



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 11:53 PM JST

PDB ID : 7C6A
Title : Crystal structure of AT2R-BRIL and SRP2070_Fab complex
Authors : Suzuki, M.; Miyagi, H.; Asada, H.; Yasunaga, M.; Suno, C.; Takahashi, Y.;
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Deposited on : 2020-05-21
Resolution : 3.40 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

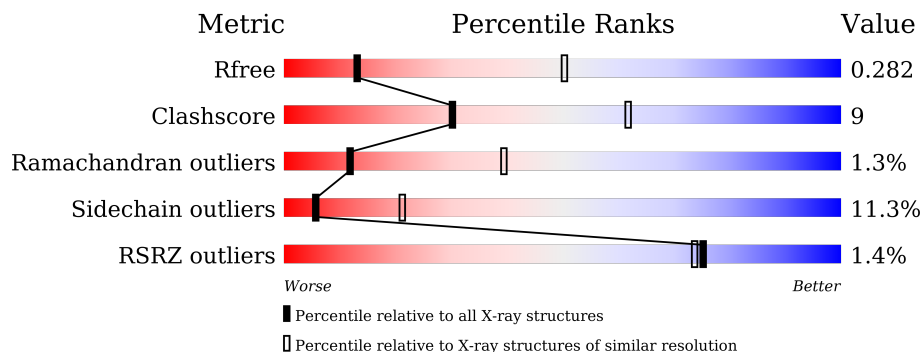
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

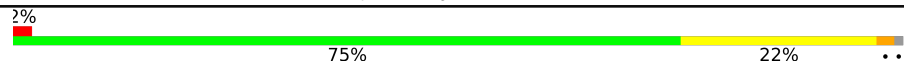
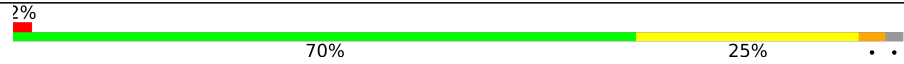


The reported resolution of this entry is 3.40 Å.

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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	L	214	 2% 75% 22% ..
2	H	224	 2% 70% 25% ..
3	A	422	 % 65% 21% • 12%
4	B	8	 75% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6352 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 IgG Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	211	1640	1020	280	334	6	0	0	0

- Molecule 2 is a protein called IgG heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	219	1672	1067	268	330	7	0	0	0

- Molecule 3 is a protein called Type-2 angiotensin II receptor, Soluble cytochrome b562, Type-2 angiotensin II receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	373	2971	1968	473	507	23	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP P50052
A	93	VAL	LEU	engineered mutation	UNP P50052
A	133	TRP	PHE	engineered mutation	UNP P50052
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	347	GLU	-	expression tag	UNP P50052
A	348	ASN	-	expression tag	UNP P50052
A	349	LEU	-	expression tag	UNP P50052
A	350	TYR	-	expression tag	UNP P50052
A	351	PHE	-	expression tag	UNP P50052
A	352	GLN	-	expression tag	UNP P50052

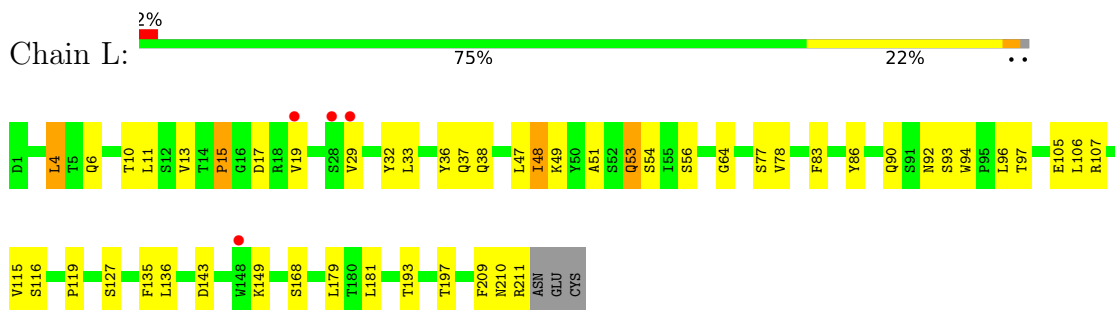
- Molecule 4 is a protein called SAR1, ILE8-ANGIOTENSIN II.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	B	8	69	46	13	10	0	0	0

