



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:23 AM UTC

PDB ID : 6N5A / pdb_00006n5a
Title : Crystal structure of an equine H7 hemagglutinin from A/equine/NY/49/73 (H7N7)
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2018-11-21
Resolution : 3.30 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

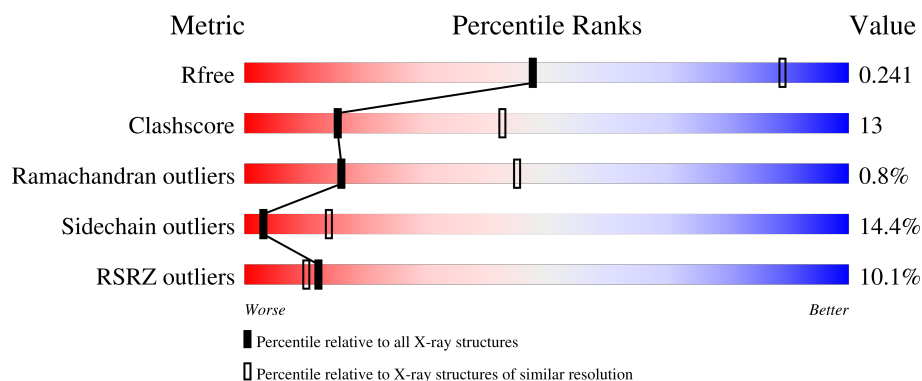
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	335	4% 56% 29% 7% 6%
2	B	186	19% 66% 21% 5% 9%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3940 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 HEMAGGLUTININ HA1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	315	2448	1531	435	467	15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP A0A348FV55
A	8	ASP	-	expression tag	UNP A0A348FV55
A	9	PRO	-	expression tag	UNP A0A348FV55
A	10	GLY	-	expression tag	UNP A0A348FV55

- Molecule 2 is a protein called HEMAGGLUTININ HA2 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	170	1390	862	247	276	5	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	179	GLU	-	expression tag	UNP A0A348FV55
B	180	SER	-	expression tag	UNP A0A348FV55
B	181	GLY	-	expression tag	UNP A0A348FV55
B	182	ARG	-	expression tag	UNP A0A348FV55
B	183	LEU	-	expression tag	UNP A0A348FV55
B	184	VAL	-	expression tag	UNP A0A348FV55
B	185	PRO	-	expression tag	UNP A0A348FV55
B	186	ARG	-	expression tag	UNP A0A348FV55

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



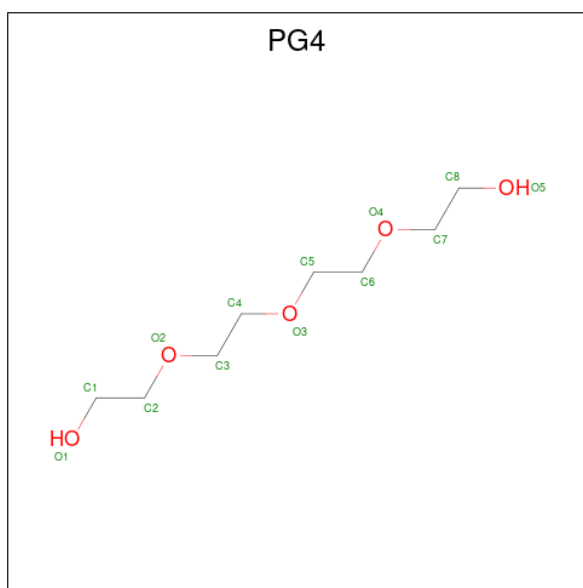
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



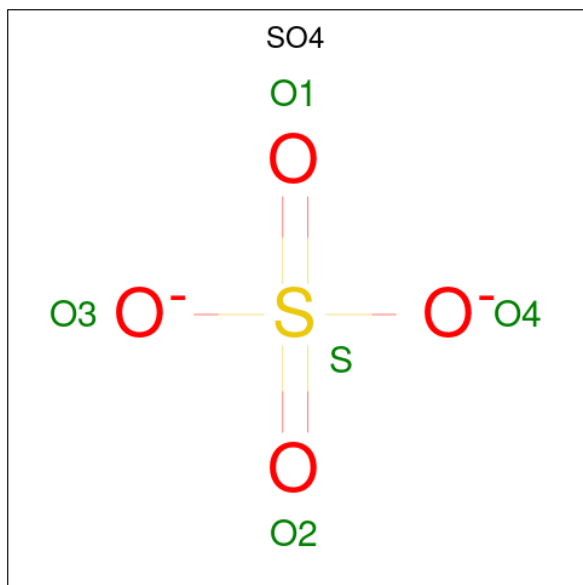
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		

