



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:03 am 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 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

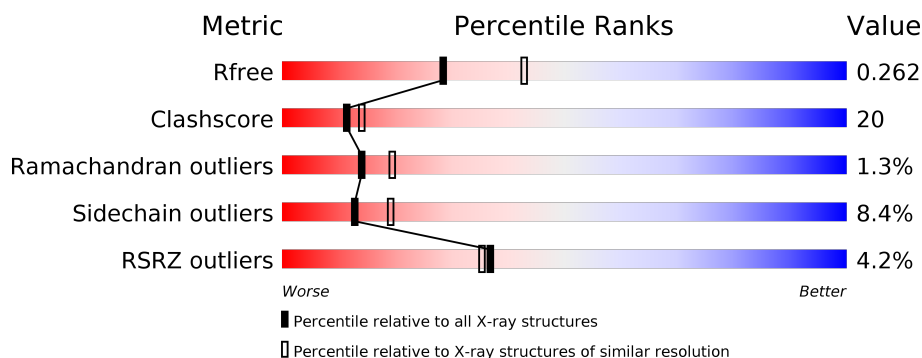
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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. 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	577	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>28%</div> <div>7%</div> </div> </div>
1	B	577	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>7%</div> </div> </div>
2	E	197	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>37%</div> <div>5%</div> </div> </div>
2	F	197	<div> <div>11%</div> <div> <div></div> <div>50%</div> <div>42%</div> <div>5%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	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 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 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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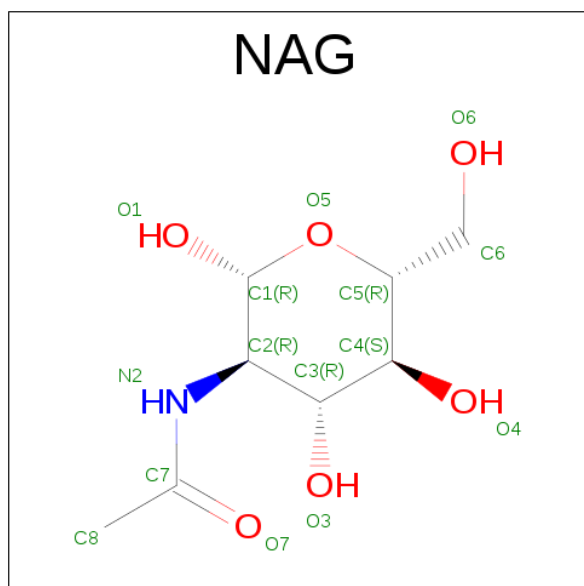
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Chain	Residue	Modelled	Actual	Comment	Reference
F	79	ASP	-	EXPRESSION TAG	UNP A4FVB9
F	80	PRO	-	EXPRESSION TAG	UNP A4FVB9
F	293	HIS	-	EXPRESSION TAG	UNP A4FVB9
F	294	HIS	-	INSERTION	UNP A4FVB9
F	295	HIS	-	EXPRESSION TAG	UNP A4FVB9
F	296	HIS	-	EXPRESSION 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		

- 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 1	Ca 1	0	0
5	E	1	Total 1	Ca 1	0	0

