



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2016 – 08:52 PM EDT

PDB ID : 5CFB
Title : Crystal Structure of Human Glycine Receptor alpha-3 Bound to Strychnine
Authors : Shaffer, P.L.; Huang, X.; Chen, H.
Deposited on : 2015-07-08
Resolution : 3.04 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20027790

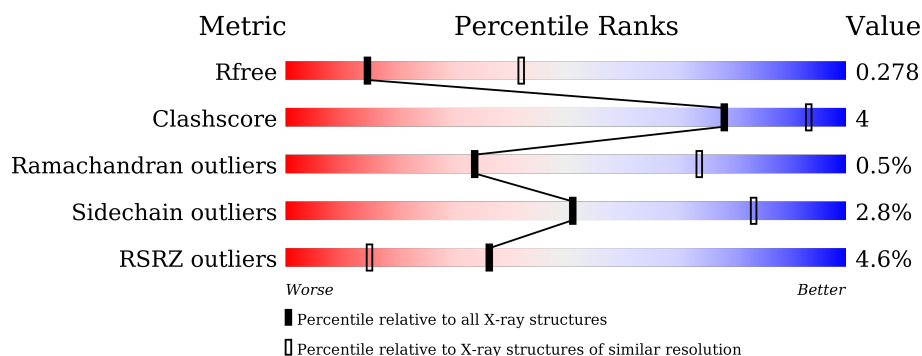
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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}	91344	1995 (3.08-3.00)
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)
RSRZ outliers	91569	2013 (3.08-3.00)

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	362	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	362	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>
1	C	362	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>
1	D	362	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>9%</div> </div> </div>
1	E	362	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13540 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 Glycine receptor subunit alpha-3, Glycine receptor subunit alpha-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2685	1748	428	490	19			
1	B	339	Total	C	N	O	S	0	0	0
			2676	1743	425	490	18			
1	C	336	Total	C	N	O	S	0	0	0
			2644	1719	421	486	18			
1	D	331	Total	C	N	O	S	0	0	0
			2626	1711	417	480	18			
1	E	339	Total	C	N	O	S	0	0	0
			2686	1752	426	490	18			

There are 55 discrepancies between the modelled and reference sequences:

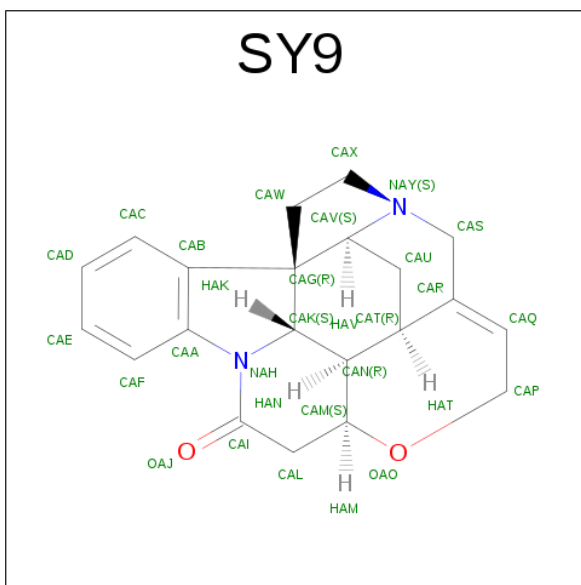
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	ALA	-	linker	UNP O75311
A	311	GLY	-	linker	UNP O75311
A	312	THR	-	linker	UNP O75311
A	355	TRP	-	expression tag	UNP O75311
A	356	SER	-	expression tag	UNP O75311
A	357	HIS	-	expression tag	UNP O75311
A	358	PRO	-	expression tag	UNP O75311
A	359	GLN	-	expression tag	UNP O75311
A	360	PHE	-	expression tag	UNP O75311
A	361	GLU	-	expression tag	UNP O75311
A	362	LYS	-	expression tag	UNP O75311
B	310	ALA	-	linker	UNP O75311
B	311	GLY	-	linker	UNP O75311
B	312	THR	-	linker	UNP O75311
B	355	TRP	-	expression tag	UNP O75311
B	356	SER	-	expression tag	UNP O75311
B	357	HIS	-	expression tag	UNP O75311
B	358	PRO	-	expression tag	UNP O75311

