/4051 (0.0%)	1.02	6/5523 (0.1%)
All	All	0.92	3/16204 (0.0%)	1.08	49/22092 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	235	GLU	CA-C	6.65	1.57	1.53
1	D	235	GLU	C-O	5.41	1.26	1.23
1	C	235	GLU	C-O	5.08	1.26	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ASN	N-CA-C	-10.54	88.36	110.80
1	D	98	PRO	N-CA-C	8.96	121.64	110.70
1	A	318	ALA	CA-C-N	8.43	128.38	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	ALA	C-N-CA	8.43	128.38	120.03
1	C	313	TYR	CA-C-N	7.16	134.60	121.70
1	C	313	TYR	C-N-CA	7.16	134.60	121.70
1	D	312	TRP	N-CA-C	7.03	121.13	108.48
1	B	62	GLY	CA-C-N	6.50	133.40	121.70
1	B	62	GLY	C-N-CA	6.50	133.40	121.70
1	B	31	PHE	CA-C-N	-6.36	113.39	120.14
1	B	31	PHE	C-N-CA	-6.36	113.39	120.14
1	B	54	GLY	CA-C-N	6.32	126.82	119.99
1	B	54	GLY	C-N-CA	6.32	126.82	119.99
1	C	302	ALA	N-CA-C	6.28	118.93	111.71
1	A	343	VAL	N-CA-C	6.28	122.39	109.34
1	B	114	ILE	N-CA-C	6.21	118.07	112.17
1	C	98	PRO	N-CA-C	6.20	118.26	110.70
1	D	305	VAL	N-CA-C	5.88	116.27	107.51
1	B	98	PRO	N-CA-C	5.87	117.86	110.70
1	C	312	TRP	CB-CA-C	-5.80	104.09	111.22
1	D	363	TYR	N-CA-C	5.50	116.95	111.07
1	D	246	PHE	N-CA-C	5.49	116.97	109.18
1	C	31	PHE	CA-C-N	5.39	126.58	119.84
1	C	31	PHE	C-N-CA	5.39	126.58	119.84
1	B	286	LEU	CA-CB-CG	5.37	135.11	116.30
1	B	319	PRO	CA-C-N	5.34	131.32	121.70
1	B	319	PRO	C-N-CA	5.34	131.32	121.70
1	A	157	LYS	N-CA-C	5.34	117.53	111.02
1	A	250	GLY	N-CA-C	5.33	118.49	111.03
1	A	132	THR	N-CA-C	-5.28	103.42	110.55
1	C	252	THR	N-CA-C	-5.25	102.51	110.39
1	A	112	GLU	N-CA-C	-5.22	106.91	113.28
1	A	114	ILE	N-CA-C	5.22	117.13	112.17
1	A	84	ALA	N-CA-C	5.16	117.66	109.24
1	B	80	GLY	N-CA-C	5.16	116.99	110.38
1	C	44	ARG	CB-CG-CD	-5.16	99.43	111.30
1	B	92	ASN	N-CA-C	5.15	116.58	111.07
1	A	80	GLY	N-CA-C	5.13	116.95	110.38
1	B	6	PRO	N-CA-C	5.11	118.52	110.80
1	C	141	ASP	N-CA-C	-5.09	102.53	109.71
1	C	70	GLN	CA-C-N	5.05	124.71	119.56
1	C	70	GLN	C-N-CA	5.05	124.71	119.56
1	B	149	LEU	CA-C-N	5.04	126.38	120.98
1	B	149	LEU	C-N-CA	5.04	126.38	120.98
1	C	185	LEU	N-CA-C	-5.04	107.12	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	ALA	N-CA-C	5.04	117.45	109.24
1	C	114	ILE	N-CA-C	5.04	116.95	112.17
1	A	121	VAL	CA-C-N	-5.03	114.77	119.85
1	A	121	VAL	C-N-CA	-5.03	114.77	119.85

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	342	CYS	Peptide
1	B	344	GLY	Peptide
1	C	91	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3930	0	3843	82	0
1	B	3930	0	3843	80	0
1	C	3930	0	3843	73	0
1	D	3930	0	3843	92	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	40	0	0	7	0
3	B	35	0	0	5	0
3	C	35	0	0	4	0
3	D	30	0	0	4	0
4	A	288	0	0	8	0
4	B	272	0	0	7	0
4	C	290	0	0	11	0
4	D	294	0	0	13	0
All	All	17060	0	15424	315	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 10.

