Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 12:10 AM EDT

PDB ID	:	2Z8V
Title	:	Structure of an IgNAR-AMA1 complex
Authors	:	Streltsov, V.A.; Henderson, K.A.; Batchelor, A.H.; Coley, A.M.; Nuttall, S.D.
Deposited on	:	2007-09-11
Resolution	:	2.35 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:

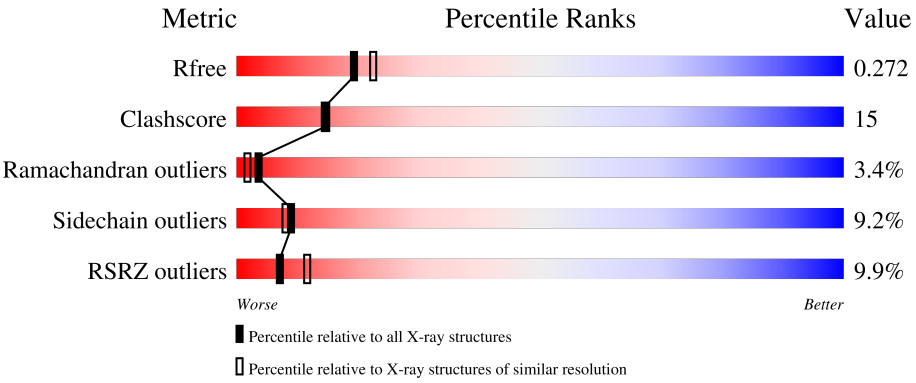
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	335	10% 68% 24% 6% •
1	B	335	12% 70% 24% 6% •
2	C	116	5% 65% 29% 6%
2	D	116	7% 69% 28% ••

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7667 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 Apical membrane antigen 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2695	1705	453	519	18			
1	B	335	Total	C	N	O	S	0	0	0
			2695	1705	453	519	18			

- Molecule 2 is a protein called New antigen receptor variable domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	116	Total	C	N	O	S	0	0	0
			900	562	157	179	2			
2	D	116	Total	C	N	O	S	0	0	0
			900	562	157	179	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	29	LEU	PHE	engineered mutation	UNP Q6X1E6
C	92	ARG	GLY	engineered mutation	UNP Q6X1E6
C	114	ALA	-	expression tag	UNP Q6X1E6
C	115	ALA	-	expression tag	UNP Q6X1E6
C	116	ALA	-	expression tag	UNP Q6X1E6
D	29	LEU	PHE	engineered mutation	UNP Q6X1E6
D	92	ARG	GLY	engineered mutation	UNP Q6X1E6
D	114	ALA	-	expression tag	UNP Q6X1E6
D	115	ALA	-	expression tag	UNP Q6X1E6
D	116	ALA	-	expression tag	UNP Q6X1E6

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	195	Total	O	0	0
			195	195		

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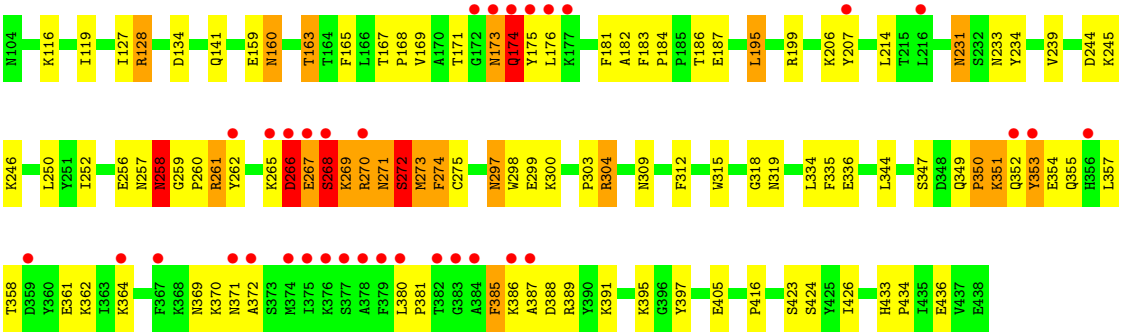
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	169	Total O 169 169	0	0
3	C	57	Total O 57 57	0	0
3	D	56	Total O 56 56	0	0

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.

