



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:58 PM GMT

PDB ID : 4N90
Title : Crystal structure of ternary complex of TRAIL, DR5, and Fab fragment from a DR5 agonist antibody
Authors : Huang, X.
Deposited on : 2013-10-18
Resolution : 3.30 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
<http://wwpdb.org/validation/2016/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:

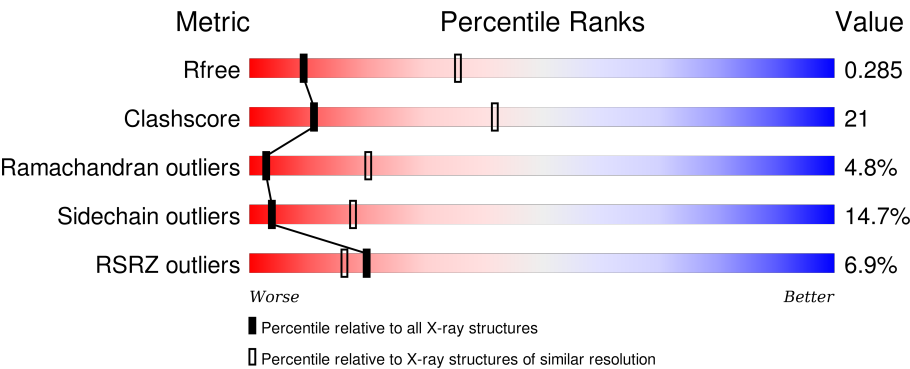
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

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 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	R	126	<div><div>2%</div><div>55%26%5%14%</div></div>
1	S	126	<div><div>4%</div><div>51%25%8%16%</div></div>
1	T	126	<div><div>3%</div><div>43%37%6%15%</div></div>
2	A	168	<div><div>4%</div><div>52%33%6%8%</div></div>
2	B	168	<div><div>4%</div><div>53%32%7%8%</div></div>

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Mol	Chain	Length	Quality of chain
2	C	168	<div><div></div><div>2%</div><div>49%</div><div>35%</div><div>8%</div><div>8%</div></div>
3	E	215	<div><div></div><div>60%</div><div>35%</div><div></div><div></div></div>
3	G	215	<div><div></div><div>21%</div><div>59%</div><div>32%</div><div>8%</div></div>
3	I	215	<div><div></div><div>19%</div><div>56%</div><div>34%</div><div>7%</div></div>
4	D	224	<div><div></div><div>46%</div><div>38%</div><div>11%</div><div></div></div>
4	F	224	<div><div></div><div>9%</div><div>49%</div><div>36%</div><div>10%</div></div>
4	H	224	<div><div></div><div>4%</div><div>45%</div><div>38%</div><div>13%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15934 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 Tumor necrosis factor receptor superfamily member 10B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	108	Total	C	N	O	S	0	0	0
			833	498	150	169	16			
1	S	106	Total	C	N	O	S	0	0	0
			814	486	145	167	16			
1	T	107	Total	C	N	O	S	0	0	0
			824	492	148	168	16			

- Molecule 2 is a protein called Tumor necrosis factor ligand superfamily member 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	155	Total	C	N	O	S	0	0	0
			1278	813	221	240	4			
2	B	155	Total	C	N	O	S	0	0	0
			1274	811	221	238	4			
2	C	154	Total	C	N	O	S	0	1	0
			1276	812	223	237	4			

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1623	1015	275	329	4			
3	G	214	Total	C	N	O	S	0	0	0
			1615	1012	271	328	4			
3	I	214	Total	C	N	O	S	0	0	0
			1615	1012	271	328	4			

- Molecule 4 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	218	Total	C	N	O	S	0	0	0
			1616	1021	269	321	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	N	O	S	0	0	0
			1575	998	258	314	5			
4	H	215	Total	C	N	O	S	0	0	0
			1590	1007	262	316	5			