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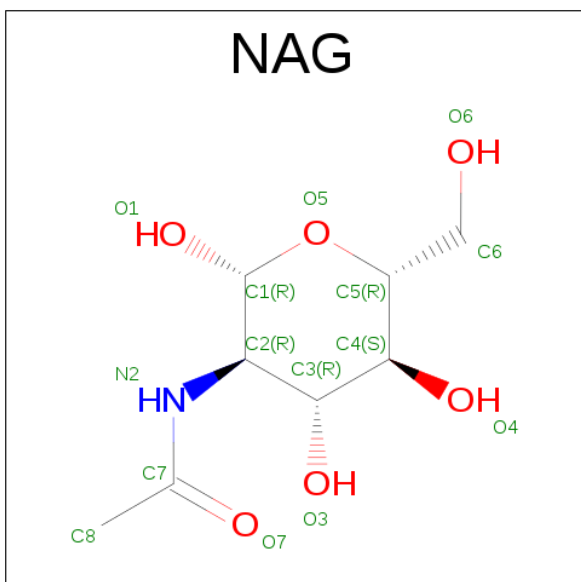
Chain	Residue	Modelled	Actual	Comment	Reference
B	359	GLN	-	expression tag	UNP O75311
B	360	PHE	-	expression tag	UNP O75311
B	361	GLU	-	expression tag	UNP O75311
B	362	LYS	-	expression tag	UNP O75311
C	310	ALA	-	linker	UNP O75311
C	311	GLY	-	linker	UNP O75311
C	312	THR	-	linker	UNP O75311
C	355	TRP	-	expression tag	UNP O75311
C	356	SER	-	expression tag	UNP O75311
C	357	HIS	-	expression tag	UNP O75311
C	358	PRO	-	expression tag	UNP O75311
C	359	GLN	-	expression tag	UNP O75311
C	360	PHE	-	expression tag	UNP O75311
C	361	GLU	-	expression tag	UNP O75311
C	362	LYS	-	expression tag	UNP O75311
D	310	ALA	-	linker	UNP O75311
D	311	GLY	-	linker	UNP O75311
D	312	THR	-	linker	UNP O75311
D	355	TRP	-	expression tag	UNP O75311
D	356	SER	-	expression tag	UNP O75311
D	357	HIS	-	expression tag	UNP O75311
D	358	PRO	-	expression tag	UNP O75311
D	359	GLN	-	expression tag	UNP O75311
D	360	PHE	-	expression tag	UNP O75311
D	361	GLU	-	expression tag	UNP O75311
D	362	LYS	-	expression tag	UNP O75311
E	310	ALA	-	linker	UNP O75311
E	311	GLY	-	linker	UNP O75311
E	312	THR	-	linker	UNP O75311
E	355	TRP	-	expression tag	UNP O75311
E	356	SER	-	expression tag	UNP O75311
E	357	HIS	-	expression tag	UNP O75311
E	358	PRO	-	expression tag	UNP O75311
E	359	GLN	-	expression tag	UNP O75311
E	360	PHE	-	expression tag	UNP O75311
E	361	GLU	-	expression tag	UNP O75311
E	362	LYS	-	expression tag	UNP O75311

- Molecule 2 is STRYCHNINE (three-letter code: SY9) (formula: C₂₁H₂₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	21	2	2		
2	B	1	Total	C	N	O	0	0
			25	21	2	2		
2	C	1	Total	C	N	O	0	0
			25	21	2	2		
2	D	1	Total	C	N	O	0	0
			25	21	2	2		
2	E	1	Total	C	N	O	0	0
			25	21	2	2		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

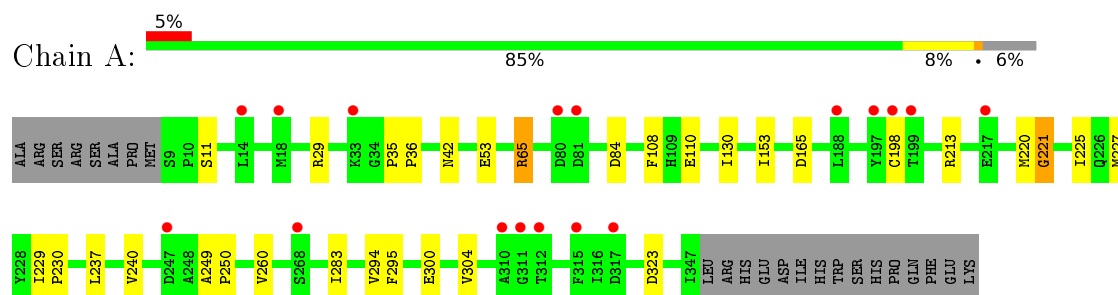


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

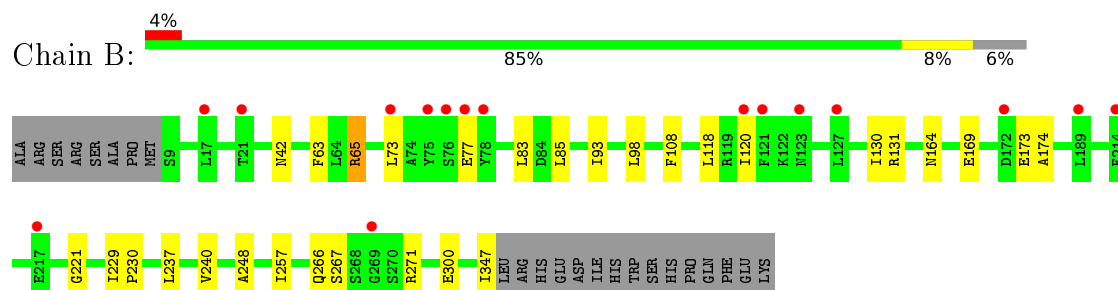
3 Residue-property plots [i](#)

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.

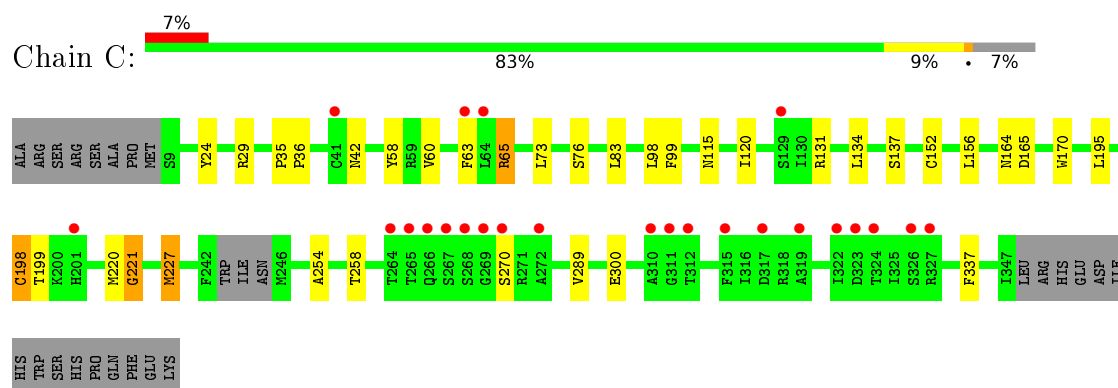
- Molecule 1: Glycine receptor subunit alpha-3, Glycine receptor subunit alpha-3



