



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2016 – 08:50 PM EDT

PDB ID : 5I74  
Title : X-ray structure of the ts3 human serotonin transporter complexed with Br-citalopram at the central site  
Authors : Coleman, J.A.; Green, E.M.; Gouaux, E.  
Deposited on : 2016-02-16  
Resolution : 3.40 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](mailto: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.

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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-20027457  
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-20027457

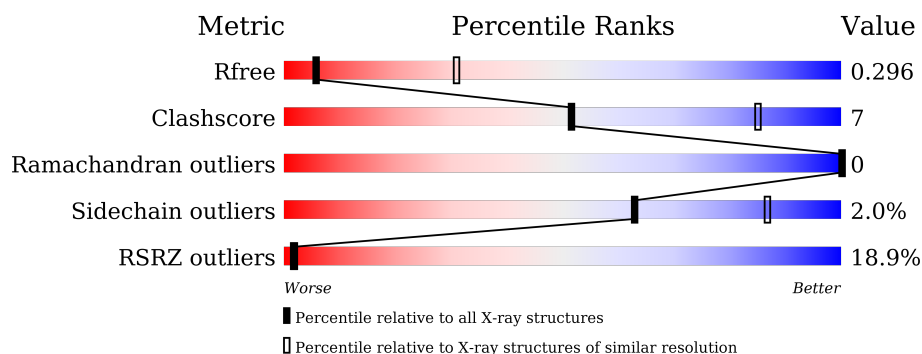
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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  $\geq 3$ , 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	549	<div> <div>12%</div> <div>82%</div> <div>16%</div> </div>
2	B	221	<div> <div>28%</div> <div>79%</div> <div>19%</div> </div>
3	C	214	<div> <div>27%</div> <div>79%</div> <div>21%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	69D	A	700	-	-	-	X
6	CLR	A	702	-	-	-	X
7	D12	A	703	-	-	-	X
8	HEX	A	704	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7610 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	542	Total	C	N	O	S	0	0	0
			4207	2809	652	722	24			

There are 11 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	110	ALA	TYR	engineered mutation	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

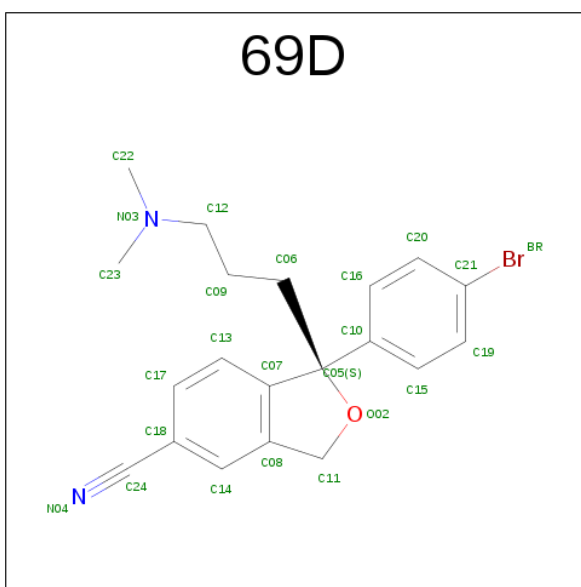
- Molecule 2 is a protein called 8B6 antibody, heavy chain.

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.

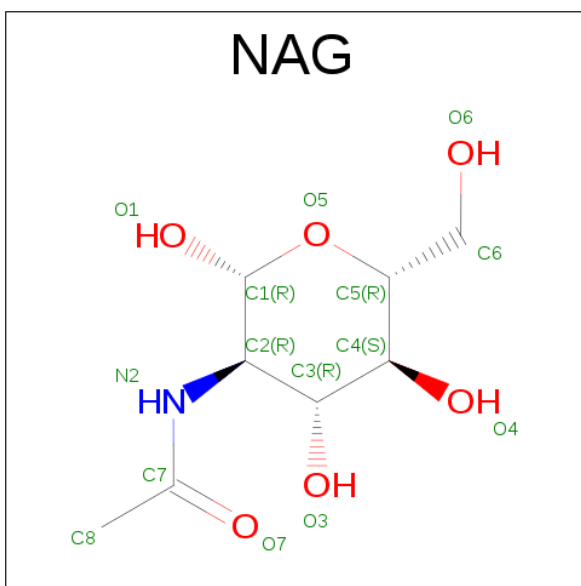
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1662	1037	280	337	8			

- Molecule 4 is (1S)-1-(4-bromophenyl)-1-[3-(dimethylamino)propyl]-1,3-dihydro-2-benzofuran-5-carbonitrile (three-letter code: 69D) (formula: C<sub>20</sub>H<sub>21</sub>BrN<sub>2</sub>O).



