



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:52 AM UTC

PDB ID : 8BGM / pdb_00008bgm
Title : Crystal structure of the OrfX1-OrfX3 complex from the PMP1 neurotoxin gene cluster
Authors : Kosenina, S.; Stenmark, P.
Deposited on : 2022-10-28
Resolution : 2.70 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

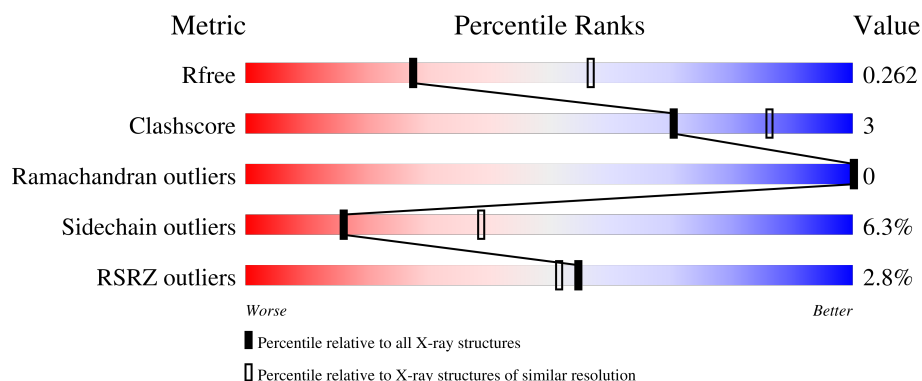
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	155	 3% 68% 15% 16%
1	C	155	 % 72% 12% 15%
2	B	491	 3% 84% 11% . .
2	D	491	 3% 85% 11% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9696 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 Toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1082	702	181	193	6			
1	C	131	Total	C	N	O	S	0	0	0
			1089	707	180	196	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP A0A5P3XKM0
A	-4	HIS	-	expression tag	UNP A0A5P3XKM0
A	-3	HIS	-	expression tag	UNP A0A5P3XKM0
A	-2	HIS	-	expression tag	UNP A0A5P3XKM0
A	-1	HIS	-	expression tag	UNP A0A5P3XKM0
A	0	HIS	-	expression tag	UNP A0A5P3XKM0
A	1	HIS	-	expression tag	UNP A0A5P3XKM0
A	2	GLU	-	expression tag	UNP A0A5P3XKM0
A	3	ASN	-	expression tag	UNP A0A5P3XKM0
A	4	LEU	-	expression tag	UNP A0A5P3XKM0
A	5	TYR	-	expression tag	UNP A0A5P3XKM0
A	6	PHE	-	expression tag	UNP A0A5P3XKM0
A	7	GLN	-	expression tag	UNP A0A5P3XKM0
A	8	GLY	-	expression tag	UNP A0A5P3XKM0
C	-5	MET	-	initiating methionine	UNP A0A5P3XKM0
C	-4	HIS	-	expression tag	UNP A0A5P3XKM0
C	-3	HIS	-	expression tag	UNP A0A5P3XKM0
C	-2	HIS	-	expression tag	UNP A0A5P3XKM0
C	-1	HIS	-	expression tag	UNP A0A5P3XKM0
C	0	HIS	-	expression tag	UNP A0A5P3XKM0
C	1	HIS	-	expression tag	UNP A0A5P3XKM0
C	2	GLU	-	expression tag	UNP A0A5P3XKM0
C	3	ASN	-	expression tag	UNP A0A5P3XKM0
C	4	LEU	-	expression tag	UNP A0A5P3XKM0
C	5	TYR	-	expression tag	UNP A0A5P3XKM0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	PHE	-	expression tag	UNP A0A5P3XKM0
C	7	GLN	-	expression tag	UNP A0A5P3XKM0
C	8	GLY	-	expression tag	UNP A0A5P3XKM0

