WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2020 – 11:22 PM BST

PDB ID	:	5I6Z
Title	:	X-ray structure of the ts2 human serotonin transporter
Authors	:	Coleman, J.A.; Green, E.M.; Gouaux, E.
Deposited on	:	2016-02-16
Resolution	:	4.53 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.
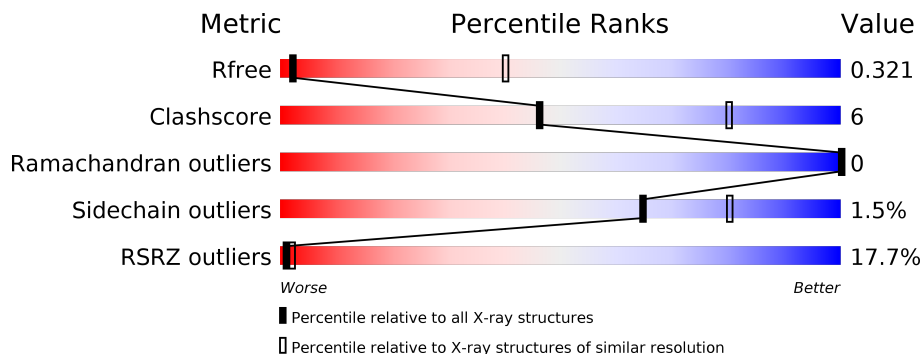
Full wwPDB X-ray Structure Validation Report

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
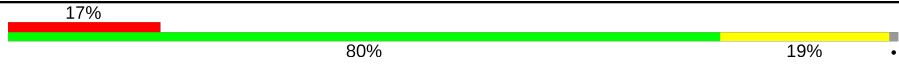*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.53 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	Percentile Ranks	Value
Rfree		0.321
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		1.5%
RSRZ outliers		17.7%

Worse ___ *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1058 (5.28-3.80)
Clashscore	141614	1126 (5.28-3.80)
Ramachandran outliers	138981	1071 (5.26-3.80)
Sidechain outliers	138945	1052 (5.26-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	549	17% / 80% / 19% / •
2	B	221	18% / 82% / 17% / •
3	C	214	20% / 85% / 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7544 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 Sodium-dependent serotonin transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			4225	2819	656	726	24			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	GLY	-	cloning artifact	UNP P31645
A	75	SER	-	cloning artifact	UNP P31645
A	291	ALA	ILE	engineered mutation	UNP P31645
A	439	SER	THR	engineered mutation	UNP P31645
A	554	ALA	CYS	engineered mutation	UNP P31645
A	580	ALA	CYS	engineered mutation	UNP P31645
A	619	LEU	-	cloning artifact	UNP P31645
A	620	VAL	-	cloning artifact	UNP P31645
A	621	PRO	-	cloning artifact	UNP P31645
A	622	ARG	-	cloning artifact	UNP P31645

- Molecule 2 is a protein called 8B6 antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1643	1038	266	331	8			

- Molecule 3 is a protein called 8B6 antibody, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1662	1037	280	337	8			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

