Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 08:16 PM EDT

PDB ID	:	4N9G
Title	:	Crystal Structure of a Computationally Designed RSV-Presenting Epitope Scaffold And Its Elicited Antibody 17HD9
Authors	:	Carrico, C.T.D.; Strong, R.K.
Deposited on	:	2013-10-21
Resolution	:	2.50 Å(reported)

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

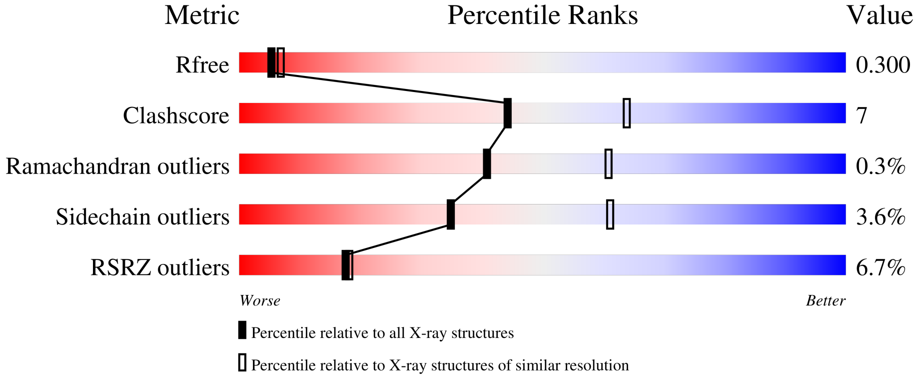
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

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

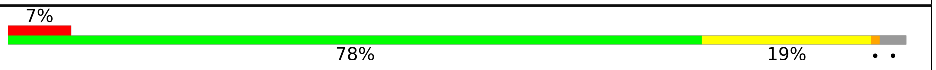
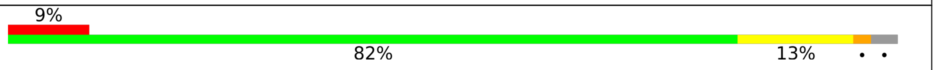
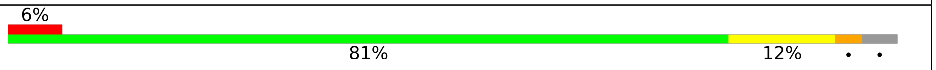
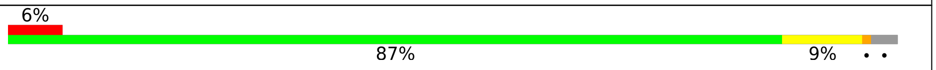
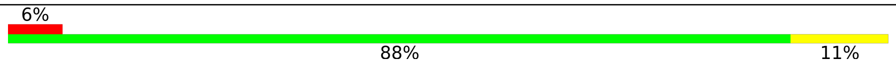
The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	230	
1	E	230	
1	H	230	
1	M	230	
2	B	215	

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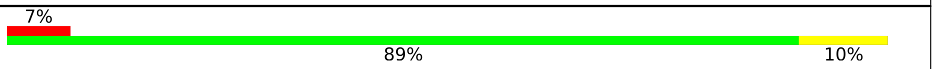
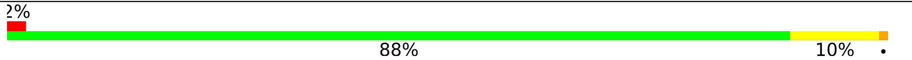
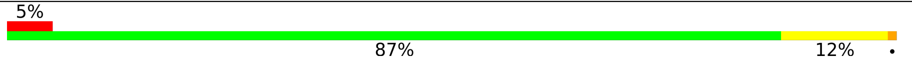
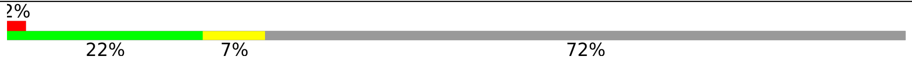
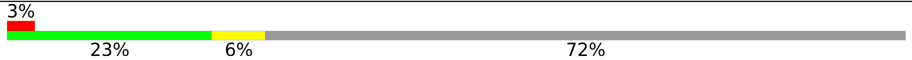
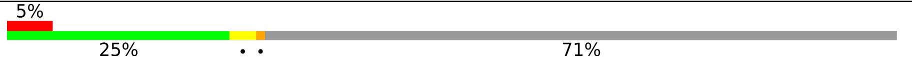
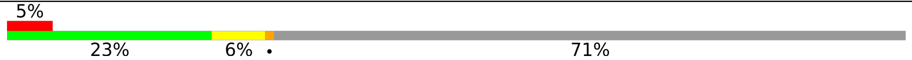
Mol	Chain	Length	Quality of chain
2	F	215	
2	L	215	
2	N	215	
3	C	123	
3	D	123	
3	Y	123	
3	Z	123	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14304 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 Antibody 17HD9, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	1656	1047	273	328	8	0	1	0
1	E	223	1664	1051	277	329	7	0	1	0
1	H	221	1650	1043	275	324	8	0	1	0
1	M	223	1653	1043	275	327	8	0	1	0

