

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 8, 2020 – 11:02 PM BST

PDB ID	:	5I6X
$\operatorname{Title}$	:	X-ray structure of the ts3 human serotonin transporter complexed with parox-
		etine at the central site
Authors	:	Coleman, J.A.; Green, E.M.; Gouaux, E.
Deposited on	:	2016-02-16
Resolution	:	3.14  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.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	÷	4.02b-467
Mogul		1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
CCP4	:	7.0.044  (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

# 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 3.14 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
$R_{free}$	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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	А	549	7% 260	%		
2	В	221	88%	119	6.	
3	С	214	89%	11	%	

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	NAG	А	704	-	-	-	Х



## 2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 7631 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	А	544	Total 4221	C 2817	N 656	О 724	S 24	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
2	В	218	Total	С	Ν	Ο	$\mathbf{S}$	0	Ο	Ο
	D	210	1643	1038	266	331	8		0	0

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

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

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





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	Λ	1	Total	С	Ν	0	0	0
	T	14	8	1	5	0	0	
4	Λ	1	Total	С	Ν	Ο	0	0
4	А		14	8	1	5		0

• Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	А	1	Total 28	С 27	0 1	0	0

• Molecule 6 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:



 $C_{24}H_{46}O_{11}).$ 



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	А	1	Total 22	C 12	O 10	0	0

• Molecule 7 is Paroxetine (three-letter code: 8PR) (formula:  $C_{19}H_{20}FNO_3$ ).



Mol	Chain	Residues		Ato	$\mathbf{ms}$			ZeroOcc	AltConf
7	А	1	Total 24	С 19	F 1	N 1	O 3	0	0

• Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	Total Cl 1 1	0	0

• Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	Total Na 1 1	0	0

• Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	1	Total O 1 1	0	0



## 3 Residue-property plots (i)

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







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	129.15Å $162.83$ Å $140.41$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	53.17 - 3.14	Depositor
Resolution (A)	82.09 - 3.14	EDS
% Data completeness	99.9(53.17-3.14)	Depositor
(in resolution range)	99.8 (82.09-3.14)	EDS
$R_{merge}$	0.13	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.57 (at 3.13 \text{\AA})$	Xtriage
Refinement program	PHENIX (DEV_2000: ???)	Depositor
B B.	0.238 , $0.270$	Depositor
$n, n_{free}$	0.240 , $0.270$	DCC
$R_{free}$ test set	1307  reflections  (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	105.9	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.26 , $83.9$	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.40, < L^2>=0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7631	wwPDB-VP
Average B, all atoms $(Å^2)$	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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, CL, NA, LMT, 8PR, 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).

Mal	Chain	Bond	lengths	Bond angles		
	Cham	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.35	0/4355	0.44	0/5955	
2	В	0.21	0/1688	0.37	0/2309	
3	С	0.21	0/1700	0.36	0/2307	
All	All	0.29	0/7743	0.41	0/10571	

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	А	4221	0	4115	150	0
2	В	1643	0	1589	14	0
3	С	1662	0	1585	12	0
4	А	28	0	26	4	0
5	А	28	0	46	4	0
6	А	22	0	20	4	0
7	А	24	0	20	4	0
8	А	1	0	0	1	0
9	А	1	0	0	0	0
10	А	1	0	0	1	0
All	All	7631	0	7401	180	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 12.

All $(180)$	$\operatorname{close}$	$\operatorname{contacts}$	within	the same	a symmetric	$\operatorname{unit}$	$\operatorname{are}$	listed	below,	sorted $\$	$\mathbf{b}\mathbf{y}$	their	$\operatorname{clash}$
magnitud	e.												