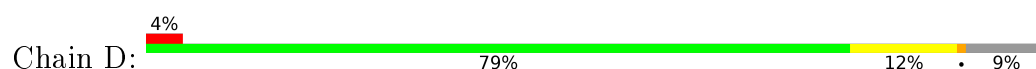
- Molecule 1: Glycine receptor subunit alpha-3, Glycine receptor subunit alpha-3

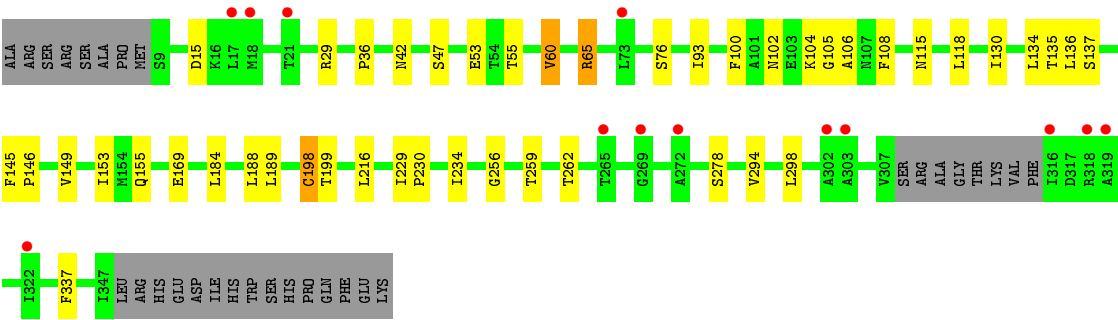


- Molecule 1: Glycine receptor subunit alpha-3, Glycine receptor subunit alpha-3

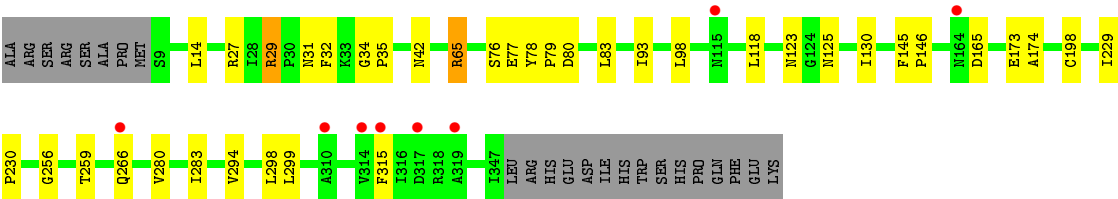
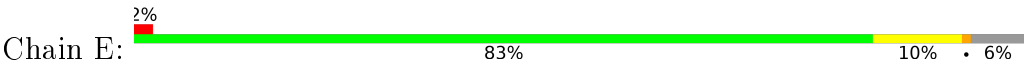


- Molecule 1: Glycine receptor subunit alpha-3, Glycine receptor subunit alpha-3





• Molecule 1: Glycine receptor subunit alpha-3,Glycine receptor subunit alpha-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.24Å 143.20Å 180.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.04 48.26 – 3.04	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-3.04) 96.9 (48.26-3.04)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.07Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.260 , 0.283 0.259 , 0.278	Depositor DCC
R_{free} test set	3426 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	97.8	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13540	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SY9, 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	0.29	0/2755	0.48	0/3759
1	B	0.29	0/2746	0.48	0/3749
1	C	0.30	0/2710	0.51	0/3696
1	D	0.36	0/2694	0.56	0/3676
1	E	0.30	0/2757	0.50	0/3762
All	All	0.31	0/13662	0.51	0/18642