All (315) 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:C:39:ARG:HG2	1:C:39:ARG:HH11	1.25	0.97
1:C:343:VAL:HB	1:C:344:GLY:HA2	1.51	0.93
1:D:11:TYR:HE2	1:D:353:ARG:HE	1.19	0.90
1:C:245:PRO:HG3	1:D:348:TRP:HB3	1.54	0.89
1:D:31:PHE:HD1	4:D:664:HOH:O	1.58	0.86
1:C:342:CYS:SG	1:C:343:VAL:N	2.48	0.86
1:A:44:ARG:HD2	3:A:506:SO4:O2	1.77	0.85
1:B:319:PRO:HA	1:B:320:ALA:HB2	1.61	0.82
1:B:70:GLN:NE2	1:B:437:VAL:HG21	1.94	0.82
1:C:243:GLY:O	1:D:348:TRP:CD1	2.36	0.78
1:D:95:ALA:CB	1:D:406:ILE:HD13	2.15	0.77
1:D:312:TRP:HH2	1:D:316:PHE:C	1.93	0.76
1:B:62:GLY:HA2	1:B:63:THR:OG1	1.84	0.76
1:B:495:HIS:HD2	4:B:853:HOH:O	1.68	0.75
1:D:284:GLN:HE22	1:D:313:TYR:HE1	1.34	0.75
1:C:169:GLN:HG3	1:C:170:ARG:H	1.52	0.75
1:D:312:TRP:CH2	1:D:316:PHE:C	2.66	0.74
1:B:5:ILE:HD12	1:B:22:TYR:CE2	2.23	0.73
1:B:96:LEU:HD21	1:B:404:VAL:HG13	1.70	0.72
1:D:270:ASN:ND2	4:D:614:HOH:O	2.21	0.72
1:B:345:SER:O	1:B:346:LYS:C	2.32	0.72
1:D:56:ILE:HG12	1:D:480:LEU:HD22	1.72	0.72
1:D:149:LEU:O	4:D:665:HOH:O	2.08	0.72
1:A:207:GLN:NE2	1:A:263:ASP:OD1	2.22	0.71
1:A:194:LYS:HB2	1:A:242:SER:HA	1.71	0.71
1:A:132:THR:O	1:A:133:TYR:HB3	1.89	0.71
1:A:243:GLY:O	1:B:348:TRP:CD1	2.45	0.70
1:D:44:ARG:HD3	3:D:502:SO4:O4	1.91	0.70
1:B:68:THR:HG23	1:B:473:LYS:HB3	1.74	0.69
1:C:165:LEU:HD22	1:C:172:VAL:HB	1.75	0.68
1:C:44:ARG:HD3	3:C:504:SO4:O1	1.94	0.67
1:B:165:LEU:HD22	1:B:172:VAL:HB	1.77	0.67
1:C:120:ARG:HB2	1:C:379:THR:HG21	1.77	0.67
1:C:313:TYR:HE2	4:C:1068:HOH:O	1.76	0.67
1:C:300:GLU:HG2	4:C:755:HOH:O	1.95	0.66
1:C:313:TYR:HB3	1:C:314:LEU:HB2	1.77	0.66
1:A:342:CYS:SG	1:A:343:VAL:N	2.69	0.65
3:A:504:SO4:O1	1:B:441:LYS:NZ	2.30	0.65
1:C:44:ARG:CD	3:C:504:SO4:O1	2.44	0.65
1:D:60:HIS:HE1	4:D:955:HOH:O	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LYS:HB2	1:B:242:SER:HA	1.79	0.64
1:B:207:GLN:NE2	1:B:263:ASP:OD1	2.30	0.64
1:D:93:ILE:O	1:D:101:GLN:HG2	1.97	0.64
1:A:328:HIS:HD2	4:A:1103:HOH:O	1.81	0.64
1:C:313:TYR:CE2	4:C:1068:HOH:O	2.49	0.64
1:D:314:LEU:HB2	1:D:343:VAL:HG12	1.79	0.64
1:B:319:PRO:CA	1:B:320:ALA:HB2	2.28	0.63
1:C:406:ILE:HG23	4:C:729:HOH:O	1.97	0.63
1:D:89:ALA:O	1:D:93:ILE:HG23	1.98	0.63
1:A:243:GLY:O	1:B:348:TRP:HD1	1.81	0.63
1:D:408:LYS:O	1:D:410:THR:HG23	2.00	0.62
1:B:31:PHE:HB3	4:B:935:HOH:O	1.99	0.62
1:A:408:LYS:HB3	1:A:410:THR:HG23	1.82	0.62
1:C:169:GLN:NE2	4:C:817:HOH:O	2.23	0.61
1:A:245:PRO:HD3	1:B:348:TRP:CG	2.36	0.61
1:D:44:ARG:CD	3:D:502:SO4:O4	2.49	0.61
1:A:209:TRP:CZ3	1:A:212:TYR:CD2	2.89	0.60
1:A:41:GLU:HG3	1:A:490:HIS:CD2	2.35	0.60
1:D:284:GLN:NE2	1:D:313:TYR:HE1	1.98	0.60
1:B:70:GLN:NE2	1:B:437:VAL:CG2	2.63	0.60
1:A:254:GLU:OE2	4:A:579:HOH:O	2.17	0.60
1:A:284:GLN:HG3	1:A:314:LEU:HD12	1.84	0.59
1:D:95:ALA:HB1	1:D:406:ILE:HD13	1.83	0.59
1:B:473:LYS:HG3	1:B:479:PHE:CE2	2.38	0.59
1:D:495:HIS:HD2	4:D:1066:HOH:O	1.84	0.59
1:A:343:VAL:HG13	1:A:344:GLY:H	1.67	0.59
1:D:12:SER:OG	3:D:499:SO4:O2	2.20	0.59
1:B:62:GLY:CA	1:B:63:THR:OG1	2.49	0.59
1:C:39:ARG:HH11	1:C:39:ARG:CG	2.10	0.59