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:461:ARG:HH11	1:A:461:ARG:HG3	1.30	0.97	
1:A:563:LEU:HD12	1:A:563:LEU:H	1.32	0.94	
1:A:573:TRP:CE3	5:A:702:CLR:H71	2.03	0.93	
1:A:393:ASP:OD2	1:A:396:GLU:OE2	1.91	0.88	
1:A:453:GLU:HG3	1:A:454:PHE:CE1	2.10	0.86	
3:C:168:TRP:HE1	3:C:197:SER:HG	1.26	0.82	
1:A:560:PRO:HA	6:A:703:LMT:H6'2	1.61	0.81	
1:A:215:GLU:O	1:A:218:ILE:HG23	1.80	0.81	
1:A:453:GLU:HG3	1:A:454:PHE:CD1	2.14	0.81	
1:A:219:THR:OG1	4:A:704:NAG:H61	1.81	0.80	
1:A:253:TRP:CZ2	1:A:254:GLN:NE2	2.52	0.78	
1:A:327:ILE:HD13	1:A:555:SER:CB	2.14	0.78	
1:A:393:ASP:OD2	1:A:396:GLU:HG2	1.83	0.77	
1:A:327:ILE:HD13	1:A:555:SER:HB2	1.67	0.76	
2:B:54:ASN:HD22	2:B:66:TRP:HE1	1.31	0.76	
1:A:461:ARG:NH1	1:A:461:ARG:HG3	1.97	0.73	
1:A:563:LEU:N	1:A:563:LEU:HD12	2.03	0.73	
1:A:393:ASP:O	1:A:395:SER:N	2.22	0.73	
1:A:458:TRP:CZ3	1:A:465:PHE:HB2	2.26	0.71	
1:A:334:PHE:CE2	1:A:502:LEU:HD23	2.26	0.70	
7:A:705:8PR:HAM	7:A:705:8PR:CAF	2.20	0.70	
1:A:142:TYR:HD2	1:A:143:HIS:CE1	2.10	0.70	
1:A:208:ASN:O	1:A:210:THR:HG23	1.92	0.69	
1:A:205:ASN:ND2	1:A:209:CYS:SG	2.66	0.69	
1:A:101:ASN:ND2	1:A:372:SER:OG	2.26	0.69	
1:A:142:TYR:HD2	1:A:143:HIS:ND1	1.92	0.68	
1:A:334:PHE:CZ	1:A:502:LEU:HD23	2.29	0.68	
6:A:703:LMT:H6D	6:A:703:LMT:O3'	1.93	0.67	
1:A:498:GLY:N	1:A:499:PRO:CD	2.57	0.67	
1:A:499:PRO:CD	1:A:500:ALA:H	2.09	0.66	
1:A:216:ASP:CG	1:A:217:ASN:H	1.99	0.66	
1:A:335:PHE:HD1	7:A:705:8PR:HAB	1.61	0.65	
1:A:453:GLU:HG3	1:A:454:PHE:HE1	1.62	0.64	
1:A:437:ASP:N	1:A:437:ASP:OD1	2.29	0.64	
1:A:437:ASP:OD2	10:A:1001:HOH:O	2.14	0.64	
1:A:215:GLU:O	1:A:218:ILE:CG2	2.47	0.63	
2:B:192:PRO:HD3	3:C:184:THR:HG22	1.81	0.63	