O6
OH

O5
HO
C1(R)   C5(R)
C2(R)   C4(S)
C3(R)
N2
HN
OH
O4
C7
OH
C8
O3
O
O7
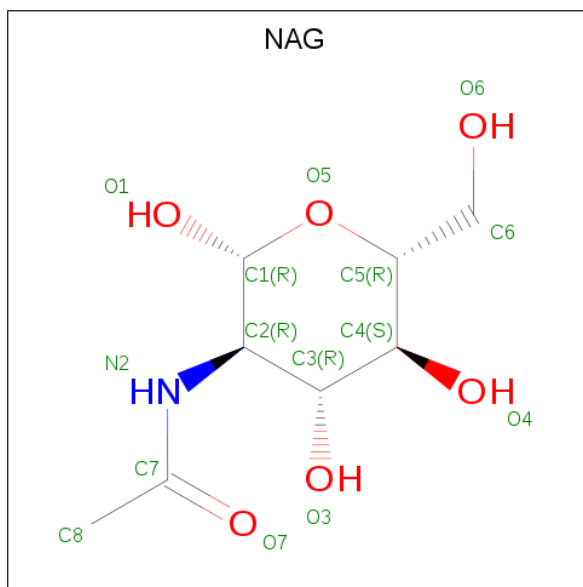
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Sodium-dependent serotonin transporter
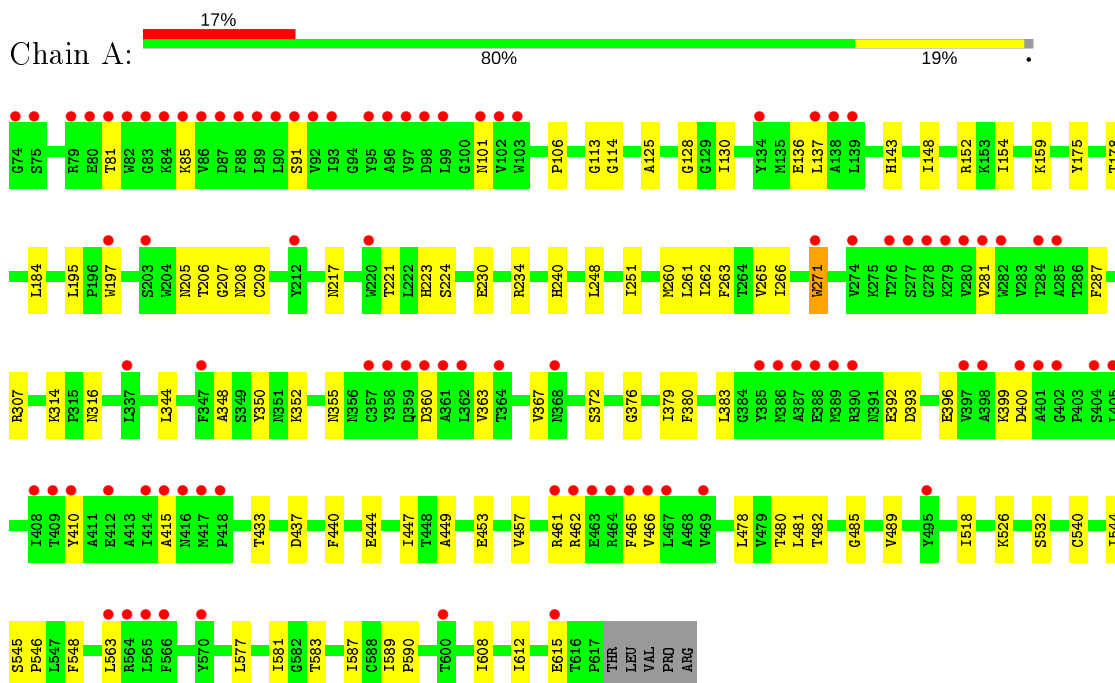
- Molecule 2: 8B6 antibody, heavy chain
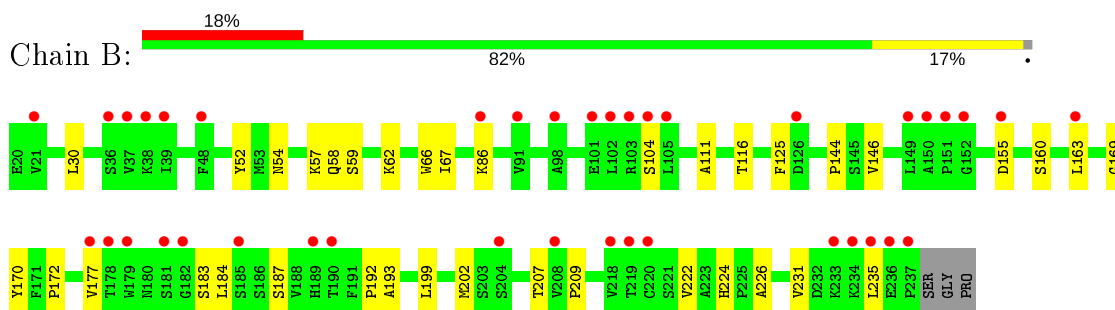
- Molecule 3: 8B6 antibody, light chain

