



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:24 PM UTC

PDB ID : 5XLB / pdb_00005xlb
Title : The structure of hemagglutinin Q226L-G228S mutant from an avian-origin H4N6 influenza virus
Authors : Song, H.; Qi, J.; Gao, G.F.
Deposited on : 2017-05-10
Resolution : 2.50 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

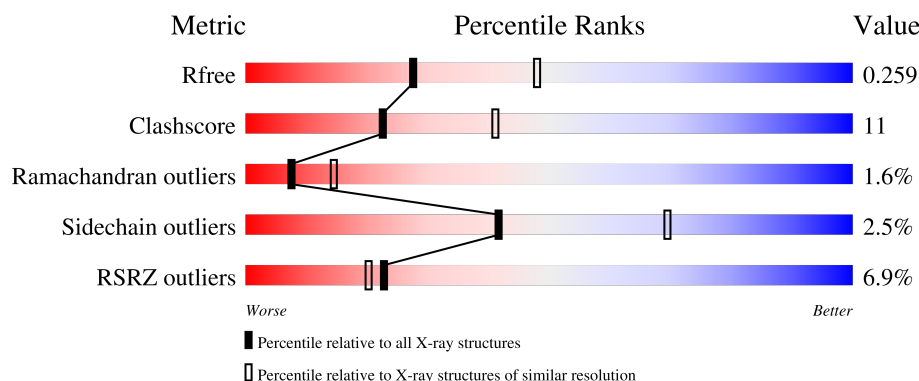
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	327	16% 69% 20% 6% ..
1	B	327	2% 84% 12% ..
2	C	176	2% 89% 9% .
2	D	176	2% 89% 8% ...

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8029 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2460	1542	436	470	12			
1	B	319	Total	C	N	O	S	0	0	0
			2460	1542	436	470	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	LEU	GLN	engineered mutation	UNP A3KF09
A	225	SER	GLY	engineered mutation	UNP A3KF09
B	223	LEU	GLN	engineered mutation	UNP A3KF09
B	225	SER	GLY	engineered mutation	UNP A3KF09

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	172	Total	C	N	O	S	0	0	0
			1404	871	250	279	4			
2	D	172	Total	C	N	O	S	0	0	0
			1404	871	250	279	4			

- 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	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		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

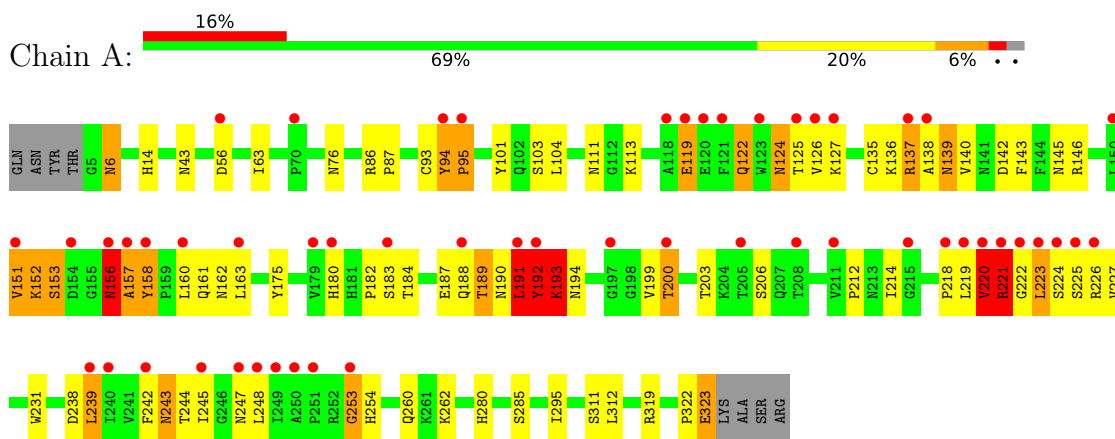
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	C	65	Total	O	0	0
			65	65		
4	B	72	Total	O	0	0
			72	72		
4	D	79	Total	O	0	0
			79	79		