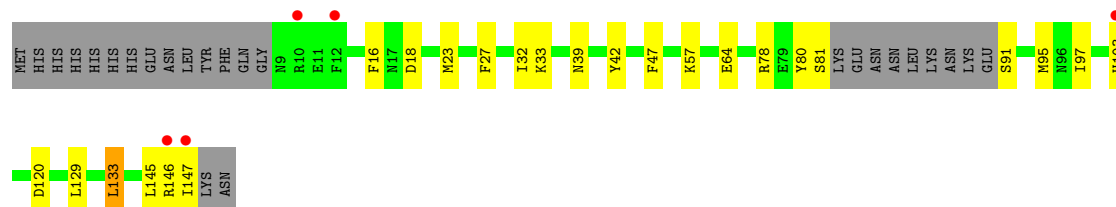
- Molecule 2 is a protein called Toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	475	Total	C	N	O	S	0	0	0
			3758	2416	600	727	15			
2	D	476	Total	C	N	O	S	0	0	0
			3767	2422	602	728	15			

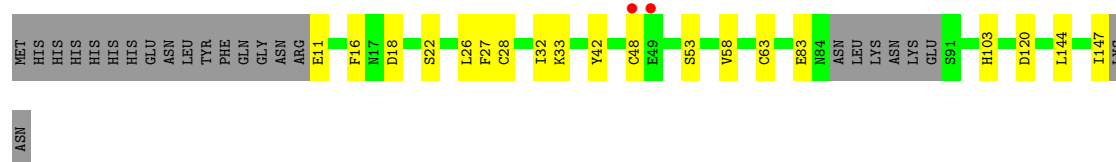
3 Residue-property plots [i](#)

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.

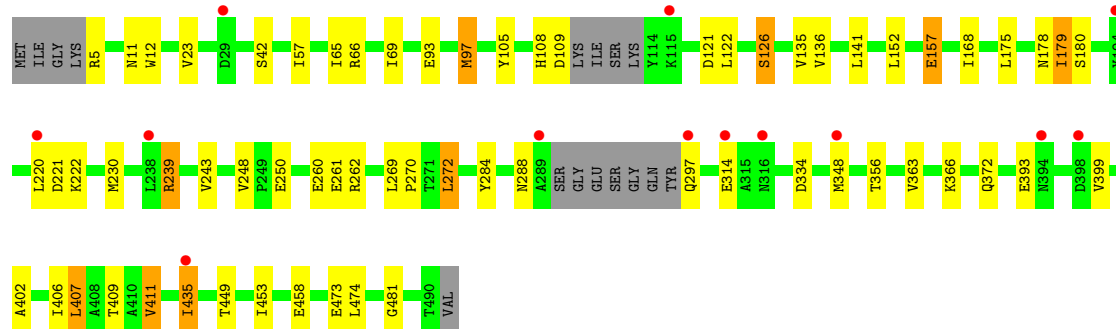
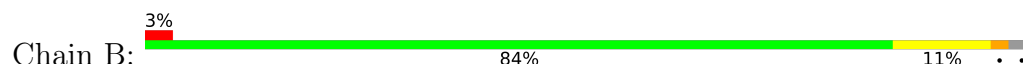
• Molecule 1: Toxin



