



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2022 – 10:14 AM JST

PDB ID : 7XNA
Title : Crystal structure of somatostatin receptor 2 (SSTR2) with peptide antagonist CYN 154806
Authors : Zhao, W.; Han, S.; Qiu, N.; Feng, W.; Lu, M.; Yang, D.; Wang, M.-W.; Wu, B.; Zhao, Q.
Deposited on : 2022-04-28
Resolution : 2.65 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 ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : ?? (??), CSD ??CSD?? (????)
Xtriage (Phenix) : 1.13
EDS : 2.29
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
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) : 2.29

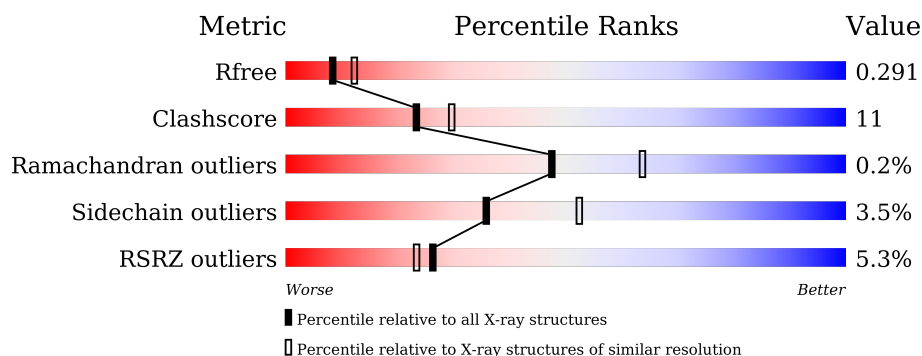
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 of 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 $\leq 5\%$. 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	583	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>21%</div> <div>•</div> <div>19%</div> </div> </div>
2	B	10	<div> <div>50%</div> <div>30%</div> <div>20%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3778 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 Somatostatin receptor type 2,Endo-1,4-beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3694	2420	602	649	23			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	expression tag	UNP P30874
A	-23	LYS	-	expression tag	UNP P30874
A	-22	THR	-	expression tag	UNP P30874
A	-21	ILE	-	expression tag	UNP P30874
A	-20	ILE	-	expression tag	UNP P30874
A	-19	ALA	-	expression tag	UNP P30874
A	-18	LEU	-	expression tag	UNP P30874
A	-17	SER	-	expression tag	UNP P30874
A	-16	TYR	-	expression tag	UNP P30874
A	-15	ILE	-	expression tag	UNP P30874
A	-14	PHE	-	expression tag	UNP P30874
A	-13	CYS	-	expression tag	UNP P30874
A	-12	LEU	-	expression tag	UNP P30874
A	-11	VAL	-	expression tag	UNP P30874
A	-10	PHE	-	expression tag	UNP P30874
A	-9	ALA	-	expression tag	UNP P30874
A	-8	ASP	-	expression tag	UNP P30874
A	-7	TYR	-	expression tag	UNP P30874
A	-6	LYS	-	expression tag	UNP P30874
A	-5	ASP	-	expression tag	UNP P30874
A	-4	ASP	-	expression tag	UNP P30874
A	-3	ASP	-	expression tag	UNP P30874
A	-2	ASP	-	expression tag	UNP P30874
A	-1	GLY	-	expression tag	UNP P30874
A	0	ALA	-	expression tag	UNP P30874
A	1	PRO	-	expression tag	UNP P30874
A	89	ASN	ASP	conflict	UNP P30874

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Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLU	VAL	conflict	UNP P30874
A	1010	PHE	ASP	conflict	UNP P09850
A	1121	ASP	ARG	conflict	UNP P09850
A	316	ASP	SER	conflict	UNP P30874
A	360	GLU	-	expression tag	UNP P30874
A	361	PHE	-	expression tag	UNP P30874
A	362	LEU	-	expression tag	UNP P30874
A	363	GLU	-	expression tag	UNP P30874
A	364	VAL	-	expression tag	UNP P30874
A	365	LEU	-	expression tag	UNP P30874
A	366	PHE	-	expression tag	UNP P30874
A	367	GLN	-	expression tag	UNP P30874
A	368	GLY	-	expression tag	UNP P30874
A	369	PRO	-	expression tag	UNP P30874
A	370	HIS	-	expression tag	UNP P30874
A	371	HIS	-	expression tag	UNP P30874
A	372	HIS	-	expression tag	UNP P30874
A	373	HIS	-	expression tag	UNP P30874
A	374	HIS	-	expression tag	UNP P30874
A	375	HIS	-	expression tag	UNP P30874
A	376	HIS	-	expression tag	UNP P30874
A	377	HIS	-	expression tag	UNP P30874
A	378	HIS	-	expression tag	UNP P30874
A	379	HIS	-	expression tag	UNP P30874