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2685	0	2603	17	0
1	B	2676	0	2585	21	0
1	C	2644	0	2561	19	0
1	D	2626	0	2542	22	0
1	E	2686	0	2603	20	0
2	A	25	0	22	0	0
2	B	25	0	22	0	0
2	C	25	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	25	0	22	0	0
2	E	25	0	22	0	0
3	A	14	0	13	2	0
3	B	14	0	13	2	0
3	C	28	0	25	1	0
3	D	28	0	25	1	0
3	E	14	0	13	0	0
All	All	13540	0	13093	96	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (96) 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:D:189:LEU:HD12	1:D:216:LEU:HD23	1.72	0.71
1:A:42:ASN:HD21	1:A:65:ARG:HD2	1.57	0.70
1:B:42:ASN:HD21	1:B:65:ARG:HD2	1.62	0.65
1:D:42:ASN:HD21	1:D:65:ARG:HD2	1.63	0.64
1:C:42:ASN:HD21	1:C:65:ARG:HD2	1.63	0.62
1:B:108:PHE:CE1	1:B:130:ILE:HD11	2.36	0.61
1:A:227:MET:HG2	1:A:283:ILE:HD11	1.86	0.58
1:B:257:ILE:HG12	1:C:258:THR:HG21	1.87	0.56
1:D:93:ILE:HD13	1:D:118:LEU:HD21	1.87	0.56
1:D:189:LEU:HD12	1:D:216:LEU:CD2	2.35	0.56
1:E:42:ASN:HD21	1:E:65:ARG:HD2	1.71	0.56
1:E:93:ILE:HD13	1:E:118:LEU:HD21	1.87	0.55
1:B:257:ILE:HG23	1:C:258:THR:HG22	1.90	0.54
1:D:55:THR:O	1:D:104:LYS:NZ	2.41	0.54
1:B:63:PHE:CZ	1:B:131:ARG:HD2	2.43	0.54
1:D:108:PHE:CE1	1:D:130:ILE:HD11	2.44	0.53
3:B:601:NAG:H3	3:B:601:NAG:H83	1.91	0.52
1:D:259:THR:HG22	1:D:294:VAL:HG13	1.92	0.52
1:C:29:ARG:NH2	1:C:35:PRO:O	2.45	0.49
1:B:63:PHE:CE1	1:B:131:ARG:HD2	2.47	0.49
1:D:100:PHE:HA	1:D:155:GLN:O	2.12	0.49
1:C:58:TYR:CE1	1:C:152:CYS:HB3	2.48	0.49
1:D:229:ILE:HB	1:D:230:PRO:HD3	1.93	0.48
1:B:173:GLU:O	1:B:174:ALA:C	2.51	0.48
1:B:108:PHE:HE1	1:B:130:ILE:HD11	1.75	0.48
1:D:105:GLY:O	1:D:135:THR:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:LEU:HG	1:E:83:LEU:HD23	1.94	0.48
1:D:256:GLY:HA3	1:D:298:LEU:HD13	1.96	0.48
1:C:36:PRO:O	3:C:502:NAG:H82	2.13	0.48
1:A:229:ILE:HB	1:A:230:PRO:HD3	1.95	0.48
1:A:225:ILE:HD12	1:E:280:VAL:HG21	1.95	0.47
1:A:304:VAL:HG21	1:A:323:ASP:OD1	2.14	0.47
1:E:259:THR:HG22	1:E:294:VAL:HG13	1.97	0.47
1:C:24:TYR:CE2	1:C:73:LEU:HD21	2.49	0.47
1:B:229:ILE:HB	1:B:230:PRO:HD3	1.96	0.47
1:A:29:ARG:NH2	1:A:35:PRO:O	2.48	0.47
1:A:36:PRO:O	3:A:502:NAG:H82	2.15	0.47
1:C:170:TRP:CD1	1:C:195:LEU:HD22	2.51	0.46
1:E:229:ILE:HB	1:E:230:PRO:HD3	1.98	0.46
1:D:189:LEU:CD1	1:D:216:LEU:CD2	2.94	0.46
3:A:502:NAG:H83	3:A:502:NAG:H3	1.98	0.46
1:D:153:ILE:HD12	1:D:155:GLN:HG3	1.98	0.46
1:C:63:PHE:CZ	1:C:131:ARG:HD2	2.52	0.45
1:C:83:LEU:HD12	1:C:120:ILE:HD11	1.97	0.45
1:C:289:VAL:HG11	1:C:337:PHE:CZ	2.52	0.45
1:E:29:ARG:NH2	1:E:35:PRO:O	2.49	0.45
1:E:77:GLU:OE1	1:E:77:GLU:N	2.49	0.45
1:B:267:SER:O	1:B:271:ARG:HG3	2.17	0.45
1:D:188:LEU:O	1:D:216:LEU:HA	2.16	0.45
1:A:260:VAL:HG22	1:A:294:VAL:HG12	1.99	0.44
1:A:153:ILE:HG22	1:A:213:ARG:HG2	1.99	0.44
1:D:60:VAL:HG12	1:D:134:LEU:HB2	1.99	0.44
1:A:249:ALA:N	1:A:250:PRO:CD	2.81	0.44
1:C:98:LEU:HD23	1:C:99:PHE:N	2.32	0.44
1:A:11:SER:HB3	1:E:27:ARG:CZ	2.48	0.44
1:B:77:GLU:N	1:B:77:GLU:OE1	2.48	0.44
1:A:29:ARG:NH1	1:A:165:ASP:OD2	2.51	0.44
1:A:237:LEU:O	1:A:240:VAL:HG22	2.17	0.43
1:C:254:ALA:O	1:C:258:THR:HG23	2.17	0.43
1:B:230:PRO:CB	1:B:266:GLN:HE22	2.31	0.43
1:B:42:ASN:ND2	1:B:65:ARG:HD2	2.32	0.43
1:E:31:ASN:O	1:E:32:PHE:C	2.56	0.43
1:B:83:LEU:HD12	1:B:120:ILE:HD11	2.01	0.43
1:B:98:LEU:HD23	1:B:98:LEU:C	2.38	0.43
1:C:289:VAL:HG11	1:C:337:PHE:CE2	2.54	0.43
1:B:85:LEU:HD23	1:B:118:LEU:HD23	2.01	0.42
1:C:156:LEU:HD12	1:C:156:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ASN:O	1:D:136:LEU:HA	2.19	0.42
1:E:256:GLY:HA3	1:E:298:LEU:HD13	2.01	0.42
1:C:220:MET:O	1:C:221:GLY:C	2.58	0.42
1:A:225:ILE:HD12	1:E:280:VAL:CG2	2.50	0.42
1:A:220:MET:O	1:A:221:GLY:C	2.58	0.42
1:B:108:PHE:CD1	1:B:130:ILE:HD11	2.54	0.42
1:B:73:LEU:HD11	1:B:93:ILE:HD11	2.01	0.42
1:D:198:CYS:O	1:D:199:THR:C	2.57	0.42
1:E:123:ASN:OD1	1:E:125:ASN:ND2	2.52	0.42
1:E:145:PHE:HA	1:E:146:PRO:HA	1.85	0.41
1:D:115:ASN:HD22	1:D:115:ASN:N	2.17	0.41
1:E:78:TYR:CG	1:E:79:PRO:HD2	2.55	0.41
1:D:36:PRO:O	3:D:503:NAG:H82	2.21	0.41
1:A:237:LEU:HD21	1:E:299:LEU:HD13	2.01	0.41
1:E:31:ASN:O	1:E:34:GLY:N	2.54	0.41
1:A:108:PHE:CE1	1:A:130:ILE:HD11	2.55	0.41
1:D:145:PHE:HA	1:D:146:PRO:HA	1.91	0.41
1:E:173:GLU:O	1:E:174:ALA:C	2.59	0.41
1:B:230:PRO:HB3	1:B:266:GLN:HE22	1.86	0.41
1:C:227:MET:SD	1:C:270:SER:HB3	2.61	0.41
1:E:98:LEU:HD23	1:E:98:LEU:C	2.41	0.41
1:B:229:ILE:HB	1:B:230:PRO:CD	2.51	0.40
1:D:106:ALA:HB1	1:D:134:LEU:HD23	2.04	0.40
1:D:234:ILE:HD11	1:D:262:THR:HG22	2.02	0.40
1:E:146:PRO:HD3	1:E:283:ILE:HB	2.01	0.40
3:B:601:NAG:H3	3:B:601:NAG:C8	2.52	0.40
1:C:60:VAL:HG12	1:C:134:LEU:HB2	2.02	0.40
1:B:237:LEU:O	1:B:240:VAL:HG22	2.20	0.40
1:C:198:CYS:O	1:C:199:THR:C	2.60	0.40

