



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:58 PM GMT

PDB ID : 4C99
Title : Mouse ZNRF3 ectodomain in complex with mouse RSPO2 Fu1-Fu2 crystal form I
Authors : Zebisch, M.; Jones, E.Y.
Deposited on : 2013-10-02
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

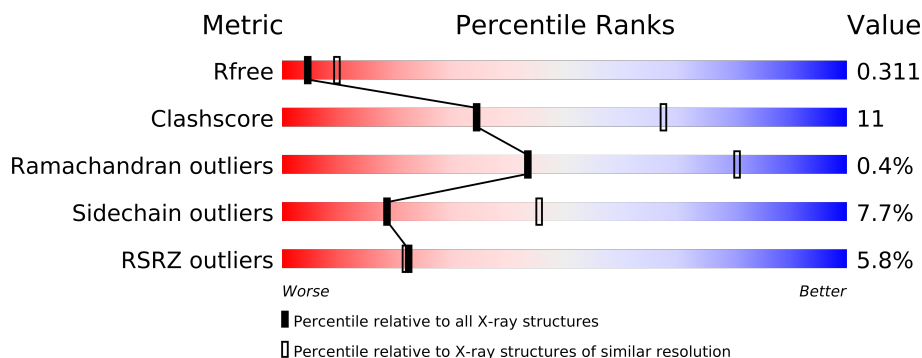
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	165	
1	C	165	
2	B	122	
2	D	122	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3968 atoms, of which 0 are hydrogen and 0 are deuterium.

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 E3 UBIQUITIN-PROTEIN LIGASE ZNR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1178	740	205	228	5			
1	C	153	Total	C	N	O	S	0	0	0
			1178	740	205	228	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	GLU	-	EXPRESSION TAG	UNP Q5SSZ7
A	51	THR	-	EXPRESSION TAG	UNP Q5SSZ7
A	52	GLY	-	EXPRESSION TAG	UNP Q5SSZ7
A	206	GLY	-	EXPRESSION TAG	UNP Q5SSZ7
A	207	THR	-	EXPRESSION TAG	UNP Q5SSZ7
A	208	LYS	-	EXPRESSION TAG	UNP Q5SSZ7
A	209	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
A	210	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
A	211	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
A	212	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
A	213	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
A	214	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
C	50	GLU	-	EXPRESSION TAG	UNP Q5SSZ7
C	51	THR	-	EXPRESSION TAG	UNP Q5SSZ7
C	52	GLY	-	EXPRESSION TAG	UNP Q5SSZ7
C	206	GLY	-	EXPRESSION TAG	UNP Q5SSZ7
C	207	THR	-	EXPRESSION TAG	UNP Q5SSZ7
C	208	LYS	-	EXPRESSION TAG	UNP Q5SSZ7
C	209	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
C	210	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
C	211	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
C	212	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
C	213	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
C	214	HIS	-	EXPRESSION TAG	UNP Q5SSZ7