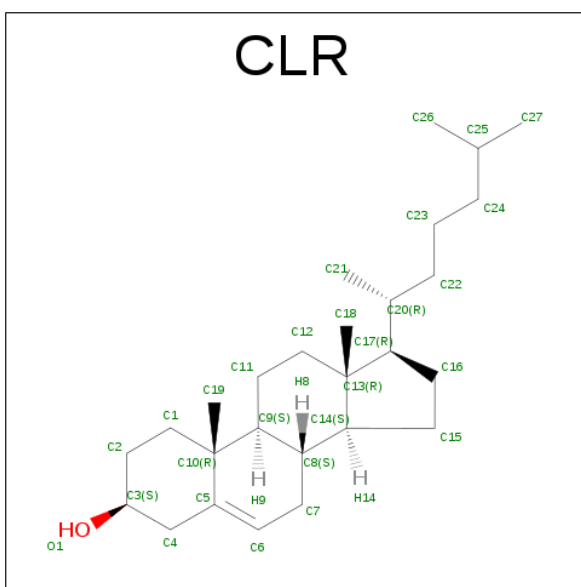
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	Br	C	N	O	0	0
			24	1	20	2	1		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



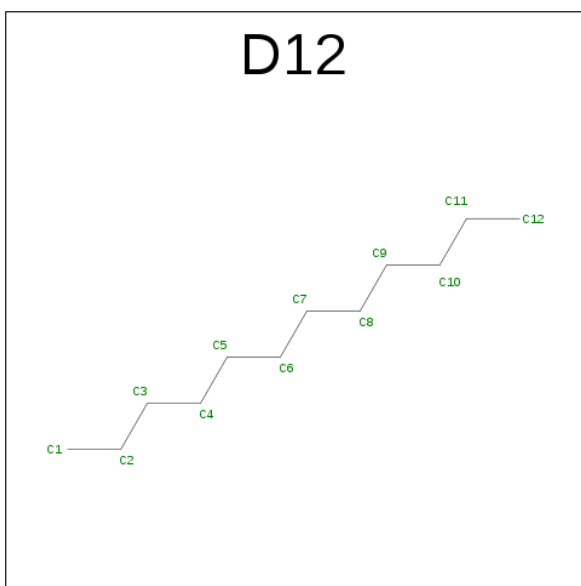
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



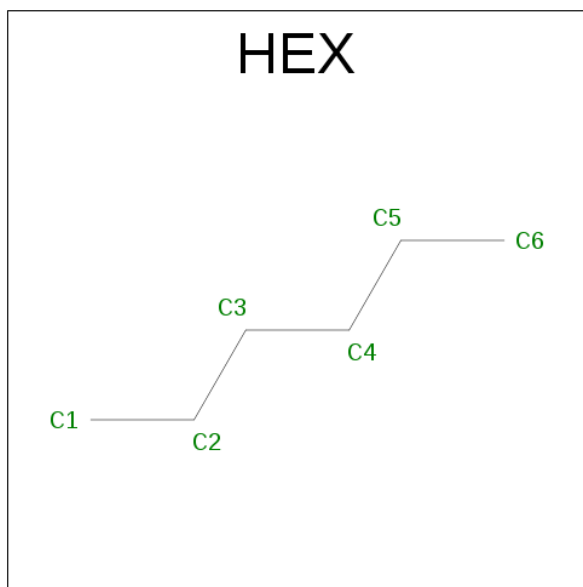
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 7 is DODECANE (three-letter code: D12) (formula:  $C_{12}H_{26}$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	C	0	0
			12	12		

- Molecule 8 is HEXANE (three-letter code: HEX) (formula:  $C_6H_{14}$ ).