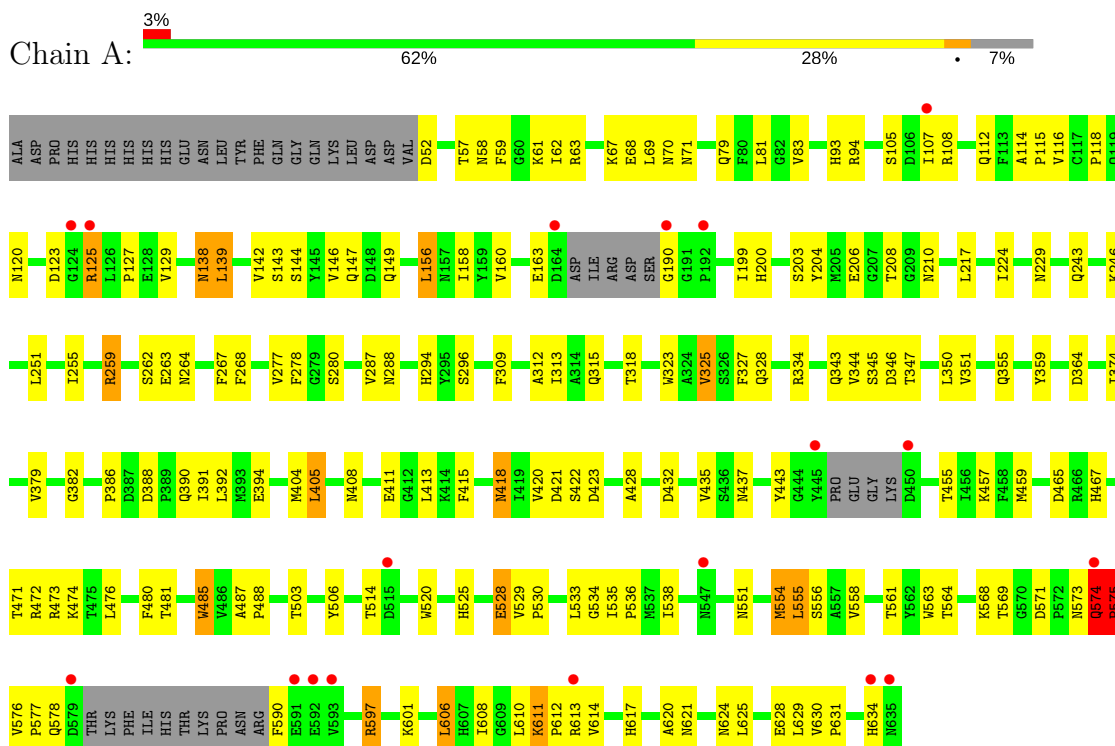
- Molecule 6 is water.