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:393:ASP:OD2	1:A:396:GLU:CG	2.47	0.63		
1:A:142:TYR:CD2	1:A:143:HIS:CE1	2.87	0.62		
1:A:363:VAL:O	1:A:367:VAL:HG23	1.98	0.62		
1:A:573:TRP:CZ3	5:A:702:CLR:H71	2.33	0.62		
3:C:171:ASP:OD2	3:C:209:HIS:ND1	2.30	0.61		
1:A:499:PRO:HD2	1:A:500:ALA:H	1.65	0.61		
1:A:453:GLU:C	1:A:454:PHE:HD1	2.04	0.61		
1:A:334:PHE:CE2	1:A:502:LEU:CD2	2.83	0.61		
1:A:396:GLU:OE1	1:A:399:LYS:HE3	2.01	0.61		
1:A:447:ILE:HD13	1:A:466:VAL:HG22	1.83	0.60		
1:A:113:GLY:HA2	1:A:316:ASN:HB3	1.82	0.60		
1:A:552:ILE:HG22	1:A:556:PHE:CE1	2.36	0.60		
1:A:455:PRO:O	1:A:457:VAL:N	2.27	0.60		
1:A:454:PHE:O	1:A:458:TRP:HB2	2.01	0.60		
1:A:91:SER:HA	1:A:281:VAL:HG11	1.83	0.59		
1:A:497:THR:C	1:A:499:PRO:HD2	2.23	0.58		
1:A:526:LYS:HD3	1:A:532:SER:HB2	1.85	0.58		
1:A:499:PRO:CG	1:A:500:ALA:N	2.67	0.57		
3:C:74:ARG:HH21	3:C:83:THR:HG22	1.70	0.57		
1:A:393:ASP:OD2	1:A:396:GLU:CD	2.43	0.57		
1:A:184:LEU:HD21	1:A:261:LEU:HD23	1.86	0.56		
1:A:546:PRO:O	1:A:550:LEU:HB2	2.05	0.56		
1:A:292:LEU:O	1:A:296:LEU:HB2	2.06	0.56		
1:A:394:VAL:O	1:A:397:VAL:HG12	2.07	0.55		
1:A:216:ASP:OD1	1:A:217:ASN:N	2.37	0.55		
2:B:86:LYS:NZ	2:B:104:SER:O	2.39	0.55		
2:B:30:LEU:HD22	2:B:172:PRO:HD3	1.89	0.55		
1:A:334:PHE:CD2	1:A:502:LEU:HD21	2.43	0.54		
1:A:495:TYR:HE1	1:A:561:PRO:HD2	1.71	0.54		
1:A:556:PHE:CD2	6:A:703:LMT:H4B	2.41	0.54		
2:B:188:VAL:HG22	2:B:206:VAL:HG23	1.89	0.54		
1:A:502:LEU:HD13	1:A:552:ILE:HB	1.91	0.53		
1:A:125:ALA:O	1:A:130:ILE:HG12	2.08	0.53		
1:A:501:VAL:HA	1:A:504:VAL:HG12	1.90	0.53		
1:A:498:GLY:N	1:A:499:PRO:HD3	2.24	0.53		
1:A:499:PRO:CG	1:A:500:ALA:H	2.22	0.53		
1:A:85:LYS:HE2	1:A:355:ASN:HD21	1.74	0.53		
1:A:453:GLU:HG3	1:A:454:PHE:HD1	1.70	0.52		
1:A:492:LEU:O	1:A:497:THR:HG23	2.10	0.52		
1:A:195:LEU:H	1:A:195:LEU:HD12	1.73	0.52		
6:A:703:LMT:H4'	6:A:703:LMT:O2B	2.09	0.52		



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:A:705:8PB:HAF	7:A:705:8PR:HAH	1.90	0.52
3:C:55:TRP:CD2	3:C:93:PHE:HB2	2.45	0.52
1:A:499:PRO:HG2	1:A:500:ALA:N	2.25	0.52
1:A:396:GLU:HA	1:A:396:GLU:OE1	2.10	0.52
1:A:362:LEU:O	1:A:366:VAL:HG23	2.10	0.51
1:A:178:THR:HG21	1:A:480:THR:HB	1.92	0.51
1:A:136:GLU:HG2	1:A:344:LEU:HB2	1.92	0.51
3:C:111:HIS:O	3:C:111:HIS:ND1	2.43	0.51
1:A:499:PRO:CD	1:A:500:ALA:N	2.73	0.50
1:A:253:TRP:CE2	1:A:254:GLN:NE2	2.79	0.50
1:A:458:TRP:O	1:A:459:ALA:HB3	2.11	0.50
3:C:135:VAL:HA	3:C:155:PHE:O	2.10	0.50
3:C:211:SER:HA	3:C:229:PHE:O	2.12	0.50
1:A:206:THR:HG23	1:A:234:ARG:NH2	2.27	0.49
1:A:122:THR:O	1:A:125:ALA:HB3	2.13	0.49
2:B:59:SER:HB2	2:B:62:LYS:HB2	1.95	0.49
1:A:219:THB:OG1	4:A:704:NAG:C6	2.56	0.49
1:A:263:PHE:O	1:A:267:TYR:HB2	2.13	0.49
1:A:478:LEU:HD23	1:A:481:LEU:HD12	1.95	0.49
1:A:425:ILE:O	1:A:429:LEU:HB2	2.13	0.48
1:A:197:TRP:HB2	1:A:228:ALA:HA	1.95	0.48
1:A:137:LEU:HD12	1:A:348:ALA:HB2	1.96	0.48
1:A:85:LYS:NZ	1:A:360:ASP:OD2	2.46	0.47
1:A:429:LEU:O	1:A:433:THR:OG1	2.16	0.47
1:A:605:LYS:O	1:A:609:ILE:CB	2.62	0.47
1:A:216:ASP:CG	1:A:217:ASN:N	2.67	0.47
1:A:152:ARG:O	1:A:615:GLU:HG2	2.14	0.47
1:A:495:TYR:CE1	1:A:561:PRO:HD2	2.48	0.47
3:C:138:PHE:HB2	3:C:153:VAL:HB	1.95	0.47
1:A:453:GLU:C	1:A:454:PHE:CD1	2.86	0.47
1:A:573:TRP:CZ3	5:A:702:CLR:C7	2.98	0.47
1:A:455:PRO:O	1:A:456:HIS:HB3	2.15	0.47
1:A:393:ASP:O	1:A:394:VAL:C	2.51	0.46
1:A:256:ALA:O	1:A:260:MET:HB2	2.15	0.46
1:A:485:GLY:O	1:A:489:VAL:HG23	2.16	0.46
1:A:336:SER:O	7:A:705:8PR:HAIA	2.15	0.46
1:A:594:ALA:O	1:A:598:ILE:CB	2.64	0.46
1:A:87:ASP:OD1	1:A:282:TRP:NE1	2.39	0.46
1:A:552:ILE:CG2	1:A:556:PHE:CE1	2.98	0.46
1:A:396:GLU:HA	1:A:399:LYS:HG3	1.98	0.45
1:A:447:ILE:HA	1:A:465:PHE:HE2	1.81	0.45