- Molecule 2 is a protein called Antibody 17HD9, Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	214	1624	1013	271	334	6	6	0	0
2	F	214	1645	1025	275	339	6	8	2	0
2	L	214	1641	1023	275	337	6	9	1	0
2	N	214	1632	1018	272	336	6	10	0	0

- Molecule 3 is a protein called Epitope Scaffold rsv_1isea_FFL_001_C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	35	263	164	42	55	2	0	0	0
3	D	35	268	165	45	56	2	0	0	0
3	Y	36	281	175	46	58	2	0	1	0
3	Z	36	268	168	43	55	2	0	0	0

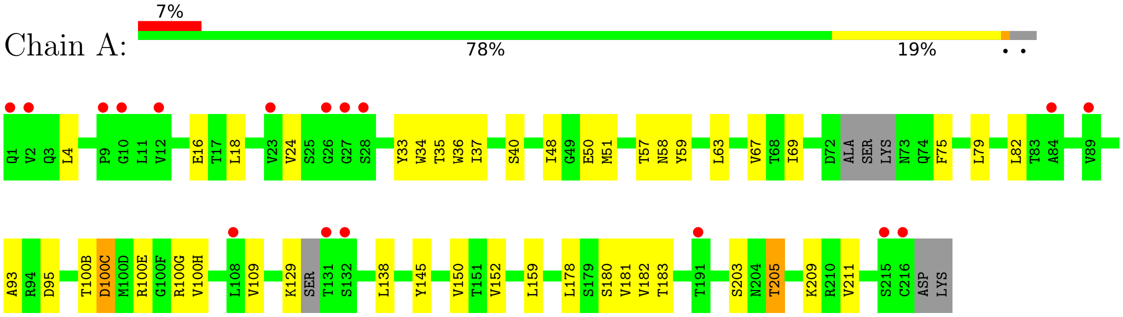
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	7	Total O 7 7	0	0
4	E	5	Total O 5 5	0	0
4	F	5	Total O 5 5	0	0
4	H	6	Total O 6 6	0	0
4	L	12	Total O 12 12	0	0
4	M	6	Total O 6 6	0	0
4	N	8	Total O 8 8	0	0
4	Z	1	Total O 1 1	0	0

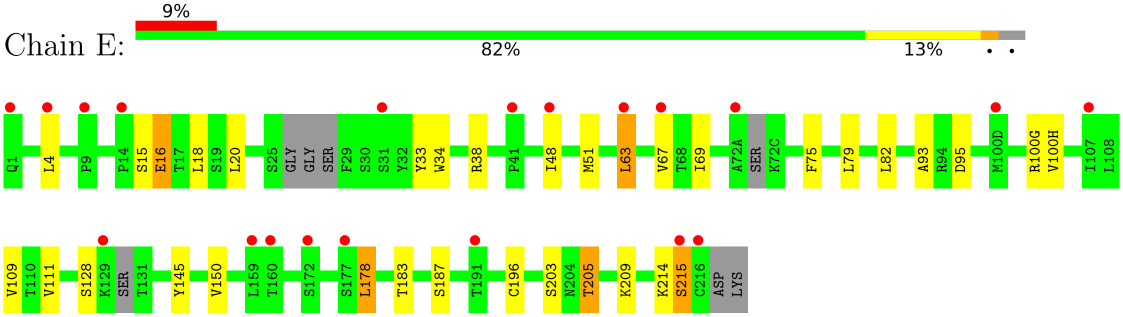
3 Residue-property plots ⓘ

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.