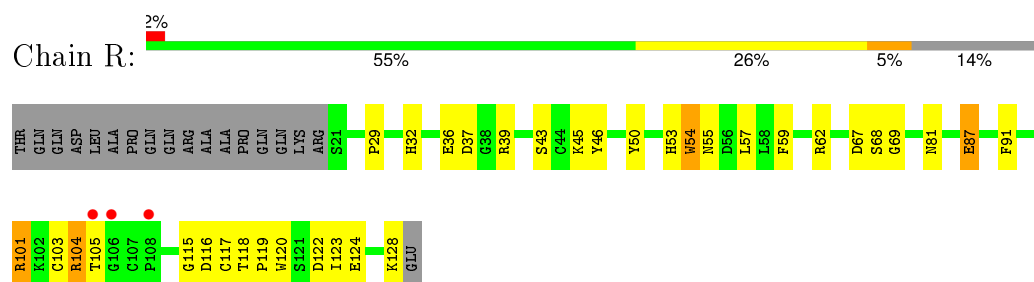
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	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 ($\text{RSRZ} > 2$). 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.

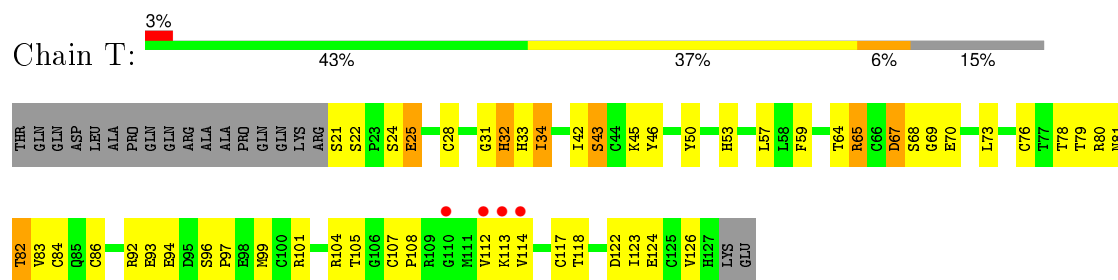
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



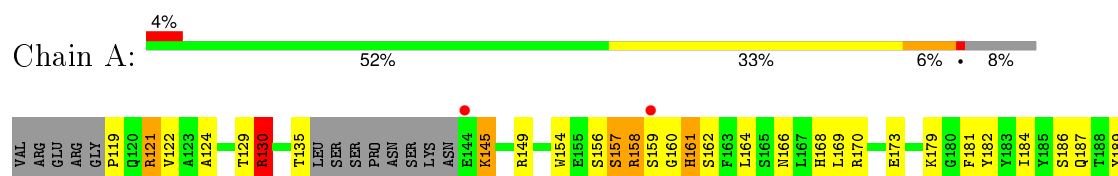
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

