



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:45 AM UTC

PDB ID : 3ALZ / pdb_00003alz
Title : Crystal structure of the measles virus hemagglutinin bound to its cellular receptor SLAM (Form I)
Authors : Hashiguchi, T.; Ose, T.; Kubota, M.; Maita, N.; Kamishikiryo, J.; Maenaka, K.; Yanagi, Y.
Deposited on : 2010-08-11
Resolution : 4.51 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

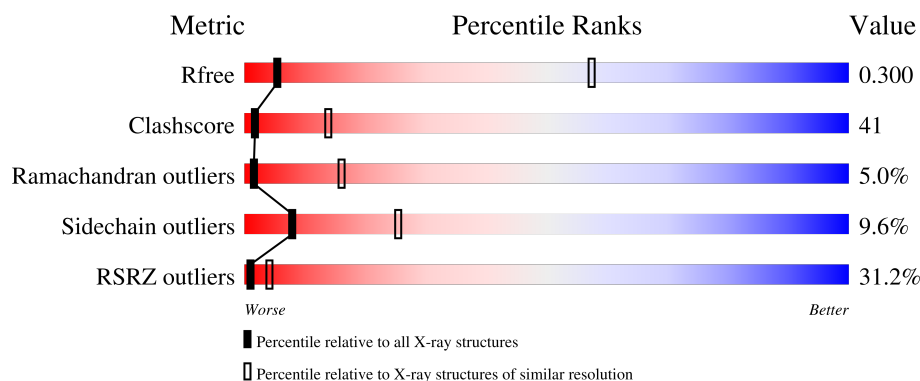
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.51 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	1131 (5.14-3.90)
Clashscore	190562	1005 (5.10-3.94)
Ramachandran outliers	187476	1061 (5.12-3.90)
Sidechain outliers	187428	1044 (5.12-3.90)
RSRZ outliers	180081	1126 (5.14-3.90)

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	481	
2	B	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	901	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4163 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	417	Total	C	N	O	S	0	0	0
			3244	2078	541	602	23			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	GLU	-	expression tag	UNP E2RZS2
A	147	THR	-	expression tag	UNP E2RZS2
A	148	GLY	-	expression tag	UNP E2RZS2
A	618	GLY	-	expression tag	UNP E2RZS2
A	619	THR	-	expression tag	UNP E2RZS2
A	620	LYS	-	expression tag	UNP E2RZS2
A	621	HIS	-	expression tag	UNP E2RZS2
A	622	HIS	-	expression tag	UNP E2RZS2
A	623	HIS	-	expression tag	UNP E2RZS2
A	624	HIS	-	expression tag	UNP E2RZS2
A	625	HIS	-	expression tag	UNP E2RZS2
A	626	HIS	-	expression tag	UNP E2RZS2

- Molecule 2 is a protein called CDw150.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	109	Total	C	N	O	S	0	0	0
			891	568	153	165	5			

There are 9 discrepancies between the modelled and reference sequences:

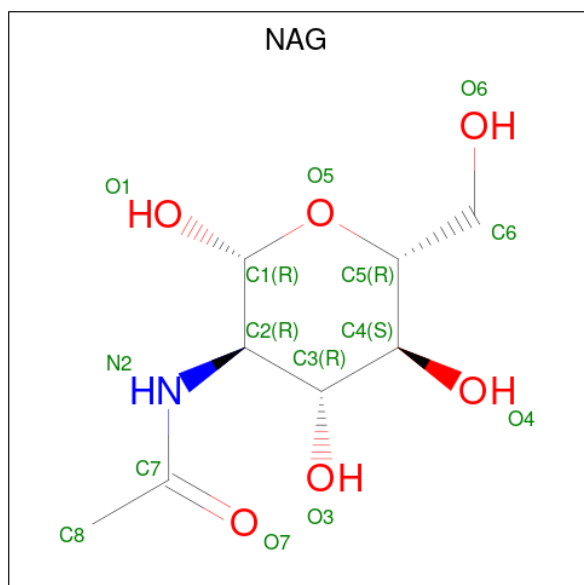
Chain	Residue	Modelled	Actual	Comment	Reference
B	141	GLY	-	expression tag	UNP Q9GJT3
B	142	THR	-	expression tag	UNP Q9GJT3
B	143	LYS	-	expression tag	UNP Q9GJT3
B	144	HIS	-	expression tag	UNP Q9GJT3

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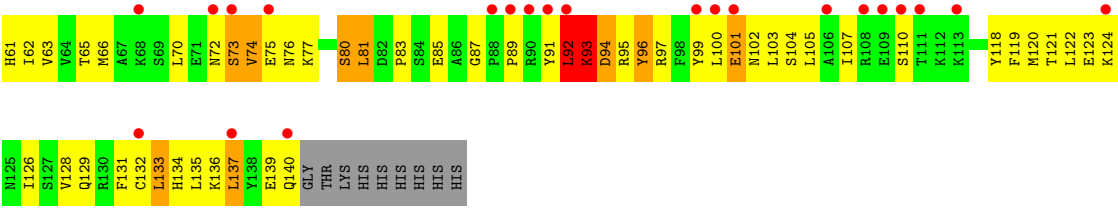
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Chain	Residue	Modelled	Actual	Comment	Reference
B	145	HIS	-	expression tag	UNP Q9GJT3
B	146	HIS	-	expression tag	UNP Q9GJT3
B	147	HIS	-	expression tag	UNP Q9GJT3
B	148	HIS	-	expression tag	UNP Q9GJT3
B	149	HIS	-	expression tag	UNP Q9GJT3