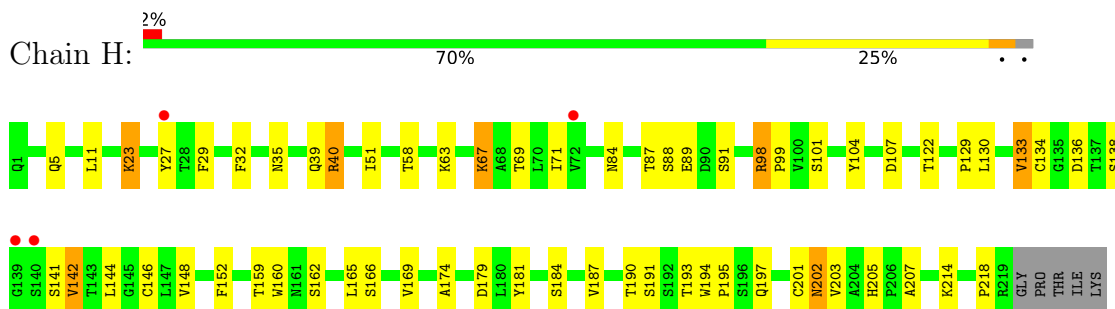
3 Residue-property plots i

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.

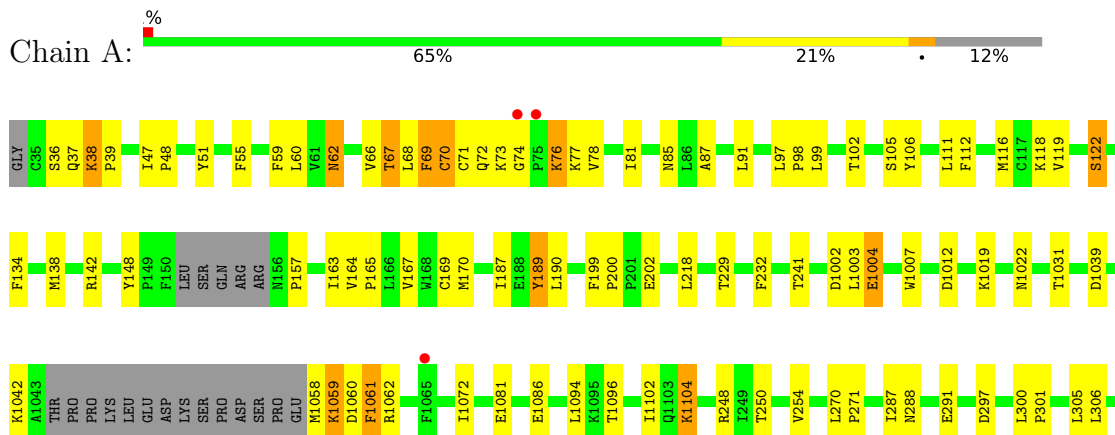
- Molecule 1: IgG Light Chain

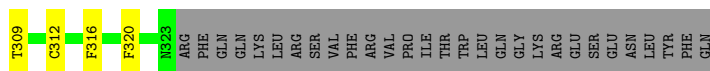


- Molecule 2: IgG heavy chain



- Molecule 3: Type-2 angiotensin II receptor, Soluble cytochrome b562, Type-2 angiotensin II receptor