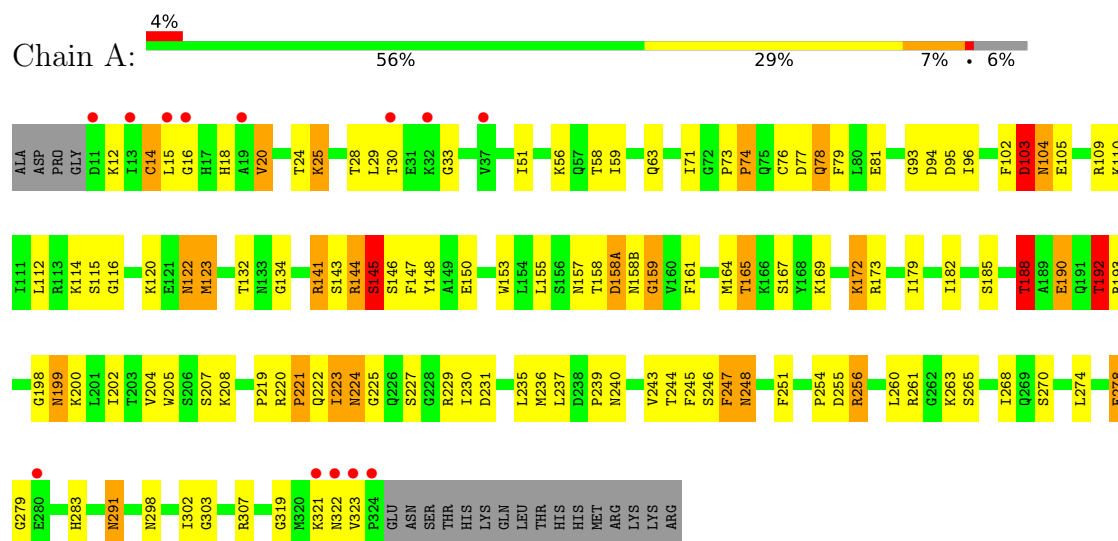
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	21	Total 21	O 21	0	0
9	B	1	Total 1	O 1	0	0

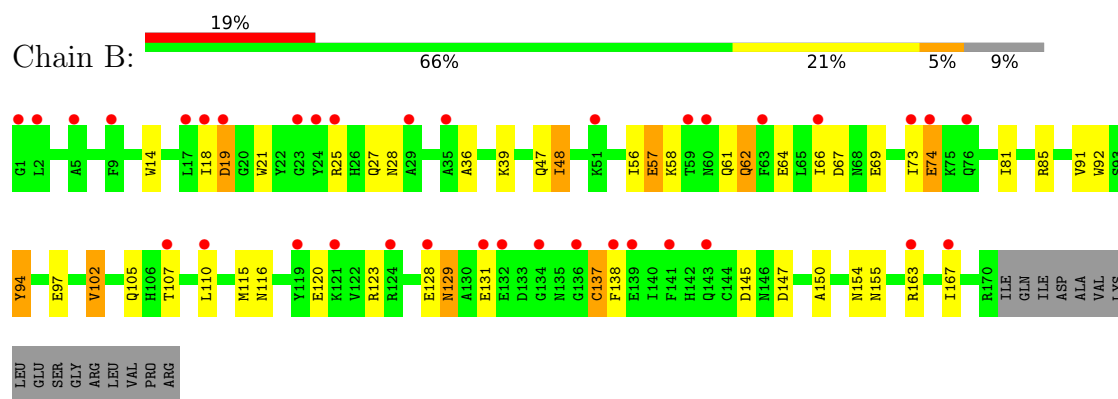
3 Residue-property plots [i](#)