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

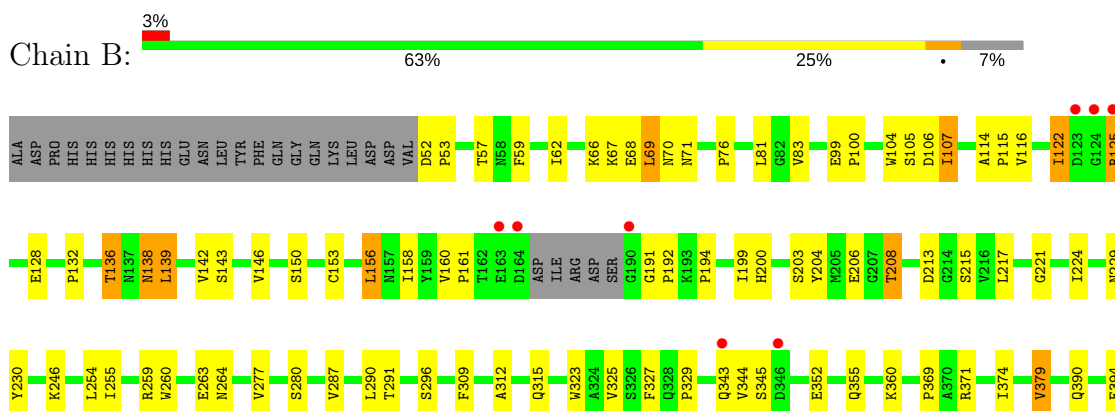
3 Residue-property plots

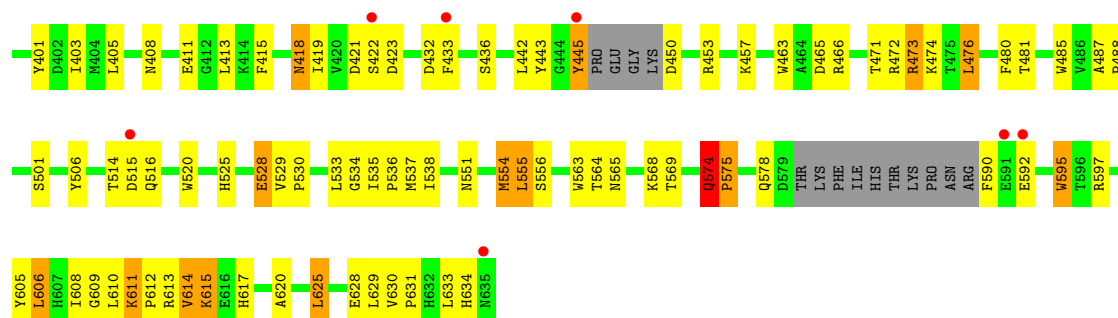
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Nlgn1 protein

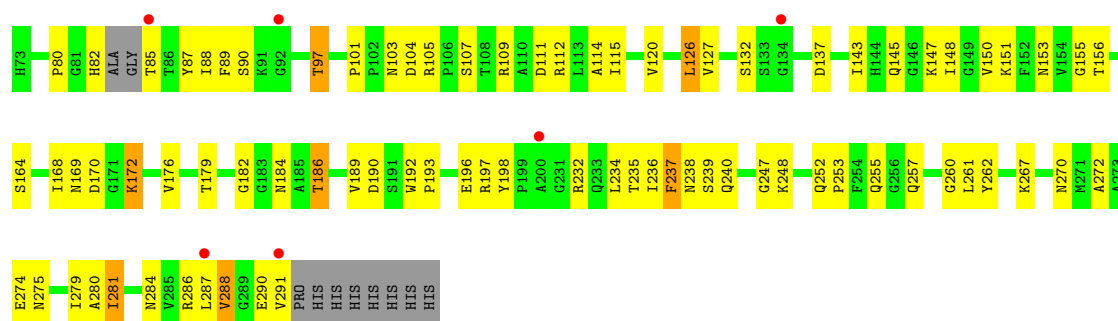


• Molecule 1: Nlgn1 protein

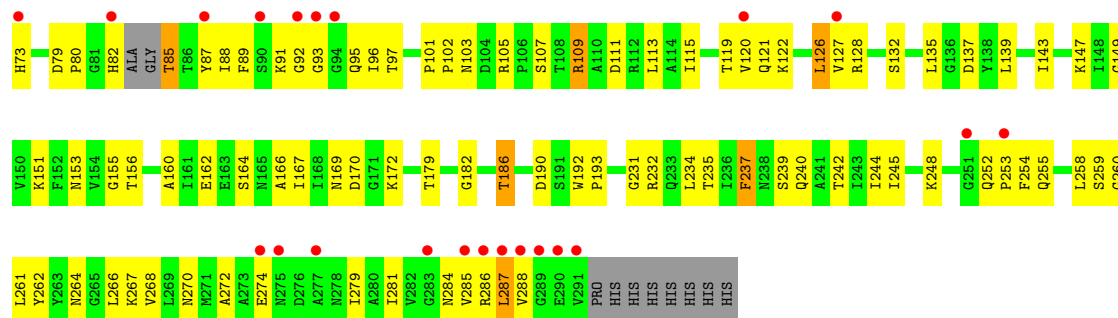




• Molecule 2: NRXN1 protein



• Molecule 2: NRXN1 protein



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 0.242 , 0.262	Depositor DCC
R_{free} test set	3783 reflections (5.08%)	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 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k	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.

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: 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 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	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

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 20.