4 Data and refinement statistics (i)

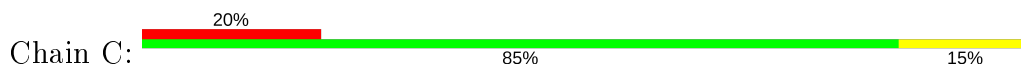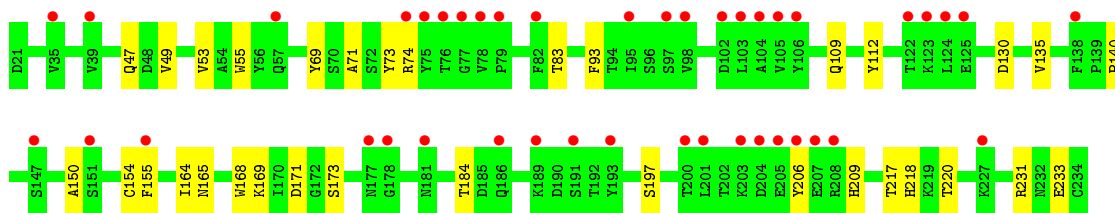| Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	129.75Å　162.81Å　140.06Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	40.50　–　4.53 82.17　–　4.53	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.50-4.53) 99.3 (82.17-4.53)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	0.97 (at 4.47Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.280　,　0.317 0.282　,　0.321	Depositor DCC
R_{free} test set	443 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	260.9	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 452.9	EDS
L-test for twinning[2]	$<|L|> = 0.34$, $<L^2> = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	7544	wwPDB-VP
Average B, all atoms (Å^2)	387.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ 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: 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	0.24	0/4359	0.38	0/5960
2	B	0.24	0/1688	0.44	0/2309
3	C	0.24	0/1700	0.45	0/2307
All	All	0.24	0/7747	0.41	0/10576

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	4225	0	4118	59	0
2	B	1643	0	1589	18	0
3	C	1662	0	1585	17	0
4	A	14	0	13	1	0
All	All	7544	0	7305	93	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 6.