- Molecule 2 is a protein called R-SPONDIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	103	Total	C	N	O	S	0	0	0
			797	484	146	148	19			
2	D	105	Total	C	N	O	S	0	0	0
			814	498	146	151	19			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	GLU	-	EXPRESSION TAG	UNP Q8BFU0
B	35	THR	-	EXPRESSION TAG	UNP Q8BFU0
B	36	GLY	-	EXPRESSION TAG	UNP Q8BFU0
B	145	THR	-	EXPRESSION TAG	UNP Q8BFU0
B	146	HIS	-	EXPRESSION TAG	UNP Q8BFU0
B	147	HIS	-	EXPRESSION TAG	UNP Q8BFU0
B	148	HIS	-	EXPRESSION TAG	UNP Q8BFU0
B	149	HIS	-	EXPRESSION TAG	UNP Q8BFU0
B	150	HIS	-	EXPRESSION TAG	UNP Q8BFU0
B	151	HIS	-	EXPRESSION TAG	UNP Q8BFU0
B	152	HIS	-	EXPRESSION TAG	UNP Q8BFU0
B	153	HIS	-	EXPRESSION TAG	UNP Q8BFU0
B	154	HIS	-	EXPRESSION TAG	UNP Q8BFU0
B	155	HIS	-	EXPRESSION TAG	UNP Q8BFU0
D	34	GLU	-	EXPRESSION TAG	UNP Q8BFU0
D	35	THR	-	EXPRESSION TAG	UNP Q8BFU0
D	36	GLY	-	EXPRESSION TAG	UNP Q8BFU0
D	145	THR	-	EXPRESSION TAG	UNP Q8BFU0
D	146	HIS	-	EXPRESSION TAG	UNP Q8BFU0
D	147	HIS	-	EXPRESSION TAG	UNP Q8BFU0
D	148	HIS	-	EXPRESSION TAG	UNP Q8BFU0
D	149	HIS	-	EXPRESSION TAG	UNP Q8BFU0
D	150	HIS	-	EXPRESSION TAG	UNP Q8BFU0
D	151	HIS	-	EXPRESSION TAG	UNP Q8BFU0
D	152	HIS	-	EXPRESSION TAG	UNP Q8BFU0
D	153	HIS	-	EXPRESSION TAG	UNP Q8BFU0
D	154	HIS	-	EXPRESSION TAG	UNP Q8BFU0
D	155	HIS	-	EXPRESSION TAG	UNP Q8BFU0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

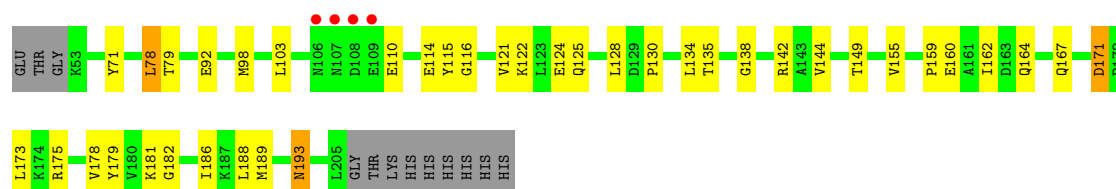
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

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.

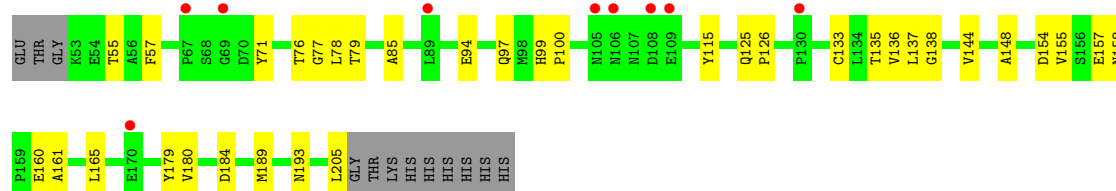
• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3

Chain A: 



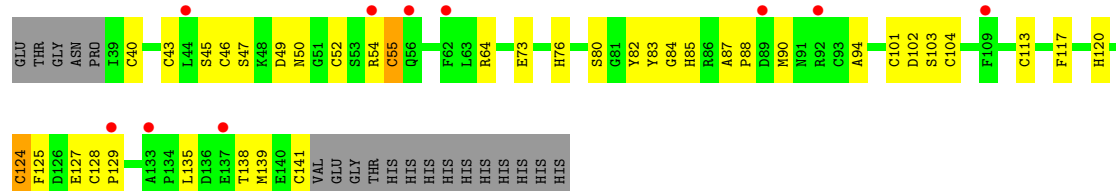
• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3

Chain C: 



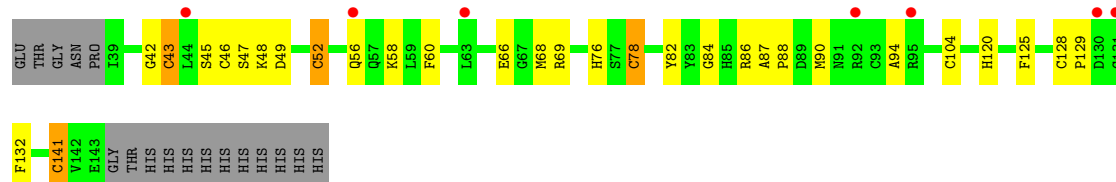
• Molecule 2: R-SPONDIN-2

Chain B: 



