



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:35 AM UTC

PDB ID : 6ID3 / pdb_00006id3
Title : Crystal structure of H7 hemagglutinin mutant H7-SGPL (A138S, V186G)
from the influenza virus A/Anhui/1/2013 (H7N9)
Authors : Gao, G.F.; Xu, Y.; Qi, J.X.
Deposited on : 2018-09-08
Resolution : 2.60 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

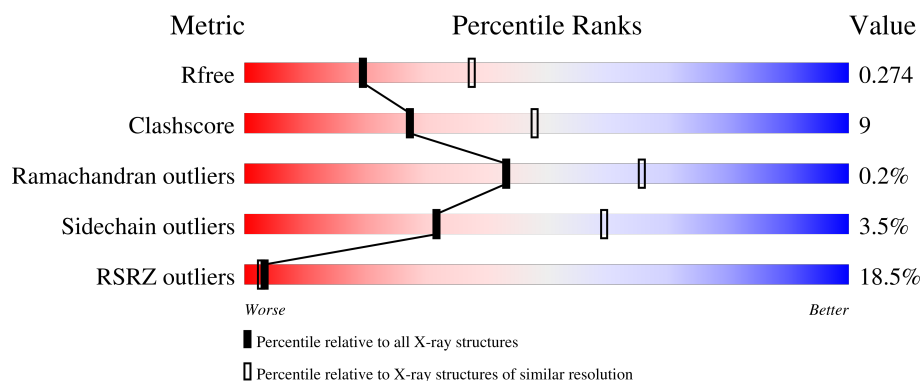
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	321	
2	B	177	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3824 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2385	1480	432	458	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	SER	ALA	engineered mutation	UNP R4NN21
A	177	GLY	VAL	engineered mutation	UNP R4NN21

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	161	1319	812	229	271	7	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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		

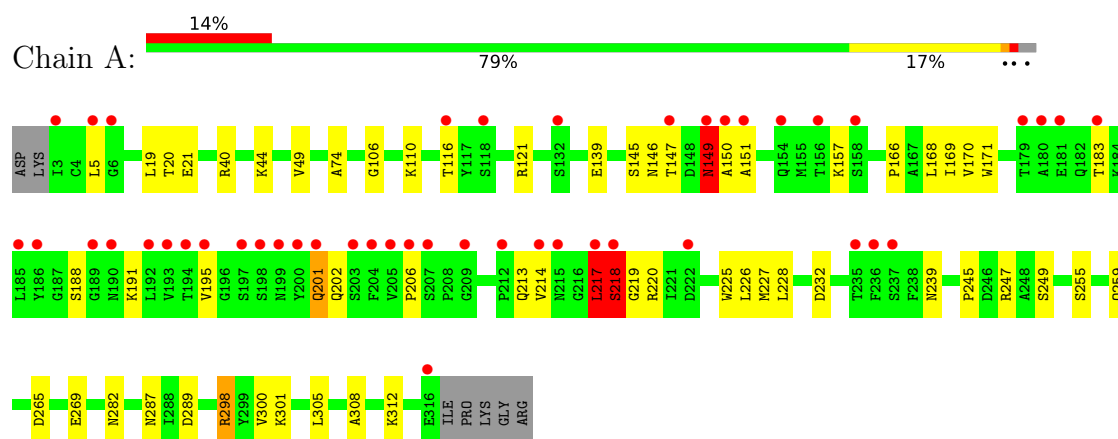
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	20	Total	O	0	0
			20	20		

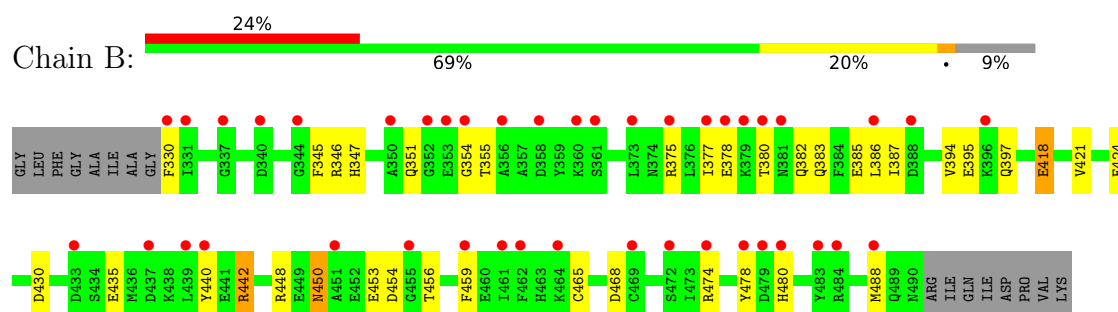
3 Residue-property plots [i](#)