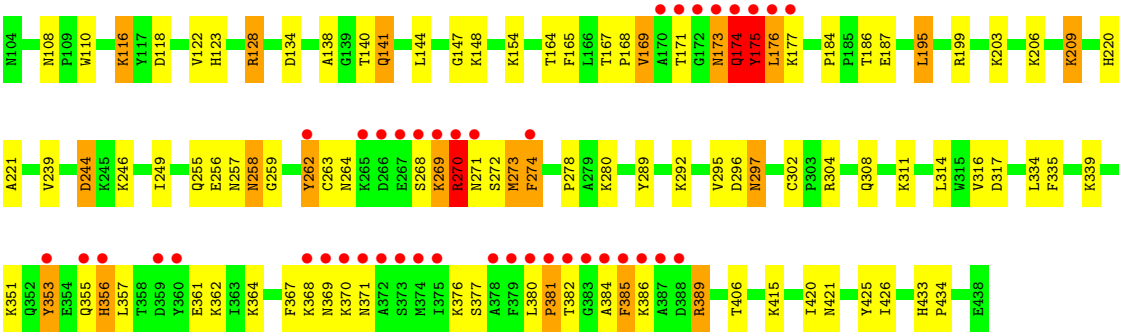
• Molecule 1: Apical membrane antigen 1

Chain A:



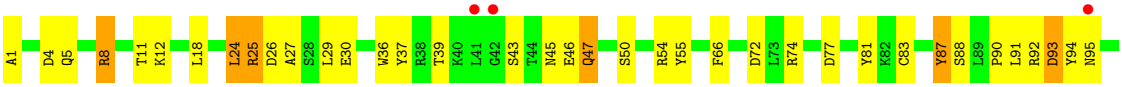
• Molecule 1: Apical membrane antigen 1

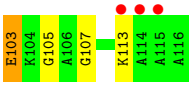
Chain B:



• Molecule 2: New antigen receptor variable domain

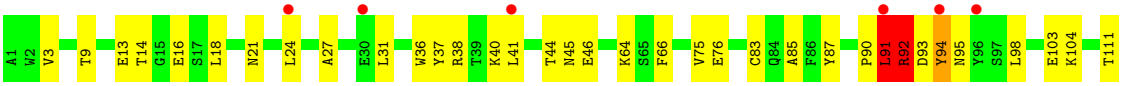
Chain C:





• Molecule 2: New antigen receptor variable domain

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	76.33Å 76.33Å 140.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.19 – 2.35 38.19 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.19-2.35) 99.9 (38.19-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.285 0.187 , 0.272	Depositor DCC
R_{free} test set	3806 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.825	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.480 for -h,-k,l 0.062 for h,-h-k,-l 0.058 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7667	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.72	0/2765	0.78	1/3740 (0.0%)
1	B	0.71	0/2765	0.80	4/3740 (0.1%)
2	C	0.58	0/914	0.78	0/1234
2	D	0.63	1/914 (0.1%)	0.76	2/1234 (0.2%)
All	All	0.69	1/7358 (0.0%)	0.79	7/9948 (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
1	A	0	1
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	92	ARG	NE-CZ	7.72	1.43	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	92	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	314	LEU	CB-CG-CD1	-5.47	101.70	111.00
1	B	144	LEU	CA-CB-CG	5.43	127.78	115.30
1	B	314	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	128	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	128	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	D	91	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	SER	Peptide
1	B	175	TYR	Peptide
1	B	273	MET	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	A	2695	0	2570	93	0
1	B	2695	0	2570	76	0
2	C	900	0	896	36	0
2	D	900	0	896	23	0
3	A	195	0	0	14	1
3	B	169	0	0	6	1
3	C	57	0	0	2	0
3	D	56	0	0	3	0
All	All	7667	0	6932	217	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 15.