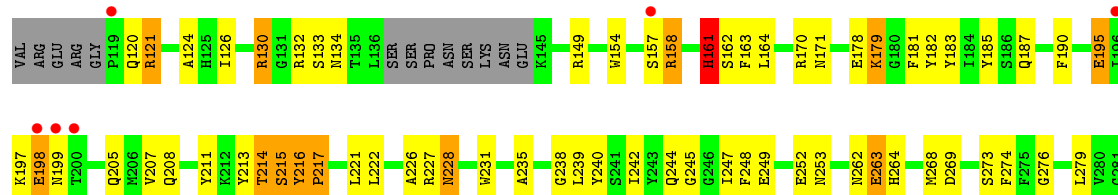


- Molecule 2: Tumor necrosis factor ligand superfamily member 10

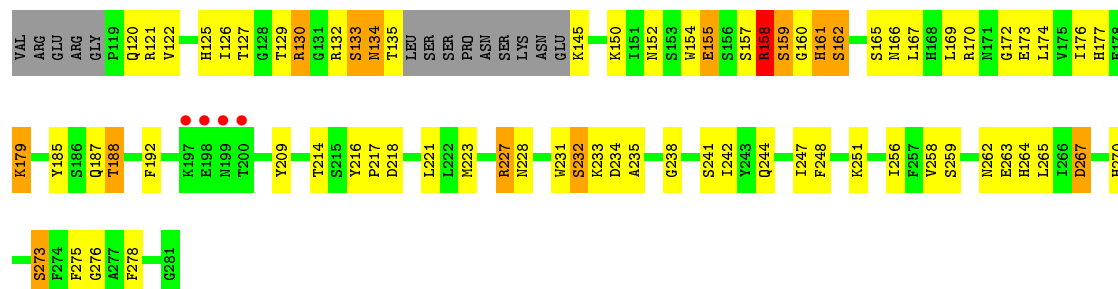




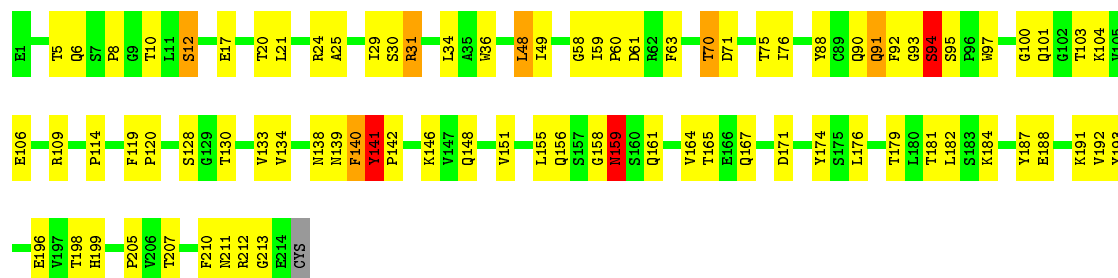
- Molecule 2: Tumor necrosis factor ligand superfamily member 10



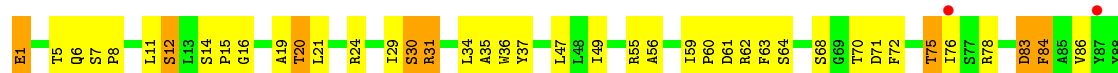
- Molecule 2: Tumor necrosis factor ligand superfamily member 10

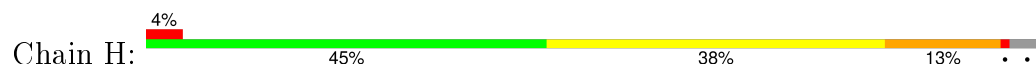


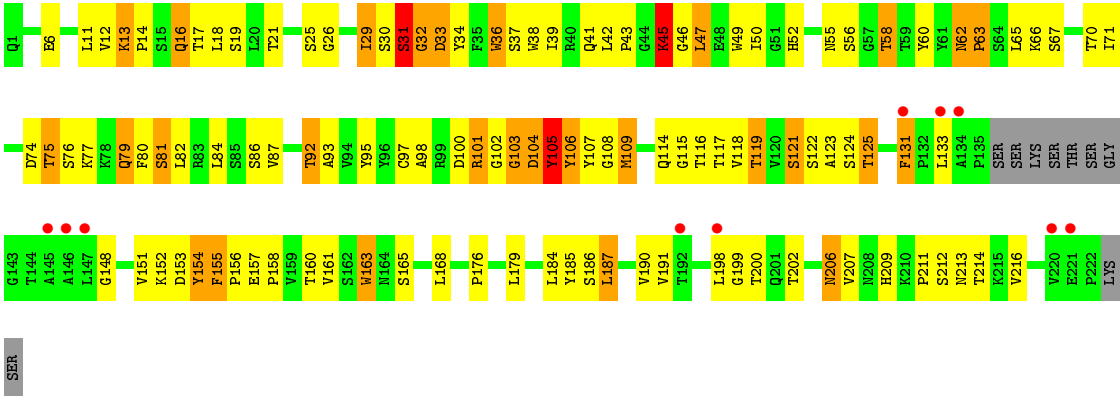
- Molecule 3: Fab light chain



- Molecule 3: Fab light chain







4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	152.01Å 152.01Å 613.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.30 49.93 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.30) 99.0 (49.93-3.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.229 , 0.286 0.229 , 0.285	Depositor DCC
R_{free} test set	3233 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 63797 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15934	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN