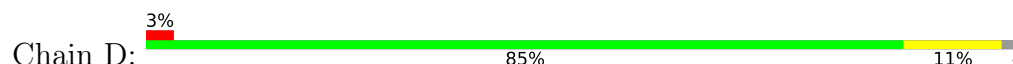
• Molecule 1: Toxin

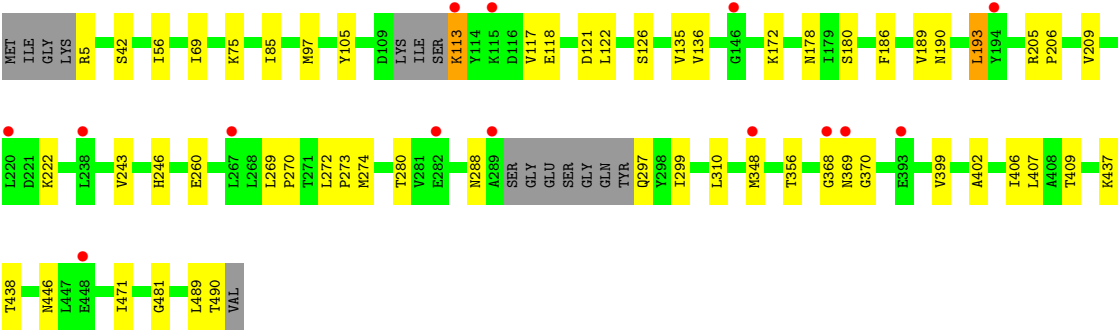


• Molecule 2: Toxin



• Molecule 2: Toxin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.02Å 126.57Å 154.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.37 – 2.70 63.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.37-2.70) 99.9 (63.37-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.222 , 0.263 0.221 , 0.262	Depositor DCC
R_{free} test set	2545 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.991	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9696	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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 30.09 % 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 1.3876e-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

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	0.70	0/1102	1.04	0/1475
1	C	0.71	0/1109	1.03	0/1484
2	B	0.70	0/3837	0.99	1/5205 (0.0%)
2	D	0.72	0/3846	0.98	2/5216 (0.0%)
All	All	0.71	0/9894	1.00	3/13380 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	369	ASN	N-CA-C	-5.92	105.77	112.87
2	B	178	ASN	N-CA-C	5.31	120.42	112.94
2	D	178	ASN	N-CA-C	5.26	120.36	112.94

There are no chirality outliers.

There are no planarity outliers.

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	A	1082	0	1095	10	0
1	C	1089	0	1101	7	0
2	B	3758	0	3702	29	0
2	D	3767	0	3715	22	0
All	All	9696	0	9613	66	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 3.