1:A:44:ARG:CD	3:A:506:SO4:O2	2.50	0.58
1:C:284:GLN:HB2	1:C:286:LEU:HD13	1.84	0.58
1:B:349:GLU:HG3	1:B:353:ARG:NH2	2.18	0.58
1:D:290:HIS:HA	1:D:293:LYS:HD2	1.86	0.58
1:D:165:LEU:HD22	1:D:172:VAL:HB	1.86	0.58
1:C:379:THR:HG22	4:C:719:HOH:O	2.03	0.58
1:D:386:ASN:HB2	1:D:387:PRO:HD2	1.86	0.58
1:B:226:GLN:HG3	3:B:502:SO4:O1	2.04	0.57
1:C:71:PRO:HB3	1:C:450:MET:HE1	1.85	0.57
1:D:207:GLN:NE2	1:D:263:ASP:OD1	2.32	0.57
1:A:253:PRO:HB2	1:A:294:VAL:HG11	1.86	0.57
1:C:343:VAL:CB	1:C:344:GLY:HA2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:GLU:HG2	1:D:353:ARG:NH1	2.18	0.57
1:A:396:ASN:HB2	4:A:745:HOH:O	2.04	0.56
1:C:284:GLN:CB	1:C:286:LEU:HD13	2.35	0.56
1:A:44:ARG:HB3	3:A:506:SO4:O2	2.05	0.56
1:C:408:LYS:O	1:C:410:THR:HG23	2.06	0.56
1:D:11:TYR:CE2	1:D:353:ARG:NE	2.64	0.56
1:B:284:GLN:HB2	1:B:286:LEU:HD13	1.86	0.56
1:D:87:ASP:HB2	1:D:129:SER:HA	1.87	0.56
1:D:463:ARG:NH2	4:D:948:HOH:O	2.38	0.56
1:A:44:ARG:NH1	3:A:506:SO4:O1	2.40	0.55
1:B:346:LYS:O	1:B:349:GLU:O	2.24	0.55
1:C:284:GLN:HG3	1:C:314:LEU:HD12	1.88	0.55
1:D:192:ASN:HB2	1:D:244:TYR:O	2.07	0.55
1:B:151:GLU:HB2	1:C:130:ILE:HD11	1.88	0.55
1:C:408:LYS:O	1:C:410:THR:CG2	2.55	0.55
1:D:312:TRP:HH2	1:D:317:LEU:N	2.04	0.55
1:C:117:ASN:HA	1:C:172:VAL:HG22	1.88	0.55
1:D:91:LEU:HD23	1:D:391:PRO:HG3	1.87	0.55
1:A:426:PHE:HB3	1:A:493:LEU:HD21	1.88	0.54
1:B:347:PHE:CE1	1:B:348:TRP:HZ3	2.24	0.54
1:C:183:THR:O	1:C:189:GLY:HA2	2.06	0.54
1:A:287:LEU:HB3	1:A:291:TRP:CD1	2.42	0.54
1:B:211:ARG:HD2	4:B:983:HOH:O	2.07	0.54
1:B:95:ALA:CB	1:B:406:ILE:HD13	2.38	0.54
1:C:39:ARG:HG2	1:C:39:ARG:NH1	2.02	0.54
1:A:266:PRO:HB2	4:A:909:HOH:O	2.07	0.54
1:B:70:GLN:HE22	1:B:437:VAL:HG21	1.68	0.54
1:C:377:GLY:C	1:C:378:TRP:CE3	2.85	0.54
1:B:232:ALA:O	1:B:233:GLU:HB2	2.09	0.53
1:D:312:TRP:CH2	1:D:316:PHE:O	2.61	0.53
1:B:371:LEU:O	1:B:433:ARG:HD2	2.08	0.53
1:D:349:GLU:OE1	1:D:353:ARG:HD2	2.07	0.53
1:A:339:SER:O	1:A:379:THR:HG22	2.08	0.53
1:B:57:GLN:HG3	1:B:481:GLU:OE1	2.08	0.53
1:C:82:GLY:HA3	1:C:118:ILE:O	2.09	0.53
1:C:245:PRO:CG	1:D:348:TRP:HB3	2.35	0.53
1:D:22:TYR:CD2	1:D:22:TYR:C	2.87	0.52
1:A:245:PRO:HD3	1:B:348:TRP:HB3	1.92	0.52
1:A:396:ASN:CB	4:A:745:HOH:O	2.58	0.52
1:A:120:ARG:NH2	1:A:234:ASN:OD1	2.35	0.52
1:A:152:GLU:HA	1:A:156:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:SER:HB3	3:D:502:SO4:O2	2.11	0.51
1:B:93:ILE:O	1:B:101:GLN:HG2	2.10	0.51
1:C:106:LYS:HG2	1:C:167:LEU:HD22	1.93	0.51
1:A:408:LYS:O	1:A:410:THR:HG23	2.09	0.51
1:B:44:ARG:CD	3:B:503:SO4:O3	2.58	0.51
1:B:19:ASN:O	1:B:103:LEU:HD12	2.11	0.51
1:D:381:TRP:HE3	1:D:381:TRP:HA	1.76	0.51
1:A:82:GLY:HA3	1:A:118:ILE:O	2.11	0.50
1:C:116:TYR:OH	1:C:420:LEU:HD13	2.11	0.50
1:D:381:TRP:HA	1:D:381:TRP:CE3	2.45	0.50
1:A:140:ASP:N	1:A:140:ASP:OD1	2.43	0.50
1:B:44:ARG:HD2	3:B:503:SO4:O3	2.12	0.50
1:B:306:HIS:ND1	3:B:505:SO4:O1	2.43	0.50
1:B:319:PRO:CA	1:B:320:ALA:CB	2.89	0.50
1:A:365:HIS:HD2	1:A:445:ASP:OD2	1.94	0.50
1:B:319:PRO:HA	1:B:320:ALA:CB	2.39	0.50
1:A:450:MET:HE3	1:A:454:GLY:HA2	1.93	0.50