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	R	0.66	3/851 (0.4%)	0.69	0/1150
1	S	0.69	3/831 (0.4%)	0.74	0/1124
1	T	0.65	1/842 (0.1%)	0.75	1/1139 (0.1%)
2	A	0.61	1/1309 (0.1%)	0.74	0/1758
2	B	0.63	0/1305	0.76	0/1753
2	C	0.66	1/1311 (0.1%)	0.81	1/1760 (0.1%)
3	E	0.60	1/1660 (0.1%)	0.80	2/2258 (0.1%)
3	G	0.52	1/1652 (0.1%)	0.72	2/2249 (0.1%)
3	I	0.55	2/1652 (0.1%)	0.78	2/2249 (0.1%)
4	D	0.62	1/1657 (0.1%)	0.87	4/2267 (0.2%)
4	F	0.63	3/1616 (0.2%)	0.77	1/2216 (0.0%)
4	H	0.64	3/1631 (0.2%)	0.80	0/2233
All	All	0.62	20/16317 (0.1%)	0.78	13/22156 (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	C	0	1
3	E	0	2
3	G	0	2
3	I	0	2
4	D	0	4
4	F	0	4
4	H	0	4
All	All	0	19

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	36	TRP	CD2-CE2	6.55	1.49	1.41
4	H	49	TRP	CD2-CE2	6.01	1.48	1.41
1	S	32	HIS	CB-CG	5.84	1.60	1.50
3	G	97	TRP	CD2-CE2	5.64	1.48	1.41
1	R	120	TRP	CD2-CE2	5.61	1.48	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	95	SER	N-CA-C	-8.99	86.72	111.00
3	E	141	TYR	N-CA-C	7.51	131.29	111.00
4	F	155	PHE	N-CA-C	6.98	129.83	111.00
3	I	95	SER	N-CA-C	-6.81	92.61	111.00
3	G	95	SER	N-CA-C	-6.54	93.33	111.00

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	155	GLU	Peptide
4	D	106	TYR	Peptide
4	D	67	SER	Peptide
3	E	140	PHE	Peptide
3	E	94	SER	Peptide

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	R	833	0	755	28	0
1	S	814	0	735	30	0
1	T	824	0	742	35	0
2	A	1278	0	1226	63	0
2	B	1274	0	1222	74	0
2	C	1276	0	1229	50	0
3	E	1623	0	1548	59	1
3	G	1615	0	1538	59	0
3	I	1615	0	1538	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1616	0	1556	89	0
4	F	1575	0	1498	63	0
4	H	1590	0	1527	91	0
5	A	1	0	0	0	0
All	All	15934	0	15114	650	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 21.

The worst 5 of 650 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:B:157:SER:HA	2:B:158:ARG:NH2	1.47	1.28
2:B:158:ARG:HH11	2:B:158:ARG:HG2	1.09	1.14
1:T:64:THR:O	1:T:82:THR:HG21	1.61	1.01
4:D:42:LEU:HB3	4:D:43:PRO:HD2	1.40	1.00
3:I:156:GLN:HB3	3:I:159:ASN:HD21	1.33	0.94

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)
3:E:17:GLU:OE1	3:E:17:GLU:OE1[12_545]	2.18	0.02