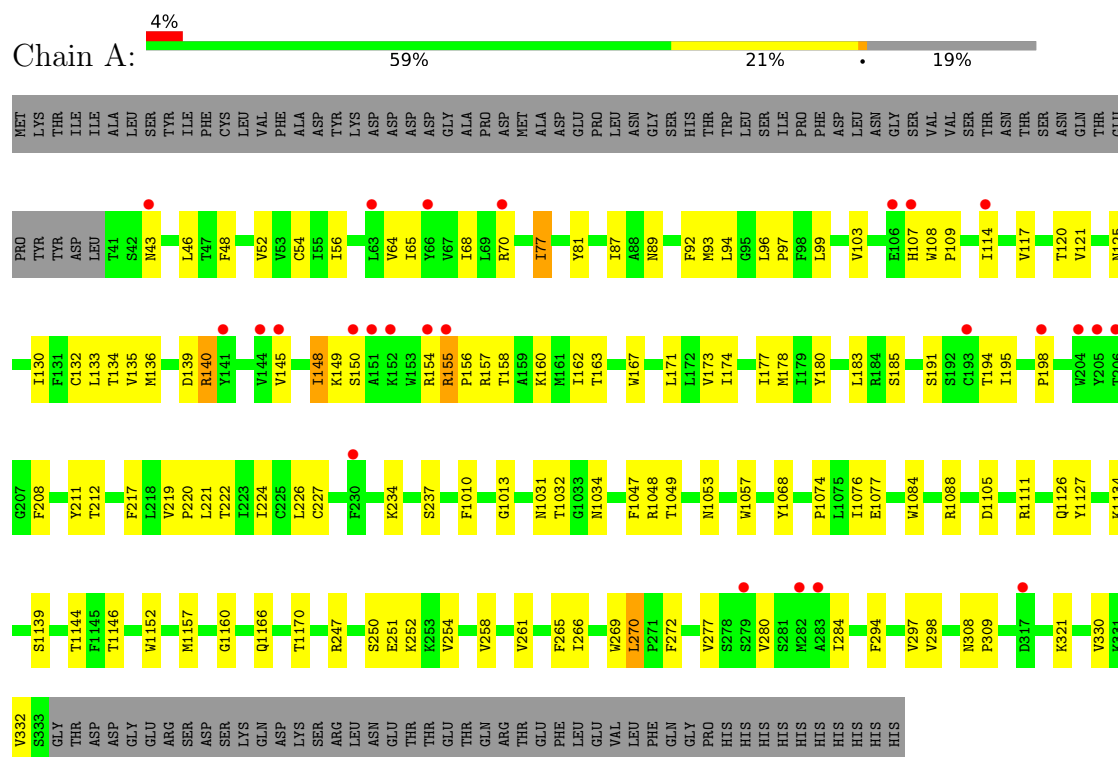
- Molecule 2 is a protein called CYN 154806.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	S	0	0	1
			84	56	12	14	2			

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: Somatostatin receptor type 2,Endo-1,4-beta-xylanase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.15Å 85.21Å 163.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.82 – 2.65 40.92 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.6 (40.82-2.65) 97.8 (40.92-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	50.02 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472, PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.220 , 0.290 0.220 , 0.291	Depositor DCC
R_{free} test set	1749 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3778	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DTR, NH2, PPN, DCY, DTY, ACE

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	0.52	0/3802	0.63	0/5196
2	B	2.33	2/33 (6.1%)	1.61	0/41
All	All	0.56	2/3835 (0.1%)	0.65	0/5237

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	THR	C-N	7.73	1.51	1.34
2	B	6	LYS	C-N	6.75	1.49	1.34

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	3694	0	3654	85	0
2	B	84	0	63	3	0
All	All	3778	0	3717	85	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 11.

