



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:57 PM UTC

PDB ID : 1BCH / pdb_00001bch
Title : MANNOSE-BINDING PROTEIN-A MUTANT (QPDWGH) COMPLEXED
WITH N-ACETYL-D-GALACTOSAMINE
Authors : Kolatkar, A.R.; Weis, W.I.
Deposited on : 1998-04-30
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

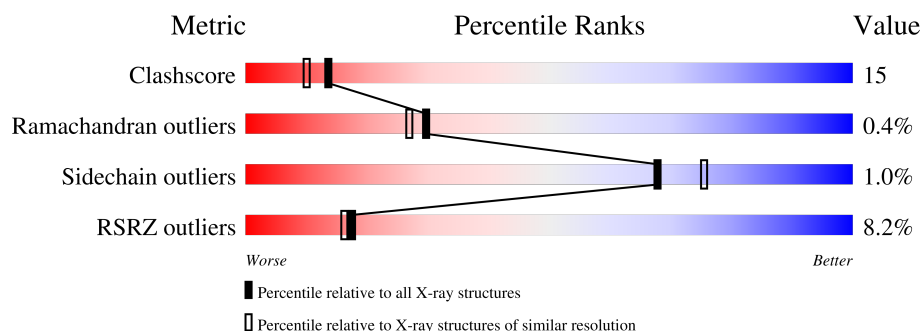
1 Overall quality at a glance

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))
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	1	154	7% 72% 27% .
1	2	154	13% 70% 29% .
1	3	154	5% 71% 29% .

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	A2G	1	1[A]	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3987 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 MANNOSE-BINDING PROTEIN-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	154	Total	C	N	O	S	0	0	0
			1196	752	206	230	8			
1	2	154	Total	C	N	O	S	0	0	0
			1196	752	206	230	8			
1	3	154	Total	C	N	O	S	0	0	0
			1196	752	206	230	8			

There are 33 discrepancies between the modelled and reference sequences:

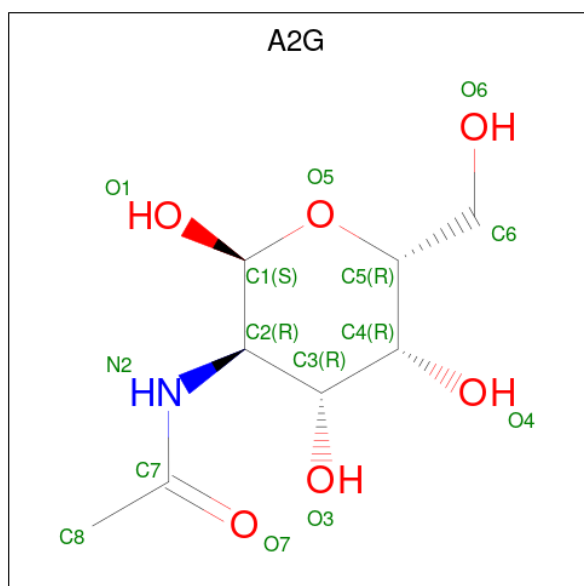
Chain	Residue	Modelled	Actual	Comment	Reference
1	185	GLN	GLU	engineered mutation	UNP P19999
1	187	ASP	ASN	engineered mutation	UNP P19999
1	189	TRP	HIS	engineered mutation	UNP P19999
1	190	TYR	GLY	engineered mutation	UNP P19999
1	191	GLY	SER	engineered mutation	UNP P19999
1	192	HIS	-	insertion	UNP P19999
1	193	GLY	-	insertion	UNP P19999
1	194	LEU	-	insertion	UNP P19999
1	195	GLY	-	insertion	UNP P19999
1	196	GLY	-	insertion	UNP P19999
1	202	HIS	THR	engineered mutation	UNP P19999
2	185	GLN	GLU	engineered mutation	UNP P19999
2	187	ASP	ASN	engineered mutation	UNP P19999
2	189	TRP	HIS	engineered mutation	UNP P19999
2	190	TYR	GLY	engineered mutation	UNP P19999
2	191	GLY	SER	engineered mutation	UNP P19999
2	192	HIS	-	insertion	UNP P19999
2	193	GLY	-	insertion	UNP P19999
2	194	LEU	-	insertion	UNP P19999
2	195	GLY	-	insertion	UNP P19999
2	196	GLY	-	insertion	UNP P19999
2	202	HIS	THR	engineered mutation	UNP P19999
3	185	GLN	GLU	engineered mutation	UNP P19999