- 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		



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	208.12Å 208.12Å 182.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.04 – 4.51 30.04 – 4.51	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.04-4.51) 99.3 (30.04-4.51)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.65 (at 4.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.326 , 0.338 0.309 , 0.300	Depositor DCC
R_{free} test set	704 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	154.8	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 220.9	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	0.83	EDS
Total number of atoms	4163	wwPDB-VP
Average B, all atoms (Å ²)	271.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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	0.54	1/3327 (0.0%)	1.03	16/4527 (0.4%)
2	B	0.55	0/908	1.12	5/1225 (0.4%)
All	All	0.54	1/4235 (0.0%)	1.05	21/5752 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	227	MET	SD-CE	5.24	1.92	1.79

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	92	LEU	N-CA-C	-13.13	96.57	112.59
2	B	48	THR	N-CA-C	-9.33	93.97	109.46
1	A	236	LYS	CA-C-N	7.76	128.17	119.32
1	A	236	LYS	C-N-CA	7.76	128.17	119.32
1	A	439	SER	N-CA-C	-6.90	104.86	113.28
1	A	347	ASP	N-CA-C	6.67	118.43	111.03
1	A	575	GLN	N-CA-C	6.24	120.19	112.58
2	B	96	TYR	N-CA-C	6.23	119.74	110.52
1	A	249	LEU	N-CA-C	-6.00	105.54	112.92
1	A	485	VAL	CA-C-N	5.96	125.72	119.76
1	A	485	VAL	C-N-CA	5.96	125.72	119.76
1	A	337	VAL	N-CA-C	5.79	114.63	108.95
1	A	456	ILE	CA-C-N	5.73	123.84	119.66
1	A	456	ILE	C-N-CA	5.73	123.84	119.66
1	A	420	THR	N-CA-C	-5.71	106.16	113.23
1	A	460	LYS	CB-CA-C	-5.70	109.98	116.54
1	A	513	ASN	N-CA-C	-5.62	103.29	110.53
2	B	81	LEU	N-CA-C	5.43	116.78	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	ASN	N-CA-C	-5.36	104.01	111.52
1	A	240	SER	N-CA-C	-5.25	99.63	110.80
1	A	212	ARG	N-CA-C	-5.21	106.60	113.17

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	3244	0	3212	251	0
2	B	891	0	908	93	1
3	A	28	0	26	0	0
All	All	4163	0	4146	339	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 41.

