



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 26, 2019 – 09:48 AM EDT

PDB ID : 6DDA
Title : Nurr1 Covalently Modified by a Dopamine Metabolite
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Deposited on : 2018-05-09
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

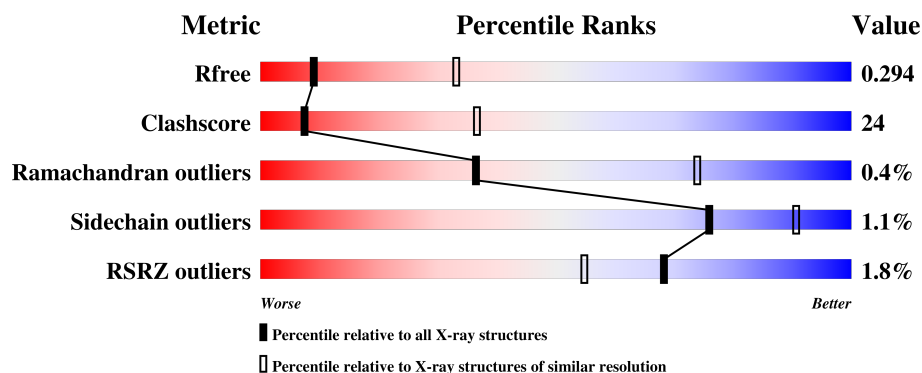
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	111664	1121 (3.22-3.18)
Clashscore	122126	1091 (3.20-3.20)
Ramachandran outliers	120053	1074 (3.20-3.20)
Sidechain outliers	120020	1073 (3.20-3.20)
RSRZ outliers	108989	1083 (3.22-3.18)

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	B	272	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>32%</div> <div>13%</div> </div> </div>
1	C	272	<div> <div>3%</div> <div> <div></div> <div>47%</div> <div>35%</div> <div>•</div> <div>17%</div> </div> </div>
2	A	272	<div> <div>%</div> <div> <div></div> <div>44%</div> <div>37%</div> <div>•</div> <div>18%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	G7J	C	605	-	-	X	X
5	BR	C	601	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5552 atoms, of which 27 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 Nuclear receptor subfamily 4 group A member 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	236	Total	C	H	N	O	S	0	0	0
			1884	1206	3	319	346	10			
1	C	225	Total	C	H	N	O	S	0	0	0
			1805	1160	3	305	328	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	327	SER	-	expression tag	UNP P43354
C	327	SER	-	expression tag	UNP P43354

- Molecule 2 is a protein called Nuclear receptor subfamily 4 group A member 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	224	Total	C	H	N	O	S	0	0	0
			1800	1156	3	303	329	9			

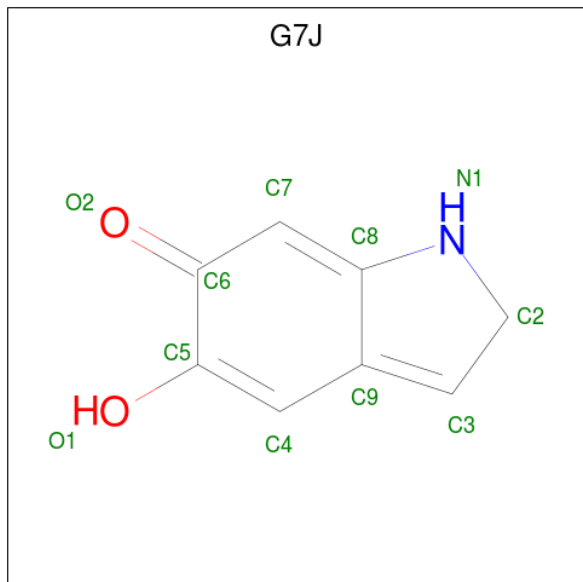
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	SER	-	expression tag	UNP P43354

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	K	0	0
			2	2		
3	A	2	Total	K	0	0
			2	2		
3	C	1	Total	K	0	0
			1	1		