All (439) 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: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	Interatomic distance (Å)	Clash overlap (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
1:A:112:GLN:NE2	6:A:876:HOH:O	2.06	0.85
2:F:192:TRP:HB3	2:F:193:PRO:HD2	1.58	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
1:B:450:ASP:HB2	6:B:707:HOH:O	1.76	0.84
2:F:287:LEU:HD12	6:F:795:HOH:O	1.78	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
1:B:421:ASP:O	1:B:423:ASP:N	2.16	0.78
2:F:166:ALA:HB3	2:F:192:TRP:CZ3	2.18	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:H	1:B:418:ASN:HD22	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:E:184:ASN:HB3	6:E:373:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:275:ASN:HB3	6:E:343:HOH:O	1.88	0.72
2:F:89:PHE:O	2:F:255:GLN:HA	1.90	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:A:437:ASN:HB3	6:A:640:HOH:O	1.92	0.69
1:B:574:GLN:HB3	1:B:575:PRO:CD	2.21	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
1:B:481:THR:HA	1:B:485:TRP:CD1	2.28	0.68
2:F:147:LYS:CD	2:F:164:SER:HA	2.14	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
1:A:93:HIS:HB3	6:A:669:HOH:O	1.94	0.67
2:E:88:ILE:HD13	2:E:257:GLN:HG2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:182:GLY:HA2	2:E:235:THR:HA	1.81	0.61
2:F:155:GLY:HA3	2:F:234:LEU:HD12	1.83	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
1:B:203:SER:O	1:B:204:TYR:HB2	2.03	0.59
2:E:120:VAL:HG22	6:E:303:HOH:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASN:HD22	1:A:138:ASN:N	2.01	0.58
2:E:115:ILE:CG2	2:E:176:VAL:CG1	2.82	0.58
1:A:467:HIS:HD2	6:A:699:HOH:O	1.85	0.58
1:A:57:THR:HA	1:A:267:PHE:CD1	2.39	0.58
2:E:80:PRO:O	2:E:260:GLY:HA3	2.03	0.58
1:A:455:THR:O	1:A:459:MET:HG2	2.04	0.58
2:F:281:ILE:HD12	2:F:281:ILE:H	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
1:A:139:LEU:CD1	1:A:139:LEU:H	2.17	0.57
2:F:151:LYS:HB2	6:F:802:HOH:O	2.03	0.57
1:A:415:PHE:CD1	1:A:480:PHE:HB2	2.39	0.56
1:B:609:GLY:O	1:B:612:PRO:HD3	2.06	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
1:A:208:THR:HG22	1:A:210:ASN:H	1.71	0.56
2:E:127:VAL:HG21	2:E:261:LEU:HD11	1.87	0.56
1:B:418:ASN:H	1:B:418:ASN:ND2	2.02	0.56
2:F:248:LYS:HA	2:F:253:PRO:HG3	1.88	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:A:200:HIS:HE1	6:A:639:HOH:O	1.90	0.55
1:B:473:ARG:NH2	1:B:520:TRP:HB2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:611:LYS:HE3	6:B:1007:HOH:O	2.08	0.54
2:F:151:LYS:CB	6:F:802:HOH:O	2.54	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: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: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: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:534:GLY:HA2	1:B:556:SER:OG	2.09	0.52
1:B:612:PRO:HB3	6:B:714:HOH:O	2.09	0.52
1:A:551:ASN:O	1:A:554:MET:HG3	2.10	0.52
2:F:160:ALA:HB1	6:F:822:HOH:O	2.09	0.52
1:A:408:ASN:HD21	1:A:528:GLU:HG3	1.73	0.52
1:A:411:GLU:HB2	1:A:481:THR:HG23	1.91	0.52
1:A:163:GLU:HG3	6:A:1044:HOH:O	2.09	0.52
1:B:630:VAL:N	1:B:631:PRO:CD	2.72	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:101:PRO:HG2	2:E:104:ASP:HB3	1.93	0.50
2:E:179:THR:HG22	6:E:312:HOH:O	2.11	0.50
3:A:1:NAG:H83	3:A:2:NAG:C6	2.41	0.50
1:B:606:LEU:HD12	1:B:608:ILE:HG12	1.93	0.50
2:E:192:TRP:CD1	2:E:192:TRP:N	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:390:GLN:O	1:A:394:GLU:HB2	2.10	0.50
1:B:568:LYS:HE2	6:B:669:HOH:O	2.09	0.50
2:E:286:ARG:NH2	6:E:386:HOH:O	2.44	0.50
2:F:137:ASP:HA	2:F:153:ASN:O	2.11	0.50