All (85) 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:A:120:THR:HG22	1:A:178:MET:HG2	1.47	0.95
1:A:155:ARG:HD3	1:A:157:ARG:H	1.38	0.87
1:A:155:ARG:HH11	1:A:156:PRO:HD2	1.53	0.72
1:A:294:PHE:O	1:A:298:VAL:HG23	1.90	0.70
1:A:77:ILE:H	1:A:77:ILE:HD13	1.57	0.68
1:A:54:CYS:HA	1:A:93:MET:HE3	1.74	0.68
1:A:77:ILE:H	1:A:77:ILE:CD1	2.07	0.68
1:A:139:ASP:OD1	1:A:154:ARG:NH1	2.28	0.66
1:A:194:THR:HA	2:B:5:DTR:HD1	1.76	0.65
1:A:134:THR:HG21	1:A:220:PRO:HB3	1.80	0.63
1:A:54:CYS:HA	1:A:93:MET:CE	2.30	0.61
1:A:272:PHE:HA	1:A:297:VAL:CG1	2.33	0.59
1:A:43:ASN:OD1	2:B:10:NH2:N	2.36	0.58
1:A:217:PHE:CE2	1:A:270:LEU:HD12	2.38	0.58
1:A:298:VAL:HG11	2:B:6:LYS:HB3	1.85	0.58
1:A:77:ILE:HD13	1:A:77:ILE:N	2.18	0.57
1:A:1152:TRP:HB3	1:A:1157:MET:HB2	1.89	0.55
1:A:208:PHE:O	1:A:212:THR:HG23	2.06	0.54
1:A:107:HIS:O	1:A:109:PRO:HD3	2.05	0.54
1:A:1074:PRO:HD2	1:A:1160:GLY:HA2	1.90	0.54
1:A:89:ASN:O	1:A:93:MET:HG2	2.08	0.54
1:A:94:LEU:O	1:A:97:PRO:HD2	2.08	0.54
1:A:114:ILE:O	1:A:117:VAL:HG12	2.09	0.52
1:A:1057:TRP:HZ3	1:A:1170:THR:HG23	1.74	0.52
1:A:254:VAL:O	1:A:258:VAL:HG23	2.10	0.51
1:A:155:ARG:HD3	1:A:157:ARG:N	2.18	0.51
1:A:64:VAL:O	1:A:68:ILE:HG13	2.10	0.51
1:A:1031:ASN:OD1	1:A:1032:THR:N	2.44	0.51
1:A:1049:THR:HG22	1:A:1144:THR:HA	1.92	0.50
1:A:155:ARG:HH11	1:A:155:ARG:HG2	1.76	0.49
1:A:92:PHE:HB2	1:A:125:ASN:HB2	1.95	0.49
1:A:145:VAL:HA	1:A:234:LYS:HD3	1.93	0.49
1:A:1127:TYR:CZ	1:A:1157:MET:HB3	2.48	0.49
1:A:65:ILE:HD13	1:A:87:ILE:HD13	1.93	0.49
1:A:150:SER:O	1:A:150:SER:OG	2.27	0.49
1:A:308:ASN:HB2	1:A:309:PRO:HD3	1.94	0.49
1:A:219:VAL:HB	1:A:220:PRO:HD3	1.95	0.48
1:A:194:THR:OG1	1:A:195:ILE:N	2.45	0.48
1:A:92:PHE:HA	1:A:121:VAL:CG1	2.43	0.48
1:A:167:TRP:O	1:A:171:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:O	1:A:284:ILE:HG13	2.12	0.48
1:A:132:CYS:O	1:A:136:MET:HG3	2.14	0.48
1:A:217:PHE:HE2	1:A:270:LEU:HD12	1.77	0.48
1:A:330:VAL:HG12	1:A:332:VAL:HG23	1.95	0.47
1:A:99:LEU:O	1:A:103:VAL:HG23	2.14	0.47
1:A:134:THR:CG2	1:A:220:PRO:HB3	2.45	0.47
1:A:1047:PHE:HA	1:A:1146:THR:HG23	1.97	0.47
1:A:155:ARG:NH1	1:A:156:PRO:HD2	2.26	0.46
1:A:185:SER:HA	1:A:191:SER:HA	1.98	0.46
1:A:1084:TRP:CD1	1:A:1134:LYS:HE2	2.51	0.46
1:A:130:ILE:HD12	1:A:265:PHE:CE1	2.50	0.46
1:A:173:VAL:O	1:A:211:TYR:OH	2.22	0.46
1:A:52:VAL:O	1:A:56:ILE:HG13	2.16	0.46
1:A:1048:ARG:NH1	1:A:1166:GLN:OE1	2.45	0.46
1:A:1077:GLU:O	1:A:1126:GLN:HA	2.16	0.45
1:A:81:TYR:CE1	1:A:135:VAL:HG11	2.52	0.45
1:A:140:ARG:NE	1:A:140:ARG:HA	2.33	0.44
1:A:1074:PRO:HG2	1:A:1076:ILE:HD12	2.00	0.44
1:A:247:ARG:CZ	1:A:252:LYS:HG3	2.48	0.44
1:A:148:ILE:HD12	1:A:149:LYS:H	1.83	0.43
1:A:96:LEU:HD12	1:A:99:LEU:HD12	1.99	0.43
1:A:108:TRP:CD1	1:A:183:LEU:HD21	2.53	0.43
1:A:81:TYR:CE1	1:A:135:VAL:CG1	3.02	0.43
1:A:1088:ARG:NH2	1:A:1105:ASP:OD2	2.51	0.43
1:A:1053:ASN:HD21	1:A:1139:SER:HA	1.83	0.43
1:A:1127:TYR:CE2	1:A:1157:MET:HB3	2.54	0.43
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.83	0.42
1:A:134:THR:HG22	1:A:224:ILE:HG13	2.00	0.42
1:A:155:ARG:CD	1:A:157:ARG:H	2.20	0.42
1:A:133:LEU:HD21	1:A:261:VAL:HG12	2.00	0.42
1:A:163:THR:O	1:A:167:TRP:HD1	2.02	0.42
1:A:222:THR:O	1:A:226:LEU:HG	2.19	0.42
1:A:174:ILE:HD12	1:A:178:MET:HG3	2.02	0.42
1:A:277:VAL:O	1:A:280:VAL:HG22	2.20	0.42
1:A:269:TRP:O	1:A:272:PHE:HB3	2.19	0.42
1:A:48:PHE:O	1:A:52:VAL:HG13	2.20	0.41
1:A:155:ARG:HG2	1:A:156:PRO:HD2	2.02	0.41
1:A:224:ILE:O	1:A:227:CYS:HB2	2.21	0.41
1:A:1010:PHE:HD2	1:A:1034:ASN:O	2.03	0.41
1:A:221:LEU:HD11	1:A:266:ILE:HG12	2.02	0.41
1:A:148:ILE:H	1:A:148:ILE:HG13	1.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ILE:HG23	1:A:195:ILE:HD11	2.03	0.40
1:A:1013:GLY:HA3	1:A:1031:ASN:HA	2.02	0.40
1:A:180:TYR:CE1	1:A:198:PRO:HD3	2.56	0.40
1:A:158:THR:O	1:A:162:ILE:HG12	2.21	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	470/583 (81%)	450 (96%)	20 (4%)	0	100	100
2	B	4/10 (40%)	2 (50%)	1 (25%)	1 (25%)	0	0
All	All	474/593 (80%)	452 (95%)	21 (4%)	1 (0%)	47	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4	TYR