• Molecule 2: R-SPONDIN-2

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.80Å 77.21Å 130.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.46 – 2.80 65.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (66.46-2.80) 99.9 (65.31-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.236 , 0.323 0.237 , 0.311	Depositor DCC
R_{free} test set	772 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	75.6	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 15477 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3968	wwPDB-VP
Average B, all atoms (Å ²)	86.0	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 31.31 % 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 1.1304e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.66	0/1198	0.79	0/1623
1	C	0.63	0/1198	0.80	0/1623
2	B	0.62	0/815	0.77	0/1089
2	D	0.67	0/832	0.90	4/1111 (0.4%)
All	All	0.65	0/4043	0.81	4/5446 (0.1%)

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
2	D	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	128	CYS	CA-CB-SG	-5.36	104.35	114.00
2	D	52	CYS	CA-CB-SG	5.35	123.63	114.00
2	D	104	CYS	CB-CA-C	-5.09	100.22	110.40
2	D	78	CYS	CA-CB-SG	-5.05	104.90	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	141	CYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1178	0	1178	27	0
1	C	1178	0	1178	30	0
2	B	797	0	698	23	0
2	D	814	0	727	13	0
3	A	1	0	0	0	0
All	All	3968	0	3781	84	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (84) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:129:PRO:HD2	2:B:141:CYS:SG	1.91	1.08
1:C:155:VAL:CG2	1:C:179:TYR:HB2	1.93	0.97
1:C:155:VAL:HG21	1:C:179:TYR:HB2	1.51	0.90
2:B:113:CYS:SG	2:B:117:PHE:HB3	2.19	0.82
2:B:113:CYS:SG	2:B:117:PHE:CB	2.74	0.76
1:A:128:LEU:HD13	2:B:45:SER:OG	1.94	0.66
1:A:124:GLU:OE1	2:B:47:SER:HB3	1.96	0.65
2:B:129:PRO:CD	2:B:141:CYS:SG	2.80	0.64
1:C:154:ASP:C	1:C:154:ASP:OD1	2.36	0.64
2:B:83:TYR:HB3	2:B:104:CYS:HB2	1.78	0.64
1:A:160:GLU:O	1:A:164:GLN:HG3	1.97	0.64
2:D:87:ALA:HB1	2:D:88:PRO:CD	2.28	0.63
1:C:155:VAL:HG12	1:C:158:ASN:O	2.00	0.60
2:B:82:TYR:HA	2:B:94:ALA:O	2.02	0.59
1:C:155:VAL:HG21	1:C:179:TYR:CB	2.29	0.59
1:A:122:LYS:O	2:B:50:ASN:ND2	2.33	0.59
1:A:155:VAL:HG21	1:A:162:ILE:CG1	2.33	0.59
2:B:113:CYS:SG	2:B:117:PHE:HB2	2.43	0.58
2:D:87:ALA:HB3	2:D:90:MET:O	2.03	0.58
1:C:57:PHE:CE1	1:C:205:LEU:HD12	2.38	0.58
1:A:149:THR:OG1	1:A:175:ARG:NH1	2.38	0.56
1:C:157:GLU:HA	1:C:157:GLU:OE1	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:49:ASP:C	2:D:69:ARG:HH22	2.10	0.56
2:D:43:CYS:HB2	2:D:45:SER:O	2.07	0.55
1:A:128:LEU:HD22	2:B:45:SER:HB2	1.86	0.55
2:D:42:GLY:O	2:D:56:GLN:HB2	2.07	0.55
1:C:85:ALA:HB2	1:C:165:LEU:O	2.07	0.55
2:D:87:ALA:HB1	2:D:88:PRO:HD2	1.88	0.54