All (66) 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)
2:D:189:VAL:HG11	2:D:209:VAL:HG11	1.68	0.74
1:A:81:SER:HA	1:A:145:LEU:HD11	1.70	0.71
1:C:16:PHE:CZ	1:C:18:ASP:HB3	2.27	0.69
1:A:47:PHE:HZ	1:A:133:LEU:HD21	1.61	0.66
2:B:230:MET:HA	2:B:230:MET:HE2	1.80	0.64
1:C:11:GLU:HB2	1:C:26:LEU:HD21	1.79	0.63
2:D:368:GLY:C	2:D:370:GLY:N	2.56	0.62
2:B:126:SER:HA	2:B:179:ILE:HD13	1.83	0.61
2:D:368:GLY:C	2:D:370:GLY:H	2.09	0.60
1:C:28:CYS:SG	1:C:48:CYS:SG	3.01	0.58
2:B:435:ILE:H	2:B:435:ILE:HD12	1.69	0.57
1:A:16:PHE:CZ	1:A:18:ASP:HB3	2.41	0.55
2:B:407:LEU:O	2:B:411:VAL:HG13	2.07	0.54
1:C:58:VAL:O	1:C:58:VAL:HG12	2.08	0.53
1:C:144:LEU:O	1:C:147:ILE:HG12	2.09	0.53
2:B:175:LEU:O	2:B:179:ILE:HG13	2.09	0.52
2:B:126:SER:HA	2:B:179:ILE:CD1	2.41	0.51
2:B:97:MET:HE2	2:B:168:ILE:HG12	1.92	0.50
2:B:372:GLN:OE1	2:B:453:ILE:HD11	2.11	0.50
2:D:56:ILE:HD11	2:D:186:PHE:HE2	1.77	0.49
2:B:12:TRP:HA	2:B:230:MET:HE3	1.95	0.48
2:D:274:MET:CE	2:D:438:THR:C	2.86	0.48
2:B:105:TYR:CZ	2:B:122:LEU:HD13	2.49	0.47
2:D:5:ARG:HH21	2:D:246:HIS:HA	1.76	0.47
2:D:269:LEU:N	2:D:270:PRO:HD2	2.29	0.47
1:A:57:LYS:N	2:B:157:GLU:OE2	2.47	0.47
1:C:32:ILE:HD12	1:C:42:TYR:HB3	1.97	0.47
2:D:471:ILE:HD12	2:D:471:ILE:O	2.14	0.47
1:A:80:TYR:O	1:A:80:TYR:CG	2.67	0.47
2:B:135:VAL:HG11	2:B:179:ILE:HD11	1.95	0.47
2:D:260:GLU:HG3	2:D:481:GLY:O	2.15	0.47
2:B:260:GLU:HG3	2:B:481:GLY:O	2.15	0.46
2:D:117:VAL:HG11	2:D:190:ASN:HD22	1.79	0.46
1:A:129:LEU:O	1:A:133:LEU:HB2	2.16	0.46
1:A:32:ILE:HD12	1:A:42:TYR:HB3	1.98	0.46
2:D:105:TYR:CZ	2:D:122:LEU:HD13	2.50	0.46
2:B:269:LEU:N	2:B:270:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:288:ASN:HA	2:D:297:GLN:O	2.15	0.45
2:B:12:TRP:HA	2:B:230:MET:CE	2.47	0.45
2:B:288:ASN:HA	2:B:297:GLN:O	2.17	0.44
2:B:105:TYR:HA	2:B:121:ASP:O	2.18	0.44
1:A:39:ASN:C	1:A:78:ARG:HG3	2.43	0.44
2:B:11:ASN:O	2:B:239:ARG:NH1	2.45	0.44
2:B:220:LEU:O	2:B:221:ASP:HB2	2.18	0.44
2:D:113:LYS:HA	2:D:113:LYS:HE2	1.99	0.44
2:B:402:ALA:O	2:B:406:ILE:HG12	2.19	0.43
2:D:105:TYR:HA	2:D:121:ASP:O	2.18	0.43
2:D:272:LEU:HB2	2:D:273:PRO:HD3	2.01	0.43
2:B:65:ILE:N	2:B:65:ILE:HD12	2.33	0.43
2:D:135:VAL:HG12	2:D:136:VAL:HG23	2.01	0.43
2:B:272:LEU:HD23	2:B:284:TYR:CG	2.54	0.43
2:B:262:ARG:HA	2:B:262:ARG:NE	2.34	0.42
2:D:489:LEU:O	2:D:490:THR:C	2.62	0.42
1:C:63:CYS:SG	2:D:85:ILE:HD12	2.59	0.42
2:D:402:ALA:O	2:D:406:ILE:HG12	2.20	0.42
2:D:471:ILE:HD12	2:D:471:ILE:C	2.45	0.42
2:B:108:HIS:O	2:B:109:ASP:C	2.63	0.42
2:B:5:ARG:NH2	2:B:248:VAL:O	2.51	0.42
2:B:57:ILE:HD11	2:B:66:ARG:HB3	2.02	0.41
2:B:97:MET:HE3	2:B:141:LEU:HD13	2.02	0.41
2:B:135:VAL:HG12	2:B:136:VAL:HG23	2.02	0.41
2:B:453:ILE:HD13	2:B:474:LEU:CD2	2.50	0.41
1:A:147:ILE:HD12	1:A:147:ILE:N	2.36	0.41
2:D:118:GLU:CB	2:D:193:LEU:HD11	2.51	0.41
1:A:95:MET:SD	1:A:97:ILE:HD12	2.60	0.41
2:D:205:ARG:HA	2:D:206:PRO:HD3	1.93	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	126/155 (81%)	120 (95%)	6 (5%)	0	100	100
1	C	127/155 (82%)	119 (94%)	8 (6%)	0	100	100
2	B	469/491 (96%)	449 (96%)	20 (4%)	0	100	100
2	D	470/491 (96%)	451 (96%)	19 (4%)	0	100	100
All	All	1192/1292 (92%)	1139 (96%)	53 (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	121/145 (83%)	112 (93%)	9 (7%)	13	32
1	C	122/145 (84%)	115 (94%)	7 (6%)	18	43
2	B	417/430 (97%)	386 (93%)	31 (7%)	13	32
2	D	418/430 (97%)	397 (95%)	21 (5%)	22	48
All	All	1078/1150 (94%)	1010 (94%)	68 (6%)	16	39