There are no symmetry-related clashes.

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	337/362 (93%)	321 (95%)	15 (4%)	1 (0%)	46	82
1	B	337/362 (93%)	314 (93%)	21 (6%)	2 (1%)	30	70
1	C	332/362 (92%)	313 (94%)	16 (5%)	3 (1%)	21	61
1	D	327/362 (90%)	309 (94%)	17 (5%)	1 (0%)	46	82
1	E	337/362 (93%)	322 (96%)	14 (4%)	1 (0%)	46	82
All	All	1670/1810 (92%)	1579 (95%)	83 (5%)	8 (0%)	34	74

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	GLY
1	B	221	GLY
1	B	248	ALA
1	C	221	GLY
1	C	76	SER
1	C	227	MET
1	D	76	SER
1	E	76	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/326 (89%)	284 (98%)	7 (2%)	57	86
1	B	289/326 (89%)	284 (98%)	5 (2%)	68	90
1	C	286/326 (88%)	279 (98%)	7 (2%)	57	86
1	D	285/326 (87%)	272 (95%)	13 (5%)	33	71
1	E	291/326 (89%)	283 (97%)	8 (3%)	52	84
All	All	1442/1630 (88%)	1402 (97%)	40 (3%)	51	83

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	65	ARG
1	A	84	ASP
1	A	110	GLU
1	A	198	CYS
1	A	295	PHE
1	A	300	GLU
1	B	65	ARG
1	B	164	ASN
1	B	169	GLU
1	B	300	GLU
1	B	347	ILE
1	C	65	ARG
1	C	115	ASN
1	C	137	SER
1	C	164	ASN
1	C	165	ASP
1	C	198	CYS
1	C	300	GLU
1	D	15	ASP
1	D	29	ARG
1	D	47	SER
1	D	53	GLU
1	D	60	VAL
1	D	65	ARG
1	D	137	SER
1	D	149	VAL
1	D	169	GLU
1	D	184	LEU
1	D	198	CYS
1	D	278	SER
1	D	337	PHE
1	E	29	ARG
1	E	65	ARG
1	E	80	ASP
1	E	130	ILE
1	E	165	ASP
1	E	198	CYS
1	E	266	GLN
1	E	315	PHE

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	125	ASN
1	A	186	GLN
1	B	42	ASN
1	B	125	ASN
1	B	186	GLN
1	B	226	GLN
1	B	266	GLN
1	C	42	ASN
1	C	125	ASN
1	D	61	ASN
1	D	69	ASN
1	D	266	GLN
1	E	66	GLN
1	E	186	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
2	SY9	A	501	-	31,31,31	1.67	6 (19%)	51,51,51	2.26	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	502	1	14,14,15	0.51	0	15,19,21	1.60	3 (20%)
2	SY9	B	501	-	31,31,31	1.56	4 (12%)	51,51,51	2.53	18 (35%)
3	NAG	B	601	1	14,14,15	0.47	0	15,19,21	1.48	3 (20%)
2	SY9	C	501	-	31,31,31	1.67	5 (16%)	51,51,51	2.29	17 (33%)
3	NAG	C	502	1,3	14,14,15	0.51	0	15,19,21	1.95	6 (40%)
3	NAG	C	503	3	14,14,15	0.47	0	15,19,21	0.66	0
2	SY9	D	501	-	31,31,31	1.64	5 (16%)	51,51,51	2.33	18 (35%)
3	NAG	D	503	1,3	14,14,15	0.38	0	15,19,21	2.76	6 (40%)
3	NAG	D	504	3	14,14,15	0.49	0	15,19,21	1.32	3 (20%)
2	SY9	E	501	-	31,31,31	1.59	5 (16%)	51,51,51	2.32	17 (33%)
3	NAG	E	601	1	14,14,15	0.43	0	15,19,21	2.97	5 (33%)