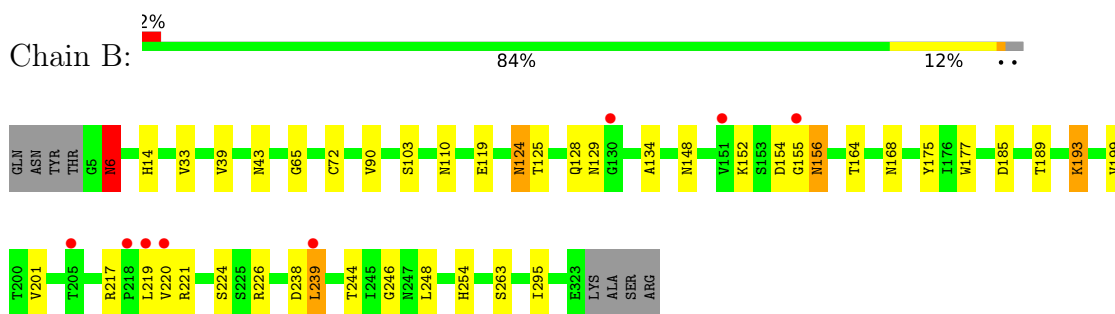
3 Residue-property plots [i](#)

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.

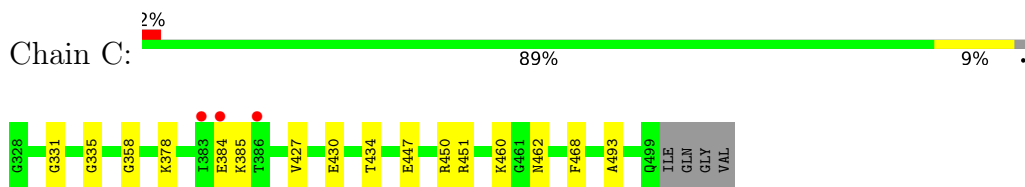
- Molecule 1: Hemagglutinin



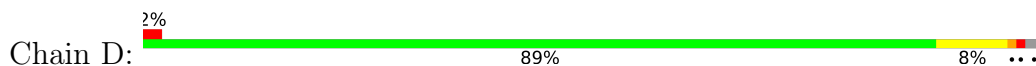
- Molecule 1: Hemagglutinin



- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	100.52Å 100.52Å 686.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.14 – 2.50 45.14 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.14-2.50) 90.0 (45.14-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.218 , 0.258 0.223 , 0.259	Depositor DCC
R_{free} test set	2398 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8029	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4335e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.60	2/2514 (0.1%)	1.10	18/3423 (0.5%)
1	B	0.35	0/2514	0.81	2/3423 (0.1%)
2	C	0.35	0/1428	0.71	1/1922 (0.1%)
2	D	0.36	0/1428	0.73	2/1922 (0.1%)
All	All	0.45	2/7884 (0.0%)	0.88	23/10690 (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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	VAL	CA-CB	7.54	1.64	1.54
1	A	140	VAL	CA-CB	5.16	1.61	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	TYR	N-CA-C	10.07	132.25	110.80
1	A	152	LYS	N-CA-C	8.57	122.32	110.24
1	B	6	ASN	CA-C-N	-8.55	111.22	119.85
1	B	6	ASN	C-N-CA	-8.55	111.22	119.85
1	A	94	TYR	CA-C-N	-7.25	110.77	119.84
1	A	94	TYR	C-N-CA	-7.25	110.77	119.84
1	A	193	LYS	CA-CB-CG	6.92	127.95	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	THR	CA-C-N	6.85	129.94	120.63
1	A	189	THR	C-N-CA	6.85	129.94	120.63
1	A	192	TYR	CA-C-N	6.79	134.51	121.54
1	A	192	TYR	C-N-CA	6.79	134.51	121.54
1	A	253	GLY	N-CA-C	6.46	119.59	110.74
2	D	384	GLU	N-CA-C	6.40	120.02	108.17
1	A	6	ASN	CA-C-N	-6.38	113.41	119.85
1	A	6	ASN	C-N-CA	-6.38	113.41	119.85
2	C	358	GLY	N-CA-C	6.23	118.36	110.38
1	A	158	TYR	CA-CB-CG	5.64	124.06	113.90
1	A	223	LEU	CA-C-O	-5.36	115.72	121.45
1	A	223	LEU	N-CA-C	-5.33	101.01	108.96
1	A	157	ALA	CA-C-N	5.26	130.18	122.98
1	A	157	ALA	C-N-CA	5.26	130.18	122.98
2	D	358	GLY	N-CA-C	5.22	117.06	110.38
1	A	140	VAL	N-CA-C	5.08	115.78	107.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	LEU	Peptide
1	A	95	PRO	Peptide