	to as pagem	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:121:TYR:OH	8:A:706:CL:CL	2.56	0.45
1:A:484:GLY:O	1:A:487:TYR:HB2	2.16	0.45
2:B:80:ASN:HB3	2:B:83:PHE:HD2	1.81	0.45
3:C:231:ARG:O	3:C:233:GLU:N	2.47	0.45
3:C:23:VAL:H	3:C:46:SER:HB3	1.81	0.45
1:A:497:THR:O	1:A:499:PRO:HD2	2.16	0.45
1:A:207:GLY:HA3	4:A:701:NAG:H82	1.98	0.45
1:A:577:LEU:O	1:A:581:ILE:HG13	2.17	0.45
1:A:266:ILE:HG22	1:A:440:PHE:HE1	1.82	0.44
1:A:499:PRO:HG2	1:A:500:ALA:H	1.81	0.44
2:B:163:LEU:O	2:B:205:SER:HA	2.17	0.44
1:A:155:CYS:HA	1:A:156:PRO:HD2	1.88	0.44
1:A:266:ILE:HG22	1:A:440:PHE:CE1	2.53	0.43
1:A:396:GLU:OE1	1:A:399:LYS:CE	2.66	0.43
1:A:540:CYS:HA	1:A:544:ILE:HB	1.99	0.43
1:A:219:THR:CG2	4:A:704:NAG:H61	2.48	0.43
1:A:279:LYS:O	1:A:282:TRP:HB2	2.19	0.43
1:A:545:SER:HB2	1:A:546:PRO:HD3	2.00	0.43
1:A:456:HIS:C	1:A:458:TRP:N	2.69	0.43
2:B:57:LYS:HB2	2:B:67:ILE:HD11	2.01	0.43
5:A:702:CLR:H231	5:A:702:CLR:H162	2.00	0.43
1:A:454:PHE:N	1:A:454:PHE:CD1	2.87	0.43
1:A:460:LYS:HG2	1:A:461:ARG:H	1.83	0.43
1:A:214:SER:OG	1:A:215:GLU:N	2.51	0.42
1:A:139:LEU:HD11	1:A:512:VAL:HG11	2.01	0.42
1:A:195:LEU:HA	1:A:196:PRO:HD3	1.84	0.42
1:A:253:TRP:CH2	1:A:254:GLN:NE2	2.88	0.42
2:B:52:TYR:HE1	2:B:71:ASN:HB2	1.85	0.42
1:A:455:PRO:C	1:A:457:VAL:N	2.72	0.42
1:A:263:PHE:HD1	1:A:266:ILE:HD11	1.85	0.42
1:A:325:VAL:HG23	1:A:326:TRP:N	2.35	0.42
3:C:165:ASN:HB3	3:C:217:THR:HB	2.01	0.42
1:A:156:PRO:O	1:A:159:LYS:HB2	2.20	0.41
1:A:281:VAL:HA	1:A:284:THR:OG1	2.20	0.41
1:A:425:ILE:O	1:A:429:LEU:CB	2.67	0.41
2:B:191:PHE:HA	2:B:192:PRO:HD3	1.87	0.41
1:A:102:VAL:HG21	1:A:434:LEU:CD1	2.50	0.41
1:A:455:PRO:C	1:A:457:VAL:H	2.19	0.41
2:B:183:SER:HA	2:B:184:LEU:HA	1.51	0.41
1:A:242:SER:HB2	1:A:248:LEU:HA	2.03	0.41
1:A:96:ALA:O	1:A:368:ASN:OD1	2.39	0.41