- Molecule 4 is 5-hydroxy-1,2-dihydro-6H-indol-6-one (three-letter code: G7J) (formula: $C_8H_7NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			17	8	6	1	2		
4	A	1	Total	C	H	N	O	0	0
			17	8	6	1	2		
4	C	1	Total	C	H	N	O	0	0
			17	8	6	1	2		

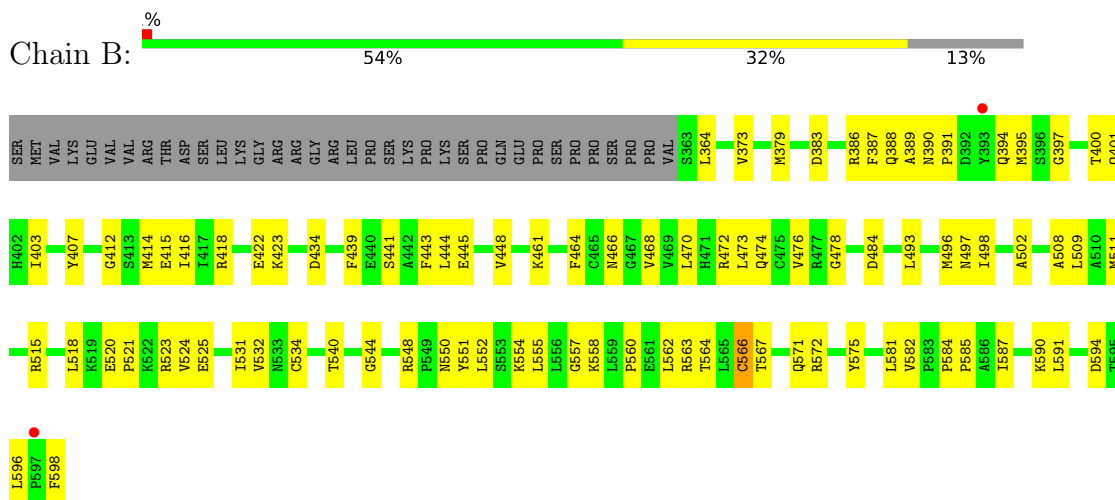
- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Br	0	0
			4	4		
5	C	3	Total	Br	0	0
			3	3		

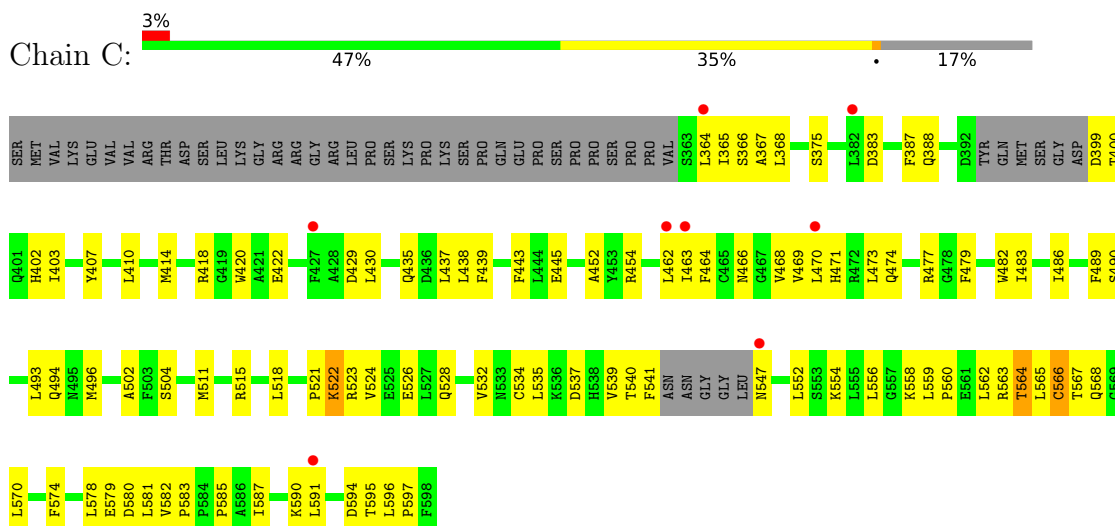
3 Residue-property plots

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

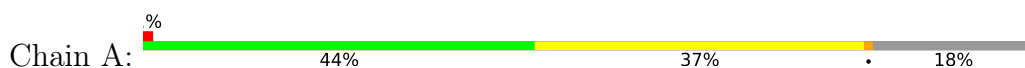
- Molecule 1: Nuclear receptor subfamily 4 group A member 2