1:D:426:PHE:HB3	1:D:493:LEU:HD21	1.94	0.50
1:C:19:ASN:HB2	4:C:516:HOH:O	2.12	0.49
1:A:120:ARG:HB2	1:A:379:THR:HG21	1.95	0.49
1:D:116:TYR:OH	1:D:420:LEU:HD13	2.11	0.49
1:C:286:LEU:HD22	1:C:287:LEU:HG	1.94	0.49
1:A:377:GLY:C	1:A:378:TRP:CE3	2.91	0.49
1:A:405:ASP:OD2	4:A:953:HOH:O	2.19	0.49
1:A:245:PRO:CG	1:B:348:TRP:HB3	2.43	0.49
1:A:389:GLY:O	1:A:396:ASN:HB3	2.13	0.49
1:B:182:PRO:HB3	1:B:184:TRP:NE1	2.28	0.49
1:C:209:TRP:O	1:C:212:TYR:HB3	2.12	0.49
1:D:19:ASN:O	1:D:103:LEU:HD12	2.13	0.49
1:C:44:ARG:HD2	3:C:504:SO4:O1	2.13	0.49
1:C:194:LYS:HB2	1:C:242:SER:HA	1.95	0.48
1:B:496:ARG:O	1:B:497:GLN:HB3	2.13	0.48
1:D:232:ALA:O	1:D:233:GLU:HB2	2.13	0.48
1:D:15:VAL:HG11	1:D:354:LEU:HD22	1.96	0.48
1:A:269:ALA:HB2	4:A:1175:HOH:O	2.14	0.48
1:D:257:ARG:HD2	1:D:298:ASP:OD2	2.14	0.48
1:B:347:PHE:CE1	1:B:348:TRP:CZ3	3.01	0.48
1:B:152:GLU:HA	1:B:156:LEU:HD12	1.95	0.48
1:C:194:LYS:NZ	4:C:527:HOH:O	2.46	0.48
1:D:95:ALA:HB3	1:D:406:ILE:HD13	1.95	0.48
1:D:347:PHE:C	1:D:347:PHE:CD2	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLY:HA2	1:B:116:TYR:CD1	2.49	0.48
1:C:67:LEU:HG	1:C:470:LEU:HD11	1.95	0.48
1:A:95:ALA:HB3	1:A:406:ILE:HG22	1.96	0.48
1:C:381:TRP:HA	1:C:381:TRP:CE3	2.48	0.48
1:B:453:ASP:OD1	1:B:455:SER:OG	2.31	0.47
1:B:41:GLU:HG3	1:B:490:HIS:CD2	2.49	0.47
1:C:245:PRO:HD3	1:D:348:TRP:CD2	2.49	0.47
1:C:256:GLN:O	1:C:260:ILE:HG13	2.15	0.47
1:D:96:LEU:HD21	1:D:404:VAL:HG13	1.97	0.47
1:B:312:TRP:CZ2	1:B:318:ALA:HB3	2.50	0.47
1:B:387:PRO:HD3	1:B:404:VAL:O	2.15	0.47
1:B:191:VAL:O	1:B:247:GLN:HA	2.15	0.47
1:C:381:TRP:HA	1:C:381:TRP:HE3	1.80	0.47
1:A:371:LEU:HD23	1:A:378:TRP:HH2	1.80	0.47
1:D:495:HIS:CD2	4:D:1066:HOH:O	2.65	0.47
1:B:146:ASN:ND2	4:B:1122:HOH:O	2.47	0.46
1:D:314:LEU:HB2	1:D:343:VAL:CG1	2.45	0.46
1:D:497:GLN:HG2	4:D:1044:HOH:O	2.14	0.46
1:A:141:ASP:OD2	1:A:146:ASN:HB2	2.15	0.46
1:D:386:ASN:HB2	1:D:387:PRO:CD	2.44	0.46
1:C:131:ARG:NH1	4:C:543:HOH:O	2.44	0.46
1:A:245:PRO:CD	1:B:348:TRP:HB3	2.46	0.46
1:C:132:THR:O	1:C:133:TYR:HB3	2.13	0.46
1:A:96:LEU:HB3	1:A:100:ALA:HB3	1.98	0.46
1:D:300:GLU:OE2	1:D:303:LYS:HE2	2.15	0.46
1:A:243:GLY:N	4:A:567:HOH:O	2.41	0.46
1:A:346:LYS:HG2	1:A:348:TRP:CH2	2.51	0.46
1:C:47:ARG:HD3	1:C:50:GLU:OE1	2.16	0.46
1:A:31:PHE:HE1	1:A:493:LEU:HD13	1.80	0.46
1:B:72:GLU:HB2	4:B:538:HOH:O	2.16	0.46
1:C:329:ARG:NH1	4:C:603:HOH:O	2.42	0.45
1:D:66:LEU:HD11	1:D:473:LYS:HB2	1.97	0.45
1:D:284:GLN:NE2	1:D:313:TYR:CE1	2.81	0.45
1:A:312:TRP:CZ2	1:A:378:TRP:CD1	3.04	0.45
1:B:381:TRP:HA	1:B:381:TRP:CE3	2.51	0.45
1:A:42:SER:HA	1:A:47:ARG:O	2.16	0.45
1:B:199:GLY:HA3	1:B:203:ASP:OD2	2.16	0.45
1:C:353:ARG:NH1	3:C:500:SO4:O1	2.50	0.45
1:D:191:VAL:O	1:D:247:GLN:HA	2.16	0.45
1:A:175:LEU:HD12	1:A:229:ALA:O	2.16	0.45
1:B:314:LEU:HB2	1:B:343:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:PHE:HB2	1:D:495:HIS:CE1	2.52	0.45
1:D:284:GLN:HB3	1:D:286:LEU:HG	1.98	0.45
1:B:351:SER:O	1:B:359:ARG:NH1	2.45	0.45
1:B:497:GLN:HB3	4:B:789:HOH:O	2.16	0.45
