



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:39 PM GMT

PDB ID : 3B3Q
Title : Crystal structure of a synaptic adhesion complex
Authors : Chen, X.; Liu, H.; Shim, A.; Focia, P.; He, X.
Deposited on : 2007-10-22
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

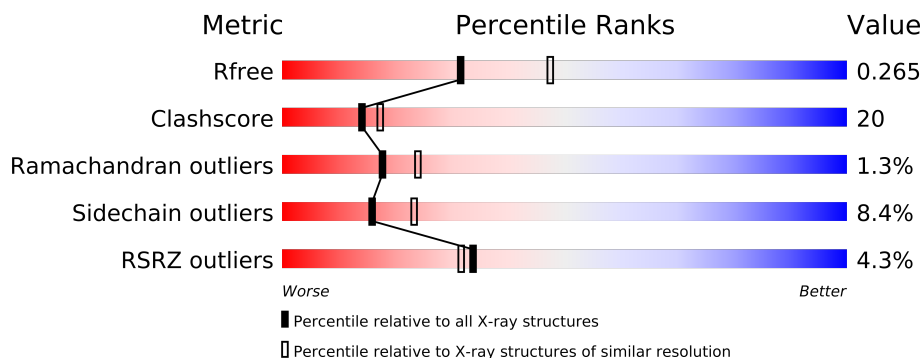
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	577	
1	B	577	
2	E	197	
2	F	197	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	CA	E	1	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12952 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Nlgn1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4219	2710	697	796	16			
1	B	536	Total	C	N	O	S	0	0	0
			4219	2710	697	796	16			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ALA	-	EXPRESSION TAG	UNP Q4KMN5
A	31	ASP	-	EXPRESSION TAG	UNP Q4KMN5
A	32	PRO	-	EXPRESSION TAG	UNP Q4KMN5
A	33	HIS	-	EXPRESSION TAG	UNP Q4KMN5
A	34	HIS	-	EXPRESSION TAG	UNP Q4KMN5
A	35	HIS	-	EXPRESSION TAG	UNP Q4KMN5
A	36	HIS	-	EXPRESSION TAG	UNP Q4KMN5
A	37	HIS	-	EXPRESSION TAG	UNP Q4KMN5
A	38	HIS	-	EXPRESSION TAG	UNP Q4KMN5
A	39	GLU	-	EXPRESSION TAG	UNP Q4KMN5
A	40	ASN	-	EXPRESSION TAG	UNP Q4KMN5
A	41	LEU	-	EXPRESSION TAG	UNP Q4KMN5
A	42	TYR	-	EXPRESSION TAG	UNP Q4KMN5
A	43	PHE	-	EXPRESSION TAG	UNP Q4KMN5
A	44	GLN	-	EXPRESSION TAG	UNP Q4KMN5
A	45	GLY	-	EXPRESSION TAG	UNP Q4KMN5
A	343	GLN	ASN	ENGINEERED MUTATION	UNP Q4KMN5
B	30	ALA	-	EXPRESSION TAG	UNP Q4KMN5
B	31	ASP	-	EXPRESSION TAG	UNP Q4KMN5
B	32	PRO	-	EXPRESSION TAG	UNP Q4KMN5
B	33	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	34	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	35	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	36	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	37	HIS	-	EXPRESSION TAG	UNP Q4KMN5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	38	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	39	GLU	-	EXPRESSION TAG	UNP Q4KMN5
B	40	ASN	-	EXPRESSION TAG	UNP Q4KMN5
B	41	LEU	-	EXPRESSION TAG	UNP Q4KMN5
B	42	TYR	-	EXPRESSION TAG	UNP Q4KMN5
B	43	PHE	-	EXPRESSION TAG	UNP Q4KMN5
B	44	GLN	-	EXPRESSION TAG	UNP Q4KMN5
B	45	GLY	-	EXPRESSION TAG	UNP Q4KMN5
B	343	GLN	ASN	ENGINEERED MUTATION	UNP Q4KMN5

- Molecule 2 is a protein called NRXN1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	187	Total	C	N	O	S	14	0	0
			1431	902	255	273	1			
2	F	187	Total	C	N	O	S	14	0	0
			1431	902	255	273	1			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	73	HIS	-	EXPRESSION TAG	UNP A4FVB9
E	74	SER	-	EXPRESSION TAG	UNP A4FVB9
E	75	ALA	-	EXPRESSION TAG	UNP A4FVB9
E	76	PHE	-	EXPRESSION TAG	UNP A4FVB9
E	77	ALA	-	EXPRESSION TAG	UNP A4FVB9
E	78	ALA	-	EXPRESSION TAG	UNP A4FVB9
E	79	ASP	-	EXPRESSION TAG	UNP A4FVB9
E	80	PRO	-	EXPRESSION TAG	UNP A4FVB9
E	293	HIS	-	EXPRESSION TAG	UNP A4FVB9
E	294	HIS	-	EXPRESSION TAG	UNP A4FVB9
E	295	HIS	-	EXPRESSION TAG	UNP A4FVB9
E	296	HIS	-	EXPRESSION TAG	UNP A4FVB9
E	297	HIS	-	EXPRESSION TAG	UNP A4FVB9
E	298	HIS	-	EXPRESSION TAG	UNP A4FVB9
E	299	HIS	-	EXPRESSION TAG	UNP A4FVB9
F	73	HIS	-	EXPRESSION TAG	UNP A4FVB9
F	74	SER	-	EXPRESSION TAG	UNP A4FVB9
F	75	ALA	-	EXPRESSION TAG	UNP A4FVB9
F	76	PHE	-	EXPRESSION TAG	UNP A4FVB9
F	77	ALA	-	EXPRESSION TAG	UNP A4FVB9
F	78	ALA	-	EXPRESSION TAG	UNP A4FVB9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	79	ASP	-	EXPRESSION TAG	UNP A4FVB9
F	80	PRO	-	EXPRESSION TAG	UNP A4FVB9
F	293	HIS	-	EXPRESSION TAG	UNP A4FVB9
F	294	HIS	-	INSERTION	UNP A4FVB9
F	295	HIS	-	EXPRESSION TAG	UNP A4FVB9
F	296	HIS	-	EXPRESSION TAG	UNP A4FVB9
F	297	HIS	-	EXPRESSION TAG	UNP A4FVB9
F	298	HIS	-	EXPRESSION TAG	UNP A4FVB9
F	299	HIS	-	EXPRESSION TAG	UNP A4FVB9

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

There are 51 discrepancies between the modelled and reference sequences:

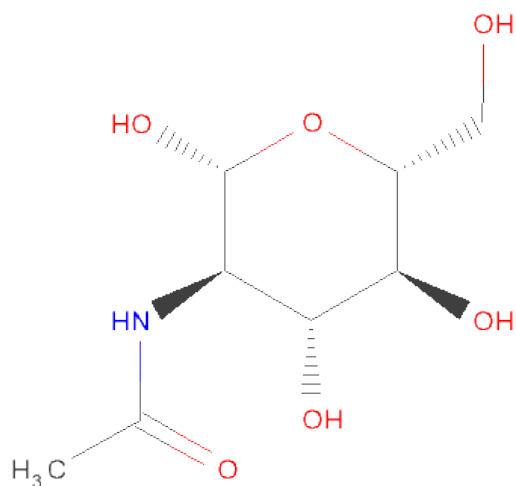
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ALA	-	EXPRESSION TAG	UNP Q4KMN5
A	31	ASP	-	EXPRESSION TAG	UNP Q4KMN5
A	32	PRO	-	EXPRESSION TAG	UNP Q4KMN5
A	33	HIS	-	EXPRESSION TAG	UNP Q4KMN5
A	34	HIS	-	EXPRESSION TAG	UNP Q4KMN5
A	35	HIS	-	EXPRESSION TAG	UNP Q4KMN5
A	36	HIS	-	EXPRESSION TAG	UNP Q4KMN5
A	37	HIS	-	EXPRESSION TAG	UNP Q4KMN5
A	38	HIS	-	EXPRESSION TAG	UNP Q4KMN5
A	39	GLU	-	EXPRESSION TAG	UNP Q4KMN5
A	40	ASN	-	EXPRESSION TAG	UNP Q4KMN5
A	41	LEU	-	EXPRESSION TAG	UNP Q4KMN5
A	42	TYR	-	EXPRESSION TAG	UNP Q4KMN5
A	43	PHE	-	EXPRESSION TAG	UNP Q4KMN5
A	44	GLN	-	EXPRESSION TAG	UNP Q4KMN5
A	45	GLY	-	EXPRESSION TAG	UNP Q4KMN5
A	343	GLN	ASN	ENGINEERED MUTATION	UNP Q4KMN5
B	30	ALA	-	EXPRESSION TAG	UNP Q4KMN5
B	31	ASP	-	EXPRESSION TAG	UNP Q4KMN5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	32	PRO	-	EXPRESSION TAG	UNP Q4KMN5
B	33	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	34	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	35	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	36	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	37	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	38	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	39	GLU	-	EXPRESSION TAG	UNP Q4KMN5
B	40	ASN	-	EXPRESSION TAG	UNP Q4KMN5
B	41	LEU	-	EXPRESSION TAG	UNP Q4KMN5
B	42	TYR	-	EXPRESSION TAG	UNP Q4KMN5
B	43	PHE	-	EXPRESSION TAG	UNP Q4KMN5
B	44	GLN	-	EXPRESSION TAG	UNP Q4KMN5
B	45	GLY	-	EXPRESSION TAG	UNP Q4KMN5
B	343	GLN	ASN	ENGINEERED MUTATION	UNP Q4KMN5
B	30	ALA	-	EXPRESSION TAG	UNP Q4KMN5
B	31	ASP	-	EXPRESSION TAG	UNP Q4KMN5
B	32	PRO	-	EXPRESSION TAG	UNP Q4KMN5
B	33	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	34	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	35	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	36	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	37	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	38	HIS	-	EXPRESSION TAG	UNP Q4KMN5
B	39	GLU	-	EXPRESSION TAG	UNP Q4KMN5
B	40	ASN	-	EXPRESSION TAG	UNP Q4KMN5
B	41	LEU	-	EXPRESSION TAG	UNP Q4KMN5
B	42	TYR	-	EXPRESSION TAG	UNP Q4KMN5
B	43	PHE	-	EXPRESSION TAG	UNP Q4KMN5
B	44	GLN	-	EXPRESSION TAG	UNP Q4KMN5
B	45	GLY	-	EXPRESSION TAG	UNP Q4KMN5
B	343	GLN	ASN	ENGINEERED MUTATION	UNP Q4KMN5

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Ca	0	0
			1	1		
5	E	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

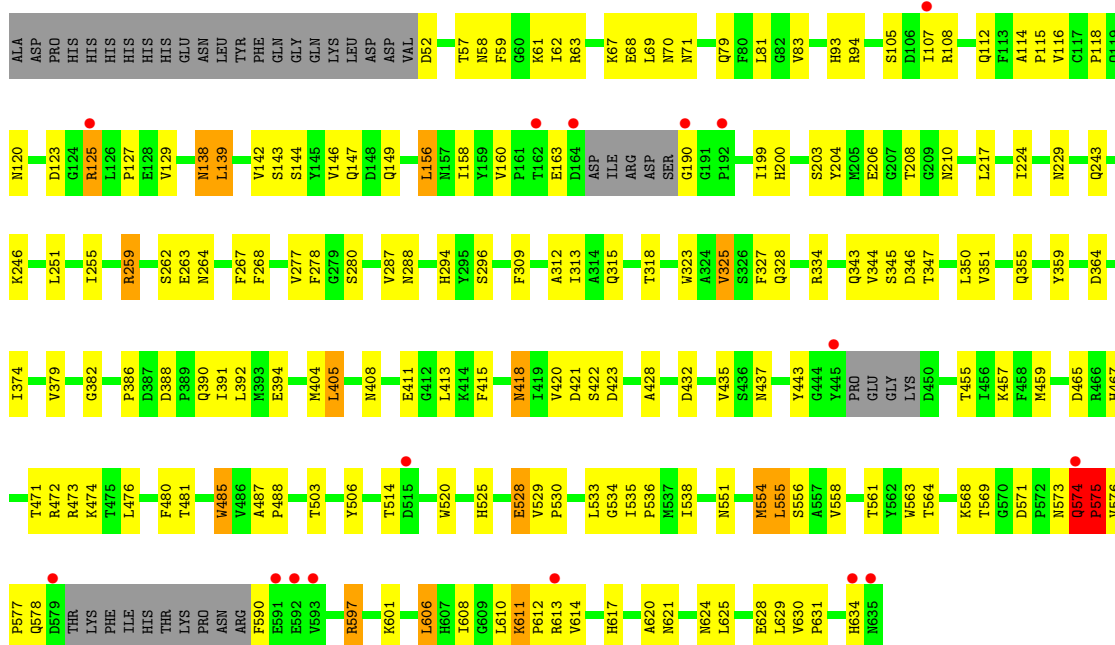
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	536	Total	O	0	0
			536	536		
6	B	598	Total	O	0	0
			598	598		
6	E	230	Total	O	0	0
			230	230		
6	F	188	Total	O	0	0
			188	188		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

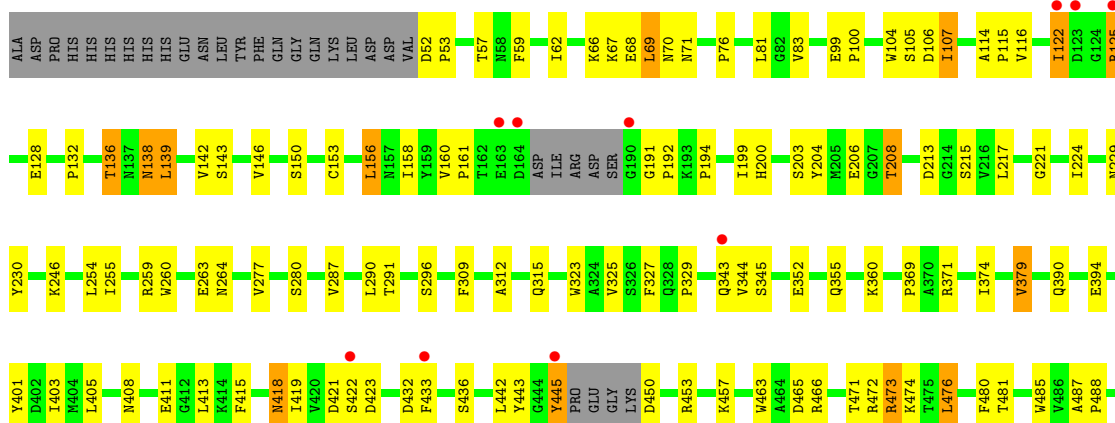
- Molecule 1: Nlgn1 protein

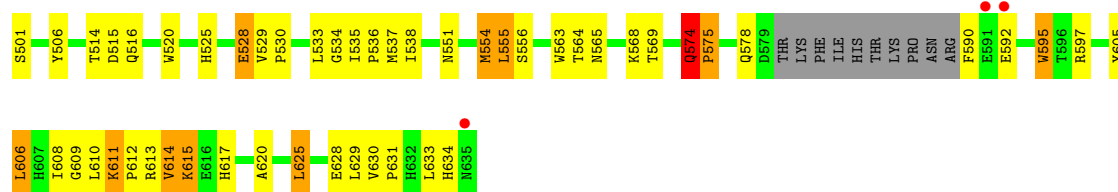
Chain A: 



- Molecule 1: Nlgn1 protein

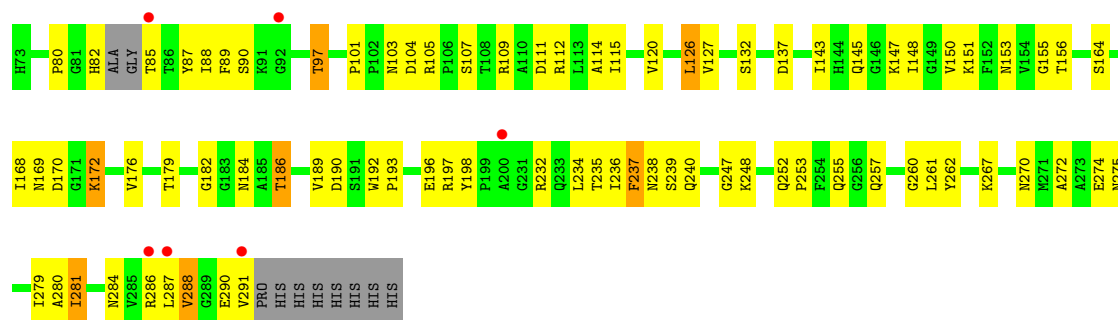
Chain B: 