1:B:371:ARG:HG3	6:B:1136:HOH:O	2.11	0.50
1:B:466:ARG:NH1	6:B:693:HOH:O	2.45	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
2:F:127:VAL:CG2	2:F:261:LEU:HD11	2.37	0.50
1:B:442:LEU:HD12	6:B:716:HOH:O	2.12	0.49
1:B:260:TRP:O	1:B:264:ASN:HB2	2.13	0.49
1:B:568:LYS:HE3	6:B:669:HOH:O	2.11	0.49
2:E:97:THR:CG2	2:E:97:THR:O	2.61	0.49
1:A:473:ARG:HG3	1:A:474:LYS:N	2.28	0.49
2:F:286:ARG:CG	6:F:795:HOH:O	2.52	0.49
1:A:138:ASN:HD22	1:A:138:ASN:H	1.60	0.49
1:B:418:ASN:HB3	6:B:807:HOH:O	2.12	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:E:89:PHE:O	2:E:255:GLN:HA	2.13	0.49
2:F:87:TYR:HD2	2:F:285:VAL:CG1	2.25	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:E:168:ILE:CG2	2:E:189:VAL:HG11	2.43	0.49
2:F:101:PRO:HB2	2:F:103:ASN:OD1	2.11	0.49
2:F:147:LYS:HG2	2:F:166:ALA:O	2.13	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:E:272:ALA:CB	2:E:279:ILE:HG21	2.42	0.48
2:F:95:GLN:HG3	6:F:719:HOH:O	2.13	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
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
2:E:115:ILE:HG22	2:E:176:VAL:HG13	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:160:VAL:HG13	1:A:224:ILE:HD13	1.96	0.47
2:E:101:PRO:HB2	2:E:103:ASN:OD1	2.14	0.47
1:B:221:GLY:O	1:B:568:LYS:NZ	2.47	0.47
1:A:114:ALA:HB1	1:A:115:PRO:HD2	1.95	0.47
1:A:57:THR:HA	1:A:267:PHE:HD1	1.77	0.47
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
2:E:252:GLN:N	2:E:253:PRO:HD3	2.29	0.47
1:A:118:PRO:HB3	1:A:359:TYR:CE1	2.49	0.47
1:A:343:GLN:HB2	6:A:932:HOH:O	2.15	0.47
1:A:443:TYR:HD2	1:A:634:HIS:CE1	2.32	0.47
1:B:418:ASN:N	1:B:418:ASN:ND2	2.61	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
3:B:2:NAG:H81	6:B:1235:HOH:O	2.15	0.47
1:B:554:MET:HE1	6:B:771:HOH:O	2.13	0.47
2:E:126:LEU:HD23	2:E:126:LEU:N	2.29	0.47
1:B:487:ALA:N	1:B:488:PRO:CD	2.78	0.47
1:B:83:VAL:HB	1:B:156:LEU:CD2	2.45	0.47
1:B:99:GLU:HG3	1:B:100:PRO:CD	2.44	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
2:F:121:GLN:OE1	2:F:255:GLN:N	2.40	0.47
1:A:144:SER:HA	1:A:147:GLN:HG2	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
2:F:113:LEU:HD11	2:F:261:LEU:HD21	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:A:529:VAL:N	1:A:530:PRO:HD2	2.29	0.46
1:B:421:ASP:C	1:B:423:ASP:N	2.66	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:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HD11	1:A:268:PHE:HZ	1.80	0.46
1:B:213:ASP:OD1	1:B:215:SER:HB2	2.16	0.46
1:B:605:TYR:CZ	1:B:615:LYS:HB2	2.51	0.46
1:B:114:ALA:HB1	1:B:115:PRO:HD2	1.98	0.46
2:F:107:SER:HA	2:F:237:PHE:O	2.16	0.46
1:B:287:VAL:O	1:B:291:THR:HG23	2.16	0.46
2:E:115:ILE:CG2	2:E:176:VAL:HG13	2.46	0.46
1:B:611:LYS:HD2	1:B:611:LYS:H	1.81	0.46
1:A:325:VAL:HG22	1:A:327:PHE:CE1	2.51	0.46
1:A:606:LEU:HD13	1:A:608:ILE:HG12	1.97	0.46
3:B:1:NAG:O4	3:B:2:NAG:H62	2.16	0.46
1:A:79:GLN:HB2	1:A:81:LEU:HD11	1.99	0.45
2:E:247:GLY:N	6:E:438:HOH:O	2.49	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:A:203:SER:O	1:A:204:TYR:HB2	2.16	0.45
1:B:390:GLN:O	1:B:394:GLU:HB2	2.17	0.45
1:B:107:ILE:HG12	6:B:926:HOH:O	2.16	0.45
2:F:79:ASP:OD1	2:F:80:PRO:HD2	2.17	0.45
1:A:143:SER:HB3	1:A:147:GLN:NE2	2.32	0.45
1:A:611:LYS:HD2	1:A:611:LYS:N	2.26	0.45
1:A:69:LEU:C	1:A:71:ASN:H	2.20	0.45
2:F:85:THR:N	6:F:746:HOH:O	2.50	0.45
1:B:634:HIS:CD2	6:B:741:HOH:O	2.70	0.45
2:E:105:ARG:HB3	2:E:240:GLN:O	2.17	0.45
2:F:102:PRO:HA	2:F:105:ARG:HE	1.82	0.45
2:F:192:TRP:HB3	2:F:193:PRO:CD	2.38	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: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