All (339) 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:558:PRO:HG2	1:A:559:ILE:HG23	1.52	0.91
2:B:74:VAL:HG13	2:B:75:GLU:H	1.33	0.91
1:A:472:TRP:HE3	1:A:472:TRP:H	1.19	0.89
1:A:473:ILE:HB	1:A:474:PRO:HD3	1.55	0.87
1:A:475:ARG:NH1	1:A:477:LYS:HD3	1.91	0.86
2:B:93:LYS:HD2	2:B:94:ASP:C	2.01	0.85
1:A:430:GLY:HA3	1:A:476:PHE:HE2	1.42	0.85
2:B:46:PRO:CG	2:B:51:ARG:HE	1.90	0.84
1:A:533:ARG:HG2	2:B:61:HIS:CD2	2.13	0.83
1:A:472:TRP:HA	1:A:476:PHE:HA	1.57	0.83
1:A:400:ALA:HB3	1:A:401:PRO:HD3	1.60	0.83
2:B:46:PRO:HG2	2:B:51:ARG:HE	1.44	0.82
1:A:216:VAL:HG22	1:A:234:VAL:HG12	1.61	0.82
1:A:562:VAL:HB	1:A:586:ALA:HB3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:TYR:O	1:A:482:LEU:HG	1.80	0.81
1:A:464:LEU:HG	1:A:465:GLY:H	1.45	0.80
2:B:89:PRO:HG2	2:B:91:TYR:CE2	2.17	0.80
2:B:77:LYS:HB3	2:B:92:LEU:HD11	1.68	0.76
2:B:95:ARG:HG3	2:B:95:ARG:HH11	1.51	0.74
2:B:74:VAL:HG13	2:B:75:GLU:N	2.03	0.73
2:B:93:LYS:HD2	2:B:94:ASP:H	1.54	0.73
1:A:570:CYS:HB3	1:A:577:LEU:HD21	1.71	0.73
2:B:35:ILE:HG13	2:B:35:ILE:O	1.89	0.73
2:B:91:TYR:HB3	2:B:93:LYS:HB3	1.70	0.72
1:A:461:ASN:HD22	1:A:461:ASN:H	1.35	0.72
2:B:139:GLU:O	2:B:140:GLN:HB2	1.88	0.72
1:A:533:ARG:HG2	2:B:61:HIS:NE2	2.04	0.72
1:A:464:LEU:HG	1:A:465:GLY:N	2.04	0.72
1:A:458:PRO:HG3	1:A:465:GLY:H	1.54	0.72
1:A:378:MET:CB	1:A:407:ILE:HG21	2.19	0.72
1:A:346:ILE:HG23	1:A:369:THR:HG21	1.72	0.71
1:A:337:VAL:HG12	1:A:423:LEU:HB3	1.72	0.71
1:A:340:SER:HB3	1:A:426:LYS:HA	1.72	0.71
2:B:103:LEU:HD13	2:B:120:MET:HE1	1.70	0.71
1:A:529:TYR:CD1	1:A:563:PRO:HG3	2.25	0.70
1:A:227:MET:HE1	1:A:294:LEU:H	1.55	0.70
1:A:544:SER:HB2	1:A:549:PHE:HB3	1.73	0.70
1:A:288:MET:HE3	1:A:299:LEU:HB3	1.73	0.70
2:B:101:GLU:CD	2:B:101:GLU:H	2.00	0.70
1:A:399:TRP:CD1	1:A:401:PRO:HD2	2.27	0.69
2:B:62:ILE:HD13	2:B:83:PRO:HD3	1.75	0.69
2:B:74:VAL:O	2:B:75:GLU:HB3	1.94	0.67
1:A:461:ASN:H	1:A:461:ASN:ND2	1.92	0.67
1:A:348:ARG:HD3	1:A:350:TYR:OH	1.95	0.66
1:A:246:LEU:O	1:A:248:GLN:N	2.28	0.66
1:A:583:CYS:O	1:A:595:THR:HA	1.96	0.66
1:A:475:ARG:O	1:A:476:PHE:HB3	1.95	0.66
1:A:481:TYR:O	1:A:482:LEU:CG	2.44	0.66
1:A:499:TYR:CD2	1:A:501:PRO:HD3	2.30	0.66
1:A:549:PHE:HD1	1:A:549:PHE:O	1.78	0.66
1:A:430:GLY:CA	1:A:476:PHE:HE2	2.09	0.66
1:A:343:ASP:OD2	1:A:346:ILE:HG13	1.97	0.65
1:A:467:ILE:O	1:A:481:TYR:HB3	1.96	0.65
1:A:216:VAL:HA	1:A:233:LEU:O	1.97	0.65
1:A:461:ASN:HD22	1:A:461:ASN:N	1.91	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:THR:O	1:A:409:SER:HB3	1.97	0.64
1:A:386:CYS:HA	1:A:390:ILE:HG13	1.79	0.64
1:A:215:ASN:CB	1:A:235:GLU:HB2	2.27	0.64
1:A:293:GLU:O	1:A:294:LEU:HB2	1.96	0.64
1:A:378:MET:HB2	1:A:407:ILE:HG21	1.79	0.64
2:B:61:HIS:CE1	2:B:63:VAL:HG22	2.33	0.64
2:B:36:VAL:HA	2:B:136:LYS:O	1.99	0.63
1:A:352:SER:N	1:A:354:HIS:NE2	2.46	0.63
1:A:294:LEU:O	1:A:326:VAL:HG12	1.99	0.63
1:A:229:GLY:N	1:A:291:LEU:HD11	2.14	0.62
2:B:93:LYS:CG	2:B:94:ASP:N	2.60	0.62
1:A:557:LEU:HD23	1:A:559:ILE:HD11	1.79	0.62
1:A:208:LEU:O	1:A:212:ARG:HG2	2.00	0.62
1:A:222:MET:HE2	1:A:291:LEU:HB2	1.82	0.62
1:A:188:CYS:O	1:A:189:SER:HB3	1.99	0.61
1:A:357:VAL:HG21	1:A:452:TYR:HE1	1.64	0.61
1:A:325:GLY:C	1:A:327:TRP:H	2.08	0.61
2:B:93:LYS:CD	2:B:94:ASP:H	2.13	0.61
1:A:396:ASN:N	1:A:397:PRO:HD3	2.15	0.61
1:A:288:MET:HE1	1:A:299:LEU:HD23	1.82	0.61
2:B:121:THR:HG23	2:B:128:VAL:HG13	1.82	0.61
1:A:288:MET:CE	1:A:299:LEU:HD23	2.30	0.61
1:A:531:THR:HG22	1:A:536:HIS:CD2	2.35	0.60
2:B:93:LYS:HD2	2:B:95:ARG:N	2.15	0.60
1:A:549:PHE:O	1:A:549:PHE:CD1	2.55	0.60
2:B:62:ILE:N	2:B:62:ILE:HD12	2.16	0.59
1:A:202:SER:O	1:A:203:LEU:HD23	2.02	0.59
1:A:314:GLY:C	1:A:315:LYS:HG3	2.27	0.59
2:B:60:ILE:O	2:B:83:PRO:HD2	2.01	0.59