All (217) 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:B:173:ASN:H	1:B:173:ASN:HD22	1.08	1.01
1:B:167:THR:HG23	1:B:175:TYR:HB2	1.40	0.99
1:A:167:THR:HG23	1:A:175:TYR:HB3	1.45	0.98
1:B:262:TYR:O	1:B:269:LYS:HA	1.65	0.96
2:C:8:ARG:HH11	2:C:8:ARG:HG3	1.39	0.86
1:B:280:LYS:O	1:B:339:LYS:HE2	1.76	0.85
1:A:364:LYS:HG2	3:A:504:HOH:O	1.76	0.84
1:B:128:ARG:NH2	1:B:256:GLU:OE1	2.11	0.83
1:B:389:ARG:HG2	1:B:389:ARG:HH21	1.43	0.82
1:B:167:THR:CG2	1:B:175:TYR:HB2	2.09	0.82
1:A:167:THR:CG2	1:A:175:TYR:HB3	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:GLY:O	1:B:263:CYS:HB2	1.83	0.79
2:D:41:LEU:HB2	3:D:136:HOH:O	1.82	0.78
2:C:103:GLU:H	2:C:103:GLU:CD	1.86	0.78
1:A:128:ARG:NH2	1:A:256:GLU:OE1	2.18	0.77
1:B:173:ASN:HD22	1:B:173:ASN:N	1.82	0.75
1:A:245:LYS:NZ	3:A:489:HOH:O	2.15	0.74
1:A:385:PHE:CE1	1:A:389:ARG:HG2	2.22	0.73
1:A:174:GLN:HG3	2:D:92:ARG:HH22	1.54	0.72
1:B:122:VAL:O	1:B:148:LYS:HE3	1.91	0.71
1:A:433:HIS:HB2	3:A:602:HOH:O	1.90	0.70
1:A:262:TYR:HA	1:A:269:LYS:O	1.94	0.68
1:B:173:ASN:H	1:B:173:ASN:ND2	1.85	0.68
1:A:349:GLN:O	1:A:351:LYS:N	2.26	0.67
2:C:37:TYR:HB3	2:C:46:GLU:HG2	1.76	0.67
1:A:159:GLU:OE1	1:A:275:CYS:HB3	1.95	0.66
1:B:268:SER:C	1:B:270:ARG:H	1.97	0.66
1:B:173:ASN:O	1:B:174:GLN:HB3	1.94	0.66
1:A:357:LEU:HD23	1:A:362:LYS:HE3	1.76	0.66
2:D:24:LEU:HD21	2:D:85:ALA:HB2	1.77	0.65
2:C:4:ASP:OD2	2:C:25:ARG:NH1	2.29	0.65
1:A:347:SER:OG	1:A:351:LYS:HE3	1.97	0.64
1:B:174:GLN:HE22	2:C:92:ARG:NH2	1.95	0.64
1:B:385:PHE:HB3	1:B:389:ARG:NH2	2.12	0.63
2:C:30:GLU:HG3	3:C:150:HOH:O	2.00	0.62
2:C:103:GLU:CD	2:C:103:GLU:N	2.53	0.62
1:B:187:GLU:O	2:C:90:PRO:HG2	2.01	0.61
1:B:351:LYS:NZ	3:B:536:HOH:O	2.32	0.61
1:A:134:ASP:HB3	1:A:141:GLN:HG2	1.83	0.61
1:A:186:THR:HA	2:D:91:LEU:HA	1.83	0.60
1:B:174:GLN:NE2	2:C:92:ARG:HH22	2.00	0.60
1:A:381:PRO:HB2	1:A:385:PHE:HD2	1.67	0.60
2:D:24:LEU:HD21	2:D:85:ALA:CB	2.31	0.60
2:D:76:GLU:HG2	3:D:121:HOH:O	2.01	0.60
1:B:406:THR:HG21	3:B:494:HOH:O	2.02	0.59
1:A:187:GLU:O	2:D:90:PRO:HG2	2.02	0.59
1:A:244:ASP:HB3	1:A:246:LYS:HG3	1.86	0.57
1:A:354:GLU:HG3	1:A:355:GLN:N	2.20	0.56
2:D:38:ARG:HD2	2:D:40:LYS:HG2	1.88	0.56
2:D:103:GLU:HG3	2:D:104:LYS:N	2.20	0.56
1:A:312:PHE:HB3	1:A:416:PRO:HB3	1.86	0.55
1:A:167:THR:HG23	1:A:175:TYR:HD1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:LEU:N	1:B:381:PRO:CD	2.70	0.55