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: HEMAGGLUTININ HA1 SUBUNIT



• Molecule 2: HEMAGGLUTININ HA2 SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	87.40Å 87.40Å 524.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.24 – 3.30 46.24 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.24-3.30) 99.7 (46.24-3.30)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.200 , 0.237 0.207 , 0.241	Depositor DCC
R_{free} test set	1015 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 97.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3940	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: SO4, PG4, PGE, NAG, PEG, EDO

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	1.11	0/2497	1.58	30/3368 (0.9%)
2	B	1.06	0/1415	1.63	1/1907 (0.1%)
All	All	1.10	0/3912	1.60	31/5275 (0.6%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	GLY	CA-C-N	-8.33	111.93	122.43
1	A	159	GLY	C-N-CA	-8.33	111.93	122.43
1	A	198	GLY	CA-C-O	-7.78	115.47	122.24
1	A	141	ARG	N-CA-C	-7.57	102.86	112.93
1	A	93	GLY	CA-C-O	-6.77	115.41	121.64
1	A	221	PRO	CB-CA-C	-6.61	102.93	111.39
1	A	161	PHE	O-C-N	6.48	126.52	121.47
1	A	122	ASN	CA-CB-CG	-6.45	106.15	112.60
1	A	248	ASN	CA-CB-CG	-6.32	106.28	112.60
1	A	188	THR	CA-CB-OG1	-6.28	100.17	109.60
1	A	110	LYS	N-CA-C	-6.20	104.52	111.28
1	A	231	ASP	CB-CA-C	5.99	119.63	109.80
1	A	199	ASN	N-CA-CB	5.86	118.60	110.17
1	A	255	ASP	N-CA-C	-5.85	105.40	113.18
1	A	103	ASP	CB-CA-C	5.83	119.48	109.51
1	A	188	THR	N-CA-C	-5.74	105.54	112.54
1	A	172	LYS	CB-CA-C	5.73	120.37	110.45
1	A	73	PRO	N-CA-C	-5.63	103.83	110.70
1	A	147	PHE	CA-C-O	-5.47	115.50	121.14
1	A	247	PHE	CA-C-O	5.47	127.11	121.10
1	A	103	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	134	GLY	CA-C-O	-5.36	116.76	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	THR	CA-CB-OG1	-5.36	101.56	109.60
1	A	192	THR	N-CA-C	-5.36	105.88	112.90
1	A	102	PHE	CA-C-O	-5.29	115.01	121.36
1	A	261	ARG	N-CA-C	-5.17	105.80	112.68
2	B	131	GLU	CB-CG-CD	5.14	121.34	112.60
1	A	95	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	158(A)	ASP	CA-C-O	-5.12	116.06	120.88
1	A	219	PRO	O-C-N	5.10	126.35	122.73
1	A	278	GLU	CB-CA-C	5.09	118.86	109.71

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	2448	0	2420	85	0
2	B	1390	0	1304	33	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	10	0	14	2	0
5	A	7	0	10	3	0
6	A	12	0	18	3	0
7	A	13	0	18	0	0
8	A	10	0	0	0	0
9	A	21	0	0	0	0
9	B	1	0	0	0	0
All	All	3940	0	3810	104	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 13.