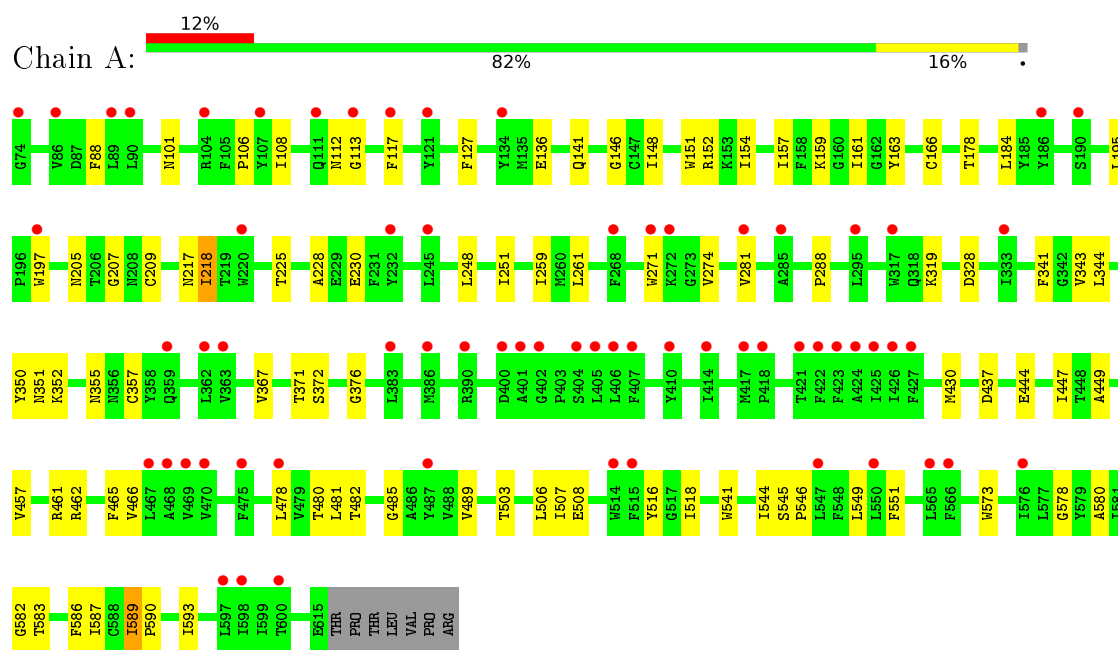


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 6 6	0	0

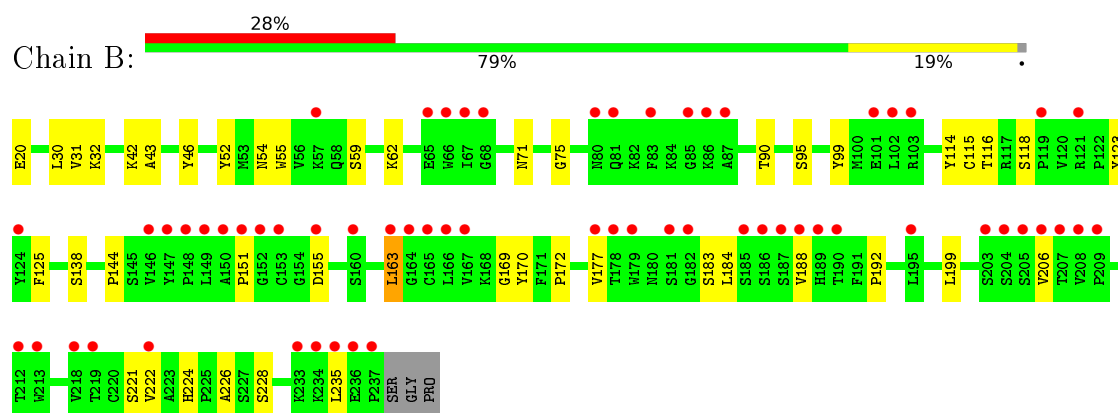
### 3 Residue-property plots

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

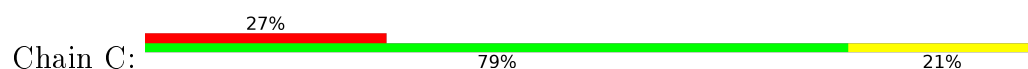
#### • Molecule 1: Sodium-dependent serotonin transporter