Atom 1	Atom D	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:234:ARG:HE	1:A:240:HIS:CG	2.38	0.41	
1:A:461:ARG:HH11	1:A:461:ARG:CG	2.12	0.41	
1:A:518:ILE:HD11	1:A:541:TRP:CE3	2.55	0.41	
1:A:577:LEU:O	1:A:580:ALA:HB3	2.21	0.41	
1:A:105:PHE:HA	1:A:108:ILE:HG22	2.02	0.41	
1:A:600:THR:HA	1:A:601:PRO:HD3	1.85	0.41	
2:B:54:ASN:ND2	2:B:69:ASN:HB3	2.35	0.41	
1:A:143:HIS:NE2	1:A:154:ILE:HD11	2.36	0.41	
1:A:400:ASP:N	1:A:400:ASP:OD1	2.50	0.41	
1:A:239:ILE:HD11	1:A:487:TYR:CE1	2.56	0.41	
1:A:263:PHE:HA	1:A:266:ILE:HG12	2.03	0.40	
1:A:459:ALA:O	1:A:460:LYS:C	2.59	0.40	
1:A:497:THR:C	1:A:499:PRO:CD	2.89	0.40	
2:B:163:LEU:HB3	2:B:235:LEU:HD22	2.03	0.40	
1:A:454:PHE:N	1:A:454:PHE:HD1	2.19	0.40	
1:A:161:ILE:HG13	1:A:589:ILE:HD12	2.03	0.40	
1:A:101:ASN:HD21	1:A:368:ASN:ND2	2.18	0.40	
1:A:458:TRP:O	1:A:459:ALA:CB	2.70	0.40	
1:A:311:PHE:CZ	1:A:395:SER:HB2	2.56	0.40	
1:A:563:LEU:HD13	1:A:570:TYR:CG	2.57	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	А	542/549~(99%)	521 (96%)	21~(4%)	0	100 100
2	В	216/221 (98%)	207~(96%)	9~(4%)	0	100 100
3	С	212/214 (99%)	200 (94%)	12~(6%)	0	100 100
All	All	970/984~(99%)	928 (96%)	42 (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.

Mol	Chain	Analysed	Rotameric	Rotameric Outliers		Percentiles		
1	А	430/462~(93%)	423~(98%)	7(2%)	62	84		
2	В	190/193~(98%)	190~(100%)	0	100	100		
3	С	189/190~(100%)	188~(100%)	1 (0%)	88	95		
All	All	809/845~(96%)	801 (99%)	8 (1%)	76	89		

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	217	ASN
1	А	260	MET
1	А	271	TRP
1	А	437	ASP
1	А	460	LYS
1	А	461	ARG
1	А	563	LEU
3	С	109	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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).

Mal	Tune	Chain	Dog	Tink	Bo	ond leng	$_{\rm sths}$	B	ond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	LMT	А	703	-	23,23,36	0.43	0	33,33,47	1.37	4 (12%)
5	CLR	А	702	-	31,31,31	0.84	0	48,48,48	1.31	4 (8%)
7	8PR	А	705	-	26,27,27	1.97	6 (23%)	33,37,37	1.73	7 (21%)
4	NAG	А	701	1	14,14,15	0.26	0	17,19,21	0.61	0
4	NAG	А	704	1	14,14,15	0.24	0	17,19,21	0.37	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
6	LMT	А	703	-	-	7/8/45/61	0/2/2/2
5	CLR	А	702	-	-	6/10/68/68	0/4/4/4
7	8PR	А	705	-	-	4/9/26/26	0/4/4/4
4	NAG	А	701	1	-	2/6/23/26	0/1/1/1
4	NAG	А	704	1	-	1/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
7	А	705	8PR	CAT-CAX	4.71	1.58	1.51
7	А	705	8PR	OAO-CAS	3.81	1.46	1.37
7	А	705	8PR	CAJ-CAX	-3.75	1.48	1.53
7	А	705	8PR	OAP-CAU	3.69	1.43	1.38



