



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:24 PM UTC

PDB ID : 1FIH / pdb_00001fih
Title : N-ACETYL GALACTOSAMINE BINDING MUTANT OF MANNOSE-BINDING PROTEIN A (QPDWG-HDRPY), COMPLEX WITH N-ACETYL GALACTOSAMINE
Authors : Feinberg, H.; Torgerson, D.; Drickamer, K.; Weis, W.I.
Deposited on : 2000-08-03
Resolution : 1.95 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

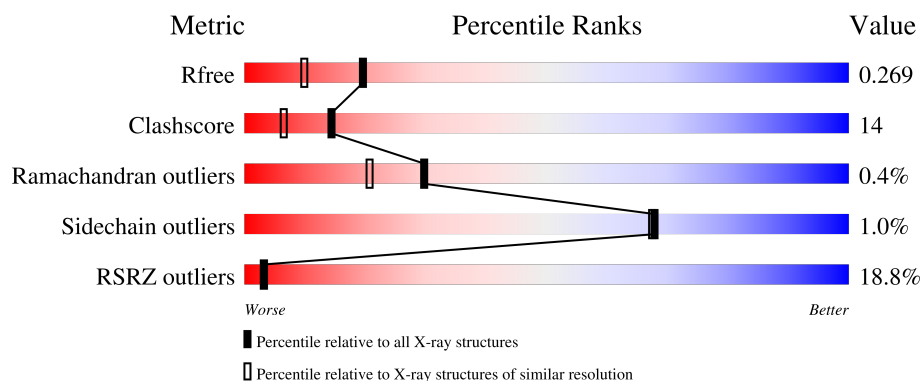
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	154	7% 77% 23%
1	B	154	33% 62% 36%
1	C	154	16% 68% 31%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3858 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	A	154	Total	C	N	O	S	0	0	0
			1205	758	207	232	8			
1	B	154	Total	C	N	O	S	0	0	0
			1205	758	207	232	8			
1	C	154	Total	C	N	O	S	0	0	0
			1205	758	207	232	8			

There are 42 discrepancies between the modelled and reference sequences:

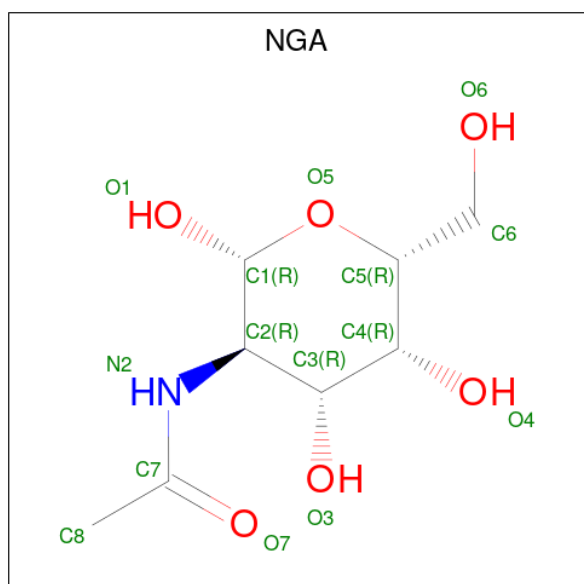
Chain	Residue	Modelled	Actual	Comment	Reference
A	185	GLN	GLU	engineered mutation	UNP P19999
A	187	ASP	ASN	engineered mutation	UNP P19999
A	189	TRP	HIS	engineered mutation	UNP P19999
A	181	TRP	-	insertion	UNP P19999
A	191	GLY	-	insertion	UNP P19999
A	192	HIS	-	insertion	UNP P19999
A	193	GLY	-	insertion	UNP P19999
A	194	LEU	-	insertion	UNP P19999
A	196	GLY	SER	engineered mutation	UNP P19999
A	202	HIS	THR	engineered mutation	UNP P19999
A	212	ASP	ILE	engineered mutation	UNP P19999
A	216	ARG	ALA	engineered mutation	UNP P19999
A	217	PRO	SER	engineered mutation	UNP P19999
A	218	TYR	HIS	engineered mutation	UNP P19999
B	185	GLN	GLU	engineered mutation	UNP P19999
B	187	ASP	ASN	engineered mutation	UNP P19999
B	189	TRP	HIS	engineered mutation	UNP P19999
B	181	TRP	-	insertion	UNP P19999
B	191	GLY	-	insertion	UNP P19999
B	192	HIS	-	insertion	UNP P19999
B	193	GLY	-	insertion	UNP P19999
B	194	LEU	-	insertion	UNP P19999
B	196	GLY	SER	engineered mutation	UNP P19999