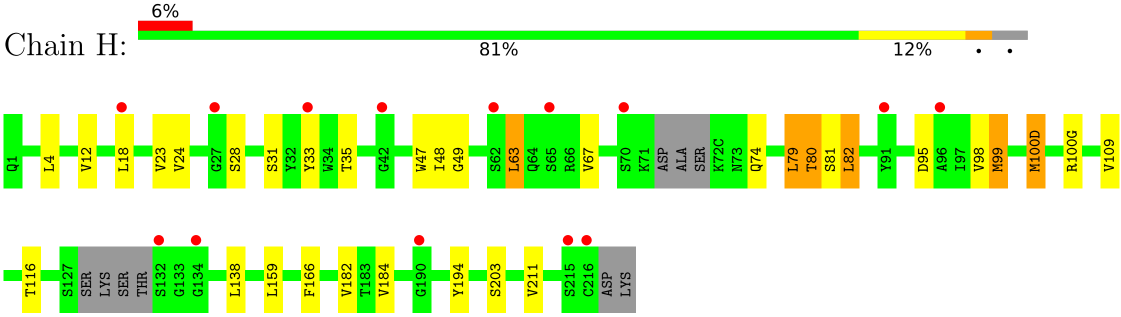
- Molecule 1: Antibody 17HD9, Heavy Chain



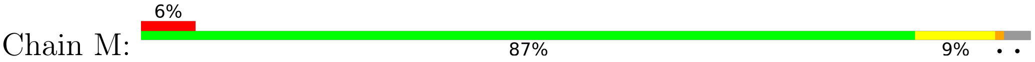
- Molecule 1: Antibody 17HD9, Heavy Chain

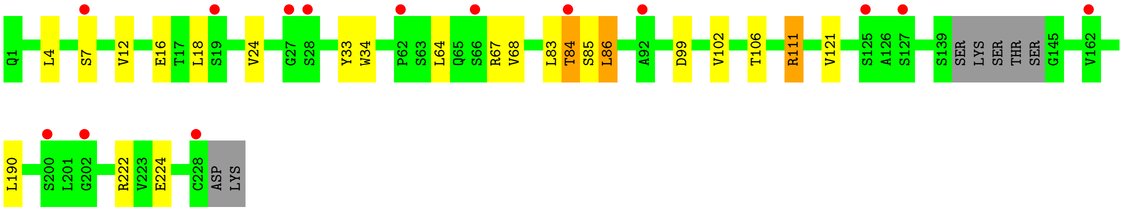


- Molecule 1: Antibody 17HD9, Heavy Chain



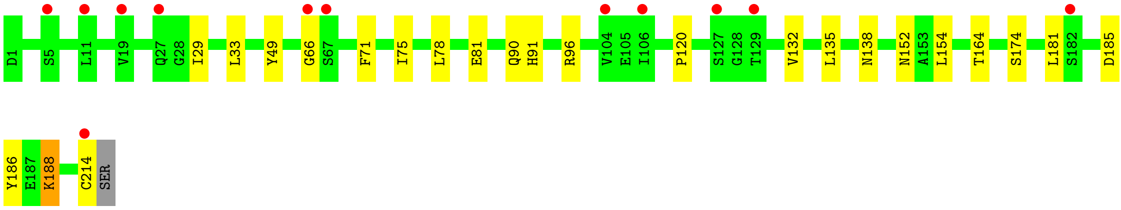
- Molecule 1: Antibody 17HD9, Heavy Chain





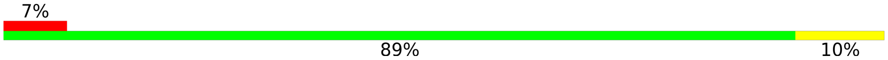
- Molecule 2: Antibody 17HD9, Light Chain

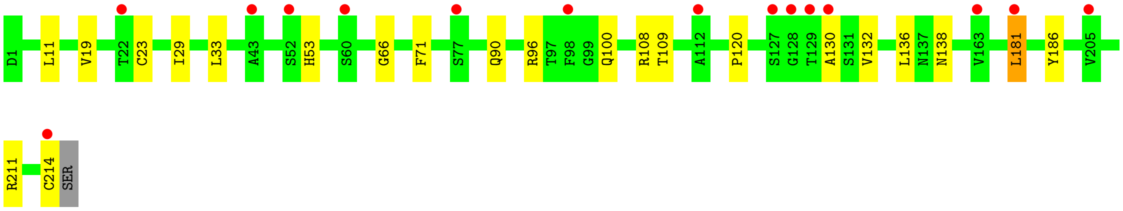
Chain B:



- Molecule 2: Antibody 17HD9, Light Chain

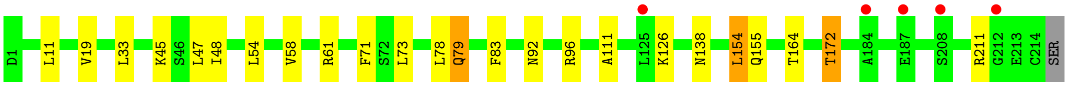
Chain F:





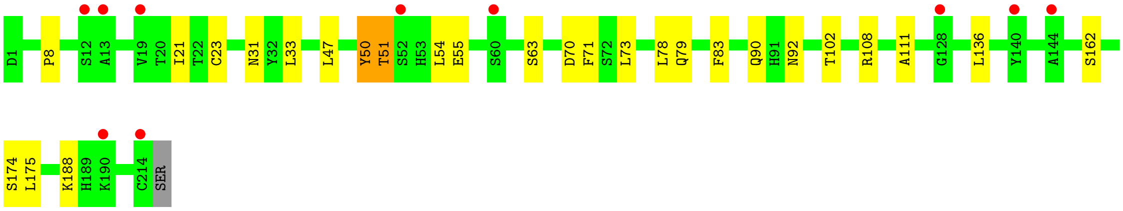
- Molecule 2: Antibody 17HD9, Light Chain

Chain L:



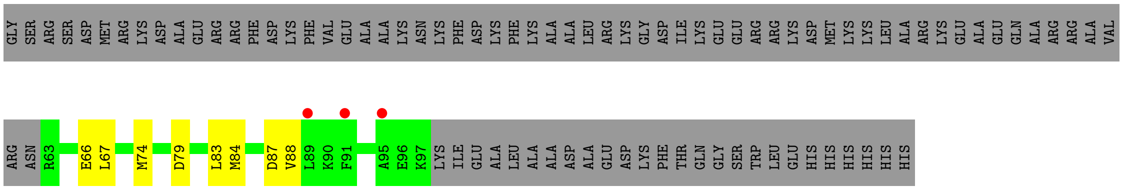
- Molecule 2: Antibody 17HD9, Light Chain

Chain N:

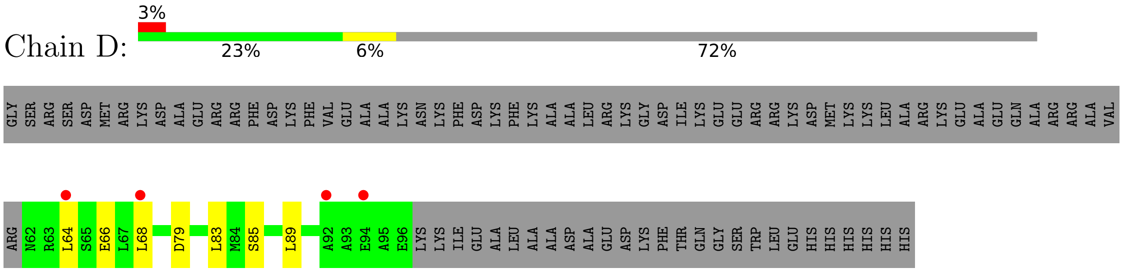


- Molecule 3: Epitope Scaffold rsv_1isea_FFL_001_C

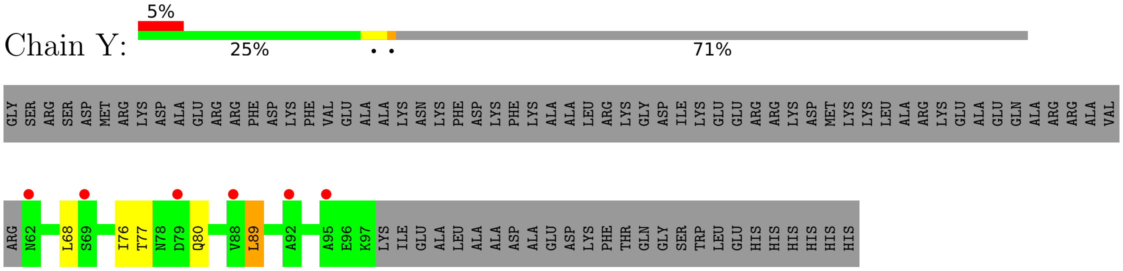
Chain C:



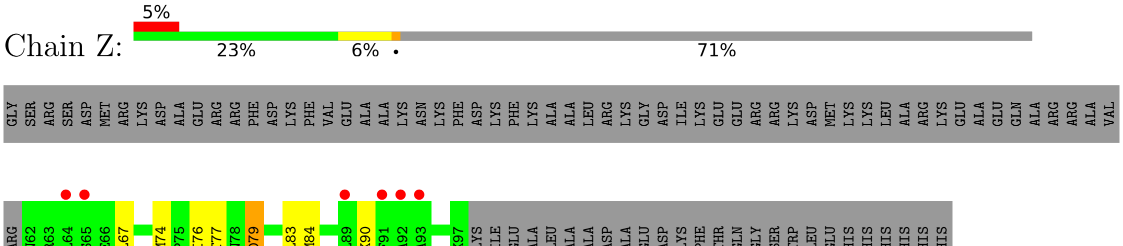
- Molecule 3: Epitope Scaffold rsv_1isea_FFL_001_C



- Molecule 3: Epitope Scaffold rsv_1isea_FFL_001_C



- Molecule 3: Epitope Scaffold rsv_1isea_FFL_001_C



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.21Å 89.27Å 104.30Å 89.99° 102.73° 89.91°	Depositor
Resolution (Å)	48.75 – 2.50 48.76 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.75-2.50) 97.3 (48.76-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.59 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.263 , 0.295 0.271 , 0.300	Depositor DCC
R_{free} test set	3829 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 7.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.430 for -h,k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	14304	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.31	0/1697	0.49	0/2319
1	E	0.30	0/1701	0.48	0/2323
1	H	0.30	0/1691	0.50	0/2308
1	M	0.31	0/1695	0.49	0/2317
2	B	0.37	1/1661 (0.1%)	0.60	1/2259 (0.0%)
2	F	0.35	0/1688	0.51	0/2294
2	L	0.68	1/1681 (0.1%)	0.60	3/2284 (0.1%)
2	N	0.37	0/1669	0.55	2/2268 (0.1%)
3	C	0.29	0/264	0.43	0/355
3	D	0.29	0/269	0.44	0/362
3	Y	0.33	0/285	0.42	0/382
3	Z	0.32	0/269	0.39	0/361
All	All	0.39	2/14570 (0.0%)	0.52	6/19832 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	211	ARG	CZ-NH2	-23.78	1.02	1.33
2	B	154	LEU	CG-CD1	-6.52	1.27	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	154	LEU	CB-CG-CD1	13.57	134.08	111.00
2	L	45	LYS	CD-CE-NZ	10.82	136.58	111.70
2	L	211	ARG	NE-CZ-NH2	8.87	124.73	120.30
2	N	79	GLN	OE1-CD-NE2	6.58	137.04	121.90
2	N	79	GLN	CG-CD-NE2	-6.15	101.94	116.70
2	L	126	LYS	CD-CE-NZ	5.82	125.08	111.70

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	1656	0	1616	41	0
1	E	1664	0	1619	25	0
1	H	1650	0	1620	27	0
1	M	1653	0	1606	15	0
2	B	1624	0	1535	12	0
2	F	1645	0	1566	13	0
2	L	1641	0	1570	18	0
2	N	1632	0	1554	20	0
3	C	263	0	257	7	0
3	D	268	0	261	4	0
3	Y	281	0	282	5	0
3	Z	268	0	264	11	0
4	A	9	0	0	0	0
4	B	7	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	H	6	0	0	0	0
4	L	12	0	0	0	0
4	M	6	0	0	0	0
4	N	8	0	0	0	0
4	Z	1	0	0	0	0
All	All	14304	0	13750	184	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 7.