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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
7	А	705	8PR	OAQ-CAV	3.22	1.43	1.38
7	А	705	8PR	CAX-CAW	-2.98	1.47	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	А	705	8PR	OAO-CAS-CAH	-3.86	101.34	119.86
7	А	705	8PR	OAO-CAS-CAD	3.60	137.66	119.94
6	А	703	LMT	C1B-O5B-C5B	3.48	120.51	113.69
7	А	705	8PR	OAQ-CAV-CAH	3.39	132.39	127.85
6	А	703	LMT	C1B-C2B-C3B	3.22	116.70	110.00
5	А	702	CLR	C8-C7-C6	-3.08	108.31	112.73
5	А	702	CLR	C9-C10-C5	2.93	114.25	109.65
6	А	703	LMT	O5B-C1B-C2B	2.70	116.06	110.35
5	А	702	CLR	C13-C14-C8	-2.62	110.50	114.38
7	А	705	8PR	CAC-CAR-CAB	-2.61	119.36	122.83
7	А	705	8PR	CAE-CAB-CAR	2.58	121.03	118.36
5	А	702	CLR	C4-C5-C10	2.34	119.52	116.42
7	A	705	8PR	OAQ-CAV-CAU	-2.32	107.14	109.78
7	A	705	8PR	OAP-CAU-CAG	2.30	132.00	127.81
6	A	703	LMT	C3B-C4B-C5B	-2.21	106.30	110.24

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	А	705	8PR	OAO-CAM-CAW-CAK
6	А	703	LMT	O5B-C1B-O1B-C4'
6	А	703	LMT	C2B-C1B-O1B-C4'
4	А	701	NAG	O5-C5-C6-O6
6	А	703	LMT	O5'-C5'-C6'-O6'
4	А	701	NAG	C4-C5-C6-O6
7	А	705	8PR	CAD-CAS-OAO-CAM
6	А	703	LMT	C3'-C4'-O1B-C1B
6	А	703	LMT	C4'-C5'-C6'-O6'
7	А	705	8PR	CAH-CAS-OAO-CAM
5	А	702	CLR	C17-C20-C22-C23
5	А	702	CLR	C21-C20-C22-C23
6	А	703	LMT	C5'-C4'-O1B-C1B
6	A	703	LMT	O5B-C5B-C6B-O6B
4	A	704	NAG	O5-C5-C6-O6
5	A	702	CLR	C20-C22-C23-C24



Mol	Chain	Res	Type	Atoms
5	А	702	CLR	C23-C24-C25-C26
7	А	705	8PR	OAO-CAM-CAW-CAX
5	А	702	CLR	C23-C24-C25-C27
5	А	702	CLR	C22-C23-C24-C25

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	А	703	LMT	4	0
5	А	702	CLR	4	0
7	А	705	8PR	4	0
4	А	701	NAG	1	0
4	А	704	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









### 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,  $95^{th}$  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	А	544/549~(99%)	0.50	41 (7%) 14 5	72, 131, 218, 322	0
2	В	218/221~(98%)	1.04	38~(17%) 1 1	73, 161, 330, 391	0
3	С	214/214~(100%)	0.84	36~(16%) 1 1	85, 176, 282, 408	0
All	All	976/984~(99%)	0.70	115 (11%) 4 2	72, 145, 269, 408	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	151	PRO	25.5
2	В	150	ALA	13.1
2	В	237	PRO	11.5
2	В	212	THR	11.1
2	В	152	GLY	10.6
2	В	236	GLU	9.0
1	А	147	CYS	7.2
2	В	235	LEU	7.1
2	В	149	LEU	6.3
2	В	209	PRO	6.3
3	С	203	LYS	6.1
2	В	155	ASP	5.5
1	А	134	TYR	5.3
1	А	146	GLY	5.1
3	С	201	LEU	4.9
2	В	208	VAL	4.5
2	В	218	VAL	4.5
2	В	173	GLU	4.4
2	В	217	THR	4.4
1	А	103	TRP	4.3
1	А	139	LEU	4.3
2	В	190	THR	4.3
3	С	40	SER	4.2