All (104) 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:A:144:ARG:O	1:A:145:SER:C	2.03	0.98
1:A:307:ARG:HG2	2:B:92:TRP:CD2	2.14	0.82
1:A:235:LEU:HD12	1:A:235:LEU:C	2.04	0.81
1:A:237:LEU:HD22	1:A:243:VAL:HG23	1.64	0.80
1:A:188:THR:O	1:A:192:THR:CG2	2.31	0.78
1:A:103:ASP:OD2	4:A:402:PGE:H6	1.84	0.77
2:B:67:ASP:OD2	2:B:85:ARG:NH2	2.23	0.71
1:A:28:THR:HB	2:B:105:GLN:OE1	1.92	0.70
1:A:116:GLY:HA2	1:A:265:SER:HB3	1.75	0.68
1:A:268:ILE:HG22	1:A:302:ILE:HD11	1.76	0.68
2:B:28:ASN:HD22	2:B:145:ASP:HA	1.60	0.67
1:A:230:ILE:HG22	1:A:230:ILE:O	1.95	0.65
2:B:163:ARG:O	2:B:167:ILE:HG22	1.96	0.65
1:A:188:THR:O	1:A:192:THR:HG23	1.97	0.65
2:B:150:ALA:O	2:B:154:ASN:HB2	1.98	0.63
1:A:96:ILE:HD12	1:A:96:ILE:C	2.25	0.62
1:A:56:LYS:NZ	1:A:279:GLY:O	2.32	0.62
1:A:182:ILE:HD12	1:A:202:ILE:HD13	1.81	0.62
1:A:159:GLY:HA3	5:A:403:PEG:H31	1.82	0.61
1:A:77:ASP:OD1	1:A:141:ARG:NH2	2.31	0.61
1:A:105:GLU:HG3	1:A:109:ARG:NH1	2.15	0.61
1:A:188:THR:O	1:A:192:THR:HG22	2.00	0.59
1:A:144:ARG:O	1:A:145:SER:O	2.19	0.59
1:A:150:GLU:CD	1:A:256:ARG:HH11	2.10	0.58
1:A:165:THR:HA	1:A:245:PHE:O	2.05	0.57
1:A:190:GLU:OE2	1:A:193:ARG:NH1	2.38	0.56
1:A:150:GLU:OE2	1:A:256:ARG:NH1	2.40	0.55
1:A:221:PRO:O	1:A:229:ARG:NH2	2.36	0.55
1:A:25:LYS:HD2	1:A:33:GLY:O	2.07	0.54
1:A:247:PHE:CD2	1:A:251:PHE:CD2	2.96	0.54
1:A:173:ARG:HG3	6:A:404:EDO:H12	1.90	0.53
1:A:172:LYS:O	1:A:239:PRO:HB3	2.08	0.53
1:A:220:ARG:HG2	1:A:229:ARG:HG3	1.91	0.53
1:A:51:ILE:HD11	1:A:270:SER:OG	2.09	0.52
1:A:222:GLN:O	1:A:223:ILE:HG12	2.09	0.52
1:A:303:GLY:O	2:B:62:GLN:HB3	2.09	0.52
2:B:66:ILE:HD12	2:B:81:ILE:HG12	1.91	0.52
2:B:129:ASN:HD22	2:B:129:ASN:N	2.08	0.52
2:B:116:ASN:O	2:B:120:GLU:HG2	2.09	0.51
1:A:14:CYS:HB2	2:B:25:ARG:O	2.10	0.51
1:A:115:SER:HB2	1:A:260:LEU:HD22	1.92	0.51
1:A:223:ILE:HA	6:A:406:EDO:H12	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LEU:HD12	1:A:236:MET:N	2.26	0.50
1:A:141:ARG:HD2	1:A:146:SER:OG	2.12	0.50
1:A:123:MET:HE2	1:A:254:PRO:HG2	1.93	0.50
1:A:223:ILE:C	1:A:225:GLY:N	2.66	0.50
1:A:20:VAL:O	1:A:322:ASN:ND2	2.34	0.50
1:A:77:ASP:CG	1:A:141:ARG:HH21	2.19	0.49
2:B:150:ALA:O	2:B:154:ASN:CB	2.61	0.48
1:A:164:MET:O	1:A:246:SER:HA	2.13	0.48
1:A:14:CYS:SG	2:B:137:CYS:HB3	2.54	0.48
1:A:141:ARG:HG3	1:A:146:SER:CB	2.44	0.47
1:A:182:ILE:CD1	1:A:202:ILE:HD13	2.45	0.47
1:A:235:LEU:C	1:A:235:LEU:CD1	2.78	0.47
1:A:307:ARG:HG2	2:B:92:TRP:CG	2.50	0.47