1:A:197:LEU:HD11	1:A:209:TRP:CD1	2.51	0.45
1:B:366:SER:O	1:B:370:ASN:ND2	2.49	0.45
1:C:207:GLN:NE2	1:C:263:ASP:OD1	2.30	0.45
1:D:273:HIS:O	1:D:276:VAL:HG23	2.17	0.45
1:D:312:TRP:HH2	1:D:316:PHE:O	1.96	0.45
1:D:371:LEU:O	1:D:433:ARG:HD2	2.16	0.45
1:B:70:GLN:CD	1:B:437:VAL:CG2	2.90	0.45
1:B:381:TRP:HA	1:B:381:TRP:HE3	1.82	0.45
1:D:285:ARG:NH1	4:D:540:HOH:O	2.50	0.45
1:A:41:GLU:HG3	1:A:490:HIS:NE2	2.32	0.44
1:A:358:ASP:HA	1:A:361:MET:HE2	1.98	0.44
1:B:5:ILE:HD12	1:B:22:TYR:CD2	2.51	0.44
1:B:59:ASN:ND2	4:B:987:HOH:O	2.50	0.44
1:C:312:TRP:HZ2	1:C:378:TRP:HE1	1.64	0.44
1:A:209:TRP:O	1:A:212:TYR:HB3	2.17	0.44
1:C:125:SER:HB3	1:C:133:TYR:CE2	2.52	0.44
1:B:284:GLN:CB	1:B:286:LEU:HD13	2.47	0.44
1:C:417:PHE:C	1:C:417:PHE:CD2	2.95	0.44
1:D:312:TRP:HH2	1:D:317:LEU:HA	1.83	0.44
1:B:23:CYS:HB2	1:B:103:LEU:HD13	2.00	0.44
1:B:56:ILE:HG12	1:B:480:LEU:HD22	1.99	0.44
1:C:199:GLY:HA3	1:C:203:ASP:OD2	2.18	0.44
1:D:236:PRO:O	1:D:250:GLY:HA2	2.18	0.44
1:B:11:TYR:CD2	1:B:353:ARG:NH1	2.86	0.44
1:D:312:TRP:HH2	1:D:317:LEU:CA	2.30	0.44
1:A:408:LYS:O	1:A:410:THR:CG2	2.66	0.44
1:C:108:TYR:CE1	1:C:402:ILE:HD12	2.53	0.44
1:D:73:GLN:O	1:D:434:VAL:HA	2.18	0.44
1:A:290:HIS:ND1	3:A:505:SO4:O3	2.51	0.44
1:A:381:TRP:HA	1:A:381:TRP:CE3	2.52	0.44
1:B:386:ASN:HB2	1:B:387:PRO:CD	2.48	0.44
1:A:245:PRO:HB2	1:A:394:VAL:HG11	2.00	0.43
1:C:110:SER:OG	1:C:112:GLU:HG2	2.17	0.43
1:A:127:ASP:OD1	1:A:127:ASP:N	2.52	0.43
1:A:298:ASP:OD1	1:A:298:ASP:C	2.60	0.43
1:C:1:ALA:HB2	1:C:27:ASP:OD1	2.18	0.43
1:D:337:PHE:CE1	1:D:377:GLY:HA3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PHE:CE1	1:A:493:LEU:HD13	2.53	0.43
1:A:312:TRP:O	1:A:313:TYR:C	2.60	0.43
1:A:423:PHE:CZ	1:A:459:VAL:HG11	2.53	0.43
1:B:337:PHE:CE1	1:B:377:GLY:HA3	2.53	0.43
1:C:123:MET:SD	1:C:178:PRO:HD3	2.58	0.43
1:A:381:TRP:HA	1:A:381:TRP:HE3	1.84	0.43
1:C:95:ALA:HB3	1:C:406:ILE:HG22	2.00	0.43
1:D:344:GLY:C	1:D:346:LYS:H	2.25	0.43
1:D:463:ARG:NH1	4:D:988:HOH:O	2.52	0.43
1:A:395:ARG:HD3	1:A:397:PHE:CZ	2.53	0.43
1:D:41:GLU:HG3	1:D:490:HIS:CD2	2.54	0.43
1:C:200:GLN:N	1:C:203:ASP:OD2	2.44	0.43
1:D:82:GLY:HA2	1:D:116:TYR:CD1	2.54	0.43
1:D:169:GLN:HG2	4:D:578:HOH:O	2.19	0.43
1:C:296:LEU:HA	1:C:302:ALA:HB2	2.00	0.43
1:A:95:ALA:CB	1:A:406:ILE:CG2	2.97	0.43
1:C:290:HIS:HB2	4:C:724:HOH:O	2.18	0.43
1:C:16:CYS:SG	1:C:48:ARG:HG3	2.59	0.42
1:D:111:GLU:HG2	1:D:169:GLN:CD	2.44	0.42
1:B:95:ALA:HB1	1:B:406:ILE:HD13	2.01	0.42
1:A:44:ARG:NH2	3:A:503:SO4:O2	2.51	0.42
1:A:370:ASN:HB3	1:A:378:TRP:HZ2	1.85	0.42
1:B:128:PHE:CZ	1:B:398:VAL:HG22	2.55	0.42
1:C:186:LYS:O	1:C:187:THR:C	2.58	0.42
1:A:135:TYR:HD1	1:A:212:TYR:HH	1.66	0.42
1:A:383:LEU:HD23	1:A:383:LEU:HA	1.86	0.42
1:A:406:ILE:HD13	1:A:406:ILE:H	1.84	0.42
1:D:70:GLN:HE22	1:D:437:VAL:HG21	1.83	0.42
1:C:120:ARG:CB	1:C:379:THR:HG21	2.46	0.42
1:D:41:GLU:HG3	1:D:490:HIS:NE2	2.34	0.42
1:A:312:TRP:HZ2	1:A:378:TRP:CD1	2.38	0.42
1:B:312:TRP:HZ2	1:B:318:ALA:HB3	1.83	0.42
1:B:252:THR:HB	1:B:253:PRO:HD2	2.01	0.41