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
2	SY9	A	501	-	-	0/0/74/74	0/0/7/7
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
2	SY9	B	501	-	-	0/0/74/74	0/0/7/7
3	NAG	B	601	1	-	0/6/23/26	0/1/1/1
2	SY9	C	501	-	-	0/0/74/74	0/0/7/7
3	NAG	C	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	503	3	-	0/6/23/26	0/1/1/1
2	SY9	D	501	-	-	0/0/74/74	0/0/7/7
3	NAG	D	503	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	504	3	-	0/6/23/26	0/1/1/1
2	SY9	E	501	-	-	0/0/74/74	0/0/7/7
3	NAG	E	601	1	-	0/6/23/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	SY9	CAP-CAQ	-6.31	1.38	1.50
2	A	501	SY9	CAP-CAQ	-6.22	1.38	1.50
2	C	501	SY9	CAP-CAQ	-6.20	1.38	1.50
2	E	501	SY9	CAP-CAQ	-6.20	1.38	1.50
2	B	501	SY9	CAP-CAQ	-5.77	1.39	1.50
2	B	501	SY9	CAK-NAH	-2.20	1.46	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	SY9	CAK-NAH	-2.20	1.46	1.49
2	A	501	SY9	CAK-NAH	-2.10	1.46	1.49
2	D	501	SY9	CAK-NAH	-2.05	1.46	1.49
2	A	501	SY9	CAL-CAM	2.13	1.58	1.53
2	E	501	SY9	CAL-CAI	2.34	1.54	1.51
2	A	501	SY9	CAL-CAI	2.44	1.54	1.51
2	C	501	SY9	CAL-CAI	2.47	1.54	1.51
2	D	501	SY9	CAL-CAI	2.59	1.55	1.51
2	C	501	SY9	CAL-CAM	2.59	1.59	1.53
2	A	501	SY9	CAQ-CAR	2.68	1.38	1.33
2	E	501	SY9	CAQ-CAR	2.69	1.38	1.33
2	D	501	SY9	CAQ-CAR	2.77	1.38	1.33
2	C	501	SY9	CAQ-CAR	2.78	1.38	1.33
2	C	501	SY9	CAI-NAH	2.80	1.40	1.36
2	E	501	SY9	CAI-NAH	2.84	1.40	1.36
2	B	501	SY9	CAQ-CAR	2.90	1.38	1.33
2	B	501	SY9	CAI-NAH	3.05	1.40	1.36
2	D	501	SY9	CAI-NAH	3.09	1.40	1.36
2	A	501	SY9	CAI-NAH	3.49	1.41	1.36