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Chain	Residue	Modelled	Actual	Comment	Reference
3	187	ASP	ASN	engineered mutation	UNP P19999
3	189	TRP	HIS	engineered mutation	UNP P19999
3	190	TYR	GLY	engineered mutation	UNP P19999
3	191	GLY	SER	engineered mutation	UNP P19999
3	192	HIS	-	insertion	UNP P19999
3	193	GLY	-	insertion	UNP P19999
3	194	LEU	-	insertion	UNP P19999
3	195	GLY	-	insertion	UNP P19999
3	196	GLY	-	insertion	UNP P19999
3	202	HIS	THR	engineered mutation	UNP P19999

- Molecule 2 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1	1	Total	C	N	O	0	1
			30	16	2	12		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	3	Total	Ca	0	0
			3	3		
3	2	3	Total	Ca	0	0
			3	3		

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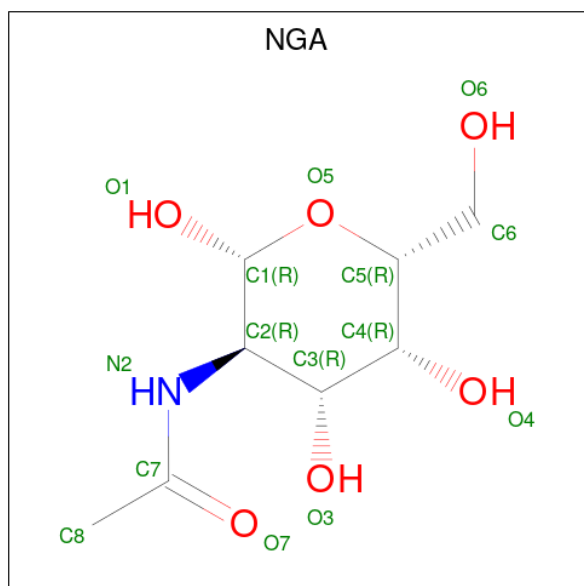
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	3	3	Total	Ca	0	0
			3	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	1	Total	Cl	0	0
			1	1		
4	2	1	Total	Cl	0	0
			1	1		
4	3	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-galactopyranose (CCD ID: NGA) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	2	1	Total	C	N	O	0	0
			15	8	1	6		
5	3	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	2	1	Total 1	Na 1	0	0

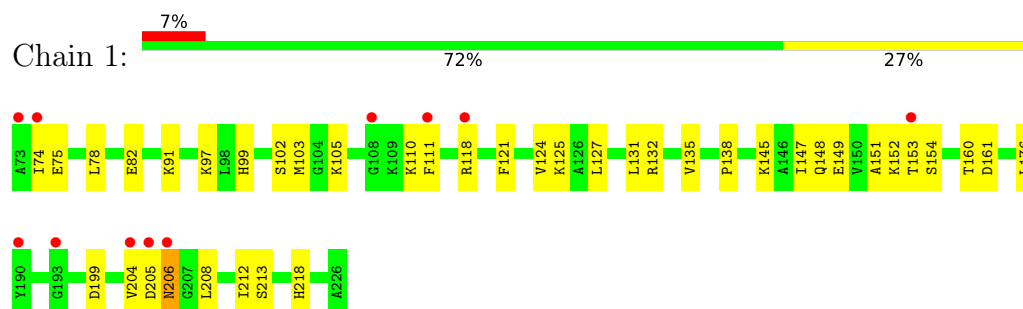
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	1	132	Total 132	O 132	0	0
7	2	85	Total 85	O 85	0	0
7	3	109	Total 109	O 109	0	0

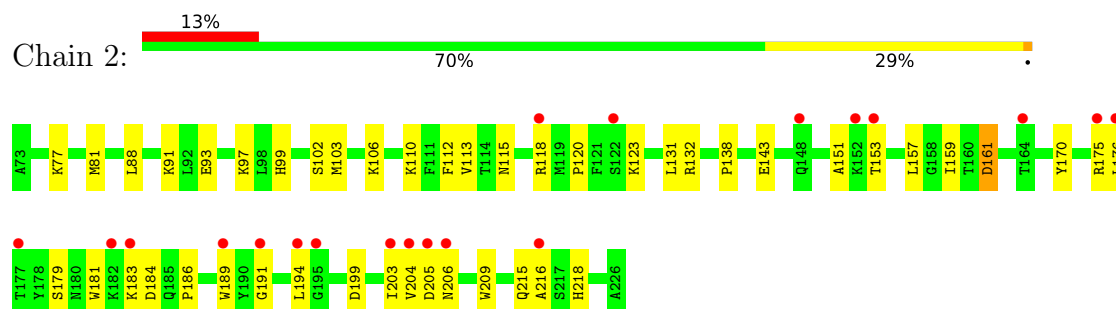
3 Residue-property plots [i](#)

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.