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 chain



• Molecule 2: Hemagglutinin HA2 chain



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	115.63Å 115.63Å 294.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.38 – 2.60 41.38 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (41.38-2.60) 98.5 (41.38-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.248 , 0.275 0.247 , 0.274	Depositor DCC
R_{free} test set	1191 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.020 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.011 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3824	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.13	0/2431	0.56	11/3287 (0.3%)
2	B	0.11	0/1342	0.43	2/1809 (0.1%)
All	All	0.12	0/3773	0.52	13/5096 (0.3%)

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	448	ARG	N-CA-C	11.20	123.47	111.03
1	A	201	GLN	N-CA-C	-10.30	88.85	110.80
1	A	149	ASN	N-CA-C	-10.10	89.29	110.80
1	A	150	ALA	CB-CA-C	-8.91	92.69	110.42
1	A	218	SER	CB-CA-C	-8.27	93.97	110.42
1	A	201	GLN	CB-CA-C	7.61	125.56	110.42
1	A	149	ASN	CB-CA-C	-7.46	95.58	110.42
2	B	448	ARG	CB-CA-C	-6.80	100.42	110.95
1	A	217	LEU	CB-CA-C	6.18	125.96	112.99
1	A	149	ASN	CA-C-N	6.07	133.12	121.54
1	A	149	ASN	C-N-CA	6.07	133.12	121.54
1	A	218	SER	CA-C-N	6.05	126.78	121.58
1	A	218	SER	C-N-CA	6.05	126.78	121.58

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	ASN	Peptide
1	A	217	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2385	0	2331	43	0
2	B	1319	0	1214	27	0
3	A	28	0	26	0	0
3	B	14	0	13	0	0
4	A	58	0	0	9	0
4	B	20	0	0	9	0
All	All	3824	0	3584	67	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 9.