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	MET
1	A	27	PHE
1	A	33	LYS
1	A	64	GLU
1	A	91	SER
1	A	103	HIS
1	A	120	ASP
1	A	133	LEU
1	A	146	ARG
2	B	23	VAL
2	B	42	SER
2	B	69	ILE
2	B	93	GLU

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Mol	Chain	Res	Type
2	B	97	MET
2	B	126	SER
2	B	152	LEU
2	B	157	GLU
2	B	179	ILE
2	B	180	SER
2	B	222	LYS
2	B	239	ARG
2	B	243	VAL
2	B	250	GLU
2	B	261	GLU
2	B	272	LEU
2	B	314	GLU
2	B	334	ASP
2	B	348	MET
2	B	356	THR
2	B	363	VAL
2	B	366	LYS
2	B	393	GLU
2	B	399	VAL
2	B	407	LEU
2	B	409	THR
2	B	411	VAL
2	B	435	ILE
2	B	449	THR
2	B	458	GLU
2	B	473	GLU
1	C	22	SER
1	C	27	PHE
1	C	33	LYS
1	C	53	SER
1	C	83	GLU
1	C	103	HIS
1	C	120	ASP
2	D	42	SER
2	D	69	ILE
2	D	75	LYS
2	D	97	MET
2	D	113	LYS
2	D	126	SER
2	D	172	LYS
2	D	180	SER

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Mol	Chain	Res	Type
2	D	193	LEU
2	D	222	LYS
2	D	243	VAL
2	D	280	THR
2	D	299	ILE
2	D	310	LEU
2	D	348	MET
2	D	356	THR
2	D	399	VAL
2	D	407	LEU
2	D	409	THR
2	D	437	LYS
2	D	446	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	24	ASN
1	A	39	ASN
1	A	122	ASN
1	A	130	ASN
2	B	6	GLN
2	B	11	ASN
2	B	178	ASN
2	B	240	GLN
2	B	278	ASN
2	B	297	GLN
2	B	358	ASN
2	B	459	ASN
2	B	480	ASN
1	C	24	ASN
1	C	39	ASN
1	C	130	ASN
2	D	11	ASN
2	D	87	ASN
2	D	89	ASN
2	D	153	ASN
2	D	178	ASN
2	D	190	ASN
2	D	235	ASN
2	D	240	GLN

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Mol	Chain	Res	Type
2	D	246	HIS
2	D	288	ASN
2	D	333	ASN
2	D	358	ASN
2	D	459	ASN
2	D	480	ASN

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 oligosaccharides 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	130/155 (83%)	0.28	5 (3%) 44 40	37, 50, 71, 95	0
1	C	131/155 (84%)	0.30	2 (1%) 72 70	40, 52, 75, 93	0
2	B	475/491 (96%)	0.19	13 (2%) 56 53	37, 51, 72, 105	0
2	D	476/491 (96%)	0.18	14 (2%) 53 50	37, 49, 72, 104	0
All	All	1212/1292 (93%)	0.21	34 (2%) 55 51	37, 50, 73, 105	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	ILE	3.5
2	D	368	GLY	3.3
2	D	146	GLY	3.2
2	D	348	MET	3.1
2	D	289	ALA	3.0
2	B	29	ASP	2.9
2	B	238	LEU	2.9
1	C	48	CYS	2.7
1	C	49	GLU	2.6
2	D	194	TYR	2.6
2	D	113	LYS	2.5
2	D	115	LYS	2.5
2	D	393	GLU	2.5
1	A	103	HIS	2.4
2	B	297	GLN	2.4
2	B	394	ASN	2.4
2	D	220	LEU	2.4
2	B	115	LYS	2.4
2	B	348	MET	2.4
2	B	194	TYR	2.3
1	A	146	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	267	LEU	2.2
2	D	238	LEU	2.2
1	A	12	PHE	2.1
1	A	10	ARG	2.1
2	B	220	LEU	2.1
2	B	316	ASN	2.1
2	B	314	GLU	2.1
2	D	448	GLU	2.1
2	B	435	ILE	2.1
2	B	398	ASP	2.0
2	B	289	ALA	2.0
2	D	282	GLU	2.0
2	D	369	ASN	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 oligosaccharides 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.