All (93) 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)
3:C:168:TRP:HE1	3:C:197:SER:HG	1.06	0.94
2:B:30:LEU:HD22	2:B:172:PRO:HD3	1.69	0.75
2:B:54:ASN:HD22	2:B:66:TRP:HE1	1.34	0.74
1:A:589:ILE:HG23	1:A:590:PRO:HD3	1.76	0.68
1:A:205:ASN:ND2	1:A:209:CYS:SG	2.68	0.67
1:A:101:ASN:ND2	1:A:372:SER:OG	2.30	0.63
2:B:192:PRO:HD3	3:C:184:THR:HG22	1.81	0.63
1:A:152:ARG:NH2	1:A:453:GLU:OE1	2.35	0.59
1:A:437:ASP:N	1:A:437:ASP:OD1	2.30	0.59
2:B:59:SER:HB2	2:B:62:LYS:HB2	1.84	0.59
1:A:113:GLY:HA2	1:A:316:ASN:HB3	1.85	0.58
1:A:175:TYR:HA	1:A:480:THR:HG21	1.85	0.58
3:C:74:ARG:HH21	3:C:83:THR:HG22	1.69	0.58
1:A:608:ILE:O	1:A:612:ILE:N	2.36	0.57
1:A:184:LEU:HD21	1:A:261:LEU:HD23	1.86	0.57
1:A:447:ILE:HD13	1:A:466:VAL:HG22	1.85	0.57
1:A:380:PHE:HA	1:A:383:LEU:HB2	1.86	0.56
1:A:85:LYS:NZ	1:A:360:ASP:OD2	2.37	0.56
1:A:85:LYS:NZ	1:A:355:ASN:OD1	2.28	0.56
2:B:193:ALA:HA	2:B:202:MET:HB3	1.89	0.54
1:A:206:THR:HG23	1:A:234:ARG:NH2	2.23	0.53
3:C:165:ASN:HB3	3:C:217:THR:HB	1.91	0.52
1:A:106:PRO:HG3	1:A:376:GLY:HA2	1.91	0.52
1:A:478:LEU:HD23	1:A:481:LEU:HD12	1.92	0.52
1:A:178:THR:HG21	1:A:480:THR:HB	1.91	0.52
3:C:47:GLN:HE21	3:C:112:TYR:HE2	1.58	0.51
3:C:49:VAL:HG13	3:C:112:TYR:CE1	2.45	0.51
1:A:251:ILE:HA	1:A:482:THR:HA	1.91	0.51
3:C:130:ASP:HB3	3:C:220:THR:HG22	1.93	0.50
1:A:262:ILE:HA	1:A:265:VAL:HG12	1.93	0.50
3:C:206:TYR:CZ	3:C:231:ARG:HG3	2.47	0.49
1:A:400:ASP:OD1	1:A:400:ASP:N	2.45	0.49
1:A:447:ILE:HA	1:A:465:PHE:HE2	1.78	0.49
1:A:234:ARG:HE	1:A:240:HIS:CG	2.30	0.49
1:A:208:ASN:HB3	1:A:224:SER:HA	1.94	0.49
2:B:86:LYS:NZ	2:B:104:SER:O	2.46	0.49
2:B:163:LEU:HB3	2:B:235:LEU:HD22	1.95	0.48
1:A:583:THR:O	1:A:587:ILE:HG23	2.14	0.48
1:A:207:GLY:HA3	4:A:700:NAG:H82	1.95	0.48
3:C:164:ILE:HB	3:C:218:HIS:HD2	1.79	0.48
1:A:125:ALA:O	1:A:130:ILE:HG12	2.13	0.48
1:A:396:GLU:OE1	1:A:399:LYS:HE3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:LYS:HD3	1:A:532:SER:HB2	1.94	0.47
2:B:183:SER:HA	2:B:184:LEU:HA	1.47	0.47
3:C:154:CYS:HB3	3:C:197:SER:HB3	1.95	0.47
3:C:169:LYS:HA	3:C:173:SER:O	2.15	0.47
1:A:148:ILE:HG13	1:A:449:ALA:HB1	1.96	0.47
1:A:307:ARG:HD3	1:A:392:GLU:HG3	1.97	0.47
1:A:444:GLU:OE1	1:A:462:ARG:NH2	2.43	0.46
1:A:287:PHE:HB3	1:A:433:THR:HG21	1.96	0.46
3:C:171:ASP:OD2	3:C:209:HIS:ND1	2.47	0.46
2:B:187:SER:OG	2:B:207:THR:O	2.34	0.46
3:C:135:VAL:HA	3:C:155:PHE:O	2.15	0.46
2:B:116:THR:OG1	2:B:125:PHE:HB3	2.15	0.46
1:A:271:TRP:HA	1:A:466:VAL:HG21	1.98	0.45
1:A:197:TRP:HE1	1:A:415:ALA:HB2	1.80	0.45
1:A:137:LEU:HD12	1:A:348:ALA:HB2	1.98	0.45
1:A:352:LYS:HB3	1:A:355:ASN:HB2	1.98	0.45
1:A:266:ILE:HG22	1:A:440:PHE:HE1	1.82	0.45
1:A:393:ASP:OD2	1:A:396:GLU:HG2	2.18	0.44
1:A:91:SER:HA	1:A:281:VAL:HG11	1.98	0.44
1:A:379:ILE:HA	1:A:410:TYR:HE2	1.82	0.44
1:A:263:PHE:HA	1:A:266:ILE:HG12	2.00	0.44
1:A:545:SER:HB2	1:A:546:PRO:HD3	2.00	0.44