2:B:121:THR:CG2	2:B:128:VAL:HG13	2.33	0.59
2:B:46:PRO:CG	2:B:51:ARG:NE	2.63	0.59
1:A:346:ILE:HG23	1:A:369:THR:CG2	2.33	0.58
1:A:400:ALA:HB3	1:A:401:PRO:CD	2.30	0.58
1:A:430:GLY:HA3	1:A:476:PHE:CE2	2.32	0.58
1:A:455:THR:HB	1:A:514:LEU:HD22	1.84	0.58
1:A:541:TYR:HB3	1:A:543:TYR:HE2	1.68	0.58
2:B:89:PRO:HG2	2:B:91:TYR:HE2	1.69	0.58
1:A:472:TRP:CZ3	1:A:473:ILE:HG13	2.39	0.58
1:A:483:PHE:HZ	1:A:524:TYR:OH	1.87	0.58
1:A:526:LEU:C	1:A:526:LEU:HD12	2.29	0.58
2:B:74:VAL:CG1	2:B:75:GLU:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:VAL:HG21	1:A:452:TYR:CE1	2.39	0.57
1:A:303:GLU:O	1:A:306:ILE:HD11	2.03	0.57
2:B:93:LYS:HD2	2:B:94:ASP:N	2.19	0.57
1:A:481:TYR:C	1:A:482:LEU:HG	2.29	0.57
1:A:318:SER:HB3	1:A:337:VAL:O	2.04	0.57
1:A:503:GLU:HG2	2:B:76:ASN:HB3	1.87	0.57
1:A:541:TYR:HB3	1:A:543:TYR:CE2	2.39	0.57
1:A:557:LEU:HB3	1:A:559:ILE:HD13	1.85	0.57
2:B:93:LYS:CG	2:B:94:ASP:H	2.16	0.57
1:A:215:ASN:HB2	1:A:235:GLU:HB2	1.86	0.57
1:A:326:VAL:HG13	1:A:327:TRP:CD1	2.40	0.57
2:B:103:LEU:HD13	2:B:120:MET:CE	2.34	0.57
1:A:570:CYS:HB3	1:A:577:LEU:CD2	2.33	0.56
1:A:238:ASN:O	1:A:239:LEU:HB2	2.06	0.56
1:A:340:SER:CB	1:A:426:LYS:HA	2.34	0.56
2:B:100:LEU:HD13	2:B:100:LEU:O	2.06	0.56
2:B:46:PRO:HG3	2:B:51:ARG:NE	2.19	0.56
1:A:458:PRO:HB2	1:A:511:SER:OG	2.05	0.56
1:A:325:GLY:C	1:A:327:TRP:N	2.61	0.56
2:B:56:MET:HB3	2:B:101:GLU:HA	1.86	0.56
1:A:314:GLY:HA3	1:A:315:LYS:HZ3	1.71	0.56
1:A:472:TRP:HE3	1:A:472:TRP:N	1.96	0.56
2:B:134:HIS:CE1	2:B:136:LYS:NZ	2.74	0.56
1:A:459:MET:SD	1:A:459:MET:C	2.89	0.56
1:A:313:SER:O	1:A:315:LYS:N	2.39	0.55
1:A:378:MET:HB2	1:A:407:ILE:HD13	1.88	0.55
1:A:389:LYS:HG3	1:A:390:ILE:N	2.21	0.55
1:A:208:LEU:HD12	1:A:212:ARG:HD3	1.89	0.55
1:A:475:ARG:O	1:A:476:PHE:CB	2.54	0.55
1:A:542:VAL:O	1:A:550:SER:HA	2.07	0.55
2:B:65:THR:HB	2:B:75:GLU:HG3	1.89	0.55
1:A:217:SER:O	1:A:218:SER:HB2	2.05	0.55
1:A:589:GLU:HG2	1:A:590:SER:H	1.73	0.54
1:A:418:SER:O	1:A:419:LEU:HD12	2.06	0.54
1:A:472:TRP:N	1:A:472:TRP:CE3	2.75	0.54
1:A:255:PHE:HD1	1:A:276:LEU:HD22	1.73	0.54
1:A:294:LEU:O	1:A:326:VAL:N	2.37	0.54
1:A:540:TYR:HE1	1:A:568:VAL:HG21	1.72	0.54
2:B:61:HIS:HE1	2:B:63:VAL:HG22	1.69	0.54
1:A:517:LEU:HB2	1:A:523:GLN:HG3	1.89	0.54
2:B:132:CYS:SG	2:B:133:LEU:N	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LEU:C	1:A:514:LEU:HD23	2.33	0.54
1:A:464:LEU:HD11	1:A:526:LEU:HD21	1.90	0.54
2:B:40:GLY:HA2	2:B:110:SER:O	2.08	0.54
1:A:473:ILE:CB	1:A:474:PRO:HD3	2.34	0.53
2:B:134:HIS:CE1	2:B:136:LYS:HZ2	2.25	0.53
1:A:255:PHE:CZ	1:A:322:VAL:HG21	2.44	0.53
1:A:499:TYR:CZ	1:A:501:PRO:HB3	2.43	0.53
1:A:242:LYS:HG3	1:A:242:LYS:O	2.08	0.53
1:A:437:HIS:CD2	1:A:459:MET:HB2	2.44	0.53
1:A:507:ASP:O	1:A:530:ASP:HA	2.09	0.52
1:A:277:GLU:O	1:A:278:GLN:HG3	2.09	0.52
2:B:36:VAL:O	2:B:37:GLN:HG2	2.09	0.52
1:A:251:MET:SD	1:A:283:ASP:HB3	2.50	0.52
1:A:262:ASN:HB2	1:A:573:TRP:CZ2	2.45	0.52
1:A:471:GLU:O	1:A:476:PHE:HA	2.09	0.52
2:B:120:MET:HE3	2:B:122:LEU:HD21	1.92	0.52
2:B:46:PRO:HD3	2:B:51:ARG:HH21	1.75	0.52
1:A:249:LEU:O	1:A:250:SER:O	2.28	0.52
1:A:378:MET:CB	1:A:407:ILE:HD13	2.40	0.52
1:A:262:ASN:HB2	1:A:573:TRP:HZ2	1.74	0.51
1:A:264:GLY:C	1:A:265:LEU:HD12	2.35	0.51
1:A:458:PRO:HG3	1:A:465:GLY:N	2.23	0.51
1:A:227:MET:HE1	1:A:294:LEU:N	2.23	0.51
1:A:385:ALA:HB2	1:A:487:ILE:HG13	1.91	0.51
1:A:554:PRO:HD2	2:B:128:VAL:HG21	1.92	0.51
1:A:392:ALA:HA	1:A:395:GLU:CD	2.35	0.51
1:A:413:LEU:HD12	1:A:427:ILE:CD1	2.40	0.51
1:A:585:LEU:N	1:A:585:LEU:HD12	2.26	0.51
1:A:308:ILE:HG23	1:A:341:THR:HG22	1.91	0.51
2:B:60:ILE:HD12	2:B:124:LYS:HA	1.92	0.51
1:A:410:TYR:CD1	1:A:478:VAL:HG11	2.45	0.51
1:A:481:TYR:O	1:A:482:LEU:CD2	2.58	0.51