1:C:312:TRP:HH2	1:C:367:ILE:HG13	1.85	0.41
1:A:95:ALA:CB	1:A:406:ILE:HG22	2.50	0.41
1:B:44:ARG:HD3	3:B:503:SO4:O3	2.19	0.41
1:A:446:ALA:HA	1:A:459:VAL:O	2.20	0.41
1:C:186:LYS:HD3	1:C:190:ALA:O	2.19	0.41
1:D:346:LYS:O	1:D:349:GLU:O	2.39	0.41
1:A:149:LEU:HB3	1:A:153:ASP:HB2	2.01	0.41
1:B:2:ARG:O	1:B:24:ASP:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:TYR:CD1	1:D:313:TYR:N	2.88	0.41
1:D:207:GLN:HE22	1:D:263:ASP:HA	1.85	0.41
1:D:348:TRP:CD1	1:D:349:GLU:HG3	2.55	0.41
1:D:405:ASP:OD2	1:D:408:LYS:HD2	2.21	0.41
1:A:165:LEU:HD22	1:A:172:VAL:HB	2.02	0.41
1:A:245:PRO:HD3	1:B:348:TRP:CB	2.51	0.41
1:B:37:PHE:CG	1:B:480:LEU:HD13	2.55	0.41
1:D:43:THR:HG23	1:D:47:ARG:HB2	2.01	0.41
1:A:176:ALA:HB2	1:A:227:PHE:CE2	2.56	0.41
1:A:371:LEU:CD2	1:A:378:TRP:HH2	2.33	0.41
1:C:370:ASN:HB3	1:C:378:TRP:HZ2	1.85	0.41
1:D:11:TYR:HE2	1:D:353:ARG:NE	2.00	0.41
1:D:70:GLN:NE2	1:D:437:VAL:HG21	2.35	0.41
1:D:95:ALA:HB3	1:D:406:ILE:CD1	2.50	0.41
1:D:194:LYS:HE3	1:D:240:LEU:O	2.21	0.41
1:D:309:ALA:HA	1:D:337:PHE:O	2.20	0.41
1:D:346:LYS:HB3	1:D:349:GLU:HB2	2.01	0.41
1:D:146:ASN:ND2	4:D:1141:HOH:O	2.54	0.41
1:A:258:ASP:O	1:A:262:ARG:HG2	2.22	0.40
1:A:284:GLN:HG3	1:A:314:LEU:HB2	2.04	0.40
1:B:373:TYR:C	1:B:374:HIS:CG	2.98	0.40
1:C:371:LEU:O	1:C:433:ARG:HD2	2.21	0.40
1:C:405:ASP:OD2	1:C:408:LYS:HE2	2.20	0.40
1:D:350:GLN:HG2	4:D:637:HOH:O	2.21	0.40
1:D:127:ASP:HB3	1:D:246:PHE:CG	2.56	0.40
1:A:209:TRP:CE3	1:A:209:TRP:HA	2.56	0.40
1:C:465:SER:HA	1:C:487:TYR:CE1	2.56	0.40
1:B:66:LEU:HB3	1:B:439:SER:HB3	2.03	0.40
1:C:184:TRP:CD1	1:C:184:TRP:H	2.39	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	495/497 (100%)	457 (92%)	32 (6%)	6 (1%)	10	8
1	B	495/497 (100%)	468 (94%)	19 (4%)	8 (2%)	7	6
1	C	495/497 (100%)	460 (93%)	31 (6%)	4 (1%)	16	16
1	D	495/497 (100%)	471 (95%)	20 (4%)	4 (1%)	16	16
All	All	1980/1988 (100%)	1856 (94%)	102 (5%)	22 (1%)	11	10

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	GLU
1	B	320	ALA
1	B	346	LYS
1	C	343	VAL
1	D	233	GLU
1	B	381	TRP
1	D	350	GLN
1	A	133	TYR
1	A	343	VAL
1	A	381	TRP
1	B	63	THR
1	C	313	TYR
1	C	381	TRP
1	D	281	LEU
1	A	281	LEU
1	A	344	GLY
1	A	345	SER
1	B	124	ALA
1	B	281	LEU
1	B	317	LEU
1	C	281	LEU
1	D	381	TRP

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	424/424 (100%)	402 (95%)	22 (5%)	21	26
1	B	424/424 (100%)	402 (95%)	22 (5%)	21	26
1	C	424/424 (100%)	397 (94%)	27 (6%)	16	19
1	D	424/424 (100%)	400 (94%)	24 (6%)	18	23
All	All	1696/1696 (100%)	1601 (94%)	95 (6%)	19	24

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	44	ARG
1	A	57	GLN
1	A	110	SER
1	A	140	ASP
1	A	165	LEU
1	A	200	GLN
1	A	271	SER
1	A	285	ARG
1	A	293	LYS
1	A	303	LYS
1	A	335	MET
1	A	346	LYS
1	A	358	ASP
1	A	379	THR
1	A	381	TRP
1	A	388	GLU
1	A	396	ASN
1	A	406	ILE
1	A	410	THR
1	A	450	MET
1	A	466	LYS
1	B	30	THR
1	B	44	ARG
1	B	47	ARG
1	B	57	GLN
1	B	59	ASN
1	B	155	LYS
1	B	169	GLN
1	B	284	GLN
1	B	286	LEU
1	B	317	LEU
1	B	321	LYS

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Mol	Chain	Res	Type