1:A:136:GLU:HG2	1:A:344:LEU:HB2	2.00	0.43
1:A:206:THR:HG23	1:A:234:ARG:HH22	1.82	0.43
3:C:140:PRO:HG2	3:C:150:ALA:HB1	1.99	0.43
1:A:266:ILE:HG22	1:A:440:PHE:CE1	2.53	0.43
2:B:58:GLN:O	2:B:111:ALA:HB1	2.18	0.43
2:B:160:SER:HA	2:B:209:PRO:HA	2.01	0.43
2:B:169:GLY:HA2	2:B:199:LEU:HB3	2.01	0.43
1:A:143:HIS:NE2	1:A:154:ILE:HD11	2.34	0.43
1:A:363:VAL:O	1:A:367:VAL:HG23	2.19	0.42
1:A:518:ILE:HA	1:A:518:ILE:HD12	1.81	0.42
1:A:114:GLY:HA3	1:A:314:LYS:O	2.20	0.42
1:A:206:THR:OG1	1:A:230:GLU:OE2	2.37	0.42
1:A:152:ARG:HE	1:A:159:LYS:HZ2	1.68	0.42
2:B:144:PRO:HB3	2:B:170:TYR:HB3	2.00	0.42
1:A:128:GLY:HA3	1:A:548:PHE:CG	2.55	0.41
3:C:69:TYR:O	3:C:73:TYR:HB2	2.20	0.41
3:C:55:TRP:CD2	3:C:93:PHE:HB2	2.55	0.41
3:C:53:VAL:HB	3:C:71:ALA:HB2	2.01	0.41
1:A:195:LEU:H	1:A:195:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:GLU:HA	1:A:399:LYS:HG3	2.03	0.41
1:A:577:LEU:O	1:A:581:ILE:HG13	2.20	0.41
1:A:485:GLY:O	1:A:489:VAL:HG23	2.21	0.40
2:B:146:VAL:HG21	2:B:231:VAL:HB	2.03	0.40
2:B:224:HIS:CE1	2:B:226:ALA:HB3	2.56	0.40
1:A:540:CYS:HA	1:A:544:ILE:HB	2.03	0.40
2:B:57:LYS:HB2	2:B:67:ILE:HD11	2.03	0.40
1:A:221:THR:HG22	1:A:223:HIS:H	1.86	0.40
2:B:177:VAL:HG22	2:B:222:VAL:HG22	2.02	0.40
1:A:81:THR:HA	1:A:350:TYR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	542/549 (99%)	519 (96%)	23 (4%)	0	100	100
2	B	216/221 (98%)	210 (97%)	6 (3%)	0	100	100
3	C	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
All	All	970/984 (99%)	932 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/463 (93%)	423 (98%)	8 (2%)	57	75
2	B	190/193 (98%)	188 (99%)	2 (1%)	73	85
3	C	189/190 (100%)	187 (99%)	2 (1%)	73	85
All	All	810/846 (96%)	798 (98%)	12 (2%)	65	80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	248	LEU
1	A	260	MET
1	A	271	TRP
1	A	457	VAL
1	A	461	ARG
1	A	563	LEU
1	A	615	GLU
2	B	52	TYR
2	B	155	ASP
3	C	109	GLN
3	C	233	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	217	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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
4	NAG	A	700	1	14,14,15	0.23	0	17,19,21	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	700	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	700	NAG	O5-C5-C6-O6
4	A	700	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	544/549 (99%)	0.66	92 (16%)	1	2	117, 324, 560, 871	0
2	B	218/221 (98%)	0.85	39 (17%)	1	2	215, 398, 628, 888	0
3	C	214/214 (100%)	0.81	42 (19%)	1	1	29, 419, 726, 919	0
All	All	976/984 (99%)	0.73	173 (17%)	1	2	29, 363, 628, 919	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	151	PRO	20.0
2	B	150	ALA	9.6
1	A	400	ASP	9.6
3	C	78	VAL	8.7
1	A	360	ASP	8.7
1	A	463	GLU	8.6
1	A	79	ARG	8.4
1	A	82	TRP	8.2
1	A	401	ALA	7.7
1	A	361	ALA	6.3
1	A	282	TRP	6.1
2	B	237	PRO	6.0
2	B	218	VAL	6.0
3	C	104	ALA	5.9
2	B	236	GLU	5.8
1	A	416	ASN	5.8
2	B	152	GLY	5.8
1	A	88	PHE	5.7