- Molecule 4: SAR1, ILE8-ANGIOTENSIN II

Chain B: 75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.23Å 131.04Å 113.80Å 90.00° 97.07° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 42.77 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-3.40) 100.0 (42.77-3.40)	Depositor EDS
R_{merge}	0.61	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.235 , 0.285 0.235 , 0.282	Depositor DCC
R_{free} test set	795 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	90.3	Xtrriage
Anisotropy	0.553	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 88.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6352	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: SAR

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	L	0.66	0/1678	0.76	0/2279
2	H	0.65	0/1720	0.77	0/2351
3	A	0.65	0/3047	0.72	0/4145
4	B	0.57	0/66	0.76	0/88
All	All	0.65	0/6511	0.74	0/8863

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
3	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	74	GLY	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	L	1640	0	1569	23	0
2	H	1672	0	1619	41	0
3	A	2971	0	3027	60	0
4	B	69	0	73	0	0
All	All	6352	0	6288	117	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 9.

All (117) 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:H:160:TRP:HB3	2:H:165:LEU:CD2	1.75	1.16
3:A:71:CYS:HB3	3:A:72:GLN:HE21	1.08	1.08
2:H:160:TRP:CB	2:H:165:LEU:HD23	1.86	1.06
2:H:160:TRP:HB3	2:H:165:LEU:HD23	1.05	1.03
3:A:71:CYS:HB3	3:A:72:GLN:NE2	1.73	1.01
2:H:160:TRP:HB2	2:H:165:LEU:HB3	1.44	0.99
3:A:71:CYS:CB	3:A:72:GLN:NE2	2.30	0.93
2:H:165:LEU:O	2:H:169:VAL:HG21	1.71	0.90
3:A:71:CYS:CB	3:A:72:GLN:HE21	1.85	0.87
2:H:160:TRP:HB2	2:H:165:LEU:CB	2.16	0.76
3:A:76:LYS:O	3:A:157:PRO:HD3	1.91	0.71
2:H:129:PRO:HG3	2:H:214:LYS:HB3	1.76	0.68
3:A:78:VAL:O	3:A:81:ILE:HG22	1.93	0.67
3:A:76:LYS:CA	3:A:157:PRO:HG3	2.25	0.66
1:L:13:VAL:HG21	1:L:78:VAL:HG11	1.79	0.64
1:L:119:PRO:HD3	2:H:133:VAL:HG13	1.80	0.64
2:H:35:ASN:HD21	2:H:99:PRO:HB3	1.63	0.63
3:A:71:CYS:HB2	3:A:72:GLN:NE2	2.11	0.63
3:A:76:LYS:HB3	3:A:157:PRO:CG	2.27	0.63
3:A:66:VAL:O	3:A:70:CYS:HB2	2.01	0.61
3:A:76:LYS:N	3:A:76:LYS:HD2	2.16	0.60
3:A:67:THR:O	3:A:71:CYS:HB2	2.03	0.59
1:L:51:ALA:O	1:L:64:GLY:HA3	2.02	0.59