1:B:168:PRO:HD2	1:B:175:TYR:CD1	2.42	0.55
2:C:29:LEU:HD12	2:C:87:TYR:HD1	1.72	0.55
1:B:368:LYS:HG2	1:B:369:ASN:HD22	1.71	0.55
2:C:1:ALA:HB2	2:C:27:ALA:HA	1.88	0.55
2:C:29:LEU:HD12	2:C:87:TYR:CD1	2.42	0.54
1:A:167:THR:HG23	1:A:175:TYR:CD1	2.42	0.54
1:B:123:HIS:CE1	1:B:147:GLY:HA3	2.43	0.54
1:B:186:THR:HG22	2:C:91:LEU:HD23	1.89	0.54
1:B:380:LEU:N	1:B:381:PRO:HD2	2.22	0.54
2:C:30:GLU:O	2:C:87:TYR:CB	2.56	0.54
2:C:24:LEU:HD22	2:C:27:ALA:HB2	1.89	0.54
1:A:351:LYS:HD3	1:B:108:ASN:O	2.07	0.54
1:A:388:ASP:HB3	1:A:391:LYS:NZ	2.23	0.54
1:A:168:PRO:HD2	1:A:175:TYR:CB	2.38	0.53
1:A:257:ASN:O	1:A:258:ASN:HB3	2.07	0.53
1:A:350:PRO:C	1:A:352:GLN:H	2.12	0.53
1:B:389:ARG:HG2	1:B:389:ARG:NH2	2.21	0.53
2:C:39:THR:HG23	2:C:45:ASN:H	1.74	0.53
2:C:8:ARG:HH11	2:C:8:ARG:CG	2.17	0.52
2:C:66:PHE:HE2	2:C:83:CYS:HB2	1.73	0.52
2:D:24:LEU:HD13	2:D:87:TYR:HE2	1.74	0.52
1:A:267:GLU:O	1:A:268:SER:C	2.47	0.52
1:B:148:LYS:HB3	1:B:295:VAL:HG13	1.90	0.52
1:B:268:SER:O	1:B:270:ARG:N	2.43	0.52
1:A:160:ASN:ND2	1:A:160:ASN:H	2.08	0.52
1:A:335:PHE:HD2	1:A:434:PRO:HB2	1.75	0.52
1:B:262:TYR:HE1	3:B:592:HOH:O	1.92	0.52
1:A:265:LYS:O	1:A:266:ASP:C	2.48	0.51
1:A:169:VAL:HG22	1:A:184:PRO:HD3	1.91	0.51
1:A:385:PHE:HE1	1:A:389:ARG:HG2	1.72	0.51
1:B:361:GLU:HA	1:B:364:LYS:HB2	1.92	0.51
1:B:169:VAL:HG22	1:B:184:PRO:HD3	1.93	0.51
1:A:351:LYS:HE2	3:A:537:HOH:O	2.10	0.50
1:B:168:PRO:HD2	1:B:175:TYR:HD1	1.74	0.50
1:A:160:ASN:HD21	1:A:275:CYS:H	1.60	0.50
1:B:262:TYR:OH	1:B:273:MET:HG2	2.11	0.50
1:A:358:THR:HG22	1:A:361:GLU:HB2	1.94	0.50
1:B:175:TYR:N	1:B:175:TYR:CD2	2.79	0.50
1:B:389:ARG:HH21	1:B:389:ARG:CG	2.20	0.50
1:A:163:THR:HG21	1:A:176:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:LEU:C	1:B:382:THR:H	2.15	0.50
2:C:54:ARG:HH22	2:C:77:ASP:CG	2.15	0.50
2:C:92:ARG:O	2:C:93:ASP:HB2	2.11	0.50
1:A:388:ASP:HB3	1:A:391:LYS:HZ2	1.77	0.50
1:A:385:PHE:O	1:A:386:LYS:HB2	2.13	0.49
1:B:257:ASN:HA	1:B:353:TYR:HE1	1.76	0.49
1:B:174:GLN:NE2	2:C:92:ARG:NH2	2.58	0.49
1:B:268:SER:C	1:B:270:ARG:N	2.66	0.49
2:C:1:ALA:O	2:C:103:GLU:HG2	2.13	0.49
2:D:103:GLU:HG3	2:D:104:LYS:H	1.76	0.49
2:C:74:ARG:O	2:C:77:ASP:HB2	2.12	0.49
1:A:395:LYS:HG3	3:A:525:HOH:O	2.12	0.48
1:B:244:ASP:HB3	1:B:246:LYS:HB2	1.94	0.48
2:C:12:LYS:HE3	2:C:18:LEU:HD23	1.95	0.48
1:A:168:PRO:HD2	1:A:175:TYR:CG	2.48	0.48