1:A:514:LEU:HD23	1:A:514:LEU:O	2.10	0.51
1:A:461:ASN:ND2	1:A:461:ASN:N	2.55	0.51
2:B:73:SER:OG	2:B:74:VAL:N	2.41	0.51
1:A:299:LEU:HD21	1:A:425:ILE:HD13	1.93	0.50
1:A:389:LYS:HG3	1:A:390:ILE:HG23	1.91	0.50
1:A:319:PHE:HB2	1:A:425:ILE:HD11	1.93	0.50
2:B:37:GLN:O	2:B:137:LEU:HA	2.11	0.50
2:B:47:LEU:HD13	2:B:120:MET:HB2	1.93	0.50
1:A:374:ASP:C	1:A:376:LEU:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:HD11	1:A:425:ILE:HD11	1.94	0.50
2:B:61:HIS:C	2:B:62:ILE:HD12	2.37	0.50
1:A:242:LYS:O	1:A:243:ARG:C	2.55	0.50
1:A:210:LEU:O	1:A:213:GLY:N	2.36	0.50
1:A:306:ILE:N	1:A:306:ILE:HD12	2.27	0.50
1:A:221:THR:HG22	1:A:230:GLY:HA3	1.93	0.49
1:A:280:VAL:HG12	1:A:282:ASN:H	1.77	0.49
1:A:249:LEU:N	1:A:249:LEU:HD22	2.27	0.49
1:A:354:HIS:ND1	1:A:367:VAL:HG12	2.26	0.49
1:A:500:LEU:CD2	1:A:502:ALA:HB3	2.42	0.49
2:B:48:THR:C	2:B:50:GLU:H	2.20	0.49
1:A:247:SER:O	1:A:248:GLN:C	2.54	0.49
1:A:259:VAL:HG12	1:A:260:ILE:N	2.26	0.49
1:A:236:LYS:HE3	1:A:238:ASN:HB3	1.95	0.49
1:A:314:GLY:HA3	1:A:315:LYS:NZ	2.27	0.49
2:B:91:TYR:CB	2:B:93:LYS:HB3	2.41	0.49
1:A:208:LEU:O	1:A:209:TYR:C	2.56	0.49
1:A:326:VAL:O	1:A:326:VAL:HG22	2.12	0.49
1:A:540:TYR:HE1	1:A:568:VAL:CG2	2.25	0.49
1:A:308:ILE:N	1:A:308:ILE:HD12	2.28	0.49
1:A:282:ASN:OD1	1:A:284:LEU:HB2	2.12	0.49
1:A:337:VAL:CG1	1:A:423:LEU:HB3	2.42	0.49
2:B:51:ARG:C	2:B:53:ASN:H	2.21	0.49
1:A:339:LEU:HD12	1:A:425:ILE:HB	1.95	0.49
2:B:85:GLU:HG3	2:B:87:GLY:H	1.77	0.48
1:A:453:TRP:CE2	1:A:522:LEU:HD13	2.48	0.48
1:A:481:TYR:O	1:A:482:LEU:HD23	2.14	0.48
2:B:43:VAL:HG21	2:B:135:LEU:HD21	1.95	0.48
1:A:263:PRO:HB2	1:A:265:LEU:HD13	1.96	0.48
1:A:513:ASN:OD1	1:A:568:VAL:HG12	2.13	0.48
1:A:540:TYR:O	1:A:552:PHE:HA	2.13	0.48
1:A:206:LEU:HD13	1:A:232:TYR:CG	2.48	0.48
1:A:399:TRP:NE1	1:A:401:PRO:HD2	2.28	0.48
2:B:93:LYS:HB2	2:B:96:TYR:HD1	1.78	0.48
1:A:293:GLU:O	1:A:295:LYS:HG2	2.13	0.48
1:A:308:ILE:HD13	1:A:348:ARG:HA	1.95	0.48
1:A:559:ILE:HG12	1:A:560:LYS:N	2.28	0.48
1:A:206:LEU:HD13	1:A:232:TYR:CD1	2.49	0.48
1:A:374:ASP:HB2	1:A:407:ILE:HB	1.96	0.48
1:A:471:GLU:OE2	1:A:477:LYS:O	2.32	0.47
2:B:99:TYR:HD1	2:B:104:SER:O	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ARG:HG3	2:B:95:ARG:NH1	2.22	0.47
1:A:475:ARG:HH12	1:A:477:LYS:HD3	1.72	0.47
1:A:301:HIS:ND1	1:A:302:GLY:N	2.62	0.47
1:A:485:VAL:HA	1:A:486:PRO:HD3	1.79	0.47
1:A:533:ARG:HG3	1:A:533:ARG:HH11	1.79	0.47
2:B:47:LEU:HA	2:B:133:LEU:HD12	1.97	0.47
2:B:126:ILE:O	2:B:126:ILE:HG13	2.15	0.47
1:A:441:MET:HE2	1:A:456:ILE:HD11	1.96	0.46
2:B:44:LEU:HD23	2:B:51:ARG:HH22	1.79	0.46
2:B:37:GLN:HB2	2:B:137:LEU:HD23	1.97	0.46
2:B:36:VAL:C	2:B:37:GLN:HG2	2.41	0.46
1:A:222:MET:HB3	1:A:355:ARG:HD3	1.98	0.46
1:A:246:LEU:C	1:A:248:GLN:N	2.74	0.46
2:B:77:LYS:NZ	2:B:80:SER:HB2	2.30	0.46
1:A:229:GLY:H	1:A:291:LEU:HD11	1.80	0.46
2:B:92:LEU:N	2:B:92:LEU:HD23	2.31	0.46
1:A:262:ASN:C	1:A:264:GLY:H	2.24	0.46
1:A:276:LEU:HD23	1:A:277:GLU:N	2.31	0.46
1:A:406:ARG:O	1:A:408:PRO:HD3	2.16	0.45
1:A:209:TYR:O	1:A:210:LEU:C	2.59	0.45
1:A:545:PRO:O	1:A:546:SER:C	2.59	0.45
1:A:215:ASN:HB3	1:A:235:GLU:HB2	1.99	0.45
1:A:454:LEU:C	1:A:454:LEU:HD23	2.41	0.45
1:A:522:LEU:O	1:A:545:PRO:HD2	2.17	0.45
1:A:533:ARG:HG3	1:A:533:ARG:NH1	2.31	0.45
1:A:554:PRO:HG3	2:B:123:GLU:OE1	2.16	0.45
1:A:252:TYR:N	1:A:252:TYR:CD2	2.85	0.45
1:A:529:TYR:CE1	1:A:563:PRO:HD3	2.51	0.45
1:A:558:PRO:HG2	1:A:559:ILE:N	2.32	0.45
2:B:51:ARG:O	2:B:53:ASN:N	2.50	0.45
1:A:194:ILE:HD12	1:A:194:ILE:N	2.32	0.45
1:A:548:SER:C	1:A:550:SER:N	2.73	0.45
1:A:386:CYS:O	1:A:386:CYS:SG	2.74	0.45
1:A:473:ILE:HB	1:A:474:PRO:CD	2.37	0.45
1:A:311:GLN:CD	1:A:311:GLN:H	2.26	0.44
1:A:418:SER:O	1:A:419:LEU:HB2	2.18	0.44