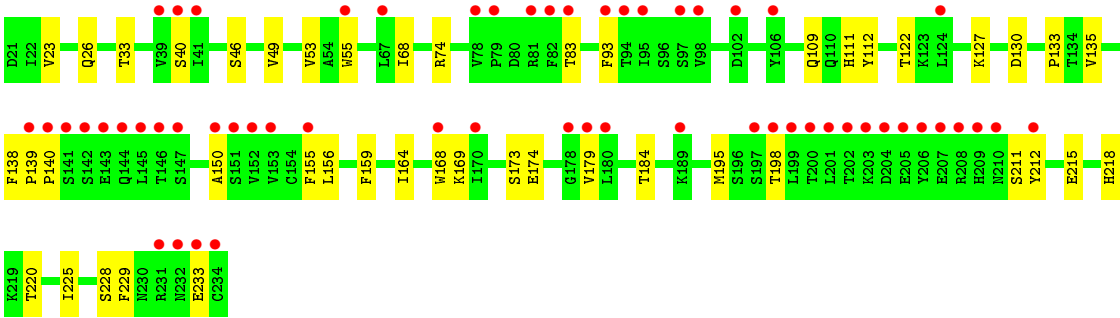
#### • Molecule 2: 8B6 antibody, heavy chain



#### • Molecule 3: 8B6 antibody, light chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.59 Å   164.00 Å   140.17 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	101.68 – 3.40 101.68 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (101.68-3.40) 99.4 (101.68-3.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 3.41 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1634)	Depositor
R, $R_{free}$	0.249   ,   0.296 0.249   ,   0.296	Depositor DCC
$R_{free}$ test set	1976 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	143.5	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 138.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	7610	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	209.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 69D, HEX, NAG, D12, CLR

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	0.25	0/4340	0.38	0/5934
2	B	0.24	0/1688	0.45	0/2309
3	C	0.25	0/1700	0.46	0/2307
All	All	0.25	0/7728	0.42	0/10550

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	4207	0	4101	50	0
2	B	1643	0	1589	28	0
3	C	1662	0	1585	24	0
4	A	24	0	0	1	0
5	A	28	0	26	2	0
6	A	28	0	46	4	0
7	A	12	0	26	1	0
8	A	6	0	14	0	0
All	All	7610	0	7387	102	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 7.