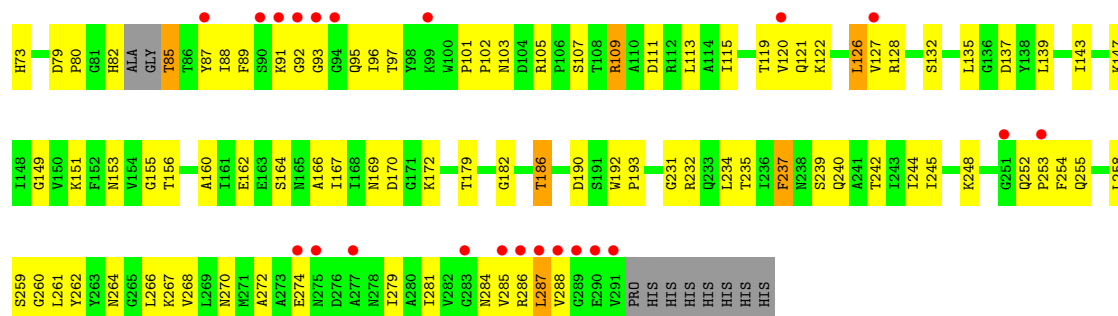
• Molecule 2: NRXN1 protein

Chain E:



• Molecule 2: NRXN1 protein

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.59Å 125.40Å 131.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.64 – 2.40 24.64 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.5 (24.64-2.40) 97.0 (24.64-2.29)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.28Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.261 0.246 , 0.265	Depositor DCC
R_{free} test set	4282 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 38.4	EDS
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 84449 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12952	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.37	0/4338	0.54	0/5922
1	B	0.39	0/4338	0.55	0/5922
2	E	0.36	0/1459	0.55	0/1977
2	F	0.42	0/1459	0.55	1/1977 (0.1%)
All	All	0.38	0/11594	0.55	1/15798 (0.0%)