Mol	Chain	Res	Type	RSRZ
3	С	116	ARG	4.1
3	С	179	VAL	4.0
3	С	193	TYR	4.0
1	А	138	ALA	3.9
2	В	163	LEU	3.8
2	В	65	GLU	3.8
3	С	106	TYR	3.8
3	С	76	THR	3.7
1	А	514	TRP	3.6
1	А	515	PHE	3.6
3	С	127	LYS	3.6
3	С	155	PHE	3.6
3	С	138	PHE	3.5
1	А	145	ASN	3.5
1	A	133	PHE	3.5
3	С	112	TYR	3.5
3	С	39	VAL	3.4
1	А	272	LYS	3.3
1	А	390	ARG	3.3
1	А	389	MET	3.3
1	А	137	LEU	3.3
3	С	174	GLU	3.2
3	С	207	GLU	3.2
2	В	66	TRP	3.2
2	В	172	PRO	3.1
1	А	140	GLY	3.1
3	С	225	ILE	3.1
3	С	95	ILE	3.0
3	С	177	ASN	3.0
1	А	231	PHE	3.0
3	С	200	THR	3.0
2	В	39	ILE	3.0
1	А	153	LYS	2.9
3	C	41	ILE	2.9
1	A	403	PRO	2.9
1	A	271	TRP	2.8
1	A	154	ILE	2.8
2	В	99	TYR	2.8
2	В	189	HIS	2.8
3	C	153	VAL	2.7
2	В	100	MET	2.7
2	В	183	SER	2.6



Mol	Chain	Res	Type	RSRZ
3	С	206	TYR	2.6
3	С	53	VAL	2.6
1	А	406	LEU	2.6
1	А	615	GLU	2.6
1	А	529	LEU	2.6
1	А	422	PHE	2.5
2	В	167	VAL	2.5
3	С	227	LYS	2.5
3	С	198	THR	2.5
2	В	144	PRO	2.5
1	А	337	LEU	2.5
3	С	214	CYS	2.4
2	В	146	VAL	2.4
2	В	121	ARG	2.4
2	В	186	SER	2.4
1	А	368	ASN	2.4
3	С	77	GLY	2.4
1	А	270	ILE	2.4
2	В	160	SER	2.4
2	В	216	GLN	2.4
1	А	345	LEU	2.4
2	В	64	LEU	2.4
1	А	151	TRP	2.4
2	В	213	TRP	2.3
1	А	462	ARG	2.3
3	С	109	GLN	2.3
1	А	148	ILE	2.3
3	С	175	ARG	2.3
3	С	117	THR	2.3
1	A	407	PHE	2.3
1	A	586	PHE	2.2
2	В	185	SER	2.2
2	B	166	LEU	2.2
3	C	228	SER	2.2
1	A	440	PHE	2.2
3	C	164	ILE	2.2
3	C	52	ALA	2.1
3	С	104	ALA	2.1
3	C	151	SER	2.1
2	В	207	THR	2.1
2	В	159	SER	2.1
2	В	38	LYS	2.1



Mol	Chain	Res	Type	RSRZ
1	А	142	TYR	2.0
1	А	220	TRP	2.0
1	А	344	LEU	2.0
1	А	317	TRP	2.0
1	А	179	ILE	2.0
1	А	342	GLY	2.0
1	А	423	PHE	2.0
3	С	124	LEU	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,  $95^{th}$  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	${f B}$ -factors( ${ m \AA}^2$ )	Q<0.9
4	NAG	А	704	14/15	0.69	1.00	274,279,284,284	0
5	CLR	А	702	28/28	0.81	0.41	184,199,204,209	0
6	LMT	А	703	22/35	0.89	0.21	$113,\!132,\!162,\!167$	0
8	CL	А	706	1/1	0.93	1.57	162, 162, 162, 162, 162	0
9	NA	А	707	1/1	0.93	0.17	$51,\!51,\!51,\!51$	1
4	NAG	А	701	14/15	0.94	0.22	64,83,132,137	0
7	8PR	А	705	24/24	0.95	0.55	85,98,114,119	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









## 6.5 Other polymers (i)

There are no such residues in this entry.