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	2460	0	2414	109	1
1	B	2460	0	2414	31	1
2	C	1404	0	1320	10	0
2	D	1404	0	1320	14	0
3	A	28	0	26	0	0
3	B	28	0	26	1	0
4	A	29	0	0	6	0
4	B	72	0	0	4	0
4	C	65	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	79	0	0	5	0
All	All	8029	0	7520	161	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 11.

All (161) 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:14:HIS:HD2	2:D:348:TRP:HA	1.15	1.05
1:A:220:VAL:O	1:A:222:GLY:N	2.00	0.94
1:A:220:VAL:HG22	1:A:221:ARG:HD3	1.45	0.94
1:A:158:TYR:H	1:A:193:LYS:HD3	1.35	0.92
1:B:244:THR:HG22	1:B:246:GLY:H	1.37	0.86
1:B:14:HIS:CD2	2:D:348:TRP:HA	2.08	0.85
1:A:218:PRO:O	1:A:221:ARG:NH2	2.10	0.84
1:A:56:ASP:OD2	4:A:702:HOH:O	1.96	0.83
1:A:220:VAL:H	1:A:221:ARG:NH1	1.75	0.83
1:A:221:ARG:HH21	1:A:224:SER:HA	1.44	0.82
2:C:385:LYS:NZ	4:C:601:HOH:O	2.10	0.82
1:B:128:GLN:HG2	1:B:148:ASN:HD21	1.44	0.81
1:A:152:LYS:NZ	1:A:189:THR:O	2.13	0.79
1:A:221:ARG:NH2	1:A:223:LEU:O	2.14	0.79
1:A:212:PRO:HG2	1:A:247:ASN:HD22	1.46	0.79
1:B:152:LYS:NZ	1:B:189:THR:O	2.16	0.78
2:D:382:LEU:O	2:D:383:ILE:C	2.26	0.77
1:A:260:GLN:OE1	1:A:262:LYS:NZ	2.17	0.77
1:A:152:LYS:HB2	1:A:192:TYR:HB3	1.68	0.73
1:A:158:TYR:CD2	1:A:192:TYR:CE2	2.76	0.73
1:A:103:SER:OG	4:A:703:HOH:O	2.06	0.73
1:A:183:SER:N	1:A:187:GLU:OE1	2.19	0.73
1:A:221:ARG:NH2	1:A:224:SER:HA	2.01	0.73
2:D:346:ASP:OD1	4:D:601:HOH:O	2.06	0.72
1:B:43:ASN:HB3	1:B:295:ILE:HD13	1.71	0.72
1:A:127:LYS:HD3	1:A:152:LYS:O	1.90	0.71
1:B:6:ASN:ND2	4:B:705:HOH:O	2.24	0.71
1:A:119:GLU:OE2	1:A:254:HIS:ND1	2.24	0.70
1:A:152:LYS:HE3	1:A:192:TYR:CB	2.22	0.69
1:A:244:THR:HG21	1:A:248:LEU:HB2	1.72	0.69
1:A:311:SER:O	4:A:704:HOH:O	2.09	0.69
1:A:212:PRO:HG2	1:A:247:ASN:ND2	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLN:HE21	1:A:247:ASN:HD21	1.41	0.68
1:A:43:ASN:HB3	1:A:295:ILE:HD13	1.76	0.67
2:D:422:ASN:OD1	4:D:602:HOH:O	2.13	0.67
1:A:152:LYS:HD3	1:A:156:ASN:OD1	1.95	0.66
2:D:456:ASN:OD1	4:D:603:HOH:O	2.15	0.65
1:A:124:ASN:HB2	1:A:161:GLN:HE21	1.61	0.65
1:A:191:LEU:HD23	1:A:192:TYR:HD1	1.63	0.64
1:A:238:ASP:OD1	1:A:239:LEU:N	2.23	0.64
1:A:226:ARG:HG2	1:A:226:ARG:HH11	1.64	0.63
1:A:191:LEU:O	1:A:192:TYR:HB3	1.98	0.62
1:A:191:LEU:HD23	1:A:192:TYR:CD1	2.34	0.62
1:A:162:ASN:HB3	1:A:243:ASN:HD21	1.64	0.62
1:A:137:ARG:HH22	1:A:145:ASN:HD22	1.48	0.62
2:D:383:ILE:HG22	2:D:384:GLU:HG3	1.81	0.61
1:A:158:TYR:HB3	1:A:193:LYS:HZ2	1.65	0.61
1:A:203:THR:HG1	1:A:206:SER:HG	1.46	0.61