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	HIS	THR	engineered mutation	UNP P19999
B	212	ASP	ILE	engineered mutation	UNP P19999
B	216	ARG	ALA	engineered mutation	UNP P19999
B	217	PRO	SER	engineered mutation	UNP P19999
B	218	TYR	HIS	engineered mutation	UNP P19999
C	185	GLN	GLU	engineered mutation	UNP P19999
C	187	ASP	ASN	engineered mutation	UNP P19999
C	189	TRP	HIS	engineered mutation	UNP P19999
C	181	TRP	-	insertion	UNP P19999
C	191	GLY	-	insertion	UNP P19999
C	192	HIS	-	insertion	UNP P19999
C	193	GLY	-	insertion	UNP P19999
C	194	LEU	-	insertion	UNP P19999
C	196	GLY	SER	engineered mutation	UNP P19999
C	202	HIS	THR	engineered mutation	UNP P19999
C	212	ASP	ILE	engineered mutation	UNP P19999
C	216	ARG	ALA	engineered mutation	UNP P19999
C	217	PRO	SER	engineered mutation	UNP P19999
C	218	TYR	HIS	engineered mutation	UNP P19999

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



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

Continued on next page...

Continued from previous page...

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

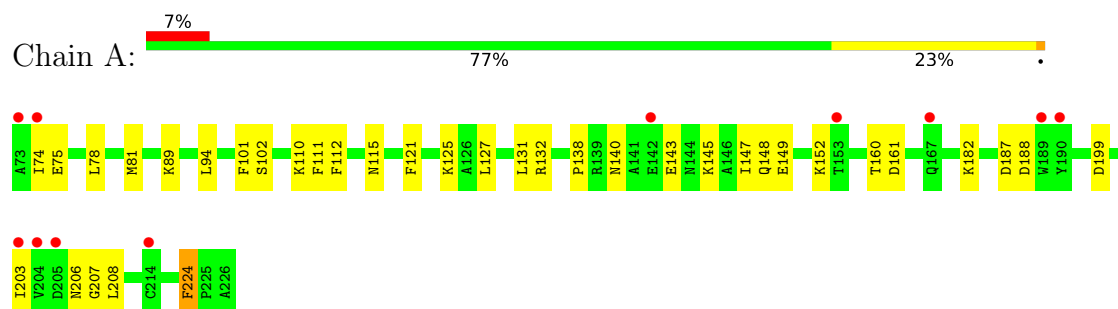
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O	0	0
			74	74		
5	B	40	Total	O	0	0
			40	40		
5	C	57	Total	O	0	0
			57	57		

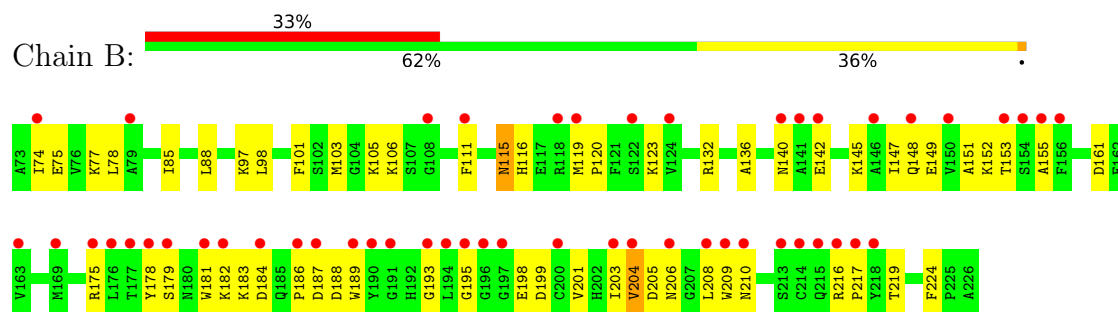
3 Residue-property plots

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.