1:L:83:PHE:CZ	1:L:106:LEU:HB2	2.39	0.58
2:H:40:ARG:NH2	2:H:89:GLU:HA	2.20	0.57
3:A:71:CYS:HB2	3:A:72:GLN:HE22	1.70	0.57
2:H:104:TYR:OH	3:A:1086:GLU:OE2	2.23	0.56
3:A:76:LYS:HA	3:A:157:PRO:HG3	1.89	0.55
1:L:149:LYS:HB2	1:L:193:THR:HB	1.88	0.54
3:A:76:LYS:HB3	3:A:157:PRO:CD	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:VAL:CG1	2:H:191:SER:HA	2.37	0.53
2:H:160:TRP:CB	2:H:165:LEU:CD2	2.62	0.53
2:H:160:TRP:CB	2:H:165:LEU:CB	2.86	0.53
2:H:194:TRP:CG	2:H:195:PRO:HA	2.44	0.53
2:H:205:HIS:CE1	2:H:207:ALA:HB3	2.45	0.52
2:H:160:TRP:O	2:H:165:LEU:HB2	2.09	0.52
3:A:62:ASN:HB3	3:A:91:LEU:HD13	1.92	0.52
3:A:164:VAL:HB	3:A:165:PRO:HD3	1.92	0.51
2:H:193:THR:OG1	2:H:194:TRP:N	2.44	0.51
3:A:199:PHE:HB3	3:A:200:PRO:HD2	1.93	0.51
2:H:67:LYS:HA	2:H:84:ASN:HD21	1.76	0.50
3:A:1059:LYS:HG2	3:A:1061:PHE:HB2	1.94	0.50
3:A:76:LYS:N	3:A:76:LYS:CD	2.74	0.49
2:H:11:LEU:HD11	2:H:152:PHE:CE2	2.48	0.49
3:A:69:PHE:CD1	3:A:69:PHE:C	2.85	0.49
3:A:37:GLN:O	3:A:39:PRO:HD3	2.13	0.49
3:A:1072:ILE:HG13	3:A:1094:LEU:HD21	1.94	0.48
3:A:316:PHE:HA	3:A:320:PHE:HB2	1.94	0.48
3:A:241:THR:HG22	3:A:241:THR:O	2.14	0.48
3:A:1004:GLU:HA	3:A:1007:TRP:HB2	1.96	0.48
3:A:250:THR:O	3:A:254:VAL:HG23	2.14	0.48
2:H:160:TRP:HB3	2:H:165:LEU:HD22	1.87	0.48
2:H:133:VAL:HG23	2:H:134:CYS:H	1.79	0.47
2:H:142:VAL:HG11	2:H:191:SER:HA	1.94	0.47
3:A:106:TYR:CE2	3:A:111:LEU:HD11	2.49	0.47
1:L:36:TYR:O	1:L:86:TYR:HA	2.15	0.47
2:H:165:LEU:HA	2:H:165:LEU:HD12	1.80	0.47
3:A:309:THR:O	3:A:312:CYS:HB3	2.16	0.46
3:A:76:LYS:HB3	3:A:157:PRO:HG3	1.96	0.46
3:A:229:THR:HA	3:A:232:PHE:HB2	1.97	0.46
3:A:106:TYR:CD2	3:A:111:LEU:HD21	2.50	0.46
3:A:62:ASN:HD21	3:A:87:ALA:HA	1.80	0.46
3:A:118:LYS:O	3:A:122:SER:OG	2.29	0.46
3:A:287:ILE:C	3:A:288:ASN:HD22	2.19	0.46
3:A:76:LYS:C	3:A:157:PRO:HG3	2.35	0.46
3:A:62:ASN:ND2	3:A:87:ALA:HB1	2.31	0.45
2:H:40:ARG:HH22	2:H:89:GLU:HA	1.81	0.45
1:L:29:VAL:C	1:L:92:ASN:HD22	2.18	0.45
1:L:4:LEU:HD11	1:L:90:GLN:HB3	1.96	0.45
3:A:55:PHE:O	3:A:59:PHE:HB2	2.17	0.45
2:H:32:PHE:CD2	2:H:98:ARG:NH2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:187:ILE:CG2	3:A:190:LEU:HB2	2.47	0.44
2:H:87:THR:O	2:H:89:GLU:N	2.50	0.44
2:H:159:THR:OG1	2:H:202:ASN:HB2	2.17	0.44
3:A:85:ASN:HB3	3:A:134:PHE:CE2	2.53	0.44