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	1
1	B	0	1
2	F	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	122	LYS	CA-CB-CG	-5.71	100.83	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	574	GLN	Peptide
1	B	574	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	F	109	ARG	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4219	0	4049	149	0
1	B	4219	0	4049	143	1
2	E	1431	0	1406	63	0
2	F	1431	0	1406	77	2
3	A	28	0	25	4	0
3	B	56	0	50	5	0
4	A	14	0	13	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	536	0	0	31	1
6	B	598	0	0	41	1
6	E	230	0	0	15	3
6	F	188	0	0	26	2
All	All	12952	0	10998	439	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (439) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:147:LYS:HD3	2:F:164:SER:HA	1.22	1.18
1:A:334:ARG:HG3	1:A:344:VAL:CG2	1.86	1.04
2:E:147:LYS:HD3	2:E:164:SER:HA	1.43	1.00
1:A:334:ARG:HG3	1:A:344:VAL:HG21	1.40	0.99
3:B:636:NAG:H62	3:B:637:NAG:H2	1.45	0.96
3:A:1:NAG:H3	3:A:2:NAG:H61	1.45	0.95
1:A:613:ARG:HD3	6:A:691:HOH:O	1.71	0.91
2:F:248:LYS:HB2	6:F:719:HOH:O	1.70	0.90
1:A:67:LYS:HE3	6:A:930:HOH:O	1.74	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:291:VAL:HB	6:E:482:HOH:O	1.75	0.86
1:B:355:GLN:HG3	6:B:875:HOH:O	1.73	0.86
2:F:192:TRP:HB3	2:F:193:PRO:HD2	1.58	0.85
1:A:112:GLN:NE2	6:A:876:HOH:O	2.06	0.85
1:A:574:GLN:HB3	1:A:575:PRO:HD2	1.56	0.84
2:F:127:VAL:HG21	2:F:261:LEU:HD11	1.59	0.84
1:A:52:ASP:N	6:A:1055:HOH:O	2.10	0.84
3:B:636:NAG:C6	3:B:637:NAG:H2	2.07	0.84
2:F:287:LEU:HD12	6:F:795:HOH:O	1.78	0.84
1:B:450:ASP:HB2	6:B:707:HOH:O	1.76	0.84
1:B:574:GLN:HB3	1:B:575:PRO:HD2	1.60	0.83
1:A:418:ASN:HD22	1:A:418:ASN:H	1.26	0.82
1:A:574:GLN:HB3	1:A:575:PRO:CD	2.09	0.82
2:F:135:LEU:HA	6:F:759:HOH:O	1.78	0.82
1:A:473:ARG:NH2	1:A:520:TRP:HB2	1.93	0.81
1:A:108:ARG:HG3	6:A:836:HOH:O	1.80	0.81
1:A:199:ILE:CD1	1:A:277:VAL:HG13	2.10	0.81
2:E:115:ILE:HD13	2:E:261:LEU:HD12	1.62	0.81
1:A:190:GLY:HA3	6:A:941:HOH:O	1.80	0.80
1:A:208:THR:HG23	1:A:229:ASN:OD1	1.81	0.80
1:A:421:ASP:O	1:A:423:ASP:N	2.15	0.80
2:F:164:SER:HB2	6:F:761:HOH:O	1.82	0.79
2:F:166:ALA:HB3	2:F:192:TRP:CZ3	2.18	0.78
1:B:421:ASP:O	1:B:423:ASP:N	2.16	0.78
2:F:170:ASP:OD1	2:F:172:LYS:HG2	1.85	0.77
1:B:466:ARG:HG2	6:B:693:HOH:O	1.84	0.77
1:A:577:PRO:HB3	6:A:1068:HOH:O	1.86	0.76
1:B:418:ASN:HD22	1:B:418:ASN:H	1.33	0.75
2:F:286:ARG:HG2	6:F:795:HOH:O	1.85	0.74
1:A:334:ARG:CG	1:A:344:VAL:HG21	2.15	0.74
2:F:80:PRO:O	2:F:260:GLY:HA3	1.85	0.74
2:F:179:THR:HB	2:F:186:THR:HB	1.70	0.74
1:A:611:LYS:HD2	1:A:611:LYS:H	1.53	0.73
2:E:192:TRP:HB3	2:E:193:PRO:HD2	1.69	0.73
1:B:146:VAL:HG12	1:B:146:VAL:O	1.89	0.73
1:B:481:THR:HA	1:B:485:TRP:HD1	1.54	0.72
1:B:125:ARG:HG3	6:B:1216:HOH:O	1.89	0.72
1:A:564:THR:O	1:A:568:LYS:HG3	1.88	0.72
2:F:160:ALA:HA	6:F:802:HOH:O	1.89	0.72
1:A:569:THR:HG21	1:A:575:PRO:HD2	1.72	0.72
2:F:89:PHE:O	2:F:255:GLN:HA	1.90	0.72
2:E:275:ASN:HB3	6:E:343:HOH:O	1.88	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:184:ASN:HB3	6:E:373:HOH:O	1.88	0.72
2:F:92:GLY:HA2	6:F:721:HOH:O	1.89	0.72
1:A:116:VAL:HG21	1:A:146:VAL:HG13	1.71	0.71
1:B:597:ARG:NH2	6:B:869:HOH:O	2.22	0.71
1:B:139:LEU:O	1:B:143:SER:OG	2.07	0.71
1:A:578:GLN:HB3	6:A:974:HOH:O	1.89	0.71
1:B:565:ASN:OD1	6:B:669:HOH:O	2.08	0.71
2:F:287:LEU:HD21	6:F:835:HOH:O	1.91	0.70
1:B:125:ARG:HB3	6:B:1216:HOH:O	1.91	0.70
1:B:208:THR:HG22	1:B:229:ASN:OD1	1.92	0.70
1:A:259:ARG:HG3	1:A:259:ARG:HH11	1.57	0.69
1:A:443:TYR:CD2	1:A:634:HIS:HE1	2.10	0.69
1:A:481:THR:HA	1:A:485:TRP:HD1	1.57	0.69
1:B:574:GLN:HB3	1:B:575:PRO:CD	2.21	0.69
1:A:437:ASN:HB3	6:A:640:HOH:O	1.92	0.69
1:A:328:GLN:NE2	6:A:671:HOH:O	2.24	0.69
1:A:334:ARG:HD3	6:A:966:HOH:O	1.92	0.68
2:F:147:LYS:CD	2:F:164:SER:HA	2.14	0.68
1:B:481:THR:HA	1:B:485:TRP:CD1	2.28	0.68
1:B:355:GLN:HB3	6:B:967:HOH:O	1.93	0.68
1:B:613:ARG:HD2	6:B:671:HOH:O	1.94	0.67
1:A:421:ASP:C	1:A:423:ASP:H	1.97	0.67
1:A:481:THR:HA	1:A:485:TRP:CD1	2.29	0.67
2:F:267:LYS:HE3	6:F:718:HOH:O	1.93	0.67
2:E:88:ILE:HD13	2:E:257:GLN:HG2	1.77	0.67
1:A:93:HIS:HB3	6:A:669:HOH:O	1.94	0.67
1:A:199:ILE:HD11	1:A:277:VAL:HG13	1.76	0.67
1:A:208:THR:CG2	1:A:229:ASN:OD1	2.42	0.67
1:B:418:ASN:N	1:B:418:ASN:HD22	1.90	0.67
2:F:244:ILE:O	2:F:244:ILE:HG22	1.95	0.67
1:A:577:PRO:HD2	6:A:1126:HOH:O	1.94	0.66
1:A:127:PRO:HG3	6:A:1011:HOH:O	1.94	0.66
1:B:255:ILE:HD11	1:B:290:LEU:HD22	1.78	0.66
2:F:270:ASN:O	2:F:274:GLU:HG2	1.96	0.66
2:F:272:ALA:CB	2:F:279:ILE:HG21	2.25	0.66
2:F:85:THR:O	2:F:85:THR:OG1	2.11	0.66
3:A:1:NAG:H83	3:A:2:NAG:H61	1.78	0.66
1:B:146:VAL:CG1	1:B:146:VAL:O	2.44	0.65
1:A:471:THR:HA	1:A:474:LYS:HD2	1.77	0.65
1:A:597:ARG:HD3	6:A:665:HOH:O	1.96	0.65
1:B:132:PRO:O	1:B:136:THR:HG23	1.97	0.65
1:B:125:ARG:CG	6:B:1216:HOH:O	2.43	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:360:LYS:HE3	6:B:933:HOH:O	1.95	0.65
2:E:238:ASN:ND2	6:E:311:HOH:O	2.19	0.65
1:A:70:ASN:HB2	1:A:538:ILE:HG23	1.79	0.65
1:B:421:ASP:C	1:B:423:ASP:H	2.00	0.65
1:B:191:GLY:HA3	6:B:965:HOH:O	1.96	0.65
2:E:281:ILE:HD12	2:E:281:ILE:H	1.62	0.65
2:F:93:GLY:HA3	6:F:805:HOH:O	1.97	0.64
1:A:146:VAL:O	1:A:146:VAL:HG12	1.97	0.64
1:B:634:HIS:HB2	6:B:1005:HOH:O	1.97	0.64
1:B:457:LYS:NZ	6:B:953:HOH:O	2.28	0.64
1:A:125:ARG:HA	6:A:706:HOH:O	1.96	0.64
1:A:139:LEU:HA	1:A:142:VAL:HB	1.80	0.63
1:A:315:GLN:HG2	1:A:506:TYR:OH	1.98	0.63
1:B:408:ASN:HD21	1:B:528:GLU:HG3	1.62	0.63
1:A:487:ALA:HB3	1:A:488:PRO:HD3	1.79	0.63
1:B:569:THR:HG21	1:B:575:PRO:HD2	1.81	0.63
1:A:277:VAL:HG12	1:A:287:VAL:HG22	1.80	0.63
1:B:125:ARG:CB	6:B:1216:HOH:O	2.44	0.62
2:E:290:GLU:HG2	6:E:324:HOH:O	1.98	0.62
1:B:564:THR:O	1:B:568:LYS:HG3	1.99	0.62
1:B:70:ASN:HB2	1:B:538:ILE:HG23	1.82	0.62
1:A:125:ARG:HD3	6:A:922:HOH:O	1.99	0.61
1:A:139:LEU:H	1:A:139:LEU:HD12	1.66	0.61
1:A:535:ILE:N	1:A:536:PRO:CD	2.63	0.61
2:F:155:GLY:HA3	2:F:234:LEU:HD12	1.83	0.61
2:E:182:GLY:HA2	2:E:235:THR:HA	1.81	0.61
1:A:597:ARG:HH11	1:A:597:ARG:HG3	1.65	0.60
1:A:125:ARG:HB3	6:A:1011:HOH:O	2.01	0.60
1:B:208:THR:CG2	1:B:229:ASN:OD1	2.50	0.60
2:F:182:GLY:HA2	2:F:235:THR:HA	1.81	0.60
2:F:87:TYR:HD2	2:F:285:VAL:HG12	1.67	0.60
1:B:535:ILE:N	1:B:536:PRO:CD	2.64	0.59
1:B:592:GLU:HG3	6:B:1153:HOH:O	2.02	0.59
2:E:90:SER:HB2	2:E:284:ASN:OD1	2.03	0.59
1:B:122:ILE:HD11	6:B:745:HOH:O	2.00	0.59
2:E:120:VAL:HG22	6:E:303:HOH:O	2.03	0.59
1:B:203:SER:O	1:B:204:TYR:HB2	2.03	0.59
1:B:568:LYS:CE	6:B:669:HOH:O	2.50	0.58
2:F:149:GLY:HA3	2:F:162:GLU:HG3	1.85	0.58
2:E:115:ILE:CG2	2:E:176:VAL:CG1	2.82	0.58
1:A:138:ASN:HD22	1:A:138:ASN:N	2.01	0.58