All (102) 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)
4:A:700:69D:O02	4:A:700:69D:C11	1.69	1.37
2:B:30:LEU:HD22	2:B:172:PRO:HD3	1.68	0.76
1:A:141:GLN:NE2	1:A:357:CYS:SG	2.61	0.74
1:A:205:ASN:ND2	1:A:209:CYS:SG	2.62	0.73
1:A:108:ILE:HD11	1:A:328:ASP:HB3	1.70	0.72
1:A:589:ILE:HG23	1:A:590:PRO:HD3	1.71	0.72
2:B:71:ASN:O	2:B:75:GLY:N	2.26	0.67
1:A:447:ILE:HD13	1:A:466:VAL:HG22	1.76	0.67
2:B:71:ASN:O	2:B:75:GLY:CA	2.42	0.67
2:B:192:PRO:HD3	3:C:184:THR:HG22	1.78	0.66
1:A:152:ARG:HH21	1:A:159:LYS:HZ1	1.47	0.62
1:A:127:PHE:HB3	1:A:544:ILE:HG21	1.81	0.62
3:C:211:SER:HA	3:C:229:PHE:O	2.00	0.61
1:A:352:LYS:HB2	1:A:355:ASN:HB2	1.83	0.61
2:B:71:ASN:O	2:B:75:GLY:HA2	2.00	0.61
1:A:444:GLU:OE1	1:A:462:ARG:NH2	2.34	0.60
2:B:30:LEU:HB2	2:B:172:PRO:HG3	1.83	0.60
3:C:135:VAL:HA	3:C:155:PHE:O	2.01	0.59
1:A:184:LEU:HD21	1:A:261:LEU:HD23	1.85	0.59
2:B:59:SER:HB2	2:B:62:LYS:HB2	1.84	0.59
3:C:49:VAL:HG13	3:C:112:TYR:CE1	2.39	0.58
5:A:701:NAG:HO3	2:B:20:GLU:N	2.02	0.57
1:A:157:ILE:HB	1:A:593:ILE:HG12	1.87	0.57
2:B:54:ASN:ND2	2:B:118:SER:OG	2.36	0.56
3:C:164:ILE:HB	3:C:218:HIS:HD2	1.71	0.56
3:C:55:TRP:HB2	3:C:68:ILE:HB	1.86	0.56
1:A:101:ASN:ND2	1:A:372:SER:OG	2.34	0.55
3:C:215:GLU:HA	3:C:225:ILE:O	2.06	0.55
1:A:148:ILE:HG13	1:A:449:ALA:HB1	1.87	0.55
1:A:207:GLY:HA3	5:A:701:NAG:H82	1.87	0.55
2:B:42:LYS:NZ	2:B:95:SER:O	2.38	0.54
2:B:224:HIS:O	2:B:228:SER:N	2.40	0.53
1:A:113:GLY:H	1:A:319:LYS:HG3	1.73	0.52
1:A:88:PHE:HE2	1:A:350:TYR:HB2	1.74	0.52
2:B:163:LEU:HB3	2:B:235:LEU:HD22	1.91	0.52
1:A:478:LEU:HD23	1:A:481:LEU:HD12	1.92	0.52
3:C:74:ARG:HH21	3:C:83:THR:HG22	1.75	0.52
1:A:580:ALA:HB1	6:A:702:CLR:H241	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ILE:HG21	1:A:481:LEU:HD11	1.93	0.50
1:A:573:TRP:CE3	6:A:702:CLR:H71	2.45	0.50
2:B:177:VAL:HA	2:B:221:SER:O	2.11	0.50
1:A:341:PHE:HD2	1:A:343:VAL:HG23	1.76	0.50
1:A:106:PRO:HG3	1:A:376:GLY:HA2	1.93	0.50
1:A:88:PHE:HZ	1:A:274:VAL:HB	1.77	0.49
3:C:130:ASP:HB3	3:C:220:THR:HG22	1.94	0.49
3:C:140:PRO:HG2	3:C:150:ALA:HB1	1.94	0.49
1:A:151:TRP:HZ2	1:A:508:GLU:HG2	1.78	0.48
2:B:151:PRO:HG3	3:C:138:PHE:HE2	1.77	0.48
3:C:212:TYR:O	3:C:228:SER:HA	2.14	0.48
2:B:116:THR:OG1	2:B:125:PHE:HB3	2.13	0.48
1:A:573:TRP:CZ3	6:A:702:CLR:H71	2.49	0.48
3:C:23:VAL:H	3:C:46:SER:HB3	1.79	0.48
1:A:178:THR:HG21	1:A:480:THR:HB	1.96	0.48
1:A:178:THR:HG22	1:A:259:ILE:HD12	1.95	0.47
1:A:583:THR:HA	1:A:586:PHE:CZ	2.49	0.47
3:C:133:PRO:HB3	3:C:159:PHE:HB3	1.97	0.47
1:A:506:LEU:HD23	1:A:549:LEU:HB2	1.96	0.47
1:A:146:GLY:HA3	1:A:449:ALA:HA	1.95	0.47
1:A:518:ILE:HD11	1:A:541:TRP:CE3	2.49	0.47