3:A:36:SER:HB2	3:A:189:TYR:CE1	2.52	0.44
1:L:49:LYS:NZ	2:H:101:SER:O	2.50	0.44
3:A:47:ILE:N	3:A:48:PRO:CD	2.80	0.44
2:H:160:TRP:CG	2:H:165:LEU:HD23	2.51	0.44
1:L:48:ILE:HD13	1:L:64:GLY:N	2.33	0.44
1:L:115:VAL:HA	1:L:135:PHE:O	2.18	0.44
1:L:49:LYS:O	1:L:53:GLN:HB2	2.18	0.43
3:A:1060:ASP:OD1	3:A:1060:ASP:C	2.57	0.43
1:L:38:GLN:HE22	2:H:39:GLN:NE2	2.16	0.43
1:L:11:LEU:HD21	1:L:19:VAL:CG2	2.48	0.43
3:A:1007:TRP:CD2	3:A:1102:ILE:HD12	2.54	0.43
1:L:179:LEU:HD11	1:L:181:LEU:HD21	2.01	0.43
1:L:209:PHE:HB3	2:H:133:VAL:HG21	2.01	0.43
3:A:163:ILE:O	3:A:167:VAL:HG23	2.19	0.42
2:H:148:VAL:HG22	2:H:203:VAL:HG21	2.02	0.42
3:A:112:PHE:HB3	3:A:116:MET:HG2	2.02	0.42
3:A:300:LEU:N	3:A:301:PRO:HD2	2.34	0.42
1:L:15:PRO:HD3	1:L:106:LEU:CD1	2.50	0.42
3:A:78:VAL:HG22	3:A:157:PRO:HA	2.02	0.42
2:H:174:ALA:HB1	2:H:181:TYR:HD2	1.85	0.42
3:A:76:LYS:CB	3:A:157:PRO:HG3	2.50	0.42
2:H:165:LEU:O	2:H:169:VAL:CG2	2.56	0.41
3:A:1061:PHE:HE1	3:A:1104:LYS:HB3	1.85	0.41
2:H:51:ILE:HB	2:H:58:THR:HG22	2.03	0.41
1:L:11:LEU:HD21	1:L:19:VAL:HG23	2.02	0.41
1:L:38:GLN:HE22	2:H:39:GLN:HE22	1.69	0.41
1:L:210:ASN:O	1:L:211:ARG:C	2.58	0.41
2:H:5:GLN:O	2:H:23:LYS:N	2.54	0.41
3:A:102:THR:O	3:A:105:SER:N	2.54	0.41
3:A:271:PRO:HG2	3:A:306:LEU:HD23	2.02	0.41
3:A:51:TYR:CD1	3:A:305:LEU:HD12	2.56	0.41
3:A:187:ILE:HD12	3:A:187:ILE:HA	1.96	0.41
2:H:27:TYR:CE1	2:H:29:PHE:HA	2.56	0.41
3:A:76:LYS:HD2	3:A:76:LYS:H	1.85	0.41
3:A:78:VAL:HG22	3:A:157:PRO:CA	2.51	0.41
3:A:270:LEU:N	3:A:271:PRO:CD	2.83	0.41
2:H:130:LEU:HD12	2:H:146:CYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:37:GLN:HB2	1:L:47:LEU:HD11	2.02	0.40
1:L:94:TRP:CZ3	1:L:96:LEU:HD21	2.56	0.40
1:L:93:SER:HA	3:A:1096:THR:HG23	2.02	0.40
2:H:35:ASN:ND2	2:H:99:PRO:HB3	2.34	0.40
3:A:97:LEU:N	3:A:98:PRO:CD	2.85	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	L	209/214 (98%)	185 (88%)	22 (10%)	2 (1%)	15	46
2	H	217/224 (97%)	190 (88%)	22 (10%)	5 (2%)	6	28
3	A	367/422 (87%)	319 (87%)	45 (12%)	3 (1%)	19	51
4	B	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
All	All	799/868 (92%)	699 (88%)	90 (11%)	10 (1%)	12	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	88	SER
2	H	91	SER
2	H	187	VAL
1	L	15	PRO
1	L	32	TYR
3	A	1061	PHE
2	H	133	VAL
2	H	218	PRO
3	A	119	VAL
3	A	38	LYS