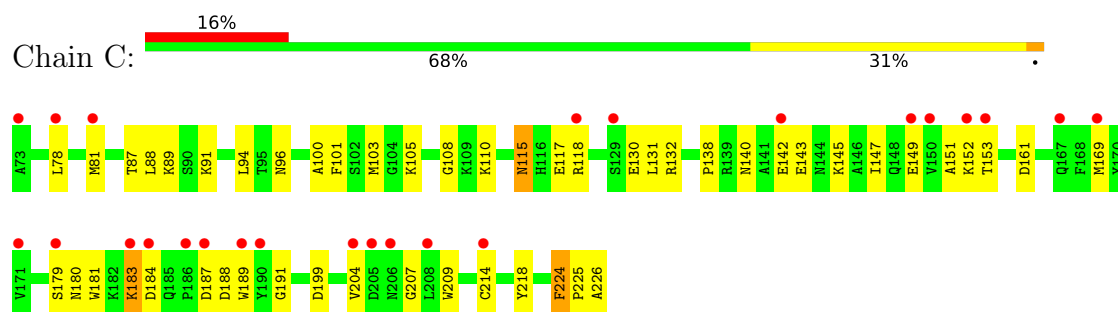
• Molecule 1: MANNOSE-BINDING PROTEIN A



• 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	81.49Å 84.55Å 98.54Å 90.00° 105.43° 90.00°	Depositor
Resolution (Å)	28.66 – 1.95 28.66 – 1.95	Depositor EDS
% Data completeness (in resolution range)	89.9 (28.66-1.95) 89.9 (28.66-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.67 (at 1.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.269 0.237 , 0.269	Depositor DCC
R_{free} test set	3622 reflections (8.30%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3858	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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: NGA, CL, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/1230	0.86	4/1657 (0.2%)
1	B	0.35	0/1230	0.81	4/1657 (0.2%)
1	C	0.39	0/1230	0.86	3/1657 (0.2%)
All	All	0.38	0/3690	0.84	11/4971 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	224	PHE	CA-C-N	6.38	126.39	119.89
1	C	224	PHE	C-N-CA	6.38	126.39	119.89
1	A	224	PHE	CA-C-N	6.00	126.01	119.89
1	A	224	PHE	C-N-CA	6.00	126.01	119.89
1	C	115	ASN	N-CA-C	-5.88	105.30	112.88
1	A	182	LYS	N-CA-C	-5.84	102.83	110.53
1	B	115	ASN	N-CA-C	-5.41	106.36	113.17
1	B	119	MET	N-CA-C	5.31	112.80	108.07
1	A	115	ASN	N-CA-C	-5.26	106.45	112.92
1	B	224	PHE	CA-C-N	5.03	124.96	119.78
1	B	224	PHE	C-N-CA	5.03	124.96	119.78

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1205	0	1172	30	0
1	B	1205	0	1172	47	0
1	C	1205	0	1172	43	0
2	A	15	0	14	0	0
2	B	15	0	13	1	0
2	C	30	0	30	4	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	74	0	0	0	0
5	B	40	0	0	6	0
5	C	57	0	0	3	0
All	All	3858	0	3573	102	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 14.