1:A:125:GLN:HB2	1:A:128:LEU:HG	1.88	0.54
2:B:135:LEU:O	2:B:139:MET:N	2.41	0.53
2:B:64:ARG:HH21	2:B:73:GLU:HG2	1.73	0.53
2:D:82:TYR:HA	2:D:94:ALA:O	2.09	0.53
1:C:97:GLN:HE22	2:D:69:ARG:HH12	1.56	0.53
1:A:135:THR:O	1:A:138:GLY:N	2.41	0.53
1:C:155:VAL:HG23	1:C:179:TYR:HB2	1.83	0.52
1:C:161:ALA:O	1:C:165:LEU:N	2.42	0.52
2:D:129:PRO:O	2:D:132:PHE:HB2	2.10	0.52
1:A:171:ASP:OD1	1:A:171:ASP:N	2.43	0.52
2:B:83:TYR:CE2	2:B:85:HIS:HB2	2.46	0.51
2:B:87:ALA:HB1	2:B:88:PRO:HD2	1.93	0.51
1:A:78:LEU:HD21	1:A:188:LEU:HB2	1.92	0.50
2:B:83:TYR:CD2	2:B:84:GLY:O	2.64	0.50
1:A:155:VAL:HG21	1:A:162:ILE:HG12	1.91	0.50
1:C:189:MET:O	1:C:193:ASN:HB2	2.11	0.50
2:B:64:ARG:NH2	2:B:73:GLU:HG2	2.26	0.50
1:C:99:HIS:ND1	1:C:100:PRO:HD2	2.27	0.49
1:A:98:MET:CE	1:A:103:LEU:HD21	2.42	0.49
1:C:193:ASN:ND2	2:D:49:ASP:OD1	2.46	0.48
1:C:126:PRO:HD3	1:C:158:ASN:HB2	1.94	0.48
1:A:182:GLY:O	1:A:186:ILE:HG12	2.14	0.48
1:C:55:THR:HG23	1:C:79:THR:HG23	1.95	0.48
1:C:144:VAL:HA	1:C:148:ALA:HB3	1.96	0.47
1:C:136:VAL:HG13	1:C:137:LEU:H	1.79	0.47
2:B:135:LEU:O	2:B:138:THR:N	2.47	0.46
1:C:76:THR:HG22	1:C:77:GLY:N	2.31	0.46
2:D:60:PHE:CZ	2:D:84:GLY:HA3	2.51	0.46
2:B:87:ALA:HB3	2:B:90:MET:O	2.16	0.46
2:D:46:CYS:SG	2:D:47:SER:N	2.89	0.45
1:C:154:ASP:HA	1:C:180:VAL:HG23	1.98	0.45
1:A:71:TYR:CE2	1:C:115:TYR:HB2	2.52	0.45
1:C:136:VAL:HG13	1:C:137:LEU:N	2.31	0.45
1:A:144:VAL:HG21	1:A:173:LEU:HD13	1.98	0.44
1:A:159:PRO:O	1:A:162:ILE:N	2.50	0.44
1:C:125:GLN:O	1:C:126:PRO:C	2.55	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:80:SER:HA	2:B:102:ASP:OD1	2.17	0.44
1:A:193:ASN:ND2	2:B:49:ASP:OD1	2.50	0.44
1:C:154:ASP:HB2	1:C:189:MET:HE3	2.01	0.43
1:C:160:GLU:H	1:C:160:GLU:CD	2.21	0.43
1:A:115:TYR:HB2	1:C:71:TYR:CE1	2.53	0.43
1:A:114:GLU:OE1	1:A:114:GLU:N	2.51	0.43
1:A:178:VAL:HG12	1:A:179:TYR:N	2.34	0.42
1:A:116:GLY:O	1:A:149:THR:HG22	2.19	0.42
1:A:98:MET:HB2	1:A:121:VAL:HG22	2.02	0.42
1:C:135:THR:O	1:C:138:GLY:N	2.52	0.42
1:A:189:MET:O	1:A:193:ASN:HB2	2.20	0.42
2:B:127:GLU:O	2:B:128:CYS:C	2.57	0.41
1:C:76:THR:HG22	1:C:77:GLY:H	1.85	0.41
1:C:57:PHE:CZ	1:C:205:LEU:HD12	2.55	0.41
2:D:120:HIS:HB3	2:D:125:PHE:CE1	2.56	0.41
1:C:135:THR:O	1:C:136:VAL:C	2.58	0.41
2:B:113:CYS:HB2	2:B:124:CYS:HB2	2.00	0.41
1:A:167:GLN:OE1	1:A:167:GLN:O	2.39	0.40
1:A:98:MET:HE3	1:A:103:LEU:HD21	2.03	0.40
1:A:110:GLU:OE2	1:A:142:ARG:NH2	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	151/165 (92%)	135 (89%)	15 (10%)	1 (1%)	30	69
1	C	151/165 (92%)	141 (93%)	10 (7%)	0	100	100
2	B	101/122 (83%)	87 (86%)	13 (13%)	1 (1%)	22	60
2	D	103/122 (84%)	93 (90%)	10 (10%)	0	100	100
All	All	506/574 (88%)	456 (90%)	48 (10%)	2 (0%)	43	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	55	CYS
1	A	130	PRO