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	L	190/193 (98%)	171 (90%)	19 (10%)	7	27
2	H	191/195 (98%)	169 (88%)	22 (12%)	5	20
3	A	319/366 (87%)	282 (88%)	37 (12%)	5	20
4	B	7/7 (100%)	5 (71%)	2 (29%)	0	1
All	All	707/761 (93%)	627 (89%)	80 (11%)	6	21

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	LEU
1	L	6	GLN
1	L	10	THR
1	L	17	ASP
1	L	33	LEU
1	L	48	ILE
1	L	53	GLN
1	L	54	SER
1	L	56	SER
1	L	77	SER
1	L	97	THR
1	L	105	GLU
1	L	107	ARG
1	L	116	SER
1	L	127	SER
1	L	136	LEU
1	L	143	ASP
1	L	168	SER
1	L	197	THR
2	H	23	LYS
2	H	40	ARG
2	H	63	LYS
2	H	67	LYS
2	H	69	THR

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Mol	Chain	Res	Type
2	H	71	ILE
2	H	98	ARG
2	H	107	ASP
2	H	122	THR
2	H	136	ASP
2	H	138	SER
2	H	141	SER
2	H	142	VAL
2	H	144	LEU
2	H	162	SER
2	H	166	SER
2	H	179	ASP
2	H	184	SER
2	H	190	THR
2	H	197	GLN
2	H	201	CYS
2	H	202	ASN
3	A	38	LYS
3	A	60	LEU
3	A	62	ASN
3	A	67	THR
3	A	68	LEU
3	A	69	PHE
3	A	70	CYS
3	A	73	LYS
3	A	76	LYS
3	A	77	LYS
3	A	99	LEU
3	A	122	SER
3	A	138	MET
3	A	142	ARG
3	A	148	TYR
3	A	169	CYS
3	A	170	MET
3	A	189	TYR
3	A	202	GLU
3	A	218	LEU
3	A	1002	ASP
3	A	1003	LEU
3	A	1004	GLU
3	A	1012	ASP
3	A	1019	LYS

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Mol	Chain	Res	Type
3	A	1022	ASN
3	A	1031	THR
3	A	1039	ASP
3	A	1042	LYS
3	A	1058	MET
3	A	1059	LYS
3	A	1062	ARG
3	A	1081	GLU
3	A	1104	LYS
3	A	248	ARG
3	A	291	GLU
3	A	297	ASP
4	B	4	TYR
4	B	8	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	53	GLN
1	L	210	ASN
2	H	35	ASN
2	H	39	GLN
2	H	82	GLN
2	H	84	ASN
2	H	177	GLN
3	A	62	ASN
3	A	72	GLN
3	A	288	ASN
3	A	310	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](#)

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
4	SAR	B	1	4	4,4,5	0.69	0	1,3,5	1.73	0

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	SAR	B	1	4	-	1/1/2/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	SAR	C-CA-N-CN

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

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	L	211/214 (98%)	0.30	4 (1%) 66 65	109, 151, 207, 224	0
2	H	219/224 (97%)	0.14	4 (1%) 68 67	91, 141, 185, 218	0
3	A	373/422 (88%)	-0.03	3 (0%) 86 85	107, 142, 193, 232	0
4	B	7/8 (87%)	-0.19	0 100 100	111, 121, 149, 156	0
All	All	810/868 (93%)	0.10	11 (1%) 75 74	91, 144, 198, 232	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	140	SER	3.8
2	H	139	GLY	3.7
1	L	148	TRP	3.3
3	A	74	GLY	2.9
1	L	28	SER	2.8
2	H	72	VAL	2.6
1	L	29	VAL	2.5
3	A	1065	PHE	2.3
3	A	75	PRO	2.2
2	H	27	TYR	2.0
1	L	19	VAL	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
4	SAR	B	1	5/6	0.88	0.25	169,170,171,174	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.