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	R	106/126 (84%)	98 (92%)	6 (6%)	2 (2%)	10	45
1	S	104/126 (82%)	90 (86%)	13 (12%)	1 (1%)	19	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	105/126 (83%)	89 (85%)	13 (12%)	3 (3%)	6	34
2	A	151/168 (90%)	129 (85%)	16 (11%)	6 (4%)	4	24
2	B	151/168 (90%)	133 (88%)	14 (9%)	4 (3%)	7	36
2	C	151/168 (90%)	132 (87%)	14 (9%)	5 (3%)	5	30
3	E	212/215 (99%)	181 (85%)	23 (11%)	8 (4%)	4	26
3	G	212/215 (99%)	177 (84%)	25 (12%)	10 (5%)	3	20
3	I	212/215 (99%)	178 (84%)	20 (9%)	14 (7%)	1	12
4	D	214/224 (96%)	175 (82%)	26 (12%)	13 (6%)	2	14
4	F	210/224 (94%)	167 (80%)	28 (13%)	15 (7%)	1	11
4	H	211/224 (94%)	162 (77%)	32 (15%)	17 (8%)	1	8
All	All	2039/2199 (93%)	1711 (84%)	230 (11%)	98 (5%)	3	20

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	119	PRO
2	A	130	ARG
2	A	161	HIS
2	B	198	GLU
2	C	158	ARG

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	R	99/114 (87%)	90 (91%)	9 (9%)	12	41
1	S	97/114 (85%)	82 (84%)	15 (16%)	3	16
1	T	98/114 (86%)	87 (89%)	11 (11%)	7	30
2	A	137/149 (92%)	120 (88%)	17 (12%)	6	25
2	B	136/149 (91%)	117 (86%)	19 (14%)	4	20
2	C	137/149 (92%)	118 (86%)	19 (14%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	179/185 (97%)	161 (90%)	18 (10%)	9	35
3	G	178/185 (96%)	152 (85%)	26 (15%)	4	18
3	I	178/185 (96%)	152 (85%)	26 (15%)	4	18
4	D	181/192 (94%)	143 (79%)	38 (21%)	1	6
4	F	175/192 (91%)	147 (84%)	28 (16%)	3	14
4	H	178/192 (93%)	142 (80%)	36 (20%)	1	6
All	All	1773/1920 (92%)	1511 (85%)	262 (15%)	4	17

5 of 262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	55	ASN
3	G	1	GLU
4	H	75	THR
4	D	70	THR
4	D	116	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	159	ASN
4	D	114	GLN
4	H	62	ASN
4	D	41	GLN
3	G	43	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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.

No monomer is involved in short contacts.

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 [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	R	108/126 (85%)	0.16	3 (2%) 56 50	39, 71, 149, 167	0
1	S	106/126 (84%)	0.31	5 (4%) 35 29	49, 71, 152, 169	0
1	T	107/126 (84%)	0.22	4 (3%) 45 38	44, 72, 139, 168	0
2	A	155/168 (92%)	-0.01	6 (3%) 43 36	32, 55, 121, 202	0
2	B	155/168 (92%)	-0.06	6 (3%) 43 36	34, 51, 109, 164	0
2	C	154/168 (91%)	-0.02	4 (2%) 59 53	34, 54, 107, 181	0
3	E	214/215 (99%)	-0.02	0 100 100	28, 55, 103, 117	0
3	G	214/215 (99%)	0.96	45 (21%) 1 1	43, 94, 158, 175	0
3	I	214/215 (99%)	0.73	41 (19%) 2 1	28, 85, 140, 154	0
4	D	218/224 (97%)	-0.13	0 100 100	36, 55, 94, 113	0
4	F	214/224 (95%)	0.45	20 (9%) 11 9	51, 92, 141, 166	0
4	H	215/224 (95%)	0.20	10 (4%) 35 29	29, 74, 113, 136	0
All	All	2074/2199 (94%)	0.25	144 (6%) 20 16	28, 68, 139, 202	0

The worst 5 of 144 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	135	CYS	10.3
2	C	199	ASN	8.6
2	A	199	ASN	7.2
3	G	149	TRP	6.8
3	G	117	PHE	6.5

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 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	ZN	A	301	1/1	0.99	0.15	-0.60	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.