1:A:467:HIS:HD2	6:A:699:HOH:O	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:80:PRO:O	2:E:260:GLY:HA3	2.03	0.58
1:A:57:THR:HA	1:A:267:PHE:CD1	2.39	0.58
1:A:455:THR:O	1:A:459:MET:HG2	2.04	0.58
2:F:281:ILE:H	2:F:281:ILE:HD12	1.69	0.58
1:B:199:ILE:HD12	1:B:277:VAL:HG13	1.85	0.57
1:A:243:GLN:HG3	1:A:246:LYS:HE2	1.87	0.57
2:E:115:ILE:HG23	2:E:176:VAL:HG12	1.85	0.57
2:E:155:GLY:HA3	2:E:234:LEU:HD12	1.86	0.57
1:A:634:HIS:HB3	6:A:681:HOH:O	2.04	0.57
2:F:272:ALA:HB2	2:F:279:ILE:HG21	1.87	0.57
2:F:151:LYS:HB2	6:F:802:HOH:O	2.03	0.57
1:A:139:LEU:CD1	1:A:139:LEU:H	2.17	0.57
1:B:609:GLY:O	1:B:612:PRO:HD3	2.06	0.56
1:A:415:PHE:CD1	1:A:480:PHE:HB2	2.39	0.56
1:A:606:LEU:CD1	1:A:608:ILE:HG12	2.35	0.56
2:F:91:LYS:O	2:F:284:ASN:ND2	2.39	0.56
1:B:200:HIS:HA	6:B:868:HOH:O	2.04	0.56
1:B:625:LEU:HD22	1:B:630:VAL:HG23	1.87	0.56
2:E:127:VAL:HG21	2:E:261:LEU:HD11	1.87	0.56
1:A:208:THR:HG22	1:A:210:ASN:H	1.71	0.56
2:F:248:LYS:HA	2:F:253:PRO:HG3	1.88	0.56
1:B:418:ASN:ND2	1:B:418:ASN:H	2.02	0.56
1:B:471:THR:HA	1:B:474:LYS:HD2	1.88	0.56
1:A:259:ARG:HG3	6:A:1058:HOH:O	2.06	0.55
2:E:112:ARG:NH1	2:E:179:THR:HG23	2.20	0.55
1:B:516:GLN:NE2	6:B:1046:HOH:O	2.39	0.55
2:E:179:THR:HB	2:E:186:THR:HB	1.88	0.55
2:F:245:ILE:HD11	2:F:268:VAL:HG11	1.88	0.55
1:B:473:ARG:NH2	1:B:520:TRP:HB2	2.21	0.55
1:A:200:HIS:HE1	6:A:639:HOH:O	1.90	0.55
1:A:617:HIS:HB3	1:A:620:ALA:HB2	1.88	0.55
2:F:82:HIS:H	2:F:259:SER:HB3	1.72	0.55
2:F:192:TRP:N	2:F:192:TRP:CD1	2.72	0.54
1:A:578:GLN:HB2	1:A:590:PHE:HB2	1.87	0.54
1:A:465:ASP:HB2	6:A:938:HOH:O	2.07	0.54
1:B:68:GLU:HG2	1:B:76:PRO:HB3	1.90	0.54
1:A:597:ARG:CD	6:A:665:HOH:O	2.54	0.54
1:A:428:ALA:HB2	1:A:472:ARG:NH1	2.22	0.54
1:A:83:VAL:HB	1:A:156:LEU:HD23	1.89	0.54
2:F:248:LYS:HD2	6:F:805:HOH:O	2.07	0.54
2:F:151:LYS:CB	6:F:802:HOH:O	2.54	0.54
1:B:611:LYS:HE3	6:B:1007:HOH:O	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.72	0.54
1:B:578:GLN:HB2	1:B:590:PHE:HB2	1.89	0.54
1:A:443:TYR:CD2	1:A:634:HIS:CE1	2.94	0.53
2:F:102:PRO:HG3	2:F:105:ARG:HH21	1.71	0.53
2:E:145:GLN:NE2	6:E:416:HOH:O	2.41	0.53
1:A:146:VAL:HG12	1:A:149:GLN:HE21	1.73	0.53
2:E:120:VAL:HA	2:E:169:ASN:O	2.08	0.53
1:B:485:TRP:CZ3	1:B:525:HIS:CE1	2.96	0.53
2:F:160:ALA:CB	6:F:802:HOH:O	2.57	0.53
1:B:116:VAL:HG12	1:B:208:THR:CG2	2.39	0.53
1:B:116:VAL:HG12	1:B:208:THR:HG21	1.91	0.53
1:A:418:ASN:HD22	1:A:418:ASN:N	2.01	0.53
1:A:473:ARG:HH22	1:A:520:TRP:HB2	1.72	0.53
1:B:277:VAL:CG1	1:B:287:VAL:HG22	2.39	0.53
2:E:112:ARG:HG3	6:E:341:HOH:O	2.09	0.53
1:A:388:ASP:HB3	1:A:391:ILE:HG12	1.90	0.53
1:A:443:TYR:HD2	1:A:634:HIS:HE1	1.56	0.52
2:F:166:ALA:HB3	2:F:192:TRP:HZ3	1.70	0.52
1:B:612:PRO:HB3	6:B:714:HOH:O	2.09	0.52
1:B:534:GLY:HA2	1:B:556:SER:OG	2.09	0.52
2:F:160:ALA:HB1	6:F:822:HOH:O	2.09	0.52
1:A:551:ASN:O	1:A:554:MET:HG3	2.10	0.52
1:A:411:GLU:HB2	1:A:481:THR:HG23	1.91	0.52
1:A:408:ASN:HD21	1:A:528:GLU:HG3	1.73	0.52
1:B:630:VAL:N	1:B:631:PRO:CD	2.72	0.52
1:A:163:GLU:HG3	6:A:1044:HOH:O	2.09	0.52
2:E:97:THR:HG22	2:E:280:ALA:HB3	1.92	0.52
1:B:128:GLU:CD	6:B:1010:HOH:O	2.48	0.51
1:A:83:VAL:HB	1:A:156:LEU:CD2	2.41	0.51
2:F:242:THR:HG21	6:F:780:HOH:O	2.09	0.51
1:B:514:THR:HG22	1:B:515:ASP:N	2.25	0.51
1:B:401:TYR:HB2	1:B:403:ILE:HD11	1.91	0.51
2:E:179:THR:HG22	6:E:312:HOH:O	2.11	0.50
2:E:101:PRO:HG2	2:E:104:ASP:HB3	1.93	0.50
3:A:1:NAG:H83	3:A:2:NAG:C6	2.41	0.50
2:E:192:TRP:CD1	2:E:192:TRP:N	2.75	0.50
1:B:606:LEU:HD12	1:B:608:ILE:HG12	1.93	0.50
1:A:473:ARG:NE	1:A:520:TRP:CE3	2.80	0.50
1:B:139:LEU:HA	1:B:142:VAL:HB	1.92	0.50
1:B:568:LYS:HE2	6:B:669:HOH:O	2.09	0.50
1:A:390:GLN:O	1:A:394:GLU:HB2	2.10	0.50
2:E:286:ARG:NH2	6:E:386:HOH:O	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:137:ASP:HA	2:F:153:ASN:O	2.11	0.50
1:B:466:ARG:NH1	6:B:693:HOH:O	2.45	0.50
1:B:371:ARG:HG3	6:B:1136:HOH:O	2.11	0.50
2:F:127:VAL:CG2	2:F:261:LEU:HD11	2.37	0.50
1:A:554:MET:HG3	1:A:555:LEU:N	2.26	0.50
1:A:94:ARG:O	1:A:355:GLN:NE2	2.44	0.50
1:B:442:LEU:HD12	6:B:716:HOH:O	2.12	0.49
1:B:568:LYS:HE3	6:B:669:HOH:O	2.11	0.49
1:B:260:TRP:O	1:B:264:ASN:HB2	2.13	0.49
2:E:97:THR:CG2	2:E:97:THR:O	2.61	0.49
2:F:286:ARG:CG	6:F:795:HOH:O	2.52	0.49
1:A:473:ARG:HG3	1:A:474:LYS:N	2.28	0.49
1:B:418:ASN:HB3	6:B:807:HOH:O	2.12	0.49
1:A:138:ASN:HD22	1:A:138:ASN:H	1.60	0.49
1:B:614:VAL:HG12	6:B:788:HOH:O	2.12	0.49
1:B:83:VAL:HB	1:B:156:LEU:HD23	1.93	0.49
2:E:197:ARG:NH1	6:E:434:HOH:O	2.36	0.49
2:F:87:TYR:HD2	2:F:285:VAL:CG1	2.25	0.49
2:E:89:PHE:O	2:E:255:GLN:HA	2.13	0.49
2:E:286:ARG:HB2	6:E:447:HOH:O	2.10	0.49
2:F:254:PHE:CE2	2:F:258:LEU:HD21	2.48	0.49
2:F:147:LYS:HG2	2:F:166:ALA:O	2.13	0.49
2:F:101:PRO:HB2	2:F:103:ASN:OD1	2.11	0.49
2:E:168:ILE:CG2	2:E:189:VAL:HG11	2.43	0.49
2:E:114:ALA:HB3	2:E:262:TYR:HB3	1.95	0.48
3:A:1:NAG:H3	3:A:2:NAG:C6	2.32	0.48
2:F:95:GLN:HG3	6:F:719:HOH:O	2.13	0.48
2:E:272:ALA:CB	2:E:279:ILE:HG21	2.42	0.48
1:A:325:VAL:HG22	1:A:327:PHE:CZ	2.48	0.48
1:A:160:VAL:HG13	1:A:224:ILE:CD1	2.43	0.48
2:E:192:TRP:HB3	2:E:193:PRO:CD	2.41	0.48
2:E:115:ILE:HG22	2:E:176:VAL:HG13	1.96	0.48
1:B:287:VAL:CG1	1:B:312:ALA:HB1	2.43	0.48
1:B:296:SER:HB2	1:B:309:PHE:CE1	2.49	0.48
1:B:371:ARG:CZ	6:B:1160:HOH:O	2.61	0.48
1:A:199:ILE:CD1	1:A:277:VAL:CG1	2.86	0.48
1:B:199:ILE:CD1	1:B:277:VAL:HG13	2.44	0.48
2:F:252:GLN:N	2:F:253:PRO:HD3	2.29	0.48
2:E:101:PRO:HB2	2:E:103:ASN:OD1	2.14	0.47
1:A:160:VAL:HG13	1:A:224:ILE:HD13	1.96	0.47
1:B:221:GLY:O	1:B:568:LYS:NZ	2.47	0.47
1:A:57:THR:HA	1:A:267:PHE:HD1	1.77	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:514:THR:HG22	1:B:515:ASP:H	1.79	0.47
1:B:617:HIS:HB3	1:B:620:ALA:HB2	1.96	0.47
1:A:114:ALA:HB1	1:A:115:PRO:HD2	1.95	0.47
2:E:252:GLN:N	2:E:253:PRO:HD3	2.29	0.47
1:B:418:ASN:N	1:B:418:ASN:ND2	2.61	0.47
1:A:443:TYR:HD2	1:A:634:HIS:CE1	2.32	0.47
1:A:343:GLN:HB2	6:A:932:HOH:O	2.15	0.47
1:A:118:PRO:HB3	1:A:359:TYR:CE1	2.49	0.47
1:B:465:ASP:OD2	1:B:465:ASP:N	2.46	0.47
1:B:277:VAL:HG12	1:B:287:VAL:HG22	1.96	0.47
1:B:329:PRO:HG3	1:B:379:VAL:HG21	1.95	0.47
1:A:287:VAL:CG1	1:A:312:ALA:HB1	2.45	0.47
1:B:554:MET:HE1	6:B:771:HOH:O	2.13	0.47
3:B:2:NAG:H81	6:B:1235:HOH:O	2.15	0.47
2:E:126:LEU:HD23	2:E:126:LEU:N	2.29	0.47
2:F:121:GLN:OE1	2:F:255:GLN:N	2.40	0.47
1:A:259:ARG:HG3	1:A:259:ARG:NH1	2.27	0.47
1:B:473:ARG:HG3	1:B:474:LYS:N	2.30	0.47
1:B:83:VAL:HB	1:B:156:LEU:CD2	2.45	0.47
1:B:487:ALA:N	1:B:488:PRO:CD	2.78	0.47
1:B:99:GLU:HG3	1:B:100:PRO:CD	2.44	0.47
2:F:113:LEU:HD11	2:F:261:LEU:HD21	1.97	0.47
1:B:371:ARG:NH2	6:B:1160:HOH:O	2.48	0.47
2:E:143:ILE:HG12	2:E:148:ILE:HD12	1.97	0.47
1:A:144:SER:HA	1:A:147:GLN:HG2	1.97	0.47