1	A	285	ALA	5.6
1	A	364	THR	5.6
3	C	75	TYR	5.6
3	C	77	GLY	5.5
1	A	87	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	36	SER	5.4
1	A	281	VAL	5.4
1	A	417	MET	5.4
1	A	357	CYS	5.2
3	C	98	VAL	5.2
3	C	193	TYR	5.0
3	C	76	THR	5.0
1	A	466	VAL	5.0
1	A	277	SER	5.0
2	B	235	LEU	4.9
1	A	358	TYR	4.7
3	C	124	LEU	4.7
1	A	83	GLY	4.6
3	C	103	LEU	4.6
1	A	418	PRO	4.5
2	B	190	THR	4.4
3	C	201	LEU	4.3
2	B	98	ALA	4.3
3	C	106	TYR	4.3
1	A	85	LYS	4.3
1	A	464	ARG	4.1
2	B	102	LEU	4.1
1	A	90	LEU	4.1
3	C	123	LYS	4.1
3	C	181	ASN	4.1
1	A	386	MET	4.1
1	A	359	GLN	4.1
1	A	414	ILE	4.1
1	A	134	TYR	4.0
2	B	179	TRP	4.0
2	B	177	VAL	4.0
2	B	37	VAL	3.9
1	A	274	VAL	3.9
1	A	84	LYS	3.9
1	A	89	LEU	3.8
1	A	81	THR	3.8
1	A	91	SER	3.8
1	A	563	LEU	3.8
3	C	178	GLY	3.7
1	A	409	THR	3.7
3	C	200	THR	3.7
1	A	74	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	415	ALA	3.6
1	A	278	GLY	3.6
1	A	462	ARG	3.6
2	B	219	THR	3.6
3	C	177	ASN	3.5
3	C	203	LYS	3.5
1	A	410	TYR	3.5
2	B	233	LYS	3.5
3	C	39	VAL	3.5
1	A	465	PHE	3.5
1	A	86	VAL	3.5
1	A	102	VAL	3.5
3	C	79	PRO	3.4
1	A	390	ARG	3.4
1	A	96	ALA	3.4
1	A	93	ILE	3.4
1	A	284	THR	3.4
1	A	404	SER	3.3
3	C	122	THR	3.3
1	A	347	PHE	3.2
1	A	564	ARG	3.2
2	B	220	CYS	3.2
1	A	97	VAL	3.1
1	A	389	MET	3.1
3	C	35	VAL	3.1
1	A	402	GLY	3.1
3	C	204	ASP	3.1
1	A	137	LEU	3.0
2	B	104	SER	3.0
1	A	99	LEU	3.0
1	A	103	TRP	3.0
2	B	103	ARG	3.0
2	B	189	HIS	3.0
1	A	495	TYR	2.9
1	A	92	VAL	2.9
3	C	82	PHE	2.9
1	A	101	ASN	2.9
1	A	95	TYR	2.9
2	B	234	LYS	2.9
3	C	74	ARG	2.9
2	B	105	LEU	2.9
2	B	182	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	155	ASP	2.9
1	A	220	TRP	2.8
1	A	388	GLU	2.8
1	A	467	LEU	2.8
1	A	197	TRP	2.8
3	C	191	SER	2.8
3	C	207	GLU	2.8
1	A	469	VAL	2.8
1	A	461	ARG	2.8
1	A	565	LEU	2.8
1	A	279	LYS	2.8
1	A	368	ASN	2.7
1	A	80	GLU	2.7
3	C	95	ILE	2.7
3	C	208	ARG	2.6
1	A	570	TYR	2.6
2	B	204	SER	2.6
1	A	405	LEU	2.5
1	A	75	SER	2.5
1	A	280	VAL	2.5
3	C	205	GLU	2.5
1	A	98	ASP	2.5
2	B	163	LEU	2.5
2	B	86	LYS	2.5
1	A	566	PHE	2.5
1	A	600	THR	2.5
2	B	91	VAL	2.4
3	C	97	SER	2.4
2	B	149	LEU	2.4
3	C	125	GLU	2.4
1	A	412	GLU	2.4
1	A	203	SER	2.4
2	B	39	ILE	2.4
2	B	181	SER	2.4
3	C	138	PHE	2.3
3	C	151	SER	2.3
1	A	139	LEU	2.3
3	C	206	TYR	2.3
2	B	208	VAL	2.3
3	C	105	VAL	2.3
1	A	212	TYR	2.3
1	A	398	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	397	VAL	2.2
2	B	38	LYS	2.2
2	B	48	PHE	2.2
3	C	147	SER	2.2
1	A	271	TRP	2.2
3	C	57	GLN	2.2
3	C	155	PHE	2.2
2	B	21	VAL	2.2
3	C	186	GLN	2.2
1	A	337	LEU	2.2
2	B	185	SER	2.2
3	C	102	ASP	2.2
2	B	126	ASP	2.1
1	A	362	LEU	2.1
1	A	276	THR	2.1
1	A	138	ALA	2.1
2	B	101	GLU	2.1
1	A	408	ILE	2.1
3	C	189	LYS	2.0
3	C	227	LYS	2.0
1	A	385	TYR	2.0
1	A	387	ALA	2.0
2	B	178	THR	2.0
1	A	615	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	700	14/15	0.89	0.34	237,303,328,328	0

6.5 Other polymers (i)

There are no such residues in this entry.