2:F:102:PRO:HA	2:F:105:ARG:NE	2.32	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:A:503:THR:H	1:A:597:ARG:NH1	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:139:LEU:CD1	1:B:139:LEU:H	2.30	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:280:SER:HA	1:A:315:GLN:O	2.18	0.43
1:A:405:LEU:N	1:A:405:LEU:CD2	2.81	0.43
1:A:62:ILE:HG22	1:A:108:ARG:HB3	1.99	0.43
1:B:369:PRO:HD2	6:B:1012:HOH:O	2.18	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:248:LYS:HG3	2:F:253:PRO:HG3	2.00	0.43
2:F:262:TYR:HA	2:F:266:LEU:O	2.18	0.43
1:A:61:LYS:HE2	6:A:1164:HOH:O	2.17	0.43
2:F:105:ARG:HB3	2:F:240:GLN:O	2.18	0.43
1:A:344:VAL:HG22	1:A:344:VAL:O	2.18	0.43
1:A:571:ASP:OD2	1:A:573:ASN:HB2	2.18	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
2:E:85:THR:OG1	2:E:87:TYR:HE1	2.01	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:125:ARG:NE	1:A:125:ARG:HA	2.34	0.43
1:A:125:ARG:HE	1:A:125:ARG:HA	1.84	0.43
1:A:485:TRP:CZ3	1:A:525:HIS:CE1	3.07	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:A:288:ASN:HD22	1:A:318:THR:HA	1.84	0.43
1:A:120:ASN:ND2	1:A:364:ASP:OD1	2.52	0.43
1:B:551:ASN:O	1:B:554:MET:HG3	2.19	0.43
1:B:194:PRO:HG2	1:B:568:LYS:HG2	2.01	0.42
2:E:82:HIS:CD2	6:E:365:HOH:O	2.71	0.42
2:F:87:TYR:CD2	2:F:96:ILE:HD11	2.54	0.42
1:A:554:MET:HG3	1:A:555:LEU:H	1.85	0.42
1:B:360:LYS:HG3	6:B:933:HOH:O	2.20	0.42
1:B:472:ARG:O	1:B:476:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ILE:CD1	1:B:290:LEU:HD22	2.49	0.42
1:B:69:LEU:C	1:B:71:ASN:H	2.22	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:A:263:GLU:HG3	1:A:264:ASN:ND2	2.34	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
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
2:E:196:GLU:OE1	2:E:198:TYR:HE1	2.01	0.42
1:A:347:THR:O	1:A:351:VAL:HG23	2.20	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:432:ASP:HA	1:A:457:LYS:HE2	2.01	0.42
1:A:630:VAL:N	1:A:631:PRO:CD	2.83	0.42
1:B:199:ILE:HG12	1:B:254:LEU:HD22	2.01	0.42
1:A:350:LEU:C	1:A:350:LEU:HD23	2.40	0.41
1:A:251:LEU:O	1:A:255:ILE:HG12	2.19	0.41
1:A:288:ASN:ND2	1:A:318:THR:HA	2.35	0.41
1:B:401:TYR:O	1:B:501:SER:HB3	2.20	0.41
2:F:170:ASP:OD2	2:F:172:LYS:HD3	2.20	0.41
2:F:97:THR:HB	6:F:803:HOH:O	2.19	0.41
1:B:506:TYR:HB3	1:B:595:TRP:CZ2	2.55	0.41
1:B:66:LYS:HG2	1:B:67:LYS:N	2.36	0.41
1:B:99:GLU:HG3	1:B:100:PRO:HD2	2.00	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:160:VAL:HA	1:B:161:PRO:HD3	1.94	0.41
1:B:230:TYR:CD1	1:B:254:LEU:HD21	2.56	0.41
1:A:294:HIS:CE1	2:E:236:ILE:HD11	2.55	0.41
2:F:111:ASP:HA	2:F:264:ASN:OD1	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:MET:CE	6:B:771:HOH:O	2.68	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:192:TRP:HD1	2:F:192:TRP:N	2.16	0.41
1:A:313:ILE:HA	1:A:404:MET:O	2.21	0.40
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: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
2:E:248:LYS:HA	2:E:253:PRO:HG3	2.02	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:O	1:B:419:ILE:HG22	2.21	0.40
1:A:628:GLU:OE2	1:B:463:TRP:CZ2	2.75	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
1:B:605:TYR:CE1	1:B:615:LYS:HB2	2.57	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	Interatomic distance (Å)	Clash overlap (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%)	22	33
1	B	528/577 (92%)	484 (92%)	40 (8%)	4 (1%)	22	33
2	E	183/197 (93%)	166 (91%)	12 (7%)	5 (3%)	6	6
2	F	183/197 (93%)	162 (88%)	16 (9%)	5 (3%)	6	6
All	All	1422/1548 (92%)	1292 (91%)	112 (8%)	18 (1%)	14	19