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	SY9	CAS-CAR-CAQ	-7.03	114.72	122.99
2	D	501	SY9	CAS-CAR-CAQ	-6.92	114.84	122.99
2	E	501	SY9	CAS-CAR-CAQ	-6.92	114.85	122.99
2	A	501	SY9	CAS-CAR-CAQ	-6.89	114.89	122.99
2	B	501	SY9	CAS-CAR-CAQ	-6.39	115.47	122.99
2	D	501	SY9	CAN-CAK-NAH	-5.54	101.87	106.09
2	E	501	SY9	CAN-CAK-NAH	-5.11	102.20	106.09
2	B	501	SY9	CAN-CAK-NAH	-5.04	102.24	106.09
2	B	501	SY9	CAN-CAT-CAR	-4.43	111.14	114.40
2	B	501	SY9	CAM-CAL-CAI	-4.35	112.30	117.12
2	A	501	SY9	CAN-CAK-NAH	-4.07	102.99	106.09
2	E	501	SY9	CAM-CAL-CAI	-3.82	112.89	117.12
2	C	501	SY9	CAN-CAK-NAH	-3.77	103.22	106.09
2	A	501	SY9	CAS-NAY-CAX	-3.69	106.55	112.56
2	D	501	SY9	CAN-CAT-CAR	-3.59	111.75	114.40
2	C	501	SY9	CAK-NAH-CAI	-3.59	115.23	119.29
2	D	501	SY9	CAK-NAH-CAI	-3.59	115.23	119.29
2	E	501	SY9	CAN-CAT-CAR	-3.57	111.77	114.40
2	D	501	SY9	CAM-CAL-CAI	-3.57	113.17	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	SY9	CAK-NAH-CAI	-3.53	115.30	119.29
2	C	501	SY9	CAM-CAL-CAI	-3.51	113.23	117.12
2	E	501	SY9	CAS-NAY-CAX	-3.37	107.06	112.56
2	B	501	SY9	CAS-NAY-CAX	-3.29	107.20	112.56
2	E	501	SY9	CAK-NAH-CAI	-3.28	115.58	119.29
3	C	502	NAG	C4-C3-C2	-3.21	106.36	111.34
2	A	501	SY9	CAK-NAH-CAI	-3.13	115.75	119.29
2	A	501	SY9	CAM-CAL-CAI	-3.04	113.75	117.12
2	B	501	SY9	OAD-CAM-CAL	-2.99	101.03	104.41
2	C	501	SY9	CAN-CAT-CAR	-2.86	112.29	114.40
2	C	501	SY9	CAS-NAY-CAX	-2.72	108.14	112.56
3	D	503	NAG	C4-C3-C2	-2.68	107.18	111.34
3	E	601	NAG	O7-C7-C8	-2.60	117.28	122.07
2	A	501	SY9	CAN-CAT-CAR	-2.55	112.52	114.40
2	D	501	SY9	CAS-NAY-CAX	-2.48	108.52	112.56
3	C	502	NAG	O7-C7-C8	-2.47	117.52	122.07
2	C	501	SY9	CAF-CAA-CAB	-2.44	119.14	121.77
2	B	501	SY9	CAW-CAG-CAB	-2.40	108.03	112.40
3	D	504	NAG	O7-C7-C8	-2.30	117.83	122.07
2	B	501	SY9	CAF-CAA-CAB	-2.30	119.30	121.77
2	D	501	SY9	CAF-CAA-CAB	-2.28	119.31	121.77
2	A	501	SY9	CAW-CAG-CAB	-2.26	108.28	112.40
2	E	501	SY9	OAJ-CAI-NAH	-2.23	120.71	122.61
3	D	503	NAG	O7-C7-C8	-2.23	117.97	122.07
3	A	502	NAG	O7-C7-C8	-2.21	118.00	122.07
2	D	501	SY9	OAJ-CAI-NAH	-2.18	120.76	122.61
2	E	501	SY9	CAF-CAA-CAB	-2.16	119.44	121.77
2	D	501	SY9	CAR-CAS-NAY	-2.16	108.85	112.92
2	A	501	SY9	CAF-CAA-CAB	-2.14	119.47	121.77
2	D	501	SY9	CAU-CAT-CAR	-2.12	106.57	109.15
2	A	501	SY9	CAR-CAS-NAY	-2.10	108.96	112.92
3	B	601	NAG	O7-C7-C8	-2.10	118.21	122.07
2	C	501	SY9	CAU-CAT-CAR	-2.08	106.62	109.15
2	A	501	SY9	CAU-CAT-CAR	-2.03	106.68	109.15
2	D	501	SY9	CAK-CAG-CAV	2.03	115.96	113.91
3	B	601	NAG	C8-C7-N2	2.05	120.03	116.10
2	E	501	SY9	CAG-CAK-CAN	2.06	118.47	117.01
3	C	502	NAG	O5-C5-C4	2.07	113.56	110.13
2	A	501	SY9	CAW-CAG-CAV	2.08	103.28	101.14
2	D	501	SY9	OAD-CAP-CAQ	2.16	116.33	111.49
2	A	501	SY9	CAS-CAR-CAT	2.18	118.74	113.91
2	C	501	SY9	CAA-NAH-CAK	2.24	110.80	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	SY9	CAS-NAY-CAV	2.26	115.09	113.03
2	D	501	SY9	CAS-CAR-CAT	2.26	118.92	113.91
2	D	501	SY9	CAG-CAK-CAN	2.31	118.64	117.01
2	B	501	SY9	CAA-NAH-CAK	2.33	110.86	109.30
2	E	501	SY9	OAQ-CAP-CAQ	2.33	116.72	111.49
2	C	501	SY9	OAQ-CAP-CAQ	2.36	116.77	111.49
2	C	501	SY9	CAK-CAG-CAV	2.44	116.37	113.91
2	B	501	SY9	CAM-CAN-CAK	2.47	109.47	107.47
3	A	502	NAG	C8-C7-N2	2.49	120.87	116.10
3	D	504	NAG	C2-N2-C7	2.50	126.35	123.11
2	D	501	SY9	CAA-NAH-CAK	2.50	110.97	109.30
2	C	501	SY9	CAP-OAQ-CAM	2.50	117.32	114.93
2	E	501	SY9	CAA-NAH-CAK	2.52	110.98	109.30
2	E	501	SY9	CAS-CAR-CAT	2.53	119.51	113.91
2	E	501	SY9	CAK-CAG-CAV	2.54	116.47	113.91
3	C	502	NAG	C1-O5-C5	2.54	115.88	112.14
2	C	501	SY9	CAL-CAI-NAH	2.58	118.01	115.23
2	C	501	SY9	CAS-CAR-CAT	2.60	119.66	113.91
2	B	501	SY9	CAL-CAI-NAH	2.64	118.08	115.23
3	D	503	NAG	C8-C7-N2	2.66	121.19	116.10
2	B	501	SY9	CAS-CAR-CAT	2.68	119.85	113.91
2	A	501	SY9	OAQ-CAP-CAQ	2.68	117.50	111.49
2	A	501	SY9	CAK-CAG-CAV	2.73	116.66	113.91
2	B	501	SY9	CAK-CAG-CAV	2.78	116.71	113.91
3	C	502	NAG	C8-C7-N2	2.78	121.43	116.10
2	C	501	SY9	CAT-CAR-CAQ	2.89	125.61	122.63