1:A:199:VAL:HG22	1:A:244:THR:HG22	1.83	0.60
1:A:188:GLN:NE2	1:A:247:ASN:HD21	1.99	0.60
1:A:244:THR:HG21	1:A:248:LEU:CB	2.32	0.58
1:A:158:TYR:N	1:A:193:LYS:HD3	2.13	0.58
1:A:219:LEU:HA	1:A:221:ARG:NH2	2.19	0.58
1:A:119:GLU:HG3	1:A:253:GLY:HA2	1.85	0.58
1:A:158:TYR:HB3	1:A:193:LYS:NZ	2.18	0.57
1:A:182:PRO:HG2	1:A:188:GLN:HG2	1.85	0.57
2:D:382:LEU:O	2:D:383:ILE:O	2.21	0.57
1:A:137:ARG:HH12	1:A:145:ASN:HB3	1.68	0.57
1:A:199:VAL:HG11	1:A:248:LEU:HD13	1.87	0.57
1:A:162:ASN:HB3	1:A:243:ASN:ND2	2.19	0.57
1:A:322:PRO:O	1:A:323:GLU:HB2	2.04	0.57
1:A:183:SER:HB3	1:A:224:SER:HB3	1.86	0.56
1:B:156:ASN:HB3	1:B:193:LYS:NZ	2.20	0.56
1:B:164:THR:OG1	3:B:601:NAG:O7	2.23	0.55
1:B:14:HIS:CE1	1:B:33:VAL:HG11	2.42	0.55
1:A:220:VAL:HG23	1:A:221:ARG:N	2.22	0.55
1:A:137:ARG:HD2	1:A:142:ASP:OD2	2.07	0.54
1:A:94:TYR:H	1:A:135:CYS:HB2	1.71	0.54
1:A:158:TYR:HD2	1:A:192:TYR:HE2	1.56	0.54
2:C:447:GLU:OE1	2:C:450:ARG:NH1	2.41	0.53
1:B:134:ALA:O	1:B:221:ARG:NH1	2.42	0.53
1:B:156:ASN:HB3	1:B:193:LYS:HZ1	1.74	0.53
1:B:14:HIS:HE1	1:B:33:VAL:HG11	1.72	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:TYR:CD1	1:A:192:TYR:N	2.77	0.52
1:B:14:HIS:CE1	1:B:33:VAL:HG21	2.45	0.52
1:B:103:SER:OG	4:B:702:HOH:O	2.19	0.51
2:C:434:THR:OG1	4:C:602:HOH:O	2.19	0.51
1:A:319:ARG:NE	4:A:701:HOH:O	1.89	0.51
1:B:220:VAL:HG12	1:B:221:ARG:HG3	1.93	0.50
1:B:39:VAL:O	4:B:703:HOH:O	2.20	0.50
1:A:152:LYS:HA	1:A:192:TYR:CD2	2.47	0.50
1:A:280:HIS:ND1	1:A:285:SER:OG	2.44	0.49
1:A:76:ASN:OD1	1:A:146:ARG:NH2	2.41	0.49
1:A:221:ARG:HH11	1:A:226:ARG:HH12	1.60	0.49
1:A:158:TYR:CD2	1:A:192:TYR:HE2	2.26	0.48
1:A:111:ASN:ND2	4:A:705:HOH:O	2.12	0.48
1:A:94:TYR:OH	1:A:225:SER:HB2	2.14	0.48
1:A:220:VAL:HG13	1:A:221:ARG:NH1	2.29	0.48
2:C:460:LYS:NZ	4:C:607:HOH:O	2.47	0.48
1:A:221:ARG:HG2	1:A:222:GLY:N	2.29	0.47
2:D:495:ASN:ND2	2:D:499:GLN:OE1	2.47	0.47
1:A:226:ARG:HH11	1:A:226:ARG:CG	2.27	0.47
1:A:188:GLN:NE2	1:A:247:ASN:ND2	2.62	0.47
1:A:192:TYR:HD1	1:A:192:TYR:N	2.13	0.47
1:A:153:SER:OG	1:A:157:ALA:N	2.48	0.47
1:A:94:TYR:N	1:A:135:CYS:HB2	2.30	0.47
1:B:238:ASP:OD1	1:B:239:LEU:N	2.42	0.46
1:A:221:ARG:NH1	1:A:226:ARG:HH12	2.13	0.46
1:A:124:ASN:HB3	1:A:125:THR:H	1.47	0.46
1:A:152:LYS:HE3	1:A:192:TYR:CA	2.45	0.46
1:A:119:GLU:CG	1:A:253:GLY:HA2	2.44	0.46
1:B:177:TRP:CE2	1:B:201:VAL:HG21	2.51	0.46
1:A:63:ILE:HG13	1:A:101:TYR:CE2	2.52	0.45
1:A:104:LEU:HB2	1:A:231:TRP:CZ3	2.51	0.45
1:A:127:LYS:HG2	1:A:151:VAL:HG23	1.98	0.45
1:A:152:LYS:HE3	1:A:192:TYR:HB3	1.97	0.45