All (184) 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:A:57[A]:THR:HG21	1:A:59:TYR:CE1	1.96	0.99
2:F:11:LEU:HD21	2:F:19:VAL:CG1	1.98	0.93
1:E:67:VAL:HG22	1:E:79:LEU:HD13	1.49	0.92
1:A:181:VAL:HG21	2:B:135:LEU:HD22	1.60	0.84
1:A:51:MET:HE2	1:A:69:ILE:HG22	1.58	0.83
1:A:63:LEU:HB3	1:A:67:VAL:HG21	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:11:LEU:HD21	2:F:19:VAL:HG11	1.63	0.81
1:E:67:VAL:HG22	1:E:79:LEU:CD1	2.13	0.78
2:N:33:LEU:O	2:N:50:TYR:O	2.03	0.77
1:A:51:MET:CE	1:A:69:ILE:HG22	2.16	0.76
1:A:138:LEU:HD13	1:A:211:VAL:HG11	1.66	0.76
2:F:11:LEU:HD21	2:F:19:VAL:HG13	1.66	0.76
1:A:67:VAL:HG22	1:A:79:LEU:HD13	1.67	0.74
1:M:4:LEU:CD2	1:M:24:VAL:HG22	2.21	0.71
1:A:50:GLU:O	1:A:57[A]:THR:HG23	1.91	0.71
3:D:68:LEU:HD21	3:D:89:LEU:HD21	1.73	0.71
1:A:18:LEU:HD13	1:A:109:VAL:HG11	1.74	0.69
1:H:31:SER:HA	1:H:99:MET:HE1	1.74	0.69
3:Z:77:THR:HG21	3:Z:79:ASP:OD2	1.93	0.69
2:L:48:ILE:HD12	2:L:73:LEU:HD12	1.76	0.68
1:E:51:MET:CE	1:E:69:ILE:HG22	2.23	0.68
2:N:33:LEU:HD13	2:N:71:PHE:CG	2.28	0.67
3:D:85:SER:O	3:D:89:LEU:HD23	1.94	0.67
1:H:18:LEU:CD1	1:H:109:VAL:HG11	2.24	0.66
2:B:164:THR:HG22	2:B:174:SER:H	1.61	0.66
1:A:57[A]:THR:HG21	1:A:59:TYR:CZ	2.31	0.65
1:E:51:MET:HE2	1:E:69:ILE:HG22	1.76	0.65
1:H:4:LEU:CD2	1:H:24:VAL:HG22	2.27	0.64
1:A:138:LEU:HD13	1:A:211:VAL:CG1	2.27	0.64
1:H:138:LEU:HD13	1:H:211:VAL:HG11	1.79	0.63
3:C:74:MET:SD	3:Z:74:MET:HE1	2.38	0.63
3:Y:68:LEU:HD21	3:Y:89:LEU:HD13	1.80	0.62
1:H:4:LEU:HD22	1:H:24:VAL:HG22	1.81	0.62
2:L:92:ASN:OD1	3:Y:77:THR:HG23	2.00	0.61
1:H:48:ILE:HG23	1:H:63:LEU:HD23	1.82	0.61
2:N:92:ASN:OD1	3:Z:77:THR:HG23	2.01	0.61
1:H:18:LEU:HB2	1:H:82:LEU:HD21	1.82	0.61
1:H:138:LEU:HD13	1:H:211:VAL:CG1	2.31	0.61
2:L:61:ARG:NE	2:L:79:GLN:HG3	2.16	0.60
1:E:18:LEU:HD13	1:E:109:VAL:HG11	1.82	0.60
1:H:98:VAL:HG22	1:H:99:MET:HE3	1.83	0.60
1:H:98:VAL:HG22	1:H:99:MET:CE	2.31	0.60
1:A:48:ILE:HG23	1:A:63:LEU:CD2	2.32	0.59
2:L:154:LEU:HG	2:L:155:GLN:N	2.17	0.59
1:H:18:LEU:HD13	1:H:109:VAL:HG11	1.85	0.58
2:F:33:LEU:HD13	2:F:71:PHE:CD1	2.39	0.58
1:A:63:LEU:HB3	1:A:67:VAL:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:GLU:OE1	2:B:81:GLU:N	2.34	0.58
2:L:61:ARG:CZ	2:L:79:GLN:HG3	2.34	0.58
1:M:64:LEU:HB3	1:M:68:VAL:HG21	1.85	0.57
1:H:116:THR:HG22	1:H:203:SER:HB3	1.86	0.56
3:C:74:MET:SD	3:Z:74:MET:CE	2.94	0.56