1:A:357:LEU:HG	1:A:362:LYS:HG2	1.94	0.48
1:B:380:LEU:O	1:B:382:THR:N	2.46	0.48
1:A:309:ASN:OD1	1:A:423:SER:HA	2.14	0.48
2:D:3:VAL:HG22	2:D:24:LEU:HD23	1.95	0.48
1:B:203:LYS:HA	1:B:209:LYS:HD2	1.95	0.47
1:A:195:LEU:O	1:A:199:ARG:HG3	2.15	0.47
1:A:336:GLU:HA	1:A:336:GLU:OE1	2.14	0.47
1:B:118:ASP:OD2	1:B:415:LYS:HD3	2.15	0.47
1:B:255:GLN:O	1:B:278:PRO:HD3	2.13	0.47
1:A:214:LEU:HD12	1:A:298:TRP:CZ2	2.50	0.47
1:B:221:ALA:HB2	1:B:249:ILE:HG12	1.96	0.47
1:B:269:LYS:O	1:B:271:ASN:N	2.46	0.47
1:A:116:LYS:O	1:A:303:PRO:HD3	2.15	0.47
1:A:334:LEU:HD22	1:A:426:ILE:HD13	1.95	0.47
1:B:353:TYR:HD1	3:B:592:HOH:O	1.97	0.47
1:B:272:SER:OG	1:B:273:MET:N	2.47	0.47
2:C:30:GLU:O	2:C:87:TYR:HB2	2.15	0.47
1:A:304:ARG:NH1	3:A:602:HOH:O	2.48	0.46
2:C:30:GLU:O	2:C:87:TYR:HB3	2.15	0.46
1:A:297:ASN:HD22	1:A:297:ASN:H	1.62	0.46
1:B:311:LYS:HB3	1:B:420:ILE:HB	1.96	0.46
2:C:72:ASP:OD2	2:C:74:ARG:NH2	2.45	0.46
1:A:159:GLU:O	1:A:265:LYS:HE3	2.16	0.46
2:D:36:TRP:CZ3	2:D:83:CYS:HB3	2.51	0.45
1:A:169:VAL:HG12	1:A:252:ILE:HD12	1.99	0.45
1:A:272:SER:OG	1:A:273:MET:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:TYR:HB3	2:D:46:GLU:HG2	1.97	0.45
1:A:119:ILE:HG21	1:A:127:ILE:HD11	1.99	0.45
1:B:171:THR:HG23	3:B:596:HOH:O	2.16	0.45
1:B:297:ASN:HD22	1:B:297:ASN:H	1.63	0.45
1:A:272:SER:N	3:A:626:HOH:O	2.49	0.45
1:A:405:GLU:HG2	1:A:424:SER:HB3	1.98	0.45
1:B:258:ASN:CG	1:B:258:ASN:O	2.55	0.45
1:A:173:ASN:HD22	1:A:173:ASN:N	2.15	0.45
2:C:5:GLN:OE1	2:C:105:GLY:HA3	2.16	0.45
1:A:261:ARG:NH1	1:A:262:TYR:HE1	2.15	0.44
2:C:47:GLN:HA	3:C:130:HOH:O	2.17	0.44
1:B:154:LYS:HG2	1:B:289:TYR:HB2	1.98	0.44
2:D:92:ARG:O	2:D:93:ASP:OD1	2.35	0.44
1:A:165:PHE:O	1:A:181:PHE:HB2	2.18	0.44
1:B:334:LEU:HD22	1:B:426:ILE:HG21	1.99	0.44
2:D:13:GLU:HB2	2:D:16:GLU:HG3	1.99	0.44
1:A:304:ARG:NH2	3:A:557:HOH:O	2.48	0.44
1:A:361:GLU:HA	1:A:364:LYS:HB2	2.00	0.44
1:A:386:LYS:C	1:A:388:ASP:H	2.21	0.44
2:C:81:TYR:O	2:C:107:GLY:HA2	2.18	0.44
2:D:38:ARG:NH1	3:D:130:HOH:O	2.51	0.44
2:C:66:PHE:CE2	2:C:83:CYS:HB2	2.51	0.44
1:B:362:LYS:O	1:B:367:PHE:HB2	2.17	0.43
1:B:199:ARG:NH1	1:B:209:LYS:O	2.46	0.43
1:B:335:PHE:HD1	1:B:434:PRO:HB2	1.83	0.43
1:A:167:THR:HG23	1:A:175:TYR:CB	2.31	0.43
1:B:220:HIS:CD2	1:B:249:ILE:HD11	2.53	0.43
1:A:187:GLU:HG2	2:D:92:ARG:HB2	2.01	0.43
1:B:316:VAL:O	1:B:317:ASP:HB2	2.18	0.43