All (102) 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:204:VAL:HG12	1:B:205:ASP:H	1.21	1.03
1:A:102:SER:HB2	1:B:103:MET:HE2	1.56	0.87
1:B:88:LEU:HD21	1:C:89:LYS:HG2	1.56	0.85
1:C:118:ARG:NH1	1:C:218:TYR:HA	1.90	0.85
1:B:201:VAL:HG13	5:B:454:HOH:O	1.77	0.83
1:C:138:PRO:HG3	1:C:147:ILE:HD12	1.64	0.76
1:B:204:VAL:HG12	1:B:205:ASP:N	2.00	0.73
1:C:110:LYS:HD3	1:C:143:GLU:OE2	1.93	0.69
1:A:78:LEU:HD22	1:C:81:MET:HE1	1.76	0.67
1:A:78:LEU:HD22	1:C:81:MET:CE	2.25	0.67
1:A:94:LEU:HD21	1:B:132:ARG:HB2	1.78	0.66
1:C:161:ASP:OD1	1:C:199:ASP:HA	1.97	0.65
1:B:161:ASP:OD1	1:B:199:ASP:HA	1.97	0.65
1:C:169:MET:HE3	5:C:455:HOH:O	1.98	0.63
1:A:121:PHE:CE2	1:A:125:LYS:HD2	2.34	0.62
1:C:118:ARG:HH11	1:C:218:TYR:HA	1.63	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:TRP:HB3	5:B:454:HOH:O	2.02	0.59
1:A:138:PRO:HG3	1:A:147:ILE:HD12	1.84	0.59
1:A:145:LYS:HD2	1:A:148:GLN:NE2	2.19	0.58
1:B:179:SER:HA	1:B:209:TRP:CH2	2.39	0.57
1:B:74:ILE:HG13	1:B:75:GLU:N	2.20	0.56
1:B:181:TRP:CZ3	1:B:186:PRO:HG3	2.40	0.56
1:B:77:LYS:HD2	1:C:78:LEU:CD2	2.35	0.56
1:B:187:ASP:OD2	2:B:227:NGA:H62	2.06	0.56
1:C:118:ARG:HH12	1:C:218:TYR:HA	1.70	0.55
1:A:74:ILE:HG23	1:A:75:GLU:N	2.21	0.55
1:C:140:ASN:OD1	1:C:142:GLU:HB3	2.06	0.55
1:A:110:LYS:HE2	1:A:143:GLU:CD	2.31	0.55
1:B:103:MET:HG3	5:B:418:HOH:O	2.08	0.53
1:C:101:PHE:N	2:C:228:NGA:O6	2.41	0.53
1:C:100:ALA:HB3	2:C:228:NGA:O6	2.08	0.53
1:A:110:LYS:HE2	1:A:143:GLU:OE2	2.10	0.52
1:A:161:ASP:OD1	1:A:199:ASP:HA	2.09	0.52
1:B:151:ALA:C	1:B:153:THR:H	2.18	0.52
1:A:89:LYS:HG2	1:C:88:LEU:HD21	1.90	0.52
1:A:140:ASN:OD1	1:A:143:GLU:HG3	2.11	0.51
1:B:181:TRP:CE3	1:B:186:PRO:HG3	2.46	0.50
1:C:151:ALA:C	1:C:153:THR:H	2.18	0.50
1:B:145:LYS:O	1:B:148:GLN:HB3	2.12	0.50
1:C:183:LYS:O	1:C:184:ASP:HB2	2.11	0.50
1:A:132:ARG:HG3	1:C:94:LEU:CD2	2.41	0.49
1:C:214:CYS:HB2	5:C:437:HOH:O	2.11	0.49
1:C:87:THR:O	1:C:91:LYS:HG3	2.13	0.49
1:C:100:ALA:HB3	2:C:228:NGA:C6	2.42	0.49
1:B:210:ASN:N	5:B:454:HOH:O	2.45	0.49
1:A:111:PHE:CE1	1:A:224:PHE:HB2	2.48	0.49
1:A:145:LYS:HA	1:A:148:GLN:HE21	1.77	0.48
1:B:183:LYS:HG3	1:B:184:ASP:OD1	2.13	0.48
1:C:189:TRP:CE2	1:C:191:GLY:HA3	2.49	0.48
1:B:77:LYS:HD2	1:C:78:LEU:HD21	1.95	0.48
1:B:98:LEU:HD21	1:C:103:MET:HE1	1.95	0.47
1:C:183:LYS:NZ	1:C:183:LYS:HB3	2.30	0.47
1:A:131:LEU:O	1:A:132:ARG:HB2	2.14	0.47
1:B:140:ASN:OD1	1:B:142:GLU:N	2.48	0.46
1:A:110:LYS:HE3	1:A:112:PHE:CZ	2.50	0.46
1:B:216:ARG:HG3	1:B:217:PRO:HD2	1.97	0.46