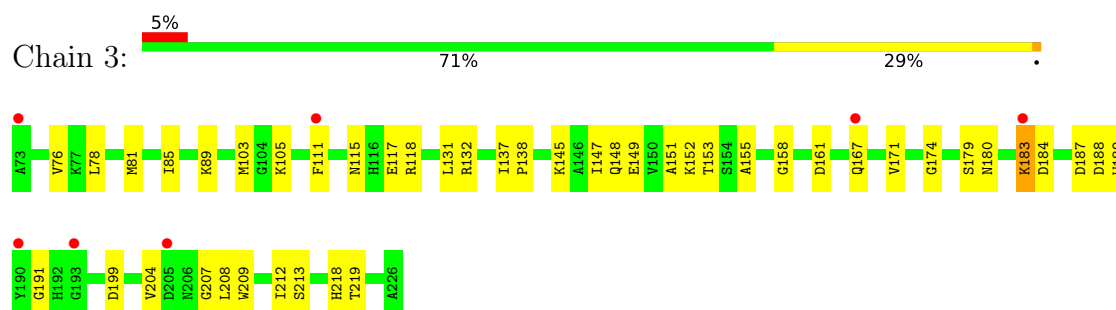
• Molecule 1: MANNOSE-BINDING PROTEIN-A



• Molecule 1: MANNOSE-BINDING PROTEIN-A



• Molecule 1: MANNOSE-BINDING PROTEIN-A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	80.49Å 85.01Å 98.71Å 90.00° 104.82° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (30.00-2.00) 96.6 (30.00-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.252 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3987	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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: CA, A2G, NGA, NA, CL

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	1	0.43	0/1220	0.92	3/1643 (0.2%)
1	2	0.40	0/1220	0.85	2/1643 (0.1%)
1	3	0.41	0/1220	0.90	2/1643 (0.1%)
All	All	0.41	0/3660	0.89	7/4929 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	174	GLY	N-CA-C	6.62	118.24	111.95
1	2	115	ASN	N-CA-C	-5.59	105.80	113.30
1	2	161	ASP	N-CA-C	-5.50	103.84	110.88
1	1	182	LYS	N-CA-C	-5.25	103.60	110.53
1	3	115	ASN	N-CA-C	-5.21	106.16	112.88
1	1	110	LYS	CA-C-N	-5.14	115.74	122.99
1	1	110	LYS	C-N-CA	-5.14	115.74	122.99