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%)	12	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	458/496 (92%)	415 (91%)	43 (9%)	10	15
2	E	150/158 (95%)	141 (94%)	9 (6%)	22	35
2	F	150/158 (95%)	140 (93%)	10 (7%)	19	30
All	All	1216/1308 (93%)	1114 (92%)	102 (8%)	13	19

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	B	634	HIS
2	E	153	ASN
2	F	284	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	14,14,15	0.77	0	15,19,21	1.59	2 (13%)
3	NAG	A	2	3	14,14,15	0.65	0	15,19,21	0.91	1 (6%)
3	NAG	B	1	1,3	14,14,15	0.68	0	15,19,21	1.32	3 (20%)
3	NAG	B	2	3	14,14,15	0.72	0	15,19,21	0.99	0
3	NAG	B	636	1,3	14,14,15	0.90	1 (7%)	15,19,21	0.95	0
3	NAG	B	637	3	14,14,15	0.81	0	15,19,21	0.82	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	636	NAG	C1-C2	2.69	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	C2-N2-C7	-2.30	119.59	122.94
3	A	2	NAG	C2-N2-C7	-2.08	119.91	122.94
3	B	1	NAG	C3-C4-C5	2.58	114.76	110.22
3	A	1	NAG	C3-C4-C5	2.65	114.88	110.22
3	B	1	NAG	C4-C3-C2	3.44	116.06	111.02
3	A	1	NAG	C4-C3-C2	4.40	117.46	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NAG	4	0
3	A	2	NAG	4	0
3	B	1	NAG	2	0
3	B	2	NAG	2	0
3	B	636	NAG	2	0
3	B	637	NAG	2	0