1:A:208:THR:HG21	1:A:210:ASN:CG	2.35	0.47
2:E:234:LEU:HD23	6:E:404:HOH:O	2.15	0.47
1:A:613:ARG:CD	6:A:691:HOH:O	2.43	0.46
1:B:421:ASP:C	1:B:423:ASP:N	2.66	0.46
1:A:529:VAL:N	1:A:530:PRO:HD2	2.29	0.46
1:A:68:GLU:HA	6:A:646:HOH:O	2.15	0.46
1:A:259:ARG:NH1	1:A:259:ARG:CG	2.79	0.46
1:A:386:PRO:HG2	1:A:392:LEU:HD11	1.97	0.46
2:E:137:ASP:HA	2:E:153:ASN:O	2.16	0.46
1:A:62:ILE:HD11	1:A:268:PHE:HZ	1.80	0.46
1:A:62:ILE:HD11	1:A:268:PHE:CZ	2.51	0.46
1:B:605:TYR:CZ	1:B:615:LYS:HB2	2.51	0.46
1:B:213:ASP:OD1	1:B:215:SER:HB2	2.16	0.46
2:F:107:SER:HA	2:F:237:PHE:O	2.16	0.46
1:B:114:ALA:HB1	1:B:115:PRO:HD2	1.98	0.46
2:E:115:ILE:CG2	2:E:176:VAL:HG13	2.46	0.46
1:B:287:VAL:O	1:B:291:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:611:LYS:HD2	1:B:611:LYS:H	1.81	0.46
1:A:606:LEU:HD13	1:A:608:ILE:HG12	1.97	0.46
1:A:325:VAL:HG22	1:A:327:PHE:CE1	2.51	0.46
3:B:1:NAG:O4	3:B:2:NAG:H62	2.16	0.46
2:E:247:GLY:N	6:E:438:HOH:O	2.49	0.45
1:A:79:GLN:HB2	1:A:81:LEU:HD11	1.99	0.45
2:F:120:VAL:HA	2:F:169:ASN:O	2.16	0.45
2:F:73:HIS:HB2	6:F:774:HOH:O	2.16	0.45
1:B:390:GLN:O	1:B:394:GLU:HB2	2.17	0.45
1:A:203:SER:O	1:A:204:TYR:HB2	2.16	0.45
2:F:79:ASP:OD1	2:F:80:PRO:HD2	2.17	0.45
1:B:107:ILE:HG12	6:B:926:HOH:O	2.16	0.45
1:A:611:LYS:HD2	1:A:611:LYS:N	2.26	0.45
2:F:85:THR:N	6:F:746:HOH:O	2.50	0.45
1:A:143:SER:HB3	1:A:147:GLN:NE2	2.32	0.45
1:A:69:LEU:C	1:A:71:ASN:H	2.20	0.45
2:F:192:TRP:HB3	2:F:193:PRO:CD	2.38	0.45
1:B:634:HIS:CD2	6:B:741:HOH:O	2.70	0.45
2:F:102:PRO:HA	2:F:105:ARG:HE	1.82	0.45
2:E:105:ARG:HB3	2:E:240:GLN:O	2.17	0.45
1:A:382:GLY:HA2	1:A:386:PRO:HA	1.99	0.45
1:B:436:SER:OG	1:B:453:ARG:HD2	2.17	0.45
2:F:128:ARG:HA	2:F:139:LEU:O	2.17	0.45
2:F:95:GLN:CG	6:F:719:HOH:O	2.65	0.44
1:A:561:THR:HB	1:A:578:GLN:HE22	1.82	0.44
2:E:87:TYR:O	2:E:257:GLN:HA	2.16	0.44
2:F:102:PRO:HA	2:F:105:ARG:NE	2.32	0.44
2:E:148:ILE:HB	2:E:168:ILE:HG12	1.99	0.44
2:E:168:ILE:HG21	2:E:189:VAL:HG11	2.00	0.44
1:B:515:ASP:OD1	1:B:515:ASP:N	2.47	0.44
1:B:411:GLU:HB2	1:B:481:THR:HG23	2.00	0.44
1:B:408:ASN:ND2	1:B:528:GLU:HG3	2.32	0.44
1:B:259:ARG:HG3	1:B:259:ARG:NH1	2.31	0.44
1:B:139:LEU:CD1	1:B:139:LEU:H	2.30	0.44
1:A:503:THR:H	1:A:597:ARG:NH1	2.15	0.44
1:A:624:ASN:HB3	1:A:628:GLU:OE2	2.18	0.44
1:B:138:ASN:HD22	1:B:138:ASN:N	2.15	0.44
1:B:443:TYR:CD2	1:B:634:HIS:HE1	2.36	0.44
1:A:597:ARG:NH1	1:A:597:ARG:HG3	2.33	0.44
1:B:160:VAL:HG13	1:B:224:ILE:HD13	1.99	0.44
1:A:62:ILE:HG22	1:A:108:ARG:HB3	1.99	0.43
1:A:280:SER:HA	1:A:315:GLN:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:369:PRO:HD2	6:B:1012:HOH:O	2.18	0.43
1:A:405:LEU:N	1:A:405:LEU:CD2	2.81	0.43
2:F:248:LYS:HG3	2:F:253:PRO:HG3	2.00	0.43
1:A:296:SER:HB2	1:A:309:PHE:CE1	2.53	0.43
2:E:270:ASN:O	2:E:274:GLU:HG2	2.18	0.43
2:F:262:TYR:HA	2:F:266:LEU:O	2.18	0.43
2:F:105:ARG:HB3	2:F:240:GLN:O	2.18	0.43
1:A:61:LYS:HE2	6:A:1164:HOH:O	2.17	0.43
1:A:344:VAL:O	1:A:344:VAL:HG22	2.18	0.43
2:E:85:THR:OG1	2:E:87:TYR:HE1	2.01	0.43
1:A:57:THR:C	1:A:59:PHE:H	2.22	0.43
1:B:259:ARG:O	1:B:263:GLU:HG2	2.19	0.43
2:E:107:SER:HA	2:E:237:PHE:O	2.18	0.43
1:A:571:ASP:OD2	1:A:573:ASN:HB2	2.18	0.43
1:B:415:PHE:CD1	1:B:480:PHE:HB2	2.54	0.43
1:B:445:TYR:CD1	1:B:445:TYR:C	2.92	0.43
1:A:590:PHE:CZ	1:A:612:PRO:HG3	2.53	0.43
1:B:514:THR:HG22	1:B:515:ASP:OD1	2.19	0.43
1:B:62:ILE:HG23	1:B:104:TRP:HZ2	1.84	0.43
1:A:485:TRP:CZ3	1:A:525:HIS:CE1	3.07	0.43
1:A:125:ARG:HE	1:A:125:ARG:HA	1.84	0.43
1:A:125:ARG:HA	1:A:125:ARG:NE	2.34	0.43
1:A:601:LYS:HD3	6:A:867:HOH:O	2.18	0.43
1:B:325:VAL:HG22	1:B:327:PHE:CZ	2.54	0.43
1:B:551:ASN:O	1:B:554:MET:HG3	2.19	0.43
1:A:120:ASN:ND2	1:A:364:ASP:OD1	2.52	0.43
1:A:288:ASN:HD22	1:A:318:THR:HA	1.84	0.43
1:B:194:PRO:HG2	1:B:568:LYS:HG2	2.01	0.42
2:F:87:TYR:CD2	2:F:96:ILE:HD11	2.54	0.42
2:E:82:HIS:CD2	6:E:365:HOH:O	2.71	0.42
1:B:360:LYS:HG3	6:B:933:HOH:O	2.20	0.42
1:A:554:MET:HG3	1:A:555:LEU:H	1.85	0.42
1:B:472:ARG:O	1:B:476:LEU:HB2	2.19	0.42
1:B:255:ILE:CD1	1:B:290:LEU:HD22	2.49	0.42
2:E:80:PRO:HA	2:E:267:LYS:NZ	2.34	0.42
2:F:82:HIS:C	6:F:840:HOH:O	2.58	0.42
1:B:69:LEU:C	1:B:71:ASN:H	2.22	0.42
1:A:554:MET:O	1:A:558:VAL:HG23	2.20	0.42
1:B:555:LEU:HA	1:B:555:LEU:HD23	1.82	0.42
1:A:263:GLU:HG3	1:A:264:ASN:ND2	2.34	0.42
2:E:170:ASP:OD1	2:E:172:LYS:HG2	2.19	0.42
1:A:63:ARG:NH2	1:A:107:ILE:HD12	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:196:GLU:OE1	2:E:198:TYR:HE1	2.01	0.42
2:E:111:ASP:O	2:E:112:ARG:HD3	2.20	0.42
2:F:119:THR:HB	2:F:254:PHE:HE1	1.85	0.42
1:A:347:THR:O	1:A:351:VAL:HG23	2.20	0.42
1:B:199:ILE:HG12	1:B:254:LEU:HD22	2.01	0.42
1:A:630:VAL:N	1:A:631:PRO:CD	2.83	0.42
1:A:432:ASP:HA	1:A:457:LYS:HE2	2.01	0.42
1:A:350:LEU:C	1:A:350:LEU:HD23	2.40	0.41
2:F:170:ASP:OD2	2:F:172:LYS:HD3	2.20	0.41
1:B:401:TYR:O	1:B:501:SER:HB3	2.20	0.41
1:A:288:ASN:ND2	1:A:318:THR:HA	2.35	0.41
1:A:251:LEU:O	1:A:255:ILE:HG12	2.19	0.41
2:F:97:THR:HB	6:F:803:HOH:O	2.19	0.41
1:B:99:GLU:HG3	1:B:100:PRO:HD2	2.00	0.41
1:B:66:LYS:HG2	1:B:67:LYS:N	2.36	0.41
1:B:506:TYR:HB3	1:B:595:TRP:CZ2	2.55	0.41
1:B:203:SER:O	1:B:204:TYR:CB	2.68	0.41
1:B:191:GLY:HA2	1:B:192:PRO:HD3	1.96	0.41
2:E:148:ILE:HG21	2:E:189:VAL:HG22	2.02	0.41
2:E:115:ILE:CG2	2:E:176:VAL:HG12	2.45	0.41
2:E:288:VAL:O	2:E:288:VAL:HG12	2.19	0.41
2:F:231:GLY:HA3	6:F:735:HOH:O	2.19	0.41
1:B:230:TYR:CD1	1:B:254:LEU:HD21	2.56	0.41
1:B:160:VAL:HA	1:B:161:PRO:HD3	1.94	0.41
2:F:111:ASP:HA	2:F:264:ASN:OD1	2.20	0.41
1:A:294:HIS:CE1	2:E:236:ILE:HD11	2.55	0.41
1:B:52:ASP:HA	1:B:53:PRO:HD3	1.92	0.41
1:B:352:GLU:HA	6:B:875:HOH:O	2.21	0.41
1:B:554:MET:HG3	1:B:555:LEU:N	2.35	0.41
1:B:554:MET:CE	6:B:771:HOH:O	2.68	0.41
2:F:126:LEU:HD21	2:F:143:ILE:HG13	2.01	0.41
1:A:534:GLY:HA2	1:A:556:SER:OG	2.20	0.41
1:B:280:SER:HA	1:B:315:GLN:O	2.21	0.41
2:F:192:TRP:HD1	2:F:192:TRP:N	2.16	0.41
1:A:421:ASP:C	1:A:423:ASP:N	2.64	0.41
1:B:125:ARG:NE	1:B:125:ARG:HA	2.36	0.41
2:E:150:VAL:CG1	2:E:151:LYS:N	2.84	0.41
2:F:169:ASN:C	6:F:793:HOH:O	2.59	0.40
2:F:169:ASN:ND2	6:F:807:HOH:O	2.45	0.40
1:A:313:ILE:HA	1:A:404:MET:O	2.21	0.40
1:A:575:PRO:O	1:A:576:VAL:C	2.59	0.40
1:A:590:PHE:HA	6:A:1000:HOH:O	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:248:LYS:HA	2:E:253:PRO:HG3	2.02	0.40
1:A:628:GLU:OE2	1:B:463:TRP:CZ2	2.75	0.40
1:A:435:VAL:HG11	1:A:457:LYS:HG3	2.04	0.40
1:B:150:SER:O	1:B:153:CYS:HB3	2.20	0.40
1:B:419:ILE:HG22	1:B:419:ILE:O	2.21	0.40
1:B:605:TYR:CE1	1:B:615:LYS:HB2	2.57	0.40
1:B:246:LYS:NZ	6:B:789:HOH:O	2.54	0.40
1:B:529:VAL:N	1:B:530:PRO:HD2	2.37	0.40
3:B:1:NAG:H3	3:B:1:NAG:H83	2.04	0.40
1:B:57:THR:C	1:B:59:PHE:H	2.24	0.40