1:A:14:CYS:SG	2:B:137:CYS:SG	3.12	0.47
1:A:200:LYS:HA	1:A:248:ASN:HD22	1.80	0.46
2:B:67:ASP:OD1	2:B:67:ASP:N	2.47	0.46
1:A:220:ARG:HB2	1:A:227:SER:O	2.15	0.46
2:B:94:TYR:C	2:B:94:TYR:CD1	2.93	0.46
1:A:103:ASP:O	1:A:104:ASN:C	2.59	0.46
1:A:159:GLY:HA3	5:A:403:PEG:C3	2.44	0.45
1:A:150:GLU:OE1	1:A:256:ARG:HD3	2.16	0.45
1:A:291:ASN:HB2	2:B:56:ILE:HG23	1.99	0.45
1:A:103:ASP:OD2	4:A:402:PGE:C6	2.62	0.45
2:B:28:ASN:ND2	2:B:145:ASP:HA	2.29	0.45
1:A:71:ILE:HD12	1:A:148:TYR:CE2	2.52	0.44
1:A:150:GLU:CD	1:A:256:ARG:NH1	2.76	0.44
2:B:19:ASP:HB3	2:B:36:ALA:HB2	1.99	0.44
2:B:73:ILE:HD12	2:B:74:GLU:H	1.82	0.44
1:A:283:HIS:HB2	1:A:298:ASN:ND2	2.32	0.44
1:A:29:LEU:HD21	2:B:102:VAL:HG23	2.00	0.44
2:B:18:ILE:C	2:B:18:ILE:HD12	2.43	0.44
1:A:112:LEU:HA	1:A:115:SER:HB3	1.98	0.43
1:A:247:PHE:CE2	1:A:251:PHE:CD2	3.05	0.43
2:B:48:ILE:HD11	2:B:107:THR:HG23	2.00	0.43
1:A:96:ILE:C	1:A:96:ILE:CD1	2.91	0.43
1:A:204:VAL:HG22	1:A:245:PHE:HD1	1.83	0.43
1:A:223:ILE:O	1:A:224:ASN:C	2.59	0.43
1:A:307:ARG:HG2	2:B:92:TRP:CE2	2.51	0.43
1:A:173:ARG:HG3	6:A:404:EDO:C1	2.47	0.43
1:A:16:GLY:HA3	2:B:14:TRP:CH2	2.53	0.43
2:B:47:GLN:CB	2:B:110:LEU:HD21	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASN:HD22	1:A:157:ASN:HA	1.58	0.42
1:A:71:ILE:O	1:A:148:TYR:HB3	2.19	0.42
1:A:169:LYS:HE3	1:A:240:ASN:HA	2.02	0.42
1:A:205:TRP:CZ2	1:A:244:THR:HG21	2.55	0.42
2:B:115:MET:HE3	2:B:115:MET:HA	2.02	0.42
1:A:247:PHE:CE2	1:A:251:PHE:CE2	3.06	0.42
1:A:12:LYS:HE2	2:B:27:GLN:HB3	2.02	0.41
1:A:74:PRO:C	1:A:76:CYS:N	2.77	0.41
2:B:28:ASN:HD22	2:B:145:ASP:CA	2.31	0.41
1:A:153:TRP:NE1	1:A:155:LEU:HD21	2.36	0.41
1:A:159:GLY:CA	5:A:403:PEG:H31	2.48	0.41
1:A:223:ILE:C	1:A:225:GLY:H	2.29	0.41
1:A:81:GLU:HG2	1:A:120:LYS:H	1.86	0.41
1:A:237:LEU:HD13	1:A:243:VAL:CG2	2.50	0.41
1:A:319:GLY:HA2	2:B:21:TRP:CH2	2.56	0.41
1:A:16:GLY:N	2:B:14:TRP:CH2	2.89	0.41
1:A:78:GLN:OE1	1:A:79:PHE:CE2	2.74	0.41
1:A:74:PRO:HA	1:A:77:ASP:OD2	2.21	0.40
1:A:268:ILE:HG22	1:A:302:ILE:CD1	2.50	0.40
2:B:123:ARG:HB2	2:B:138:PHE:CZ	2.56	0.40
1:A:150:GLU:OE1	1:A:150:GLU:HA	2.22	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	313/335 (93%)	286 (91%)	25 (8%)	2 (1%)	21	52
2	B	168/186 (90%)	152 (90%)	14 (8%)	2 (1%)	10	37
All	All	481/521 (92%)	438 (91%)	39 (8%)	4 (1%)	16	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	SER
2	B	74	GLU
1	A	224	ASN
2	B	57	GLU