2	E	501	SY9	CAT-CAR-CAQ	2.93	125.64	122.63
2	E	501	SY9	CAL-CAI-NAH	3.00	118.47	115.23
3	D	504	NAG	C8-C7-N2	3.08	122.00	116.10
2	B	501	SY9	OAQ-CAP-CAQ	3.23	118.73	111.49
2	D	501	SY9	CAL-CAI-NAH	3.29	118.78	115.23
2	D	501	SY9	CAT-CAR-CAQ	3.50	126.23	122.63
3	B	601	NAG	C2-N2-C7	3.54	127.71	123.11
3	E	601	NAG	C8-C7-N2	3.55	122.91	116.10
2	A	501	SY9	CAL-CAI-NAH	3.63	119.15	115.23
2	A	501	SY9	CAT-CAR-CAQ	3.63	126.37	122.63
2	E	501	SY9	OAQ-CAM-CAN	3.79	117.16	114.44
3	A	502	NAG	C2-N2-C7	3.89	128.17	123.11
3	C	502	NAG	C2-N2-C7	4.40	128.83	123.11
3	E	601	NAG	O5-C5-C4	4.43	117.46	110.13
3	E	601	NAG	C2-N2-C7	4.50	128.95	123.11
3	D	503	NAG	C2-N2-C7	4.55	129.03	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	503	NAG	O5-C5-C4	4.57	117.70	110.13
2	C	501	SY9	OAO-CAM-CAN	4.93	117.98	114.44
3	D	503	NAG	C1-O5-C5	6.85	122.21	112.14
2	B	501	SY9	OAO-CAM-CAN	6.86	119.37	114.44
2	E	501	SY9	CAA-NAH-CAI	7.03	132.65	125.40
2	C	501	SY9	CAA-NAH-CAI	7.07	132.68	125.40
2	B	501	SY9	CAA-NAH-CAI	7.15	132.77	125.40
2	A	501	SY9	CAA-NAH-CAI	7.30	132.93	125.40
2	D	501	SY9	CAA-NAH-CAI	7.40	133.03	125.40
3	E	601	NAG	C1-O5-C5	8.09	124.03	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	2	0
3	B	601	NAG	2	0
3	C	502	NAG	1	0
3	D	503	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	339/362 (93%)	-0.05	17 (5%) 32 13	65, 126, 174, 207	0
1	B	339/362 (93%)	0.07	16 (4%) 35 14	77, 119, 164, 182	0
1	C	336/362 (92%)	0.09	24 (7%) 19 6	71, 115, 216, 247	0
1	D	331/362 (91%)	-0.03	13 (3%) 43 18	36, 116, 199, 233	0
1	E	339/362 (93%)	-0.15	8 (2%) 62 32	68, 116, 196, 232	0
All	All	1684/1810 (93%)	-0.01	78 (4%) 36 15	36, 119, 190, 247	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	322	ILE	9.9
1	C	324	THR	7.6
1	C	323	ASP	6.7
1	C	326	SER	5.1
1	D	316	ILE	4.4
1	C	317	ASP	4.3
1	A	311	GLY	4.2
1	B	120	ILE	3.9
1	D	319	ALA	3.8
1	C	319	ALA	3.8
1	A	310	ALA	3.7
1	C	310	ALA	3.7
1	E	314	VAL	3.7
1	A	312	THR	3.6
1	C	265	THR	3.6
1	D	318	ARG	3.6
1	C	64	LEU	3.5
1	C	268	SER	3.5
1	D	303	ALA	3.3
1	A	197	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	272	ALA	3.1
1	C	63	PHE	3.0
1	B	73	LEU	2.9
1	C	312	THR	2.9
1	C	269	GLY	2.9
1	E	317	ASP	2.9
1	B	121	PHE	2.9
1	B	123	ASN	2.8
1	B	76	SER	2.8
1	C	264	THR	2.8
1	A	317	ASP	2.8
1	D	302	ALA	2.7
1	E	310	ALA	2.7
1	B	77	GLU	2.7
1	E	315	PHE	2.7
1	C	267	SER	2.7
1	C	311	GLY	2.7
1	C	266	GLN	2.6
1	D	265	THR	2.6
1	B	127	LEU	2.6
1	C	270	SER	2.6
1	B	214	PHE	2.6
1	B	21	THR	2.6
1	A	81	ASP	2.6
1	B	78	TYR	2.6
1	C	315	PHE	2.5
1	D	322	ILE	2.5
1	C	129	SER	2.5
1	E	319	ALA	2.5
1	B	172	ASP	2.4
1	C	327	ARG	2.4
1	A	217	GLU	2.4
1	D	269	GLY	2.4
1	B	75	TYR	2.4
1	A	80	ASP	2.3
1	B	269	GLY	2.3
1	B	217	GLU	2.3
1	A	14	LEU	2.3
1	E	164	ASN	2.3
1	A	198	CYS	2.3
1	A	18	MET	2.3
1	A	315	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	115	ASN	2.2
1	A	268	SER	2.2
1	B	189	LEU	2.2
1	A	247	ASP	2.2
1	A	188	LEU	2.1
1	B	17	LEU	2.1
1	C	201	HIS	2.1
1	A	33	LYS	2.1
1	D	17	LEU	2.1
1	D	73	LEU	2.1
1	A	199	THR	2.0
1	D	21	THR	2.0
1	D	18	MET	2.0
1	C	41	CYS	2.0
1	D	272	ALA	2.0
1	E	266	GLN	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 carbohydrates 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. 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(\AA^2)	Q<0.9
3	NAG	E	601	14/15	0.68	0.31	1.09	153,165,179,184	0
2	SY9	E	501	25/25	0.96	0.29	0.31	114,119,125,126	0
2	SY9	B	501	25/25	0.97	0.30	0.19	101,105,112,114	0
2	SY9	C	501	25/25	0.98	0.25	0.06	95,102,112,122	0
2	SY9	A	501	25/25	0.98	0.26	0.01	103,108,114,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	D	503	14/15	0.88	0.22	-0.12	114,127,133,146	0
2	SY9	D	501	25/25	0.98	0.22	-0.41	91,103,108,112	0
3	NAG	C	502	14/15	0.92	0.13	-	114,127,132,136	0
3	NAG	D	504	14/15	0.86	0.25	-	151,159,165,166	0
3	NAG	A	502	14/15	0.87	0.21	-	123,135,145,146	0
3	NAG	C	503	14/15	0.93	0.21	-	135,140,143,144	0
3	NAG	B	601	14/15	0.82	0.19	-	126,143,148,154	0

6.5 Other polymers [i](#)

There are no such residues in this entry.