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	1	1196	0	1167	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1196	0	1167	46	0
1	3	1196	0	1167	39	0
2	1	30	0	20	0	0
3	1	3	0	0	0	0
3	2	3	0	0	0	0
3	3	3	0	0	0	0
4	1	1	0	0	0	0
4	2	1	0	0	0	0
4	3	1	0	0	0	0
5	2	15	0	14	0	0
5	3	15	0	13	0	0
6	2	1	0	0	0	0
7	1	132	0	0	1	0
7	2	85	0	0	2	0
7	3	109	0	0	1	1
All	All	3987	0	3548	105	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (105) 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)
1:2:120:PRO:HD2	1:2:123:LYS:HG3	1.57	0.87
1:3:118:ARG:HH11	1:3:218:HIS:HA	1.44	0.81
1:1:103:MET:HA	1:1:103:MET:HE2	1.64	0.79
1:1:121:PHE:CE2	1:1:125:LYS:HD2	2.19	0.78
1:3:138:PRO:HG3	1:3:147:ILE:HD12	1.67	0.77
1:1:74:ILE:HG23	1:1:75:GLU:HG3	1.67	0.77
1:2:88:LEU:HD21	1:3:89:LYS:HG2	1.67	0.74
1:3:118:ARG:NH1	1:3:218:HIS:HA	2.02	0.74
1:1:105:LYS:HG3	1:1:111:PHE:HB3	1.70	0.72
1:2:81:MET:HE3	1:3:85:ILE:HD12	1.73	0.71
1:2:102:SER:HB2	1:3:103:MET:HE2	1.75	0.68
1:2:161:ASP:OD1	1:2:199:ASP:HA	1.96	0.66
1:1:161:ASP:OD1	1:1:199:ASP:HA	1.97	0.65
1:1:74:ILE:HG23	1:1:75:GLU:N	2.13	0.63
1:1:145:LYS:HD2	1:1:148:GLN:NE2	2.14	0.61
1:2:194:LEU:HG	1:2:215:GLN:NE2	2.15	0.60
1:3:153:THR:HG23	1:3:219:THR:OG1	2.00	0.60
1:3:76:VAL:HG23	7:3:257:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:160:THR:HB	1:1:199:ASP:O	2.02	0.59
1:3:161:ASP:OD1	1:3:199:ASP:HA	2.01	0.59
1:3:105:LYS:HG3	1:3:111:PHE:HB3	1.84	0.59
1:1:97:LYS:HG2	1:2:131:LEU:HD21	1.85	0.57
1:3:151:ALA:C	1:3:153:THR:H	2.13	0.57
1:3:155:ALA:HB2	1:3:219:THR:HB	1.87	0.57
1:3:167:GLN:HE21	1:3:167:GLN:HA	1.70	0.56
1:1:205:ASP:O	1:1:206:ASN:HB3	2.04	0.56
1:2:91:LYS:HB3	1:2:91:LYS:NZ	2.21	0.56
1:1:206:ASN:HD21	1:1:208:LEU:HD12	1.69	0.56
1:2:181:TRP:CE3	1:2:186:PRO:HG3	2.42	0.55
1:2:91:LYS:HB3	1:2:91:LYS:HZ2	1.71	0.55
1:2:203:ILE:HG22	1:2:204:VAL:N	2.20	0.55
1:1:204:VAL:HG23	1:1:206:ASN:OD1	2.06	0.54
1:2:183:LYS:O	1:2:184:ASP:HB2	2.07	0.54
1:2:106:LYS:HD2	1:3:117:GLU:HG3	1.90	0.53
1:1:206:ASN:ND2	1:1:208:LEU:HD12	2.24	0.52
1:1:205:ASP:O	1:1:206:ASN:CB	2.57	0.52
1:1:151:ALA:C	1:1:153:THR:H	2.18	0.52
1:1:138:PRO:HG3	1:1:147:ILE:HD12	1.91	0.52
1:2:99:HIS:HD2	7:2:237:HOH:O	1.92	0.52
1:2:118:ARG:NH2	1:2:218:HIS:ND1	2.58	0.52
1:2:181:TRP:CZ3	1:2:186:PRO:HG3	2.44	0.51
1:2:189:TRP:CE2	1:2:191:GLY:HA3	2.46	0.50
1:1:127:LEU:C	1:1:127:LEU:HD23	2.36	0.50
1:2:179:SER:HA	1:2:209:TRP:CH2	2.48	0.49
1:3:158:GLY:C	1:3:171:VAL:HG13	2.37	0.49
1:2:194:LEU:HG	1:2:215:GLN:HE21	1.76	0.49
1:1:145:LYS:HA	1:1:148:GLN:HE21	1.76	0.49
1:2:176:LEU:HD21	1:2:179:SER:HB3	1.93	0.49