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	270/288 (94%)	228 (84%)	42 (16%)	2	12
2	B	146/160 (91%)	128 (88%)	18 (12%)	4	19
All	All	416/448 (93%)	356 (86%)	60 (14%)	3	14

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	CYS
1	A	15	LEU
1	A	18	HIS
1	A	20	VAL
1	A	24	THR
1	A	25	LYS
1	A	30	THR
1	A	59	ILE
1	A	63	GLN
1	A	74	PRO
1	A	78	GLN
1	A	94	ASP
1	A	103	ASP
1	A	104	ASN
1	A	114	LYS
1	A	122	ASN
1	A	123	MET
1	A	132	THR
1	A	143	SER

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Mol	Chain	Res	Type
1	A	144	ARG
1	A	145	SER
1	A	158	THR
1	A	158(A)	ASP
1	A	158(B)	ASN
1	A	165	THR
1	A	167	SER
1	A	179	ILE
1	A	185	SER
1	A	188	THR
1	A	190	GLU
1	A	192	THR
1	A	199	ASN
1	A	207	SER
1	A	208	LYS
1	A	223	ILE
1	A	256	ARG
1	A	263	LYS
1	A	274	LEU
1	A	278	GLU
1	A	291	ASN
1	A	321	LYS
1	A	323	VAL
2	B	19	ASP
2	B	39	LYS
2	B	48	ILE
2	B	57	GLU
2	B	58	LYS
2	B	61	GLN
2	B	62	GLN
2	B	64	GLU
2	B	69	GLU
2	B	91	VAL
2	B	94	TYR
2	B	97	GLU
2	B	102	VAL
2	B	128	GLU
2	B	129	ASN
2	B	137	CYS
2	B	147	ASP
2	B	155	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	276(A)	ASN
2	B	28	ASN
2	B	61	GLN
2	B	129	ASN
2	B	142	HIS
2	B	146	ASN

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](#)

10 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	$\# Z > 2$
8	SO4	A	408	-	4,4,4	0.46	0	6,6,6	0.28	0
5	PEG	A	403	-	6,6,6	0.42	0	5,5,5	0.44	0
6	EDO	A	404	-	3,3,3	0.19	0	2,2,2	0.36	0
6	EDO	A	406	-	3,3,3	0.30	0	2,2,2	0.29	0
6	EDO	A	405	-	3,3,3	0.18	0	2,2,2	0.12	0
8	SO4	A	409	-	4,4,4	0.32	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	401	1	14,14,15	0.77	0	17,19,21	2.01	6 (35%)
4	PGE	A	402	-	9,9,9	0.46	0	8,8,8	0.40	0
7	PG4	A	407	-	12,12,12	0.60	0	11,11,11	0.45	0
3	NAG	B	201	2	14,14,15	0.96	1 (7%)	17,19,21	2.07	7 (41%)

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
5	PEG	A	403	-	-	3/4/4/4	-
6	EDO	A	404	-	-	1/1/1/1	-
6	EDO	A	406	-	-	1/1/1/1	-
6	EDO	A	405	-	-	0/1/1/1	-
3	NAG	A	401	1	-	2/6/23/26	0/1/1/1
4	PGE	A	402	-	-	4/7/7/7	-
7	PG4	A	407	-	-	4/10/10/10	-
3	NAG	B	201	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	NAG	O4-C4	2.05	1.48	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAG	C1-O5-C5	4.75	118.55	112.19
3	B	201	NAG	C4-C3-C2	4.24	117.23	111.02
3	B	201	NAG	C3-C4-C5	-3.60	103.70	110.23
3	A	401	NAG	C1-C2-N2	-3.47	104.96	110.43
3	B	201	NAG	C2-N2-C7	3.30	127.32	122.90
3	A	401	NAG	C8-C7-N2	-2.51	111.96	116.12
3	A	401	NAG	O7-C7-C8	2.46	126.43	122.05
3	A	401	NAG	O5-C5-C4	-2.37	105.07	110.83
3	B	201	NAG	C1-C2-N2	-2.29	106.83	110.43
3	B	201	NAG	O5-C5-C6	2.27	112.07	107.66
3	A	401	NAG	C6-C5-C4	2.26	118.57	113.02
3	B	201	NAG	O4-C4-C3	2.19	115.53	110.38
3	B	201	NAG	C8-C7-N2	-2.16	112.53	116.12