All (5) 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	Distance(Å)	Clash(Å)
1:B:343:GLN:OE1	6:F:749:HOH:O[4_455]	1.64	0.56
6:A:912:HOH:O	6:F:764:HOH:O[4_445]	1.77	0.43
6:B:1124:HOH:O	6:E:499:HOH:O[4_545]	1.84	0.36
2:F:172:LYS:NZ	6:E:335:HOH:O[2_555]	2.10	0.10
2:F:172:LYS:CE	6:E:335:HOH:O[2_555]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	528/577 (92%)	480 (91%)	44 (8%)	4 (1%)	27	39
1	B	528/577 (92%)	484 (92%)	40 (8%)	4 (1%)	27	39
2	E	183/197 (93%)	166 (91%)	12 (7%)	5 (3%)	8	7
2	F	183/197 (93%)	162 (88%)	16 (9%)	5 (3%)	8	7
All	All	1422/1548 (92%)	1292 (91%)	112 (8%)	18 (1%)	18	24

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	SER
1	A	422	SER
1	A	575	PRO
1	B	345	SER
1	B	422	SER
1	B	575	PRO
2	E	156	THR
2	E	239	SER
2	F	156	THR
2	F	239	SER
1	B	595	TRP
2	E	132	SER
1	A	58	ASN
2	F	190	ASP
2	F	132	SER
2	E	190	ASP
2	E	288	VAL
2	F	288	VAL