All (67) 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)
2:B:430:ASP:OD2	4:B:601:HOH:O	2.01	0.78
1:A:298:ARG:NH2	4:A:705:HOH:O	2.17	0.76
1:A:308:ALA:O	4:A:701:HOH:O	2.04	0.74
2:B:435:GLU:O	4:B:602:HOH:O	2.07	0.72
1:A:213:GLN:HA	1:A:217:LEU:O	1.87	0.72
1:A:20:THR:HG22	1:A:21:GLU:HG3	1.72	0.71
1:A:232:ASP:OD2	4:A:702:HOH:O	2.10	0.70
2:B:418:GLU:OE1	4:B:603:HOH:O	2.11	0.69
2:B:345:PHE:O	2:B:355:THR:HA	1.93	0.68
2:B:488:MET:O	4:B:604:HOH:O	2.12	0.67
1:A:214:VAL:N	1:A:217:LEU:O	2.27	0.67
1:A:121:ARG:NH1	1:A:145:SER:O	2.30	0.65
1:A:217:LEU:HA	1:A:218:SER:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:ARG:NH2	2:B:424:GLU:OE2	2.32	0.62
1:A:217:LEU:HB3	1:A:219:GLY:H	1.62	0.62
2:B:386:LEU:O	4:B:605:HOH:O	2.16	0.61
1:A:239:ASN:O	4:A:704:HOH:O	2.16	0.60
2:B:346:ARG:HA	2:B:354:GLY:O	2.03	0.59
1:A:217:LEU:HA	1:A:218:SER:CB	2.34	0.58
1:A:151:ALA:O	4:A:706:HOH:O	2.18	0.57
1:A:110:LYS:NZ	1:A:139:GLU:OE2	2.35	0.56
1:A:170:VAL:HG22	1:A:225:TRP:HB3	1.88	0.56
2:B:380:THR:HG22	2:B:382:GLN:H	1.71	0.55
1:A:213:GLN:CA	1:A:217:LEU:O	2.55	0.54
1:A:217:LEU:HB3	1:A:219:GLY:N	2.23	0.54
2:B:450:ASN:N	2:B:450:ASN:OD1	2.41	0.53
1:A:169:ILE:O	1:A:225:TRP:HA	2.10	0.52
1:A:305:LEU:HB3	2:B:421:VAL:HG21	1.92	0.51
1:A:282:ASN:HB3	2:B:377:ILE:HG23	1.92	0.51
1:A:5:LEU:HD11	2:B:440:TYR:HA	1.94	0.51
1:A:106:GLY:HA2	1:A:255:SER:HB3	1.92	0.50
1:A:116:THR:O	1:A:157:LYS:NZ	2.44	0.50
1:A:287:ASN:ND2	1:A:300:VAL:O	2.41	0.50
2:B:330:PHE:HB2	2:B:456:THR:HA	1.93	0.49
1:A:218:SER:H	1:A:220:ARG:HH12	1.58	0.49
2:B:450:ASN:ND2	2:B:478:TYR:OH	2.45	0.49
1:A:49:VAL:HG23	1:A:74:ALA:HB2	1.96	0.48
1:A:289:ASP:OD1	4:A:707:HOH:O	2.20	0.48
1:A:121:ARG:NH1	1:A:146:ASN:O	2.46	0.47
2:B:378:GLU:O	4:B:606:HOH:O	2.20	0.47
1:A:139:GLU:OE1	1:A:247:ARG:HD3	2.14	0.47
1:A:201:GLN:O	1:A:202:GLN:HB2	2.12	0.47
1:A:168:LEU:HB3	1:A:249:SER:HB2	1.95	0.47
1:A:213:GLN:HA	1:A:217:LEU:C	2.40	0.46
1:A:170:VAL:O	1:A:245:PRO:HB3	2.16	0.46
2:B:347:HIS:HD2	2:B:474:ARG:HH12	1.62	0.46
2:B:397:GLN:NE2	4:B:607:HOH:O	2.33	0.45
1:A:147:THR:O	1:A:149:ASN:N	2.48	0.45
1:A:40:ARG:HD2	1:A:265:ASP:HB2	1.98	0.45
2:B:453:GLU:HG2	2:B:459:PHE:HE2	1.82	0.44
1:A:259:GLN:NE2	4:A:717:HOH:O	2.50	0.44
1:A:147:THR:C	1:A:149:ASN:H	2.25	0.44
1:A:301:LYS:NZ	4:A:718:HOH:O	2.51	0.43
2:B:442:ARG:HH11	2:B:442:ARG:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:PRO:HA	1:A:228:LEU:O	2.18	0.43
1:A:171:TRP:CZ2	1:A:195:VAL:HG21	2.53	0.43
1:A:183:THR:HG22	1:A:188:SER:HA	2.01	0.43
2:B:351:GLN:HE21	2:B:351:GLN:HB3	1.62	0.43
4:A:709:HOH:O	2:B:345:PHE:HD2	2.02	0.42
1:A:44:LYS:HD3	1:A:269:GLU:HB2	2.02	0.41
2:B:346:ARG:HH21	2:B:355:THR:HG21	1.85	0.41
1:A:191:LYS:HB2	1:A:206:PRO:HG3	2.01	0.41
2:B:383:GLN:NE2	2:B:385:GLU:OE2	2.39	0.41
1:A:147:THR:O	1:A:149:ASN:O	2.38	0.41
2:B:395:GLU:OE2	2:B:397:GLN:HB3	2.21	0.41
2:B:397:GLN:HG3	4:B:607:HOH:O	2.21	0.40
2:B:394:VAL:HB	4:B:611:HOH:O	2.21	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	312/321 (97%)	292 (94%)	19 (6%)	1 (0%)	36	58
2	B	159/177 (90%)	149 (94%)	10 (6%)	0	100	100
All	All	471/498 (95%)	441 (94%)	29 (6%)	1 (0%)	43	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	SER

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	261/269 (97%)	255 (98%)	6 (2%)	44	71
2	B	141/152 (93%)	133 (94%)	8 (6%)	18	40
All	All	402/421 (96%)	388 (96%)	14 (4%)	32	59