1:A:218:ILE:HD13	1:A:218:ILE:H	1.80	0.46
1:A:447:ILE:HA	1:A:465:PHE:HE2	1.80	0.46
1:A:197:TRP:HB2	1:A:228:ALA:HA	1.97	0.46
2:B:144:PRO:HB3	2:B:170:TYR:HB3	1.98	0.45
1:A:288:PRO:HA	1:A:430:MET:HG3	1.98	0.45
2:B:188:VAL:HG22	2:B:206:VAL:HB	1.98	0.44
1:A:251:ILE:HA	1:A:482:THR:HA	1.99	0.44
1:A:583:THR:O	1:A:587:ILE:HG23	2.18	0.43
6:A:702:CLR:H162	6:A:702:CLR:H231	2.00	0.43
1:A:163:TYR:O	1:A:166:CYS:HB2	2.19	0.43
1:A:136:GLU:HG2	1:A:344:LEU:HD12	2.00	0.43
1:A:485:GLY:O	1:A:489:VAL:HG23	2.18	0.43
2:B:32:LYS:HG2	2:B:138:SER:HA	2.00	0.43
3:C:26:GLN:NE2	3:C:122:THR:OG1	2.52	0.43
1:A:195:LEU:H	1:A:195:LEU:HD12	1.82	0.43
2:B:183:SER:HA	2:B:184:LEU:HA	1.50	0.42
2:B:90:THR:OG1	2:B:99:TYR:HB2	2.19	0.42
3:C:179:VAL:HA	3:C:198:THR:O	2.19	0.42
1:A:112:ASN:O	1:A:117:PHE:HB2	2.20	0.42
1:A:154:ILE:HG23	1:A:516:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:TRP:HA	2:B:114:TYR:O	2.19	0.42
2:B:123:TYR:HB3	3:C:111:HIS:HB2	2.01	0.42
3:C:169:LYS:HA	3:C:173:SER:O	2.19	0.42
3:C:156:LEU:HD13	3:C:195:MET:HG3	2.01	0.42
2:B:54:ASN:O	2:B:115:CYS:HA	2.20	0.42
1:A:225:THR:OG1	1:A:230:GLU:OE2	2.28	0.41
1:A:367:VAL:O	1:A:371:THR:OG1	2.30	0.41
1:A:545:SER:HB2	1:A:546:PRO:HD3	2.02	0.41
3:C:33:THR:O	3:C:127:LYS:N	2.39	0.41
1:A:503:THR:O	1:A:507:ILE:HG12	2.21	0.41
1:A:578:GLY:O	1:A:582:GLY:N	2.48	0.41
2:B:224:HIS:CE1	2:B:226:ALA:HB3	2.55	0.41
3:C:40:SER:HA	3:C:93:PHE:O	2.20	0.41
2:B:177:VAL:HG22	2:B:222:VAL:HG22	2.02	0.41
2:B:169:GLY:HA2	2:B:199:LEU:HB3	2.03	0.41
2:B:52:TYR:HE1	2:B:71:ASN:HB2	1.85	0.41
3:C:168:TRP:O	3:C:174:GLU:HA	2.21	0.41
1:A:161:ILE:HD11	1:A:507:ILE:HG22	2.04	0.40
2:B:43:ALA:HB1	2:B:46:TYR:CE1	2.56	0.40
7:A:703:D12:H52	7:A:703:D12:H21	1.93	0.40
3:C:212:TYR:HB2	3:C:229:PHE:CE1	2.55	0.40
3:C:139:PRO:HB3	3:C:229:PHE:CE2	2.56	0.40
1:A:141:GLN:OE1	1:A:351:ASN:ND2	2.55	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	540/549 (98%)	519 (96%)	21 (4%)	0	100	100
2	B	216/221 (98%)	209 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
All	All	968/984 (98%)	927 (96%)	41 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	428/462 (93%)	418 (98%)	10 (2%)	58	85
2	B	190/193 (98%)	187 (98%)	3 (2%)	70	89
3	C	189/190 (100%)	186 (98%)	3 (2%)	70	89
All	All	807/845 (96%)	791 (98%)	16 (2%)	63	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	218	ILE
1	A	248	LEU
1	A	271	TRP
1	A	281	VAL
1	A	437	ASP
1	A	457	VAL
1	A	461	ARG
1	A	551	PHE
1	A	589	ILE
2	B	31	VAL
2	B	155	ASP
2	B	163	LEU
3	C	53	VAL
3	C	109	GLN
3	C	233	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	26	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](#)