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	128/138 (93%)	121 (94%)	7 (6%)	30	65
1	C	128/138 (93%)	124 (97%)	4 (3%)	52	86
2	B	86/108 (80%)	74 (86%)	12 (14%)	5	15
2	D	89/108 (82%)	79 (89%)	10 (11%)	9	25
All	All	431/492 (88%)	398 (92%)	33 (8%)	18	45

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	79	THR
1	A	92	GLU
1	A	134	LEU
1	A	171	ASP
1	A	181	LYS
1	A	193	ASN
2	B	40	CYS
2	B	43	CYS
2	B	46	CYS
2	B	52	CYS
2	B	54	ARG
2	B	55	CYS
2	B	76	HIS
2	B	101	CYS
2	B	103	SER
2	B	120	HIS
2	B	124	CYS
2	B	125	PHE
1	C	78	LEU
1	C	94	GLU

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Mol	Chain	Res	Type
1	C	133	CYS
1	C	184	ASP
2	D	43	CYS
2	D	48	LYS
2	D	52	CYS
2	D	58	LYS
2	D	66	GLU
2	D	68	MET
2	D	76	HIS
2	D	78	CYS
2	D	86	ARG
2	D	141	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
2	B	85	HIS
2	B	100	ASN
2	B	120	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	153/165 (92%)	0.16	4 (2%) 53 54	38, 71, 117, 182	0
1	C	153/165 (92%)	0.32	9 (5%) 22 21	44, 77, 139, 184	0
2	B	103/122 (84%)	0.40	10 (9%) 8 7	63, 101, 136, 162	0
2	D	105/122 (86%)	0.19	7 (6%) 17 16	57, 82, 123, 143	0
All	All	514/574 (89%)	0.26	30 (5%) 22 22	38, 81, 130, 184	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	ASN	7.7
1	C	106	ASN	6.4
1	A	107	ASN	6.3
2	D	130	ASP	5.2
1	A	108	ASP	4.9
2	B	44	LEU	4.2
1	A	109	GLU	4.0
1	C	170	GLU	4.0
1	C	108	ASP	3.8
2	D	56	GLN	3.8
2	B	133	ALA	3.2
2	B	137	GLU	3.1
2	B	89	ASP	3.1
1	C	69	GLY	2.8
2	D	131	GLY	2.8
2	B	129	PRO	2.7
2	B	56	GLN	2.7
2	B	109	PHE	2.7
2	D	95	ARG	2.5
1	C	109	GLU	2.4
2	D	44	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	92	ARG	2.3
2	D	63	LEU	2.2
1	C	130	PRO	2.2
1	C	105	ASN	2.2
1	C	67	PRO	2.1
1	C	89	LEU	2.1
2	B	62	PHE	2.0
2	B	54	ARG	2.0
2	D	92	ARG	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q < 0.9
3	CL	A	1206	1/1	0.22	1.06	79,79,79,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.