1:A:243:ASN:HD22	1:A:243:ASN:HA	1.57	0.45
2:D:366:LYS:HG2	4:D:604:HOH:O	2.15	0.45
1:A:122:GLN:N	1:A:163:LEU:HD21	2.32	0.45
1:A:152:LYS:HE3	1:A:192:TYR:HB2	1.98	0.45
1:A:244:THR:CG2	1:A:248:LEU:HB2	2.44	0.45
1:A:137:ARG:O	1:A:137:ARG:HG2	2.16	0.45
1:A:113:LYS:NZ	4:A:707:HOH:O	2.36	0.44
1:A:221:ARG:CZ	1:A:223:LEU:O	2.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ASN:HA	1:B:263:SER:O	2.18	0.44
1:A:221:ARG:NE	1:A:223:LEU:O	2.51	0.44
1:A:137:ARG:HH22	1:A:145:ASN:ND2	2.13	0.44
1:A:191:LEU:O	1:A:192:TYR:CB	2.64	0.44
1:B:154:ASP:C	1:B:156:ASN:H	2.26	0.44
1:A:312:LEU:HB3	2:C:427:VAL:HG21	1.99	0.43
1:A:142:ASP:CG	1:A:143:PHE:H	2.27	0.43
1:B:199:VAL:HG11	1:B:248:LEU:HD13	1.99	0.43
1:A:136:LYS:HD3	1:A:139:ASN:C	2.43	0.43
1:B:119:GLU:OE1	1:B:175:TYR:OH	2.34	0.43
1:A:86:ARG:HA	1:A:87:PRO:HD3	1.90	0.43
1:A:94:TYR:CE2	1:A:227:VAL:HG23	2.54	0.43
1:A:152:LYS:HD3	1:A:156:ASN:HB3	2.01	0.43
1:A:188:GLN:HE21	1:A:247:ASN:ND2	2.12	0.43
2:D:468:PHE:O	2:D:493:ALA:HA	2.19	0.43
1:A:152:LYS:HE2	1:A:156:ASN:HB3	2.01	0.43
1:B:175:TYR:CE2	1:B:254:HIS:HB3	2.54	0.42
1:A:200:THR:OG1	1:A:243:ASN:HB2	2.19	0.42
1:A:94:TYR:HE2	1:A:180:HIS:CD2	2.37	0.42
1:A:160:LEU:HD23	1:A:245:ILE:HG22	2.01	0.42
1:B:199:VAL:HG22	1:B:244:THR:HG23	2.01	0.42
1:B:124:ASN:HB3	1:B:125:THR:H	1.55	0.42
1:B:217:ARG:HB2	1:B:224:SER:O	2.19	0.42
2:D:451:ARG:HD2	4:D:625:HOH:O	2.19	0.42
1:A:119:GLU:CD	1:A:253:GLY:HA2	2.45	0.42
2:C:331:GLY:O	2:C:335:GLY:HA3	2.20	0.42
1:B:128:GLN:HB3	1:B:129:ASN:ND2	2.35	0.42
1:A:127:LYS:N	1:A:127:LYS:HD2	2.35	0.42
1:B:65:GLY:HA2	1:B:72:CYS:HB3	2.02	0.42
1:A:152:LYS:HB2	1:A:191:LEU:O	2.19	0.41
1:B:226:ARG:NE	4:B:716:HOH:O	2.53	0.41
1:A:182:PRO:O	1:A:214:ILE:HA	2.20	0.41
2:C:378:LYS:NZ	2:C:430:GLU:OE1	2.41	0.41
2:D:383:ILE:HG22	2:D:384:GLU:N	2.34	0.41
1:A:175:TYR:CE2	1:A:254:HIS:HB3	2.55	0.41
2:C:447:GLU:O	2:C:451:ARG:HG3	2.21	0.41
1:B:185:ASP:O	1:B:189:THR:OG1	2.19	0.41
2:D:447:GLU:OE1	2:D:450:ARG:NH1	2.53	0.41
1:A:152:LYS:CD	1:A:156:ASN:HB3	2.50	0.41
2:C:462:ASN:OD1	2:C:462:ASN:N	2.52	0.41
1:A:153:SER:HB3	1:A:157:ALA:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:VAL:CG2	1:A:221:ARG:N	2.84	0.41
1:A:93:CYS:HA	1:A:135:CYS:HA	2.03	0.40
1:A:193:LYS:HB2	1:A:194:ASN:H	1.29	0.40
1:A:126:VAL:HG11	1:A:158:TYR:CE2	2.57	0.40
1:A:162:ASN:HA	1:A:242:PHE:O	2.21	0.40
2:C:468:PHE:O	2:C:493:ALA:HA	2.21	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)
1:A:156:ASN:ND2	1:B:155:GLY:O[14_1144]	2.13	0.07