1:B:377:SER:HB2	1:B:380:LEU:HD13	2.00	0.43
1:B:433:HIS:CG	1:B:434:PRO:HD2	2.53	0.43
2:D:94:TYR:HB3	2:D:95:ASN:H	1.53	0.43
1:A:369:ASN:HB3	1:A:371:ASN:H	1.84	0.43
1:B:108:ASN:OD1	1:B:110:TRP:HB2	2.19	0.43
1:A:335:PHE:CD2	1:A:434:PRO:HB2	2.52	0.43
1:B:368:LYS:HG2	1:B:369:ASN:ND2	2.33	0.43
2:C:29:LEU:HB2	2:C:87:TYR:CD1	2.53	0.43
1:B:311:LYS:HG3	1:B:425:TYR:CD2	2.55	0.42
1:A:271:ASN:O	1:A:272:SER:HB3	2.19	0.42
2:D:66:PHE:CE2	2:D:83:CYS:HB2	2.54	0.42
1:A:206:LYS:CE	3:A:570:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PRO:HG3	3:B:504:HOH:O	2.19	0.42
1:A:315:TRP:CZ2	1:A:318:GLY:HA2	2.54	0.42
1:A:351:LYS:HA	3:A:516:HOH:O	2.18	0.42
1:A:239:VAL:HG23	1:A:250:LEU:HD11	2.00	0.42
1:A:259:GLY:HA2	1:A:260:PRO:HD3	1.90	0.42
1:A:231:ASN:ND2	1:A:231:ASN:H	2.17	0.42
1:B:257:ASN:HD21	1:B:357:LEU:HD11	1.84	0.42
1:A:168:PRO:HA	1:A:182:ALA:O	2.20	0.42
1:A:262:TYR:OH	1:A:353:TYR:HE1	2.03	0.42
1:B:140:THR:OG1	1:B:376:LYS:HE3	2.19	0.42
2:D:75:VAL:HG12	2:D:112:VAL:O	2.20	0.42
1:A:433:HIS:CB	3:A:602:HOH:O	2.57	0.41
1:A:206:LYS:HE2	3:A:570:HOH:O	2.20	0.41
1:A:163:THR:HA	3:A:597:HOH:O	2.21	0.41
1:B:195:LEU:O	1:B:199:ARG:HG3	2.20	0.41
2:D:27:ALA:HB3	2:D:64:LYS:NZ	2.35	0.41
1:A:234:TYR:CD2	1:A:234:TYR:C	2.93	0.41
1:A:344:LEU:HB3	1:A:397:TYR:HB2	2.03	0.41
1:A:183:PHE:HA	1:A:184:PRO:HD2	1.89	0.41
1:A:273:MET:HG3	1:A:273:MET:O	2.20	0.41
1:B:165:PHE:CE1	1:B:239:VAL:HG21	2.55	0.41
1:B:173:ASN:N	1:B:173:ASN:ND2	2.55	0.41
1:A:256:GLU:OE2	1:A:258:ASN:ND2	2.53	0.41
1:A:267:GLU:O	1:A:269:LYS:N	2.54	0.41
2:C:54:ARG:NH2	2:C:55:TYR:HE1	2.19	0.41
2:C:92:ARG:NE	2:C:93:ASP:OD2	2.45	0.41
1:A:270:ARG:HD3	1:A:270:ARG:HA	1.75	0.41
1:A:297:ASN:H	1:A:297:ASN:ND2	2.18	0.41
1:A:358:THR:HG23	1:A:361:GLU:H	1.85	0.41
1:A:381:PRO:CB	1:A:385:PHE:HD2	2.32	0.41
1:B:134:ASP:HB3	1:B:141:GLN:HG3	2.03	0.41
1:B:355:GLN:HB3	1:B:356:HIS:H	1.52	0.41
1:A:269:LYS:O	1:A:270:ARG:CB	2.69	0.41
1:A:265:LYS:HB3	1:B:296:ASP:OD2	2.21	0.40
1:A:300:LYS:HE2	3:A:457:HOH:O	2.19	0.40
1:B:116:LYS:HE3	1:B:302:CYS:O	2.21	0.40
1:B:174:GLN:HG2	1:B:174:GLN:O	2.21	0.40
1:B:257:ASN:ND2	1:B:357:LEU:HD11	2.36	0.40
2:C:36:TRP:CZ3	2:C:83:CYS:HB3	2.57	0.40
2:D:24:LEU:HD11	2:D:31:LEU:HD13	2.03	0.40
1:A:265:LYS:O	1:A:267:GLU:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:92:ARG:O	2:C:93:ASP:CB	2.70	0.40