6 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	$\# Z  > 2$
4	69D	A	700	-	24,26,26	6.20	10 (41%)	31,37,37	3.35	10 (32%)
5	NAG	A	701	1	14,14,15	0.20	0	15,19,21	0.44	0
6	CLR	A	702	-	31,31,31	0.80	0	48,48,48	1.24	4 (8%)
7	D12	A	703	-	11,11,11	0.11	0	10,10,10	0.32	0
8	HEX	A	704	-	5,5,5	0.15	0	4,4,4	0.55	0
5	NAG	A	705	1	14,14,15	0.23	0	15,19,21	0.29	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	69D	A	700	-	-	0/15/27/27	0/3/3/3
5	NAG	A	701	1	-	0/6/23/26	0/1/1/1
6	CLR	A	702	-	-	0/10/68/68	0/4/4/4
7	D12	A	703	-	-	0/9/9/9	0/0/0/0
8	HEX	A	704	-	-	0/3/3/3	0/0/0/0
5	NAG	A	705	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	69D	C05-C07	-13.26	1.32	1.52
4	A	700	69D	C17-C18	-11.44	1.14	1.39
4	A	700	69D	C17-C13	-10.18	1.18	1.38
4	A	700	69D	C14-C18	-3.16	1.34	1.39
4	A	700	69D	C08-C07	-2.38	1.35	1.39
4	A	700	69D	C13-C07	-2.07	1.36	1.39
4	A	700	69D	C18-C24	3.46	1.53	1.44
4	A	700	69D	C11-C08	6.10	1.59	1.50
4	A	700	69D	C14-C08	11.42	1.59	1.39
4	A	700	69D	O02-C11	17.44	1.69	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	69D	C13-C07-C08	-10.89	108.94	120.78
4	A	700	69D	C13-C07-C05	-5.52	122.59	130.96
4	A	700	69D	C14-C08-C07	-4.28	117.33	121.10
4	A	700	69D	C09-C06-C05	-4.14	107.83	115.23
4	A	700	69D	C18-C14-C08	-3.18	116.39	120.70
6	A	702	CLR	C8-C7-C6	-2.87	108.34	112.76
6	A	702	CLR	C13-C14-C8	-2.48	110.50	114.36
4	A	700	69D	C09-C12-N03	-2.33	108.03	113.83
4	A	700	69D	C17-C18-C14	-2.24	116.71	119.79
6	A	702	CLR	C4-C5-C10	2.17	119.56	116.41
6	A	702	CLR	C9-C10-C5	2.65	114.22	109.67
4	A	700	69D	C17-C13-C07	4.78	130.24	121.94
4	A	700	69D	C11-C08-C14	6.33	142.67	129.40
4	A	700	69D	C13-C17-C18	8.00	130.38	120.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	69D	1	0
5	A	701	NAG	2	0
6	A	702	CLR	4	0
7	A	703	D12	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	542/549 (98%)	0.61	66 (12%)	5 5	106, 163, 232, 359	0
2	B	218/221 (98%)	1.45	61 (27%)	1 1	110, 221, 445, 538	0
3	C	214/214 (100%)	1.81	57 (26%)	1 1	137, 240, 585, 730	0
All	All	974/984 (98%)	1.06	184 (18%)	2 2	106, 178, 402, 730	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	151	PRO	25.8
3	C	202	THR	21.5
3	C	206	TYR	18.4
2	B	150	ALA	14.9
2	B	188	VAL	13.5
3	C	151	SER	12.8
2	B	237	PRO	12.2
3	C	201	LEU	12.2
3	C	233	GLU	12.0
3	C	152	VAL	11.3
3	C	209	HIS	10.8
3	C	204	ASP	10.7
2	B	152	GLY	10.5
3	C	200	THR	10.3
3	C	232	ASN	10.2
3	C	205	GLU	10.1
2	B	187	SER	10.1
3	C	142	SER	10.0
3	C	141	SER	9.9
2	B	204	SER	9.8
3	C	207	GLU	9.6
2	B	179	TRP	9.0
3	C	143	GLU	8.8