1:1:82:GLU:HB2	1:3:81:MET:CE	2.43	0.49
1:3:189:TRP:CZ2	1:3:191:GLY:HA3	2.47	0.49
1:1:102:SER:HB2	1:2:103:MET:HE2	1.95	0.48
1:2:110:LYS:HE3	1:2:112:PHE:CZ	2.47	0.48
1:2:175:ARG:HG3	1:2:175:ARG:HH11	1.79	0.48
1:2:93:GLU:HG3	1:2:97:LYS:HZ2	1.79	0.48
1:3:145:LYS:O	1:3:149:GLU:HG3	2.13	0.48
1:3:183:LYS:O	1:3:184:ASP:HB2	2.13	0.47
1:3:189:TRP:CE2	1:3:191:GLY:HA3	2.50	0.47
1:3:167:GLN:HA	1:3:167:GLN:NE2	2.30	0.46
1:1:118:ARG:NH2	1:1:218:HIS:ND1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:88:LEU:HD11	1:3:89:LYS:HG3	1.98	0.46
1:2:204:VAL:HG12	1:2:205:ASP:N	2.31	0.46
1:1:118:ARG:HH22	1:1:154:SER:HB3	1.80	0.45
1:2:93:GLU:HG3	1:2:97:LYS:NZ	2.30	0.45
1:3:151:ALA:O	1:3:152:LYS:HB2	2.16	0.45
1:1:74:ILE:CG2	1:1:75:GLU:N	2.79	0.45
1:1:97:LYS:HG2	1:2:131:LEU:CD2	2.46	0.45
1:2:120:PRO:HA	1:2:216:ALA:O	2.16	0.45
1:1:212:ILE:HG13	1:1:213:SER:N	2.32	0.45
1:3:179:SER:HA	1:3:209:TRP:CH2	2.52	0.45
1:2:81:MET:HE1	1:3:81:MET:HB2	1.99	0.44
1:3:212:ILE:HG13	1:3:213:SER:N	2.32	0.44
1:1:99:HIS:HD2	7:1:240:HOH:O	2.01	0.44
1:2:77:LYS:HD2	1:3:78:LEU:HD23	2.00	0.44
1:1:131:LEU:O	1:1:132:ARG:HB2	2.16	0.44
1:3:148:GLN:OE1	1:3:207:GLY:HA3	2.18	0.44
1:1:91:LYS:HE2	1:1:91:LYS:HB3	1.88	0.43
1:2:81:MET:HE1	1:3:81:MET:CB	2.48	0.43
1:2:120:PRO:HD2	1:2:123:LYS:CG	2.38	0.43
1:1:206:ASN:ND2	1:1:208:LEU:HG	2.33	0.43
1:1:74:ILE:HG23	1:1:75:GLU:H	1.80	0.43
1:1:183:LYS:O	1:1:184:ASP:HB2	2.19	0.43
1:2:157:LEU:HD21	1:2:203:ILE:HD11	2.00	0.43
1:2:132:ARG:N	1:2:132:ARG:HD2	2.33	0.43
1:2:138:PRO:HD3	1:2:157:LEU:HD22	2.00	0.43
1:1:78:LEU:HD21	1:3:78:LEU:HD13	1.99	0.43
1:3:131:LEU:O	1:3:132:ARG:HB2	2.19	0.42
1:2:110:LYS:HE2	1:2:143:GLU:CD	2.44	0.42
1:2:157:LEU:HD21	1:2:203:ILE:CD1	2.50	0.42
1:2:203:ILE:CG2	1:2:204:VAL:N	2.82	0.42
1:1:182:LYS:HA	1:1:208:LEU:HD13	2.00	0.42
1:2:77:LYS:HD2	1:3:78:LEU:CD2	2.49	0.42
1:3:180:ASN:ND2	1:3:208:LEU:HA	2.34	0.42
1:2:151:ALA:C	1:2:153:THR:H	2.28	0.41
1:2:91:LYS:HZ2	1:2:91:LYS:CB	2.31	0.41
1:3:187:ASP:O	1:3:188:ASP:C	2.62	0.41
1:2:113:VAL:HG23	7:2:308:HOH:O	2.19	0.41
1:3:155:ALA:CB	1:3:219:THR:HB	2.49	0.41
1:3:137:ILE:HA	1:3:138:PRO:HD3	1.90	0.41
1:1:124:VAL:HG12	1:1:135:VAL:HG22	2.02	0.41
1:2:204:VAL:HB	1:2:206:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:181:TRP:CD2	1:2:186:PRO:HG3	2.56	0.41
1:3:151:ALA:C	1:3:153:THR:N	2.79	0.41
1:3:167:GLN:HE21	1:3:167:GLN:CA	2.29	0.41
1:2:159:ILE:CD1	1:2:170:TYR:CD1	3.04	0.41
1:1:82:GLU:HB2	1:3:81:MET:HE2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:3:265:HOH:O	7:3:265:HOH:O[2_556]	2.09	0.11