1:A:274:ASN:ND2	1:A:324:LEU:HG	2.32	0.44
2:B:66:MET:HE3	2:B:66:MET:HB3	1.85	0.44
1:A:250:SER:O	1:A:251:MET:HB2	2.16	0.44
1:A:458:PRO:HB3	1:A:464:LEU:HA	1.98	0.44
2:B:32:CYS:O	2:B:33:PRO:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:SER:OG	1:A:440:GLY:HA2	2.18	0.44
1:A:400:ALA:CB	1:A:401:PRO:CD	2.96	0.44
1:A:508:VAL:HG13	1:A:528:THR:HG23	2.00	0.44
1:A:558:PRO:HG2	1:A:559:ILE:H	1.84	0.43
2:B:81:LEU:C	2:B:81:LEU:HD12	2.43	0.43
2:B:93:LYS:HD3	2:B:96:TYR:N	2.33	0.43
1:A:340:SER:HB2	1:A:424:LYS:HD3	2.01	0.43
1:A:343:ASP:OD2	1:A:345:VAL:HB	2.19	0.43
1:A:196:GLY:HA3	1:A:553:TYR:CZ	2.54	0.43
1:A:276:LEU:HD23	1:A:276:LEU:C	2.43	0.43
1:A:379:GLU:HA	1:A:407:ILE:HD11	2.01	0.43
1:A:551:TYR:CD1	1:A:551:TYR:N	2.87	0.43
2:B:66:MET:HG3	2:B:118:TYR:CZ	2.54	0.43
1:A:299:LEU:HD11	1:A:425:ILE:CD1	2.48	0.43
1:A:362:GLN:HB3	1:A:364:LYS:HE2	1.99	0.43
1:A:395:GLU:O	1:A:396:ASN:HB2	2.19	0.43
1:A:533:ARG:NH2	1:A:554:PRO:HB3	2.34	0.43
2:B:44:LEU:CD2	2:B:51:ARG:HH22	2.32	0.43
2:B:97:ARG:HG2	2:B:99:TYR:OH	2.19	0.43
1:A:327:TRP:O	1:A:328:LYS:C	2.61	0.42
1:A:443:LEU:HD22	1:A:452:TYR:HB3	2.01	0.42
1:A:475:ARG:HD2	1:A:475:ARG:C	2.44	0.42
2:B:44:LEU:HG	2:B:51:ARG:NH2	2.34	0.42
2:B:62:ILE:N	2:B:62:ILE:CD1	2.82	0.42
1:A:236:LYS:HA	1:A:237:PRO:HD3	1.75	0.42
1:A:540:TYR:CE1	1:A:568:VAL:HG21	2.54	0.42
1:A:548:SER:O	1:A:550:SER:N	2.53	0.42
1:A:385:ALA:C	1:A:387:LYS:H	2.28	0.42
1:A:233:LEU:HD23	1:A:253:ARG:HA	2.01	0.42
1:A:371:ARG:HH11	1:A:429:SER:HB3	1.84	0.42
1:A:374:ASP:CG	1:A:375:LYS:H	2.27	0.42
1:A:538:VAL:HG23	1:A:557:LEU:HD11	2.01	0.42
1:A:400:ALA:O	1:A:401:PRO:C	2.63	0.42
1:A:422:GLU:O	1:A:423:LEU:C	2.63	0.42
1:A:337:VAL:O	1:A:337:VAL:HG23	2.19	0.42
1:A:546:SER:OG	1:A:547:ARG:N	2.53	0.42
1:A:562:VAL:CB	1:A:586:ALA:HB3	2.39	0.42
1:A:392:ALA:HA	1:A:395:GLU:HG2	2.02	0.41
1:A:470:LEU:HD11	1:A:476:PHE:CE1	2.55	0.41
1:A:559:ILE:H	1:A:559:ILE:CD1	2.32	0.41
1:A:487:ILE:HG22	1:A:490:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:SER:O	2:B:61:HIS:N	2.53	0.41
1:A:229:GLY:HA3	1:A:291:LEU:HD21	2.02	0.41
1:A:348:ARG:HD3	1:A:350:TYR:CZ	2.56	0.41
1:A:466:VAL:CG1	1:A:468:ASN:HD21	2.34	0.41
1:A:488:LYS:O	1:A:489:GLU:C	2.64	0.41
1:A:418:SER:O	1:A:419:LEU:CB	2.67	0.41
1:A:486:PRO:HA	1:A:495:HIS:ND1	2.36	0.41
2:B:51:ARG:C	2:B:53:ASN:N	2.77	0.41
2:B:51:ARG:HA	2:B:51:ARG:HD3	1.33	0.41
2:B:91:TYR:C	2:B:93:LYS:H	2.21	0.41
2:B:103:LEU:CD1	2:B:120:MET:HE1	2.47	0.41
2:B:97:ARG:NH2	2:B:99:TYR:HE2	2.17	0.41
1:A:392:ALA:HA	1:A:395:GLU:OE1	2.21	0.41
2:B:70:LEU:HA	2:B:70:LEU:HD12	1.83	0.41
1:A:470:LEU:HD13	1:A:478:VAL:CG2	2.50	0.41
1:A:570:CYS:HA	1:A:578:TRP:O	2.21	0.41
2:B:36:VAL:O	2:B:37:GLN:CG	2.69	0.41
2:B:65:THR:OG1	2:B:119:PHE:HB2	2.21	0.41
1:A:221:THR:OG1	1:A:569:GLU:OE1	2.30	0.41
1:A:255:PHE:CD1	1:A:276:LEU:HD22	2.55	0.41
1:A:524:TYR:CD2	1:A:524:TYR:N	2.89	0.41
1:A:579:CYS:O	1:A:599:MET:HA	2.20	0.41
1:A:228:TYR:HB3	1:A:260:ILE:HD11	2.03	0.40
2:B:43:VAL:HG22	2:B:107:ILE:HB	2.03	0.40
2:B:101:GLU:HG2	2:B:102:ASN:ND2	2.37	0.40
1:A:334:GLN:HE21	1:A:334:GLN:HB3	1.67	0.40
1:A:358:ILE:HA	1:A:362:GLN:O	2.21	0.40
2:B:100:LEU:HD13	2:B:100:LEU:C	2.46	0.40
1:A:500:LEU:HD22	1:A:502:ALA:HB3	2.02	0.40
1:A:562:VAL:HG23	1:A:586:ALA:O	2.21	0.40
2:B:93:LYS:HB2	2:B:96:TYR:H	1.86	0.40
1:A:248:GLN:O	1:A:248:GLN:HG2	2.20	0.40
1:A:308:ILE:N	1:A:308:ILE:CD1	2.85	0.40
2:B:129:GLN:HG2	2:B:131:PHE:CE1	2.56	0.40
1:A:343:ASP:C	1:A:345:VAL:H	2.29	0.40
1:A:374:ASP:CG	1:A:375:LYS:N	2.80	0.40
1:A:395:GLU:O	1:A:395:GLU:HG3	2.21	0.40
2:B:93:LYS:HG3	2:B:94:ASP:N	2.35	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)
2:B:99:TYR:OH	2:B:99:TYR:OH[8_555]	2.16	0.04