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	317/327 (97%)	289 (91%)	18 (6%)	10 (3%)	3	4
1	B	317/327 (97%)	300 (95%)	13 (4%)	4 (1%)	9	18
2	C	170/176 (97%)	159 (94%)	10 (6%)	1 (1%)	21	38
2	D	170/176 (97%)	161 (95%)	8 (5%)	1 (1%)	21	38
All	All	974/1006 (97%)	909 (93%)	49 (5%)	16 (2%)	7	14

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	221	ARG
1	B	124	ASN
2	D	383	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	138	ALA
1	A	156	ASN
1	A	193	LYS
1	B	6	ASN
1	B	156	ASN
1	A	6	ASN
1	B	193	LYS
1	A	153	SER
1	A	192	TYR
2	C	384	GLU
1	A	220	VAL
1	A	95	PRO

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	276/283 (98%)	260 (94%)	16 (6%)	18	38
1	B	276/283 (98%)	272 (99%)	4 (1%)	59	81
2	C	147/150 (98%)	147 (100%)	0	100	100
2	D	147/150 (98%)	146 (99%)	1 (1%)	76	89
All	All	846/866 (98%)	825 (98%)	21 (2%)	42	69

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	119	GLU
1	A	122	GLN
1	A	137	ARG
1	A	139	ASN
1	A	156	ASN
1	A	184	THR
1	A	190	ASN
1	A	191	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	192	TYR
1	A	200	THR
1	A	220	VAL
1	A	221	ARG
1	A	239	LEU
1	A	243	ASN
1	A	323	GLU
1	B	90	VAL
1	B	168	ASN
1	B	219	LEU
1	B	239	LEU
2	D	384	GLU