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	1	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	18	14
1	2	152/154 (99%)	146 (96%)	6 (4%)	0	100	100
1	3	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	18	14
All	All	456/462 (99%)	438 (96%)	16 (4%)	2 (0%)	30	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	206	ASN
1	3	204	VAL

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	1	128/128 (100%)	125 (98%)	3 (2%)	44	49
1	2	128/128 (100%)	128 (100%)	0	100	100
1	3	128/128 (100%)	127 (99%)	1 (1%)	73	80
All	All	384/384 (100%)	380 (99%)	4 (1%)	68	75

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	149	GLU
1	1	152	LYS
1	1	176	LEU
1	3	183	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	96	ASN
1	1	99	HIS
1	1	116	HIS
1	1	148	GLN
1	2	80	ASN
1	2	96	ASN
1	2	99	HIS
1	2	180	ASN
1	2	215	GLN
1	3	80	ASN
1	3	96	ASN
1	3	99	HIS
1	3	167	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 17 ligands modelled in this entry, 13 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A2G	1	1[B]	3	15,15,15	0.43	0	21,21,21	0.56	0
5	NGA	2	1	3	15,15,15	0.53	0	21,21,21	0.61	0
2	A2G	1	1[A]	3	15,15,15	0.42	0	21,21,21	0.57	0
5	NGA	3	1	3	15,15,15	0.46	0	21,21,21	0.70	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	A2G	1	1[B]	3	-	0/6/26/26	0/1/1/1
5	NGA	2	1	3	-	2/6/26/26	0/1/1/1
2	A2G	1	1[A]	3	1/1/6/7	0/6/26/26	0/1/1/1
5	NGA	3	1	3	-	1/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	1	1[A]	A2G	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	2	1	NGA	O5-C5-C6-O6
5	2	1	NGA	C4-C5-C6-O6
5	3	1	NGA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	1	154/154 (100%)	0.40	11 (7%) 22 20	20, 31, 44, 57	0
1	2	154/154 (100%)	0.87	20 (12%) 7 6	24, 38, 58, 71	0
1	3	154/154 (100%)	0.64	7 (4%) 38 37	23, 35, 49, 57	0
All	All	462/462 (100%)	0.64	38 (8%) 17 16	20, 35, 52, 71	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	204	VAL	7.2
1	2	205	ASP	6.7
1	1	205	ASP	4.0
1	1	204	VAL	3.8
1	2	194	LEU	3.6
1	2	206	ASN	3.5
1	3	183	LYS	3.3
1	3	73	ALA	3.2
1	2	195	GLY	3.2
1	1	111	PHE	3.2
1	2	176	LEU	3.0
1	2	177	THR	2.9
1	1	190	TYR	2.8
1	2	189	TRP	2.8
1	1	118	ARG	2.7
1	2	148	GLN	2.7
1	1	74	ILE	2.5
1	2	164	THR	2.5
1	2	216	ALA	2.4
1	2	118	ARG	2.4
1	2	175	ARG	2.4
1	3	111	PHE	2.4
1	1	206	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	3	205	ASP	2.4
1	3	167	GLN	2.3
1	3	190	TYR	2.3
1	2	122	SER	2.2
1	1	73	ALA	2.2
1	1	108	GLY	2.2
1	2	153	THR	2.2
1	1	193	GLY	2.1
1	2	203	ILE	2.1
1	3	193	GLY	2.1
1	1	153	THR	2.1
1	2	191	GLY	2.1
1	2	182	LYS	2.1
1	2	152	LYS	2.0
1	2	183	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($\text{\AA}^2$)	Q<0.9
4	CL	2	4	1/1	0.71	0.25	61,61,61,61	0
5	NGA	3	1	15/15	0.74	0.17	43,46,50,51	0
5	NGA	2	1	15/15	0.82	0.13	39,42,47,50	0
2	A2G	1	1[B]	15/15	0.89	0.14	19,21,23,25	15
2	A2G	1	1[A]	15/15	0.89	0.14	23,25,26,29	15
4	CL	3	4	1/1	0.95	0.13	39,39,39,39	0
3	CA	2	2	1/1	0.96	0.07	35,35,35,35	0
3	CA	2	3	1/1	0.96	0.05	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	3	2	1/1	0.97	0.05	35,35,35,35	0
4	CL	1	4	1/1	0.97	0.13	43,43,43,43	0
3	CA	1	3	1/1	0.98	0.03	25,25,25,25	0
3	CA	3	227	1/1	0.98	0.03	27,27,27,27	0
3	CA	2	227	1/1	0.98	0.03	34,34,34,34	0
3	CA	1	227	1/1	0.98	0.03	26,26,26,26	0
6	NA	2	5	1/1	0.98	0.09	36,36,36,36	0
3	CA	1	2	1/1	0.99	0.03	28,28,28,28	0
3	CA	3	3	1/1	0.99	0.02	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.