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	217	LEU
1	A	226	LEU
1	A	227	MET
1	A	298	ARG
1	A	312	LYS
2	B	387	ILE
2	B	418	GLU
2	B	442	ARG
2	B	450	ASN
2	B	454	ASP
2	B	465	CYS
2	B	468	ASP
2	B	480	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	374	ASN

5.3.3 RNA ⓘ

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](#)

3 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	A	601	1	14,14,15	0.31	0	17,19,21	0.46	0
3	NAG	A	602	1	14,14,15	0.29	0	17,19,21	0.49	0
3	NAG	B	501	2	14,14,15	0.30	0	17,19,21	0.47	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	A	601	1	-	1/6/23/26	0/1/1/1
3	NAG	A	602	1	-	2/6/23/26	0/1/1/1
3	NAG	B	501	2	-	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 (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAG	O5-C5-C6-O6
3	A	602	NAG	C4-C5-C6-O6
3	A	601	NAG	O5-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	A	314/321 (97%)	0.66	46 (14%) 6 4	33, 64, 114, 137	0
2	B	161/177 (90%)	1.26	42 (26%) 1 1	36, 101, 154, 183	0
All	All	475/498 (95%)	0.86	88 (18%) 3 3	33, 71, 142, 183	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	433	ASP	6.0
2	B	330	PHE	5.0
1	A	180	ALA	5.0
2	B	480	HIS	4.8
2	B	451	ALA	4.7
2	B	350	ALA	4.6
2	B	488	MET	4.5
1	A	158	SER	4.3
2	B	379	LYS	4.2
2	B	380	THR	4.1
1	A	207	SER	4.1
2	B	331	ILE	4.0
2	B	464	LYS	4.0
1	A	218	SER	3.9
1	A	212	PRO	3.9
1	A	183	THR	3.7
2	B	354	GLY	3.6
2	B	462	PHE	3.6
1	A	205	VAL	3.5
1	A	156	THR	3.5
1	A	154	GLN	3.5
1	A	199	ASN	3.4
1	A	316	GLU	3.4
1	A	214	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	388	ASP	3.3
1	A	215	ASN	3.3
2	B	352	GLY	3.2
1	A	204	PHE	3.1
1	A	190	ASN	3.1
1	A	150	ALA	3.1
1	A	200	TYR	3.1
1	A	217	LEU	3.1
2	B	483	TYR	3.0
1	A	203	SER	3.0
2	B	361	SER	3.0
1	A	236	PHE	3.0
1	A	237	SER	2.9
1	A	201	GLN	2.9
1	A	3	ILE	2.9
2	B	344	GLY	2.9
2	B	461	ILE	2.9
1	A	6	GLY	2.9
1	A	192	LEU	2.9
2	B	375	ARG	2.8
1	A	132	SER	2.8
2	B	337	GLY	2.8
1	A	151	ALA	2.8
2	B	469	CYS	2.7
2	B	358	ASP	2.7
1	A	193	VAL	2.7
2	B	437	ASP	2.7
2	B	459	PHE	2.7
2	B	396	LYS	2.6
1	A	5	LEU	2.6
1	A	195	VAL	2.6
2	B	386	LEU	2.5
2	B	484	ARG	2.5
1	A	179	THR	2.5
1	A	194	THR	2.5
1	A	149	ASN	2.4
2	B	381	ASN	2.4
2	B	472	SER	2.4
1	A	147	THR	2.4
1	A	222	ASP	2.4
2	B	353	GLU	2.4
2	B	378	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	198	SER	2.4
1	A	189	GLY	2.3
2	B	478	TYR	2.3
2	B	356	ALA	2.3
1	A	186	TYR	2.3
1	A	197	SER	2.2
2	B	377	ILE	2.2
1	A	206	PRO	2.2
1	A	118	SER	2.2
2	B	360	LYS	2.2
2	B	439	LEU	2.2
2	B	455	GLY	2.2
2	B	440	TYR	2.1
2	B	479	ASP	2.1
1	A	185	LEU	2.1
2	B	474	ARG	2.1
2	B	373	LEU	2.1
1	A	181	GLU	2.1
1	A	235	THR	2.1
1	A	209	GLY	2.1
2	B	340	ASP	2.0
1	A	116	THR	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	A	602	14/15	0.43	0.15	90,106,114,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	601	14/15	0.58	0.21	109,119,124,132	0
3	NAG	B	501	14/15	0.82	0.13	60,73,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.