1	B	335	MET
1	B	348	TRP
1	B	366	SER
1	B	381	TRP
1	B	394	VAL
1	B	470	LEU
1	B	473	LYS
1	B	480	LEU
1	B	481	GLU
1	B	493	LEU
1	B	497	GLN
1	C	39	ARG
1	C	57	GLN
1	C	61	THR
1	C	69	LEU
1	C	73	GLN
1	C	98	PRO
1	C	111	GLU
1	C	200	GLN
1	C	204	ILE
1	C	226	GLN
1	C	286	LEU
1	C	303	LYS
1	C	335	MET
1	C	342	CYS
1	C	343	VAL
1	C	345	SER
1	C	346	LYS
1	C	347	PHE
1	C	350	GLN
1	C	370	ASN
1	C	379	THR
1	C	381	TRP
1	C	395	ARG
1	C	397	PHE
1	C	410	THR
1	C	457	VAL
1	C	464	SER
1	D	39	ARG
1	D	44	ARG
1	D	93	ILE
1	D	110	SER

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Mol	Chain	Res	Type
1	D	111	GLU
1	D	118	ILE
1	D	165	LEU
1	D	169	GLN
1	D	212	TYR
1	D	262	ARG
1	D	286	LEU
1	D	312	TRP
1	D	335	MET
1	D	347	PHE
1	D	350	GLN
1	D	379	THR
1	D	381	TRP
1	D	394	VAL
1	D	420	LEU
1	D	480	LEU
1	D	481	GLU
1	D	489	ILE
1	D	493	LEU
1	D	497	GLN

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	59	ASN
1	A	73	GLN
1	A	145	HIS
1	A	200	GLN
1	A	223	HIS
1	A	274	HIS
1	A	328	HIS
1	A	365	HIS
1	A	396	ASN
1	A	495	HIS
1	A	497	GLN
1	B	57	GLN
1	B	59	ASN
1	B	60	HIS
1	B	146	ASN
1	B	200	GLN
1	B	223	HIS
1	B	274	HIS

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Mol	Chain	Res	Type
1	B	350	GLN
1	B	362	GLN
1	B	495	HIS
1	C	274	HIS
1	D	59	ASN
1	D	60	HIS
1	D	70	GLN
1	D	146	ASN
1	D	169	GLN
1	D	311	HIS
1	D	328	HIS
1	D	350	GLN
1	D	362	GLN
1	D	495	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	504	-	4,4,4	0.51	0	6,6,6	0.18	0
3	SO4	C	504	-	4,4,4	0.36	0	6,6,6	0.53	0
3	SO4	D	504	-	4,4,4	0.44	0	6,6,6	0.33	0
3	SO4	D	503	-	4,4,4	0.51	0	6,6,6	0.33	0
3	SO4	B	502	-	4,4,4	0.63	0	6,6,6	0.50	0
3	SO4	C	503	-	4,4,4	0.58	0	6,6,6	0.30	0
3	SO4	B	499	-	4,4,4	0.34	0	6,6,6	0.57	0
3	SO4	A	505	-	4,4,4	0.53	0	6,6,6	0.25	0
3	SO4	D	501	-	4,4,4	0.50	0	6,6,6	0.40	0
3	SO4	B	504	-	4,4,4	0.51	0	6,6,6	0.23	0
3	SO4	A	506	-	4,4,4	0.28	0	6,6,6	0.44	0
3	SO4	A	502	-	4,4,4	0.47	0	6,6,6	0.23	0
3	SO4	A	500	-	4,4,4	0.53	0	6,6,6	0.56	0
3	SO4	A	499	-	4,4,4	0.36	0	6,6,6	0.34	0
3	SO4	C	499	-	4,4,4	0.38	0	6,6,6	0.41	0
2	NAG	B	498	1	14,14,15	0.63	0	17,19,21	1.57	4 (23%)
3	SO4	D	500	-	4,4,4	0.38	0	6,6,6	0.48	0
3	SO4	B	501	-	4,4,4	0.44	0	6,6,6	0.35	0
3	SO4	A	503	-	4,4,4	0.49	0	6,6,6	0.41	0
3	SO4	B	500	-	4,4,4	0.38	0	6,6,6	0.24	0
2	NAG	D	498	1	14,14,15	0.58	0	17,19,21	2.60	4 (23%)
3	SO4	C	502	-	4,4,4	0.44	0	6,6,6	0.39	0
3	SO4	A	501	-	4,4,4	0.44	0	6,6,6	0.38	0
2	NAG	A	498	1	14,14,15	0.75	0	17,19,21	1.34	2 (11%)
3	SO4	C	505	-	4,4,4	0.49	0	6,6,6	0.32	0
3	SO4	D	502	-	4,4,4	0.42	0	6,6,6	0.52	0
3	SO4	C	501	-	4,4,4	0.45	0	6,6,6	0.72	0
3	SO4	D	499	-	4,4,4	0.39	0	6,6,6	0.50	0
3	SO4	B	505	-	4,4,4	0.54	0	6,6,6	0.31	0
2	NAG	C	498	1	14,14,15	0.96	1 (7%)	17,19,21	1.77	5 (29%)
3	SO4	B	503	-	4,4,4	0.42	0	6,6,6	0.81	0
3	SO4	C	500	-	4,4,4	0.36	0	6,6,6	0.37	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	NAG	B	498	1	-	0/6/23/26	0/1/1/1
2	NAG	A	498	1	-	0/6/23/26	0/1/1/1