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Mol	Chain	Res	Type	RSRZ
3	C	150	ALA	8.5
3	C	203	LYS	8.3
3	C	199	LEU	7.9
2	B	186	SER	7.6
3	C	231	ARG	7.3
3	C	39	VAL	7.2
2	B	190	THR	7.1
2	B	182	GLY	7.0
2	B	208	VAL	6.8
3	C	95	ILE	6.5
1	A	401	ALA	6.5
1	A	423	PHE	6.5
3	C	208	ARG	6.5
1	A	422	PHE	6.4
3	C	146	THR	6.1
2	B	219	THR	6.1
2	B	185	SER	6.0
2	B	155	ASP	5.9
2	B	163	LEU	5.8
1	A	514	TRP	5.8
3	C	153	VAL	5.8
2	B	149	LEU	5.6
3	C	144	GLN	5.5
3	C	212	TYR	5.4
2	B	153	CYS	5.4
2	B	218	VAL	5.2
3	C	198	THR	5.2
3	C	82	PHE	5.2
2	B	189	HIS	5.0
3	C	94	THR	5.0
2	B	148	PRO	4.9
3	C	170	ILE	4.9
2	B	235	LEU	4.9
1	A	426	ILE	4.9
2	B	102	LEU	4.8
2	B	66	TRP	4.8
1	A	417	MET	4.7
3	C	106	TYR	4.7
2	B	233	LYS	4.6
2	B	236	GLU	4.4
3	C	98	VAL	4.4
3	C	139	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	418	PRO	4.4
2	B	166	LEU	4.3
2	B	207	THR	4.3
1	A	245	LEU	4.2
1	A	113	GLY	4.1
3	C	93	PHE	4.1
1	A	74	GLY	4.1
2	B	80	ASN	4.0
1	A	317	TRP	3.9
2	B	209	PRO	3.9
2	B	212	THR	3.9
2	B	86	LYS	3.9
1	A	407	PHE	3.8
1	A	414	ILE	3.7
2	B	87	ALA	3.7
3	C	210	ASN	3.6
3	C	124	LEU	3.5
1	A	598	ILE	3.5
2	B	205	SER	3.5
3	C	78	VAL	3.5
1	A	427	PHE	3.5
1	A	425	ILE	3.4
2	B	83	PHE	3.4
3	C	41	ILE	3.4
2	B	65	GLU	3.4
2	B	181	SER	3.4
1	A	424	ALA	3.4
2	B	177	VAL	3.3
2	B	165	CYS	3.3
1	A	547	LEU	3.3
2	B	146	VAL	3.3
1	A	134	TYR	3.2
2	B	167	VAL	3.2
1	A	86	VAL	3.2
1	A	220	TRP	3.2
1	A	405	LEU	3.2
2	B	164	GLY	3.1
2	B	195	LEU	3.1
2	B	206	VAL	3.1
1	A	487	TYR	3.1
1	A	406	LEU	3.1
1	A	359	GLN	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	281	VAL	3.1
2	B	124	TYR	3.0
1	A	190	SER	3.0
1	A	515	PHE	3.0
3	C	40	SER	3.0
3	C	197	SER	2.9
3	C	81	ARG	2.9
1	A	400	ASP	2.9
3	C	145	LEU	2.8
1	A	232	TYR	2.8
3	C	79	PRO	2.8
2	B	103	ARG	2.8
1	A	197	TRP	2.7
1	A	402	GLY	2.7
3	C	189	LYS	2.7
1	A	107	TYR	2.7
1	A	271	TRP	2.7
1	A	469	VAL	2.6
1	A	186	TYR	2.6
2	B	121	ARG	2.6
1	A	295	LEU	2.6
3	C	155	PHE	2.5
1	A	90	LEU	2.5
1	A	478	LEU	2.5
3	C	140	PRO	2.5
3	C	179	VAL	2.5
1	A	104	ARG	2.5
1	A	386	MET	2.5
2	B	147	TYR	2.5
3	C	83	THR	2.5
1	A	468	ALA	2.4
1	A	565	LEU	2.4
1	A	597	LEU	2.4
3	C	178	GLY	2.4
2	B	178	THR	2.4
3	C	55	TRP	2.4
3	C	97	SER	2.4
1	A	600	THR	2.4
2	B	81	GLN	2.3
1	A	576	ILE	2.3
1	A	362	LEU	2.3
1	A	111	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	272	LYS	2.3
1	A	467	LEU	2.3
2	B	68	GLY	2.3
2	B	57	LYS	2.3
2	B	160	SER	2.3
1	A	390	ARG	2.3
1	A	121	TYR	2.3
2	B	67	ILE	2.3
1	A	410	TYR	2.3
1	A	404	SER	2.2
1	A	383	LEU	2.2
1	A	566	PHE	2.2
2	B	119	PRO	2.2
3	C	102	ASP	2.2
2	B	203	SER	2.2
2	B	85	GLY	2.2
1	A	475	PHE	2.2
1	A	285	ALA	2.2
1	A	421	THR	2.2
3	C	168	TRP	2.2
1	A	117	PHE	2.2
3	C	147	SER	2.1
1	A	550	LEU	2.1
3	C	234	CYS	2.1
2	B	101	GLU	2.1
1	A	89	LEU	2.1
1	A	268	PHE	2.1
3	C	67	LEU	2.1
1	A	363	VAL	2.1
1	A	333	ILE	2.1
1	A	470	VAL	2.0
2	B	234	LYS	2.0
2	B	213	TRP	2.0
2	B	222	VAL	2.0
3	C	180	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	CLR	A	702	28/28	0.55	1.59	6.51	166,215,229,239	0
4	69D	A	700	24/24	0.90	0.46	3.38	119,155,185,275	0
7	D12	A	703	12/12	0.73	0.53	1.74	100,111,126,134	0
8	HEX	A	704	6/6	0.80	0.41	1.15	77,106,122,136	0
5	NAG	A	705	14/15	0.67	0.26	1.12	341,346,348,350	0
5	NAG	A	701	14/15	0.92	0.18	-0.57	99,122,205,206	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.