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:A:579:HOH:O	3:B:440:HOH:O[2_555]	2.19	0.01

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	333/335 (99%)	294 (88%)	25 (8%)	14 (4%)	3 1
1	B	333/335 (99%)	287 (86%)	33 (10%)	13 (4%)	3 1
2	C	114/116 (98%)	107 (94%)	6 (5%)	1 (1%)	17 17
2	D	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	8 6
All	All	894/902 (99%)	792 (89%)	72 (8%)	30 (3%)	3 2

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	266	ASP
1	A	268	SER
1	A	272	SER
1	A	273	MET
1	B	174	GLN
1	B	177	LYS
1	B	274	PHE
1	B	381	PRO

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Mol	Chain	Res	Type
1	B	384	ALA
1	A	274	PHE
1	A	372	ALA
1	B	169	VAL
1	B	176	LEU
1	B	269	LYS
1	B	270	ARG
1	B	356	HIS
2	C	93	ASP
2	D	94	TYR
1	A	171	THR
1	B	371	ASN
2	D	92	ARG
1	A	258	ASN
1	A	387	ALA
1	B	353	TYR
1	A	271	ASN
1	A	350	PRO
1	A	351	LYS
1	B	138	ALA
1	A	380	LEU

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	296/296 (100%)	272 (92%)	24 (8%)	11	11
1	B	296/296 (100%)	271 (92%)	25 (8%)	11	10
2	C	97/97 (100%)	83 (86%)	14 (14%)	3	3
2	D	97/97 (100%)	88 (91%)	9 (9%)	9	8
All	All	786/786 (100%)	714 (91%)	72 (9%)	9	8

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	163	THR
1	A	173	ASN
1	A	174	GLN
1	A	195	LEU
1	A	207	TYR
1	A	231	ASN
1	A	233	ASN
1	A	258	ASN
1	A	261	ARG
1	A	266	ASP
1	A	267	GLU
1	A	268	SER
1	A	269	LYS
1	A	270	ARG
1	A	274	PHE
1	A	297	ASN
1	A	299	GLU
1	A	304	ARG
1	A	319	ASN
1	A	353	TYR
1	A	370	LYS
1	A	385	PHE
1	A	436	GLU
1	B	116	LYS
1	B	141	GLN
1	B	164	THR
1	B	173	ASN
1	B	174	GLN
1	B	175	TYR
1	B	176	LEU
1	B	195	LEU
1	B	206	LYS
1	B	209	LYS
1	B	244	ASP
1	B	258	ASN
1	B	262	TYR
1	B	264	ASN
1	B	270	ARG
1	B	274	PHE
1	B	292	LYS
1	B	297	ASN
1	B	304	ARG

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Mol	Chain	Res	Type
1	B	308	GLN
1	B	370	LYS
1	B	385	PHE
1	B	386	LYS
1	B	389	ARG
1	B	421	ASN
2	C	8	ARG
2	C	11	THR
2	C	24	LEU
2	C	25	ARG
2	C	26	ASP
2	C	43	SER
2	C	47	GLN
2	C	50	SER
2	C	87	TYR
2	C	88	SER
2	C	94	TYR
2	C	95	ASN
2	C	103	GLU
2	C	113	LYS
2	D	9	THR
2	D	14	THR
2	D	18	LEU
2	D	21	ASN
2	D	44	THR
2	D	45	ASN
2	D	91	LEU
2	D	98	LEU
2	D	111	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	173	ASN
1	A	210	ASN
1	A	231	ASN
1	A	233	ASN
1	A	257	ASN
1	A	264	ASN
1	A	285	GLN
1	A	297	ASN