- Molecule 1: Nuclear receptor subfamily 4 group A member 2



- Molecule 2: Nuclear receptor subfamily 4 group A member 2



P560	R477	TYR	SER
E561	G478	GLN	MET
L562	F479	MET	VAL
R563		LYS	LYS
T564	W482	GLY	GLU
L565	I483	ASP	VAL
C566		D399	VAL
T567	I486	T400	ARG
Q568		Q401	THR
	F489	H402	ASP
R572	S490		SER
L573	S491	F406	LEU
F574	W492		LYS
L575	L493	L409	GLY
L576	Q494	L410	ARG
R577	W495	T411	ARG
L578	W496	Q412	GLY
		S413	ARG
L581	F503	M414	LEU
V582		E415	PRO
P583	I506	I416	SER
P584		T417	LYS
	L509	R418	PRO
I587	A510		LYS
L588	M511	G426	SER
D588			PRO
R590	L518	D436	GLN
	K519		GLU
L593	E520	F439	PRO
	P521	E440	SER
	K522		PRO
	R523	F443	PRO
	V524	L444	SER
	E525	E445	PRO
	E526	L446	PRO
	L527		PRO
	Q528	L449	VAL
			S363
	V532		L364
	N533	A452	L365
	C534	Y453	
		R454	V369
	F541	S455	R370
	ASN	W456	
	ASN	P457	N376
	GLY		P377
	GLY	R461	A378
	LEU	L462	M379
	ASN	I463	T380
		F464	S381
	R548	Q465	L382
	P549	M466	D383
	N550	G467	Y384
	Y551	V468	S385
	L552	V469	R386
		L470	F387
	L555		Q388
	L556	L473	A389
	G557	Q474	N390
	K558	C475	P391
	L559	V476	D392

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	80.59Å 80.59Å 225.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.29 – 3.20 43.89 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.29-3.20) 88.0 (43.89-3.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.49 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.250 , 0.294 0.250 , 0.294	Depositor DCC
R_{free} test set	1450 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å ²)	85.7	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 90.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5552	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0667e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, OCS, BR, G7J

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	B	0.43	2/1921 (0.1%)	0.70	0/2601
1	C	0.43	3/1839 (0.2%)	0.61	0/2488
2	A	0.47	3/1824 (0.2%)	0.71	0/2466
All	All	0.44	8/5584 (0.1%)	0.67	0/7555

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	566	CYS	N-CA	-7.30	1.31	1.46
1	C	566	CYS	N-CA	-7.29	1.31	1.46
1	B	566	CYS	N-CA	-7.27	1.31	1.46
1	C	564	THR	C-N	6.18	1.48	1.34
1	C	566	CYS	CA-CB	-6.10	1.40	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	564	THR	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1881	3	1886	88	1
1	C	1802	3	1817	90	1
2	A	1797	3	1808	87	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
4	A	11	6	0	1	0
4	B	11	6	0	0	0
4	C	11	6	0	5	0
5	A	4	0	0	0	0
5	C	3	0	0	5	0
All	All	5525	27	5511	261	1

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 24.

The worst 5 of 261 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:B:388:GLN:H	1:B:474:GLN:HE22	1.03	1.01
5:C:601:BR:BR	5:C:602:BR:BR	2.94	0.96
1:C:596:LEU:HD12	1:C:597:PRO:HD2	1.52	0.92
1:C:522:LYS:O	1:C:526:GLU:HG2	1.75	0.85
1:C:563:ARG:HD2	4:C:605:G7J:C7	2.06	0.85

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:GLN:NE2	1:C:387:PHE:O[6_455]	2.19	0.01