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	A	397/507 (78%)	384 (97%)	13 (3%)	38	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	4/4 (100%)	3 (75%)	1 (25%)	0	0
All	All	401/511 (78%)	387 (96%)	14 (4%)	36	52

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	77	ILE
1	A	140	ARG
1	A	148	ILE
1	A	155	ARG
1	A	160	LYS
1	A	237	SER
1	A	1068	TYR
1	A	1111	ARG
1	A	250	SER
1	A	251	GLU
1	A	270	LEU
1	A	321	LYS
2	B	4	TYR

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

Mol	Chain	Res	Type
1	A	1034	ASN
1	A	304	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	472/583 (80%)	0.30	25 (5%) 26 23	35, 59, 80, 101	0
2	B	4/10 (40%)	0.14	0 100 100	64, 64, 70, 76	0
All	All	476/593 (80%)	0.30	25 (5%) 26 23	35, 59, 80, 101	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	ALA	4.1
1	A	141	TYR	3.7
1	A	204	TRP	3.7
1	A	150	SER	3.7
1	A	279	SER	3.4
1	A	70	ARG	3.4
1	A	205	TYR	2.9
1	A	145	VAL	2.7
1	A	151	ALA	2.5
1	A	114	ILE	2.5
1	A	282	MET	2.5
1	A	154	ARG	2.4
1	A	317	ASP	2.3
1	A	193	CYS	2.3
1	A	198	PRO	2.3
1	A	66	TYR	2.3
1	A	155	ARG	2.3
1	A	144	VAL	2.2
1	A	107	HIS	2.2
1	A	63	LEU	2.2
1	A	206	THR	2.2
1	A	43	ASN	2.2
1	A	230	PHE	2.1
1	A	106	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	152	LYS	2.0

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	DTR	B	5	14/15	0.84	0.34	64,71,78,81	0
2	PPN	B	2	14/15	0.90	0.29	70,74,80,80	0
2	DTY	B	9	12/13	0.91	0.45	62,69,72,74	0
2	DCY	B	3	6/7	0.94	0.14	65,73,75,79	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.