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Mol	Chain	Res	Type
1	A	369	ASN
1	A	407	GLN
1	B	173	ASN
1	B	174	GLN
1	B	210	ASN
1	B	233	ASN
1	B	257	ASN
1	B	264	ASN
1	B	297	ASN
1	B	352	GLN
1	B	369	ASN
1	B	421	ASN
2	D	47	GLN
2	D	60	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	335/335 (100%)	0.49	34 (10%) 7 11	49, 58, 86, 102	0
1	B	335/335 (100%)	0.59	41 (12%) 4 7	48, 58, 85, 102	0
2	C	116/116 (100%)	0.29	6 (5%) 27 39	50, 59, 65, 68	0
2	D	116/116 (100%)	0.31	8 (6%) 16 24	50, 59, 65, 70	0
All	All	902/902 (100%)	0.48	89 (9%) 7 11	48, 59, 81, 102	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	THR	15.3
1	B	379	PHE	11.9
1	A	383	GLY	8.4
1	B	175	TYR	7.9
1	A	380	LEU	7.8
1	A	268	SER	7.7
1	B	171	THR	7.3
1	B	382	THR	7.2
1	B	383	GLY	6.9
1	B	378	ALA	6.7
1	B	385	PHE	6.6
1	A	174	GLN	6.1
1	A	386	LYS	6.0
1	A	387	ALA	5.9
1	B	375	ILE	5.7
1	A	175	TYR	5.6
1	A	173	ASN	5.5
1	A	375	ILE	5.3
1	B	174	GLN	4.8
1	B	270	ARG	4.7
1	A	172	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	373	SER	4.6
1	A	372	ALA	4.4
1	A	377	SER	4.4
1	A	376	LYS	4.2
1	B	372	ALA	4.2
1	B	173	ASN	4.0
1	A	352	GLN	4.0
1	A	371	ASN	4.0
1	A	378	ALA	3.9
1	B	267	GLU	3.9
1	B	271	ASN	3.9
2	C	42	GLY	3.7
1	A	177	LYS	3.7
1	B	359	ASP	3.6
1	B	374	MET	3.5
1	A	176	LEU	3.5
1	A	384	ALA	3.5
1	B	368	LYS	3.4
2	C	114	ALA	3.4
1	A	374	MET	3.4
1	B	381	PRO	3.4
1	B	356	HIS	3.4
1	B	170	ALA	3.3
2	C	115	ALA	3.3
2	D	96	TYR	3.3
1	B	380	LEU	3.2
1	B	176	LEU	3.2
1	B	262	TYR	3.1
1	B	370	LYS	3.1
2	C	95	ASN	3.0
1	A	216	LEU	3.0
2	D	94	TYR	2.9
1	B	386	LYS	2.9
1	B	384	ALA	2.9
1	B	387	ALA	2.9
1	B	353	TYR	2.9
1	A	262	TYR	2.8
1	B	388	ASP	2.8
2	D	30	GLU	2.8
2	D	91	LEU	2.7
1	A	353	TYR	2.7
2	C	41	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	270	ARG	2.6
1	A	379	PHE	2.6
1	B	172	GLY	2.6
1	B	268	SER	2.5
2	D	113	LYS	2.5
1	B	269	LYS	2.4
2	D	24	LEU	2.3
2	D	116	ALA	2.3
1	B	371	ASN	2.3
1	B	177	LYS	2.3
1	B	274	PHE	2.3
1	B	355	GLN	2.3
1	A	266	ASP	2.3
2	D	41	LEU	2.3
2	C	113	LYS	2.2
1	A	267	GLU	2.2
1	A	265	LYS	2.1
1	B	369	ASN	2.1
1	A	356	HIS	2.1
1	B	360	TYR	2.1
1	A	367	PHE	2.1
1	A	359	ASP	2.0
1	B	266	ASP	2.0
1	A	364	LYS	2.0
1	A	207	TYR	2.0
1	B	265	LYS	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 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.