1:B:182:LYS:HZ3	1:B:183:LYS:NZ	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD23	1:B:78:LEU:HD11	1.97	0.45
1:B:111:PHE:HZ	5:B:418:HOH:O	1.98	0.45
1:B:175:ARG:HG3	1:B:175:ARG:HH11	1.79	0.45
1:C:181:TRP:HA	1:C:209:TRP:HB2	1.99	0.45
1:B:204:VAL:HG23	1:B:208:LEU:O	2.16	0.45
1:A:110:LYS:HE3	1:A:112:PHE:HZ	1.82	0.45
1:B:181:TRP:HA	1:B:209:TRP:HB2	1.98	0.44
1:C:187:ASP:O	1:C:188:ASP:C	2.60	0.44
1:B:181:TRP:CH2	1:B:186:PRO:HG3	2.52	0.44
1:A:78:LEU:HD22	1:C:81:MET:HE3	1.98	0.44
1:A:132:ARG:HG3	1:C:94:LEU:HD21	2.00	0.43
1:B:155:ALA:HB2	1:B:219:THR:HB	2.00	0.43
1:A:81:MET:HG3	1:B:85:ILE:CD1	2.48	0.43
1:B:193:GLY:C	1:B:195:GLY:H	2.26	0.43
1:B:105:LYS:HG3	1:B:111:PHE:HB2	1.99	0.43
1:B:155:ALA:H	1:B:203:ILE:HG22	1.83	0.43
1:A:74:ILE:CG2	1:A:75:GLU:N	2.81	0.43
1:C:151:ALA:O	1:C:152:LYS:HB2	2.19	0.42
1:B:178:TYR:CD1	1:B:178:TYR:C	2.97	0.42
1:A:160:THR:HB	1:A:199:ASP:O	2.19	0.42
1:B:187:ASP:O	1:B:188:ASP:C	2.63	0.42
1:C:96:ASN:ND2	5:C:446:HOH:O	2.51	0.42
1:C:145:LYS:O	1:C:149:GLU:HG3	2.19	0.42
1:B:120:PRO:HD2	1:B:123:LYS:HG3	2.01	0.42
1:C:179:SER:HA	1:C:209:TRP:CH2	2.55	0.42
1:A:127:LEU:C	1:A:127:LEU:HD23	2.45	0.42
1:C:131:LEU:O	1:C:132:ARG:HB2	2.19	0.42
1:B:106:LYS:HD2	1:C:117:GLU:HG3	2.01	0.41
1:C:118:ARG:NH1	1:C:118:ARG:HG2	2.35	0.41
1:A:206:ASN:HD22	1:A:208:LEU:HG	1.84	0.41
1:A:187:ASP:O	1:A:188:ASP:C	2.63	0.41
1:A:203:ILE:HD11	1:A:207:GLY:HA2	2.02	0.41
1:B:149:GLU:HB2	5:B:453:HOH:O	2.20	0.41
1:B:182:LYS:NZ	1:B:183:LYS:NZ	2.68	0.41
1:B:189:TRP:O	1:B:198:GLU:HG3	2.20	0.41
1:C:180:ASN:ND2	1:C:207:GLY:O	2.51	0.41
1:B:97:LYS:HE3	1:C:130:GLU:HG2	2.03	0.41
1:B:136:ALA:HB1	1:B:147:ILE:HD13	2.03	0.41
1:C:108:GLY:O	1:C:226:ALA:HB1	2.21	0.41
1:A:101:PHE:CD1	1:B:115:ASN:HB3	2.56	0.41
1:B:101:PHE:CD1	1:C:115:ASN:HB3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:PHE:HA	1:C:225:PRO:HD3	1.86	0.41
1:C:189:TRP:CZ2	1:C:191:GLY:HA3	2.56	0.40
1:B:116:HIS:CE1	1:B:152:LYS:HE2	2.56	0.40
1:C:105:LYS:HD3	2:C:228:NGA:H61	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	152/154 (99%)	147 (97%)	5 (3%)	0	100	100
1	B	152/154 (99%)	140 (92%)	11 (7%)	1 (1%)	18	10
1	C	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	18	10
All	All	456/462 (99%)	434 (95%)	20 (4%)	2 (0%)	30	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	204	VAL
1	B	204	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	129/129 (100%)	127 (98%)	2 (2%)	55	52
1	B	129/129 (100%)	128 (99%)	1 (1%)	73	74
1	C	129/129 (100%)	128 (99%)	1 (1%)	73	74
All	All	387/387 (100%)	383 (99%)	4 (1%)	68	67