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

Mol	Chain	Res	Type
1	A	42	GLN
1	A	190	ASN
1	A	194	ASN
1	A	243	ASN
1	A	247	ASN
2	C	342	GLN
2	C	452	GLN
1	B	14	HIS
1	B	58	GLN
1	B	194	ASN
2	D	387	ASN
2	D	452	GLN
2	D	495	ASN

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](#)

4 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	NAG	B	602	1	14,14,15	0.40	0	17,19,21	0.55	0
3	NAG	B	601	1	14,14,15	0.44	0	17,19,21	0.44	0
3	NAG	A	601	1	14,14,15	0.39	0	17,19,21	0.52	0
3	NAG	A	602	1	14,14,15	0.54	0	17,19,21	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
3	NAG	B	602	1	-	2/6/23/26	0/1/1/1
3	NAG	B	601	1	-	2/6/23/26	0/1/1/1
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1
3	NAG	A	602	1	-	0/6/23/26	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
3	B	602	NAG	O5-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	602	NAG	C4-C5-C6-O6
3	B	601	NAG	C4-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	A	601	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/327 (97%)	0.88	53 (16%) 4 3	28, 78, 148, 207	0
1	B	319/327 (97%)	0.14	8 (2%) 58 54	25, 50, 91, 120	0
2	C	172/176 (97%)	-0.19	3 (1%) 69 65	28, 40, 67, 129	0
2	D	172/176 (97%)	-0.30	4 (2%) 61 57	24, 37, 52, 142	0
All	All	982/1006 (97%)	0.25	68 (6%) 23 20	24, 49, 120, 207	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	TYR	6.9
2	D	383	ILE	6.4
1	A	123	TRP	4.9
1	A	191	LEU	4.9
2	C	383	ILE	4.4
1	A	247	ASN	4.2
1	A	218	PRO	4.2
1	A	219	LEU	4.1
1	A	220	VAL	4.1
1	A	95	PRO	4.1
1	A	121	PHE	3.9
1	A	222	GLY	3.9
1	A	192	TYR	3.9
1	A	119	GLU	3.6
1	A	223	LEU	3.5
1	A	157	ALA	3.4
1	A	251	PRO	3.4
1	A	221	ARG	3.4
1	B	155	GLY	3.2
2	D	385	LYS	3.1
1	A	118	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	226	ARG	3.0
1	A	225	SER	3.0
1	B	220	VAL	2.9
1	A	205	THR	2.9
1	B	205	THR	2.9
1	A	200	THR	2.8
1	A	239	LEU	2.7
1	A	120	GLU	2.7
1	A	126	VAL	2.7
1	B	130	GLY	2.7
2	C	386	THR	2.6
1	A	245	ILE	2.6
1	A	125	THR	2.5
1	B	218	PRO	2.5
1	A	163	LEU	2.4
1	A	188	GLN	2.4
2	C	384	GLU	2.4
2	D	499	GLN	2.4
1	A	179	VAL	2.4
1	A	240	ILE	2.4
1	A	249	ILE	2.4
1	A	242	PHE	2.4
2	D	384	GLU	2.4
1	A	208	THR	2.3
1	A	56	ASP	2.3
1	A	197	GLY	2.3
1	A	215	GLY	2.3
1	A	253	GLY	2.3
1	A	211	VAL	2.3
1	A	150	LEU	2.3
1	A	248	LEU	2.3
1	A	151	VAL	2.3
1	A	158	TYR	2.2
1	A	183	SER	2.2
1	A	154	ASP	2.2
1	B	151	VAL	2.2
1	A	224	SER	2.2
1	A	127	LYS	2.2
1	A	156	ASN	2.1
1	A	250	ALA	2.1
1	A	137	ARG	2.1
1	A	160	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	239	LEU	2.1
1	A	70	PRO	2.1
1	A	180	HIS	2.1
1	A	138	ALA	2.0
1	B	219	LEU	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
3	NAG	B	601	14/15	0.58	0.15	91,96,98,100	0
3	NAG	A	601	14/15	0.67	0.13	102,105,111,118	0
3	NAG	A	602	14/15	0.90	0.08	44,48,54,55	0
3	NAG	B	602	14/15	0.94	0.08	34,38,43,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.