2	NAG	C	498	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	498	1	1/1/5/7	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	498	NAG	C1-C2	2.32	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	498	NAG	C1-O5-C5	8.79	123.97	112.19
2	C	498	NAG	C1-O5-C5	3.86	117.35	112.19
2	B	498	NAG	O5-C1-C2	-3.31	106.18	111.29
2	D	498	NAG	C1-C2-N2	-3.25	105.31	110.43
2	C	498	NAG	O5-C1-C2	-3.09	106.51	111.29
2	C	498	NAG	C1-C2-N2	2.95	115.09	110.43
2	A	498	NAG	O5-C1-C2	-2.64	107.21	111.29
2	B	498	NAG	C3-C4-C5	-2.61	105.49	110.23
2	B	498	NAG	O4-C4-C5	2.52	115.53	109.32
2	D	498	NAG	O4-C4-C5	2.41	115.26	109.32
2	A	498	NAG	C1-O5-C5	2.37	115.37	112.19
2	B	498	NAG	C1-O5-C5	2.37	115.36	112.19
2	C	498	NAG	C8-C7-N2	2.17	119.71	116.12
2	C	498	NAG	O7-C7-C8	-2.09	118.33	122.05
2	D	498	NAG	O3-C3-C4	-2.06	105.52	110.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	498	NAG	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	498	NAG	O5-C5-C6-O6
2	D	498	NAG	C4-C5-C6-O6
2	C	498	NAG	C4-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	SO4	1	0
3	C	504	SO4	3	0
3	B	502	SO4	1	0
3	A	505	SO4	1	0
3	A	506	SO4	4	0
3	A	503	SO4	1	0
3	D	502	SO4	3	0
3	D	499	SO4	1	0
3	B	505	SO4	1	0
3	B	503	SO4	3	0
3	C	500	SO4	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	497/497 (100%)	-1.44	0 100 100	9, 23, 41, 49	1 (0%)
1	B	497/497 (100%)	-1.47	0 100 100	5, 23, 39, 62	1 (0%)
1	C	497/497 (100%)	-1.43	0 100 100	10, 23, 42, 49	1 (0%)
1	D	497/497 (100%)	-1.45	0 100 100	5, 22, 40, 60	1 (0%)
All	All	1988/1988 (100%)	-1.45	0 100 100	5, 23, 40, 62	4 (0%)

There are no RSRZ outliers to report.

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
2	NAG	B	498	14/15	0.98	0.04	32,34,36,38	0
3	SO4	A	504	5/5	0.98	0.06	67,67,67,67	0
3	SO4	A	505	5/5	0.98	0.04	68,68,68,68	0
3	SO4	B	504	5/5	0.98	0.06	64,65,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	505	5/5	0.98	0.05	63,63,64,64	0
3	SO4	C	503	5/5	0.98	0.04	55,55,56,56	0
3	SO4	D	504	5/5	0.98	0.06	60,61,61,61	0
2	NAG	A	498	14/15	0.99	0.03	21,27,30,33	0
2	NAG	C	498	14/15	0.99	0.03	21,28,31,31	0
3	SO4	A	506	5/5	0.99	0.06	44,44,46,47	0
3	SO4	B	500	5/5	0.99	0.03	41,42,43,44	0
3	SO4	B	501	5/5	0.99	0.03	36,39,42,42	0
3	SO4	B	502	5/5	0.99	0.04	43,45,46,47	0
3	SO4	B	503	5/5	0.99	0.03	45,47,48,49	0
2	NAG	D	498	14/15	0.99	0.04	29,33,34,34	0
3	SO4	A	501	5/5	0.99	0.04	37,38,39,40	0
3	SO4	C	499	5/5	0.99	0.03	34,35,36,38	0
3	SO4	C	501	5/5	0.99	0.03	35,36,37,38	0
3	SO4	C	502	5/5	0.99	0.03	46,48,48,49	0
3	SO4	A	502	5/5	0.99	0.03	46,47,48,49	0
3	SO4	C	504	5/5	0.99	0.04	39,41,43,44	0
3	SO4	C	505	5/5	0.99	0.06	59,59,61,63	0
3	SO4	D	500	5/5	0.99	0.03	37,37,39,41	0
3	SO4	D	501	5/5	0.99	0.03	40,41,42,43	0
3	SO4	D	502	5/5	0.99	0.04	42,43,45,45	0
3	SO4	D	503	5/5	0.99	0.05	48,49,50,52	0
3	SO4	A	503	5/5	0.99	0.07	58,59,59,62	0
3	SO4	B	499	5/5	1.00	0.02	30,31,32,34	0
3	SO4	A	499	5/5	1.00	0.02	27,29,30,33	0
3	SO4	C	500	5/5	1.00	0.02	30,31,32,33	0
3	SO4	A	500	5/5	1.00	0.02	30,31,33,33	0
3	SO4	D	499	5/5	1.00	0.02	28,28,32,33	0

6.5 Other polymers

There are no such residues in this entry.