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

Mol	Chain	Res	Type
1	A	149	GLU
1	A	152	LYS
1	B	206	ASN
1	C	183	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	99	HIS
1	A	116	HIS
1	A	148	GLN
1	A	206	ASN
1	B	80	ASN
1	B	96	ASN
1	B	116	HIS
1	B	148	GLN
1	B	215	GLN
1	C	96	ASN
1	C	148	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 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	NGA	B	227	3	15,15,15	0.48	0	21,21,21	0.55	0
2	NGA	A	227	3	15,15,15	0.50	0	21,21,21	0.65	0
2	NGA	C	227	3	15,15,15	0.45	0	21,21,21	0.62	0
2	NGA	C	228	-	15,15,15	0.52	0	21,21,21	0.60	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	NGA	B	227	3	-	2/6/26/26	0/1/1/1
2	NGA	A	227	3	-	2/6/26/26	0/1/1/1
2	NGA	C	227	3	-	2/6/26/26	0/1/1/1
2	NGA	C	228	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	227	NGA	O5-C5-C6-O6
2	B	227	NGA	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	227	NGA	C4-C5-C6-O6
2	A	227	NGA	C4-C5-C6-O6
2	C	227	NGA	O5-C5-C6-O6
2	A	227	NGA	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	227	NGA	1	0
2	C	228	NGA	4	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	154/154 (100%)	0.72	11 (7%)	22 25	21, 32, 46, 56	0
1	B	154/154 (100%)	1.70	51 (33%)	1 0	23, 44, 65, 73	0
1	C	154/154 (100%)	1.06	25 (16%)	4 5	23, 36, 52, 62	0
All	All	462/462 (100%)	1.16	87 (18%)	3 3	21, 37, 60, 73	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	VAL	7.4
1	A	204	VAL	5.2
1	B	203	ILE	5.1
1	B	176	LEU	4.9
1	A	190	TYR	4.6
1	B	214	CYS	4.6
1	C	208	LEU	4.4
1	B	181	TRP	3.9
1	B	216	ARG	3.9
1	B	208	LEU	3.8
1	B	196	GLY	3.8
1	B	189	TRP	3.8
1	B	195	GLY	3.7
1	B	118	ARG	3.5
1	B	191	GLY	3.5
1	C	190	TYR	3.5
1	B	163	VAL	3.5
1	B	218	TYR	3.5
1	B	177	THR	3.5
1	B	154	SER	3.4
1	B	122	SER	3.4
1	C	204	VAL	3.4
1	C	167	GLN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	141	ALA	3.4
1	B	74	ILE	3.3
1	B	182	LYS	3.2
1	B	124	VAL	3.2
1	B	194	LEU	3.2
1	B	111	PHE	3.1
1	C	149	GLU	3.0
1	B	187	ASP	3.0
1	A	74	ILE	3.0
1	C	169	MET	2.9
1	C	206	ASN	2.9
1	B	217	PRO	2.9
1	B	206	ASN	2.8
1	A	167	GLN	2.8
1	B	200	CYS	2.8
1	B	178	TYR	2.8
1	B	190	TYR	2.7
1	B	142	GLU	2.7
1	A	73	ALA	2.7
1	C	187	ASP	2.7
1	C	214	CYS	2.6
1	C	183	LYS	2.6
1	B	209	TRP	2.6
1	B	175	ARG	2.6
1	C	152	LYS	2.5
1	C	73	ALA	2.5
1	C	81	MET	2.5
1	B	155	ALA	2.5
1	B	169	MET	2.5
1	C	153	THR	2.4
1	B	150	VAL	2.4
1	C	118	ARG	2.4
1	C	205	ASP	2.4
1	B	119	MET	2.4
1	B	156	PHE	2.4
1	C	184	ASP	2.4
1	B	148	GLN	2.4
1	A	214	CYS	2.4
1	C	129	SER	2.3
1	C	171	VAL	2.3
1	C	189	TRP	2.3
1	C	78	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	153	THR	2.3
1	B	140	ASN	2.3
1	B	153	THR	2.3
1	B	146	ALA	2.3
1	B	197	GLY	2.3
1	B	213	SER	2.3
1	C	179	SER	2.3
1	A	142	GLU	2.3
1	B	184	ASP	2.3
1	B	215	GLN	2.2
1	A	205	ASP	2.2
1	B	210	ASN	2.1
1	B	108	GLY	2.1
1	C	142	GLU	2.1
1	B	179	SER	2.1
1	B	193	GLY	2.1
1	B	186	PRO	2.1
1	B	79	ALA	2.1
1	C	150	VAL	2.0
1	C	186	PRO	2.0
1	A	189	TRP	2.0
1	A	203	ILE	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
2	NGA	C	228	15/15	0.67	0.16	63,66,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NGA	B	227	15/15	0.74	0.18	55,58,60,61	0
2	NGA	C	227	15/15	0.81	0.15	40,44,47,48	0
2	NGA	A	227	15/15	0.88	0.11	31,36,41,43	0
4	CL	B	416	1/1	0.91	0.14	65,65,65,65	0
3	CA	B	2	1/1	0.93	0.12	42,42,42,42	0
3	CA	C	2	1/1	0.95	0.08	36,36,36,36	0
3	CA	B	3	1/1	0.96	0.05	49,49,49,49	0
4	CL	A	415	1/1	0.97	0.10	42,42,42,42	0
4	CL	C	417	1/1	0.97	0.13	43,43,43,43	0
3	CA	A	2	1/1	0.98	0.07	28,28,28,28	0
3	CA	B	1	1/1	0.98	0.10	43,43,43,43	0
3	CA	C	3	1/1	0.99	0.02	30,30,30,30	0
3	CA	A	1	1/1	0.99	0.02	25,25,25,25	0
3	CA	C	1	1/1	0.99	0.03	32,32,32,32	0
3	CA	A	3	1/1	0.99	0.04	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.