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	413/481 (86%)	322 (78%)	71 (17%)	20 (5%)	2	16
2	B	107/149 (72%)	84 (78%)	17 (16%)	6 (6%)	1	15
All	All	520/630 (82%)	406 (78%)	88 (17%)	26 (5%)	1	16

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	LEU
1	A	241	SER
1	A	250	SER
1	A	476	PHE
1	A	512	SER
2	B	60	ILE
2	B	73	SER
2	B	74	VAL
2	B	93	LYS
1	A	240	SER
1	A	247	SER
1	A	314	GLY
1	A	397	PRO
1	A	474	PRO
1	A	490	ALA
2	B	52	ILE
2	B	94	ASP
1	A	222	MET
1	A	251	MET
1	A	489	GLU

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Mol	Chain	Res	Type
1	A	481	TYR
1	A	400	ALA
1	A	549	PHE
1	A	390	ILE
1	A	401	PRO
1	A	226	GLY

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	365/420 (87%)	333 (91%)	32 (9%)	9	29
2	B	103/137 (75%)	90 (87%)	13 (13%)	4	17
All	All	468/557 (84%)	423 (90%)	45 (10%)	8	25

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	THR
1	A	217	SER
1	A	235	GLU
1	A	246	LEU
1	A	248	GLN
1	A	249	LEU
1	A	257	VAL
1	A	275	TYR
1	A	294	LEU
1	A	296	LEU
1	A	305	SER
1	A	310	TYR
1	A	315	LYS
1	A	342	ASP
1	A	357	VAL
1	A	401	PRO
1	A	413	LEU

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Mol	Chain	Res	Type
1	A	419	LEU
1	A	449	ASN
1	A	459	MET
1	A	461	ASN
1	A	464	LEU
1	A	471	GLU
1	A	472	TRP
1	A	479	SER
1	A	484	THR
1	A	500	LEU
1	A	510	LEU
1	A	526	LEU
1	A	559	ILE
1	A	577	LEU
1	A	605	SER
2	B	34	LYS
2	B	38	GLN
2	B	45	LEU
2	B	48	THR
2	B	51	ARG
2	B	52	ILE
2	B	80	SER
2	B	92	LEU
2	B	93	LYS
2	B	101	GLU
2	B	105	LEU
2	B	133	LEU
2	B	137	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	GLN
1	A	262	ASN
1	A	278	GLN
1	A	320	GLN
1	A	334	GLN
1	A	361	ASN
1	A	362	GLN
1	A	383	GLN
1	A	384	GLN
1	A	461	ASN

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Mol	Chain	Res	Type
1	A	468	ASN
1	A	575	GLN
1	A	596	HIS
2	B	37	GLN
2	B	102	ASN
2	B	125	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](#)

2 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	801	1	14,14,15	1.06	1 (7%)	17,19,21	0.81	1 (5%)
3	NAG	A	901	1	14,14,15	0.57	0	17,19,21	0.91	1 (5%)

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	801	1	-	4/6/23/26	0/1/1/1
3	NAG	A	901	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	NAG	C1-C2	3.32	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	NAG	C2-N2-C7	-2.47	119.60	122.90
3	A	801	NAG	C3-C4-C5	-2.00	106.60	110.23