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	B	234/272 (86%)	226 (97%)	7 (3%)	1 (0%)	36	74
1	C	219/272 (80%)	209 (95%)	10 (5%)	0	100	100
2	A	217/272 (80%)	209 (96%)	6 (3%)	2 (1%)	19	60
All	All	670/816 (82%)	644 (96%)	23 (3%)	3 (0%)	36	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	551	TYR
2	A	379	MET
1	B	379	MET

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	Outliers	Percentiles	
1	B	209/243 (86%)	207 (99%)	2 (1%)	78	92
1	C	201/243 (83%)	198 (98%)	3 (2%)	67	88
2	A	199/242 (82%)	197 (99%)	2 (1%)	78	92
All	All	609/728 (84%)	602 (99%)	7 (1%)	76	90

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	566	CYS
1	C	568	GLN
1	C	522	LYS
1	B	566	CYS
1	C	566	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	474	GLN
1	C	376	ASN
1	C	402	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
2	OCS	A	465	2	7,8,9	0.87	0	8,11,13	1.31	1 (12%)

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	OCS	A	465	2	-	2/4/7/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	465	OCS	OD2-SG-CB	2.18	109.21	105.74

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	465	OCS	CA-CB-SG-OD2
2	A	465	OCS	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	G7J	A	607	2	11,12,12	1.32	1 (9%)	11,17,17	1.38	2 (18%)
4	G7J	B	602	1	11,12,12	1.33	1 (9%)	11,17,17	1.40	2 (18%)
4	G7J	C	605	1	11,12,12	1.33	1 (9%)	11,17,17	1.40	2 (18%)

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	G7J	A	607	2	-	-	0/2/2/2
4	G7J	B	602	1	-	-	0/2/2/2
4	G7J	C	605	1	-	-	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	G7J	C2-N1	2.10	1.48	1.44
4	A	607	G7J	C2-N1	2.09	1.48	1.44
4	C	605	G7J	C2-N1	2.08	1.48	1.44

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	G7J	C4-C9-C8	-3.14	116.65	120.21
4	C	605	G7J	C4-C9-C8	-3.12	116.68	120.21
4	A	607	G7J	C4-C9-C8	-3.09	116.72	120.21
4	C	605	G7J	C9-C8-N1	-2.56	103.08	106.82
4	B	602	G7J	C9-C8-N1	-2.56	103.08	106.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	607	G7J	1	0
4	C	605	G7J	5	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(Å ²)	Q<0.9
1	B	236/272 (86%)	-0.03	2 (0%) 86 78	72, 101, 147, 174	0
1	C	225/272 (82%)	0.28	8 (3%) 42 28	84, 142, 191, 236	0
2	A	223/272 (81%)	0.10	2 (0%) 84 76	64, 103, 171, 215	0
All	All	684/816 (83%)	0.12	12 (1%) 68 55	64, 121, 176, 236	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	598	PHE	3.8
1	B	597	PRO	3.4
1	B	393	TYR	3.1
1	C	547	ASN	2.9
1	C	364	LEU	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	OCS	A	465	9/10	0.96	0.15	78,80,93,94	3

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. 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	G7J	C	605	11/11	0.65	0.86	10,89,103,107	17
3	K	C	604	1/1	0.70	0.24	152,152,152,152	0
3	K	A	606	1/1	0.85	0.46	121,121,121,121	0
5	BR	A	603	1/1	0.87	0.12	91,91,91,91	1
4	G7J	A	607	11/11	0.88	0.32	10,89,103,107	17
3	K	A	605	1/1	0.89	0.22	112,112,112,112	0
4	G7J	B	602	11/11	0.89	0.36	10,89,103,107	17
3	K	B	601	1/1	0.92	0.26	87,87,87,87	0
5	BR	C	603	1/1	0.92	0.10	151,151,151,151	1
5	BR	A	604	1/1	0.93	0.11	122,122,122,122	1
5	BR	A	601	1/1	0.93	0.11	78,78,78,78	1
5	BR	A	602	1/1	0.94	0.14	95,95,95,95	1
5	BR	C	602	1/1	0.96	0.13	132,132,132,132	1
5	BR	C	601	1/1	0.96	0.34	135,135,135,135	1
3	K	B	603	1/1	0.98	0.12	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.