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	14,14,15	0.72	0	15,19,21	1.46	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	-3.96	105.22	111.02
4	A	636	NAG	C2-N2-C7	-2.40	119.45	122.94
4	A	636	NAG	C3-C4-C5	-2.14	106.45	110.22

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.

No monomer is involved in short contacts.

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%)	-0.19	18 (3%) 46 44	30, 54, 95, 146	0
1	B	536/577 (92%)	-0.23	15 (2%) 53 51	27, 50, 97, 146	0
2	E	187/197 (94%)	-0.16	6 (3%) 48 46	32, 60, 101, 137	3 (1%)
2	F	187/197 (94%)	0.59	22 (11%) 5 4	45, 72, 105, 139	3 (1%)
All	All	1446/1548 (93%)	-0.10	61 (4%) 37 35	27, 57, 101, 146	6 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	291	VAL	7.4
2	F	287	LEU	6.0
2	F	288	VAL	5.9
2	F	92	GLY	5.8
1	A	579	ASP	5.0
1	A	445	TYR	4.9
2	F	275	ASN	4.4
1	A	591	GLU	4.2
2	F	290	GLU	4.2
2	F	94	GLY	4.1
1	A	635	ASN	4.1
1	B	591	GLU	4.0
1	B	592	GLU	3.9
2	F	289	GLY	3.9
1	A	192	PRO	3.9
2	F	90	SER	3.9
1	B	124	GLY	3.8
1	A	107	ILE	3.7
1	B	445	TYR	3.7
1	B	422	SER	3.4
2	F	285	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	127	VAL	3.3
2	E	92	GLY	3.2
1	B	164	ASP	3.2
1	B	163	GLU	3.1
1	A	515	ASP	3.1
2	E	85	THR	3.1
1	B	125	ARG	3.0
1	A	592	GLU	3.0
2	F	251	GLY	3.0
1	A	634	HIS	2.9
2	E	291	VAL	2.9
2	F	87	TYR	2.9
2	F	120	VAL	2.8
1	A	125	ARG	2.8
2	F	277	ALA	2.8
1	B	123	ASP	2.7
1	A	574	GLN	2.7
1	A	613	ARG	2.6
1	A	190	GLY	2.6
2	F	82	HIS	2.6
1	B	190	GLY	2.6
2	E	287	LEU	2.5
2	F	274	GLU	2.4
1	B	515	ASP	2.4
1	B	635	ASN	2.3
2	F	286	ARG	2.3
2	F	253	PRO	2.3
1	A	593	VAL	2.3
2	F	73	HIS	2.2
1	B	346	ASP	2.2
2	F	283	GLY	2.2
1	B	343	GLN	2.2
2	F	93	GLY	2.2
2	E	134	GLY	2.1
1	A	547	ASN	2.1
1	B	433	PHE	2.1
1	A	124	GLY	2.1
1	A	164	ASP	2.1
1	A	450	ASP	2.0
2	E	200	ALA	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](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	B	2	14/15	0.61	0.35	-	99,100,102,103	0
3	NAG	A	2	14/15	0.73	0.46	-	100,102,106,108	0
3	NAG	B	637	14/15	0.48	0.66	-	111,113,113,113	0
3	NAG	B	636	14/15	0.51	0.60	-	103,106,108,109	0
3	NAG	A	1	14/15	0.78	0.29	-	96,98,100,101	0
3	NAG	B	1	14/15	0.84	0.17	-	93,97,98,99	0

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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	CA	E	1	1/1	0.75	0.36	7.09	30,30,30,30	1
5	CA	F	2	1/1	0.84	0.20	1.85	33,33,33,33	1
4	NAG	A	636	14/15	0.63	0.47	-	98,102,105,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.