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	PGE	C3-C4-O3-C5
4	A	402	PGE	O2-C3-C4-O3
3	A	401	NAG	O5-C5-C6-O6
3	A	401	NAG	C4-C5-C6-O6
4	A	402	PGE	O3-C5-C6-O4
5	A	403	PEG	O1-C1-C2-O2
7	A	407	PG4	O1-C1-C2-O2
7	A	407	PG4	O3-C5-C6-O4
6	A	404	EDO	O1-C1-C2-O2
6	A	406	EDO	O1-C1-C2-O2
4	A	402	PGE	C1-C2-O2-C3
5	A	403	PEG	C1-C2-O2-C3
7	A	407	PG4	C3-C4-O3-C5
7	A	407	PG4	O4-C7-C8-O5
5	A	403	PEG	C4-C3-O2-C2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	PEG	3	0
6	A	404	EDO	2	0
6	A	406	EDO	1	0
4	A	402	PGE	2	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	315/335 (94%)	-0.03	13 (4%)	41	27	23, 49, 138, 204	0
2	B	170/186 (91%)	1.23	36 (21%)	2	2	54, 136, 183, 194	0
All	All	485/521 (93%)	0.41	49 (10%)	12	10	23, 80, 170, 204	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	141	PHE	4.7
2	B	60	ASN	4.6
2	B	59	THR	4.6
2	B	23	GLY	4.4
2	B	76	GLN	4.3
2	B	74	GLU	4.0
2	B	29	ALA	4.0
2	B	73	ILE	3.9
1	A	13	ILE	3.5
2	B	24	TYR	3.3
2	B	2	LEU	3.2
2	B	132	GLU	3.1
2	B	124	ARG	3.1
2	B	143	GLN	3.0
1	A	16	GLY	2.9
2	B	1	GLY	2.9
2	B	138	PHE	2.9
2	B	110	LEU	2.9
1	A	37	VAL	2.9
2	B	9	PHE	2.8
1	A	19	ALA	2.8
2	B	5	ALA	2.8
2	B	163	ARG	2.8
1	A	324	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	323	VAL	2.7
1	A	32	LYS	2.6
2	B	51	LYS	2.6
2	B	121	LYS	2.5
2	B	128	GLU	2.5
1	A	280	GLU	2.5
2	B	18	ILE	2.4
2	B	139	GLU	2.4
2	B	63	PHE	2.4
2	B	167	ILE	2.3
2	B	25	ARG	2.3
2	B	35	ALA	2.3
2	B	119	TYR	2.3
2	B	17	LEU	2.3
2	B	19	ASP	2.2
2	B	131	GLU	2.2
1	A	11	ASP	2.2
2	B	107	THR	2.2
1	A	15	LEU	2.2
2	B	134	GLY	2.2
1	A	321	LYS	2.2
1	A	30	THR	2.2
2	B	136	GLY	2.1
2	B	66	ILE	2.1
1	A	322	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	NAG	B	201	14/15	0.66	0.20	95,117,130,134	0
6	EDO	A	404	4/4	0.81	0.29	84,94,97,100	0
3	NAG	A	401	14/15	0.85	0.12	74,94,114,122	0
6	EDO	A	405	4/4	0.88	0.35	53,54,56,56	0
7	PG4	A	407	13/13	0.88	0.22	74,94,140,143	0
5	PEG	A	403	7/7	0.91	0.15	57,70,84,101	0
4	PGE	A	402	10/10	0.91	0.18	45,75,78,91	0
6	EDO	A	406	4/4	0.95	0.14	43,45,51,61	0
8	SO4	A	408	5/5	0.98	0.08	42,49,51,55	5
8	SO4	A	409	5/5	0.98	0.13	52,58,61,65	5

6.5 Other polymers [i](#)

There are no such residues in this entry.