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	458/496 (92%)	418 (91%)	40 (9%)	15	22
1	B	458/496 (92%)	415 (91%)	43 (9%)	13	18
2	E	150/158 (95%)	141 (94%)	9 (6%)	27	41
2	F	150/158 (95%)	140 (93%)	10 (7%)	23	35
All	All	1216/1308 (93%)	1114 (92%)	102 (8%)	16	23

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	SER
1	A	123	ASP
1	A	125	ARG
1	A	129	VAL
1	A	138	ASN

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Mol	Chain	Res	Type
1	A	139	LEU
1	A	156	LEU
1	A	158	ILE
1	A	206	GLU
1	A	217	LEU
1	A	259	ARG
1	A	262	SER
1	A	278	PHE
1	A	323	TRP
1	A	325	VAL
1	A	346	ASP
1	A	374	ILE
1	A	379	VAL
1	A	405	LEU
1	A	413	LEU
1	A	418	ASN
1	A	420	VAL
1	A	476	LEU
1	A	485	TRP
1	A	514	THR
1	A	528	GLU
1	A	533	LEU
1	A	554	MET
1	A	555	LEU
1	A	563	TRP
1	A	574	GLN
1	A	575	PRO
1	A	597	ARG
1	A	606	LEU
1	A	610	LEU
1	A	611	LYS
1	A	614	VAL
1	A	621	ASN
1	A	625	LEU
1	A	629	LEU
1	B	69	LEU
1	B	81	LEU
1	B	105	SER
1	B	106	ASP
1	B	107	ILE
1	B	122	ILE
1	B	125	ARG

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Mol	Chain	Res	Type
1	B	136	THR
1	B	138	ASN
1	B	139	LEU
1	B	156	LEU
1	B	158	ILE
1	B	206	GLU
1	B	208	THR
1	B	217	LEU
1	B	323	TRP
1	B	344	VAL
1	B	374	ILE
1	B	379	VAL
1	B	405	LEU
1	B	413	LEU
1	B	418	ASN
1	B	432	ASP
1	B	433	PHE
1	B	445	TYR
1	B	473	ARG
1	B	476	LEU
1	B	528	GLU
1	B	533	LEU
1	B	537	MET
1	B	554	MET
1	B	555	LEU
1	B	563	TRP
1	B	574	GLN
1	B	606	LEU
1	B	610	LEU
1	B	611	LYS
1	B	614	VAL
1	B	615	LYS
1	B	625	LEU
1	B	628	GLU
1	B	629	LEU
1	B	633	LEU
2	E	97	THR
2	E	109	ARG
2	E	126	LEU
2	E	172	LYS
2	E	186	THR
2	E	232	ARG

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Mol	Chain	Res	Type
2	E	237	PHE
2	E	281	ILE
2	E	287	LEU
2	F	85	THR
2	F	88	ILE
2	F	109	ARG
2	F	115	ILE
2	F	126	LEU
2	F	167	ILE
2	F	186	THR
2	F	232	ARG
2	F	237	PHE
2	F	287	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	147	GLN
1	A	288	ASN
1	A	418	ASN
1	A	607	HIS
1	A	634	HIS
1	B	138	ASN
1	B	222	ASN
1	B	288	ASN
1	B	418	ASN
1	B	437	ASN
1	B	634	HIS
2	E	153	ASN
2	F	284	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 carbohydrates 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	1	1,3	12,14,15	0.85	0	15,19,21	1.22	2 (13%)
3	NAG	A	2	3	12,14,15	0.49	0	15,19,21	0.79	0
3	NAG	B	1	1,3	12,14,15	0.77	0	15,19,21	1.10	2 (13%)
3	NAG	B	2	3	12,14,15	0.59	0	15,19,21	0.88	0
3	NAG	B	636	1,3	12,14,15	0.65	0	15,19,21	1.04	2 (13%)
3	NAG	B	637	3	12,14,15	0.58	0	15,19,21	0.73	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	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	1/1/1/1
3	NAG	B	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	1/1/1/1
3	NAG	B	636	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	637	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	NAG	C3-C4-C5	2.62	114.88	110.20
3	B	1	NAG	C3-C4-C5	2.55	114.76	110.20
3	A	1	NAG	C4-C3-C2	2.51	117.46	111.32
3	B	636	NAG	O5-C5-C4	-2.33	107.69	110.65
3	B	636	NAG	C3-C2-N2	-2.15	108.48	111.76
3	B	1	NAG	C2-N2-C7	-2.09	119.59	123.09

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	NAG	C1-C2-C3-C4-C5-O5
3	B	2	NAG	C1-C2-C3-C4-C5-O5

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	636	1	12,14,15	0.50	0	15,19,21	1.15	3 (20%)

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
4	NAG	A	636	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	636	NAG	C4-C3-C2	-2.49	105.22	111.32
4	A	636	NAG	C2-N2-C7	-2.17	119.45	123.09
4	A	636	NAG	C3-C4-C5	-2.10	106.45	110.20

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	636	NAG	O7-C7-N2-C2

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	536/577 (92%)	-0.12	16 (2%) 48 45	30, 54, 95, 146	0
1	B	536/577 (92%)	-0.18	13 (2%) 56 54	27, 50, 97, 146	0
2	E	187/197 (94%)	-0.07	6 (3%) 45 43	32, 60, 101, 137	3 (1%)
2	F	187/197 (94%)	0.58	22 (11%) 5 5	45, 72, 105, 139	3 (1%)
All	All	1446/1548 (93%)	-0.04	57 (3%) 34 35	27, 57, 101, 146	6 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	291	VAL	8.7
2	F	288	VAL	6.2
2	F	92	GLY	6.1
2	F	287	LEU	5.3
1	A	445	TYR	5.1
2	F	94	GLY	4.7
2	F	275	ASN	4.5
2	F	90	SER	4.4
1	A	579	ASP	4.2
1	A	591	GLU	4.1
1	A	107	ILE	3.9
2	F	127	VAL	3.8
1	B	164	ASP	3.8
2	E	291	VAL	3.7
1	A	574	GLN	3.7
1	A	635	ASN	3.6
1	B	592	GLU	3.5
2	F	289	GLY	3.5
1	B	591	GLU	3.5
1	A	192	PRO	3.4
2	F	290	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	251	GLY	3.3
1	B	433	PHE	3.3
1	B	163	GLU	3.2
2	E	85	THR	3.2
2	F	285	VAL	3.1
1	B	445	TYR	3.1
2	F	87	TYR	3.1
1	A	164	ASP	3.0
2	E	92	GLY	3.0
1	A	592	GLU	2.9
1	A	125	ARG	2.8
1	A	515	ASP	2.8
1	B	635	ASN	2.8
2	F	286	ARG	2.7
1	B	422	SER	2.6
2	E	200	ALA	2.6
2	F	253	PRO	2.6
2	F	120	VAL	2.5
1	A	190	GLY	2.5
2	F	93	GLY	2.4
2	F	99	LYS	2.4
2	F	277	ALA	2.4
2	E	286	ARG	2.4
1	B	190	GLY	2.4
1	B	123	ASP	2.3
1	B	125	ARG	2.2
1	A	613	ARG	2.2
1	A	634	HIS	2.2
1	B	122	ILE	2.2
1	A	162	THR	2.2
2	F	274	GLU	2.2
2	F	91	LYS	2.2
2	E	287	LEU	2.1
1	A	593	VAL	2.1
1	B	343	GLN	2.0
2	F	283	GLY	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	1	14/15	0.30	0.42	96,98,100,101	0
3	NAG	B	1	14/15	0.16	-2.33	93,97,98,99	0
3	NAG	B	637	14/15	0.61	-	111,113,113,113	0
3	NAG	B	636	14/15	0.53	-	103,106,108,109	0
3	NAG	B	2	14/15	0.37	-	99,100,102,103	0
3	NAG	A	2	14/15	0.48	-	100,102,106,108	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	CA	E	1	1/1	0.37	7.99	30,30,30,30	1
5	CA	F	2	1/1	0.17	1.94	33,33,33,33	1
4	NAG	A	636	14/15	0.50	-	98,102,105,107	0

6.5 Other polymers

There are no such residues in this entry.