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	NAG	C8-C7-N2-C2
3	A	801	NAG	O7-C7-N2-C2
3	A	901	NAG	C8-C7-N2-C2
3	A	901	NAG	O7-C7-N2-C2
3	A	901	NAG	O5-C5-C6-O6
3	A	901	NAG	C4-C5-C6-O6
3	A	801	NAG	C4-C5-C6-O6
3	A	801	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	417/481 (86%)	1.65	128 (30%) 1 4	133, 239, 403, 704	0
2	B	109/149 (73%)	1.75	36 (33%) 1 4	217, 307, 452, 581	0
All	All	526/630 (83%)	1.67	164 (31%) 1 4	133, 254, 414, 704	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	SER	13.9
1	A	282	ASN	9.2
2	B	56	MET	7.6
1	A	549	PHE	5.5
1	A	421	VAL	5.5
2	B	52	ILE	5.4
1	A	422	GLU	5.3
2	B	55	SER	5.3
1	A	246	LEU	5.2
2	B	57	ASN	5.2
1	A	218	SER	5.1
1	A	439	SER	5.1
2	B	68	LYS	5.1
2	B	90	ARG	5.0
1	A	556	ARG	4.9
2	B	49	HIS	4.8
1	A	286	ASN	4.8
1	A	237	PRO	4.6
2	B	42	ASP	4.5
1	A	247	SER	4.5
1	A	249	LEU	4.5
1	A	452	TYR	4.4
1	A	341	THR	4.4
1	A	212	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	313	SER	4.2
1	A	499	TYR	4.1
1	A	283	ASP	4.1
1	A	285	SER	4.0
1	A	388	GLY	4.0
2	B	89	PRO	4.0
2	B	54	THR	4.0
1	A	225	GLN	4.0
1	A	428	ALA	4.0
2	B	99	TYR	4.0
1	A	580	ARG	3.9
1	A	420	THR	3.9
1	A	407	ILE	3.8
1	A	243	ARG	3.7
2	B	58	LYS	3.6
1	A	216	VAL	3.6
1	A	474	PRO	3.6
1	A	405	ASN	3.6
1	A	248	GLN	3.6
2	B	88	PRO	3.6
2	B	108	ARG	3.5
1	A	188	CYS	3.5
1	A	190	GLY	3.5
2	B	72	ASN	3.5
2	B	91	TYR	3.5
1	A	475	ARG	3.4
1	A	534	VAL	3.4
2	B	101	GLU	3.4
1	A	438	GLY	3.4
1	A	219	ILE	3.3
1	A	572	THR	3.3
1	A	588	SER	3.3
1	A	597	SER	3.2
1	A	236	LYS	3.2
2	B	124	LYS	3.2
2	B	48	THR	3.2
1	A	593	HIS	3.1
1	A	397	PRO	3.1
2	B	32	CYS	3.1
1	A	255	PHE	3.1
1	A	311	GLN	3.1
2	B	34	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	575	GLN	3.1
1	A	320	GLN	3.1
1	A	426	LYS	3.1
1	A	241	SER	3.0
1	A	442	ASP	3.0
1	A	569	GLU	3.0
1	A	492	GLY	3.0
1	A	235	GLU	3.0
1	A	302	GLY	2.9
1	A	317	VAL	2.9
1	A	230	GLY	2.9
1	A	414	SER	2.9
1	A	377	ARG	2.9
1	A	300	CYS	2.8
1	A	606	CYS	2.8
2	B	109	GLU	2.8
1	A	424	LYS	2.8
1	A	472	TRP	2.8
1	A	265	LEU	2.8
1	A	238	ASN	2.8
1	A	596	HIS	2.8
1	A	473	ILE	2.8
2	B	51	ARG	2.7
2	B	132	CYS	2.7
1	A	481	TYR	2.7
1	A	339	LEU	2.7
1	A	385	ALA	2.7
2	B	44	LEU	2.7
1	A	217	SER	2.7
1	A	301	HIS	2.6
1	A	378	MET	2.6
1	A	532	SER	2.6
2	B	140	GLN	2.6
1	A	470	LEU	2.6
2	B	106	ALA	2.6
1	A	455	THR	2.6
1	A	570	CYS	2.6
2	B	110	SER	2.6
1	A	375	LYS	2.5
1	A	284	LEU	2.5
1	A	445	LYS	2.5
1	A	550	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	278	GLN	2.5
1	A	450	ASN	2.5
1	A	335	SER	2.5
1	A	448	HIS	2.5
1	A	310	TYR	2.4
1	A	595	THR	2.4
1	A	557	LEU	2.4
2	B	137	LEU	2.4
1	A	214	TYR	2.4
1	A	491	GLY	2.4
1	A	337	VAL	2.4
2	B	73	SER	2.4
2	B	100	LEU	2.4
2	B	75	GLU	2.3
1	A	191	PRO	2.3
1	A	239	LEU	2.3
1	A	381	CYS	2.3
1	A	449	ASN	2.3
1	A	565	GLU	2.3
1	A	389	LYS	2.3
1	A	336	TRP	2.3
1	A	540	TYR	2.3
1	A	490	ALA	2.3
1	A	221	THR	2.2
2	B	113	LYS	2.2
1	A	464	LEU	2.2
1	A	208	LEU	2.2
1	A	198	PHE	2.2
1	A	489	GLU	2.2
1	A	242	LYS	2.2
1	A	443	LEU	2.2
1	A	355	ARG	2.2
1	A	432	GLY	2.2
1	A	599	MET	2.2
1	A	334	GLN	2.2
1	A	579	CYS	2.2
1	A	197	GLN	2.1
1	A	574	ASP	2.1
2	B	111	THR	2.1
1	A	356	GLY	2.1
1	A	374	ASP	2.1
1	A	229	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	402	LEU	2.1
1	A	604	VAL	2.1
1	A	434	LEU	2.1
1	A	390	ILE	2.1
1	A	427	ILE	2.1
1	A	342	ASP	2.1
1	A	460	LYS	2.1
1	A	273	THR	2.1
1	A	312	GLY	2.0
1	A	425	ILE	2.0
1	A	431	PHE	2.0
2	B	92	LEU	2.0
1	A	435	ILE	2.0
2	B	35	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
3	NAG	A	901	14/15	0.17	0.41	331,344,355,356	0
3	NAG	A	801	14/15	0.82	0.30	288,301,315,319	0

6.5 Other polymers [i](#)

There are no such residues in this entry.