1:A:48:ILE:HG23	1:A:63:LEU:HD22	1.88	0.56
2:F:108:ARG:NH1	2:F:109:THR:O	2.38	0.56
1:A:57[A]:THR:CG2	1:A:59:TYR:CE1	2.80	0.56
1:E:15:SER:O	1:E:16:GLU:HB2	2.06	0.55
2:B:185:ASP:HA	2:B:188:LYS:HE2	1.89	0.55
2:L:54:LEU:HD11	2:L:58:VAL:CG1	2.37	0.54
1:M:64:LEU:HB3	1:M:68:VAL:CG2	2.37	0.54
2:N:31:ASN:HB3	2:N:51:THR:HG22	1.89	0.54
2:B:29:ILE:HD11	2:B:71:PHE:CE1	2.42	0.54
2:L:33:LEU:HD22	2:L:71:PHE:CG	2.41	0.54
2:L:138:ASN:HA	2:L:172:THR:HG23	1.87	0.54
3:C:87:ASP:CB	3:Z:67:LEU:HD11	2.38	0.54
1:A:203:SER:OG	1:A:205:THR:HG23	2.07	0.53
1:A:51:MET:HE2	1:A:69:ILE:CG2	2.36	0.53
3:C:87:ASP:HB2	3:Z:67:LEU:HD11	1.90	0.53
1:H:33:TYR:HB2	1:H:95:ASP:HB3	1.91	0.53
3:C:67:LEU:HD23	3:C:88:VAL:CG1	2.39	0.52
2:L:11:LEU:HD21	2:L:19:VAL:HG13	1.92	0.52
2:B:49:TYR:O	2:B:91:HIS:NE2	2.42	0.52
1:M:18:LEU:CD2	1:M:121:VAL:HG11	2.40	0.52
2:B:75:ILE:HG21	2:B:78:LEU:HD12	1.92	0.52
1:M:12:VAL:HG21	1:M:18:LEU:HD13	1.91	0.51
1:E:178:LEU:C	1:E:178:LEU:HD12	2.31	0.51
1:M:18:LEU:HB2	1:M:86:LEU:HD21	1.93	0.51
2:N:63:SER:O	2:N:73:LEU:HD12	2.09	0.51
3:Z:79:ASP:O	3:Z:83:LEU:HD13	2.09	0.51
1:E:63:LEU:HD23	1:E:67:VAL:HG21	1.92	0.51
1:A:35:THR:CG2	1:A:93:ALA:HB3	2.41	0.51
1:A:51:MET:HG3	1:A:57[B]:THR:HG22	1.92	0.50
2:N:136:LEU:HD13	2:N:175:LEU:HD22	1.94	0.50
3:Z:77:THR:CG2	3:Z:79:ASP:OD2	2.59	0.50
1:A:67:VAL:CG2	1:A:79:LEU:HD13	2.40	0.50
1:A:178:LEU:C	1:A:178:LEU:HD12	2.32	0.50
1:H:33:TYR:CE2	1:H:98:VAL:HA	2.47	0.49
2:L:138:ASN:HA	2:L:172:THR:CG2	2.41	0.49
1:A:4:LEU:CD2	1:A:24:VAL:HG22	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:THR:HG22	1:A:93:ALA:O	2.11	0.49
1:A:159:LEU:HD21	1:A:182:VAL:HG21	1.94	0.49
1:E:214:LYS:O	1:E:215:SER:C	2.51	0.49
2:F:120:PRO:HD3	2:F:132:VAL:HG22	1.94	0.49
1:A:100(B):THR:O	1:A:100(C):ASP:HB2	2.13	0.49
1:A:4:LEU:HD21	1:A:34:TRP:CZ3	2.48	0.48
1:M:18:LEU:CD1	1:M:121:VAL:HG11	2.44	0.48
1:E:145:TYR:CE1	1:E:150:VAL:HG23	2.47	0.48
1:E:15:SER:O	1:E:16:GLU:CB	2.61	0.48
2:L:78:LEU:HD21	2:L:83:PHE:CE2	2.49	0.48
2:N:78:LEU:HD21	2:N:83:PHE:CE2	2.49	0.48
3:D:68:LEU:HD21	3:D:89:LEU:CD2	2.43	0.47
1:A:36:TRP:O	1:A:37:ILE:HD13	2.14	0.47
1:H:80:THR:CG2	1:H:81:SER:N	2.78	0.47
1:E:63:LEU:O	1:E:67:VAL:HG23	2.14	0.47
1:M:190:LEU:C	1:M:190:LEU:HD12	2.34	0.47
1:E:196:CYS:SG	1:E:209:LYS:HB3	2.55	0.47
3:Z:76:ILE:CD1	3:Z:84:MET:HE1	2.45	0.47
1:E:51:MET:HE1	1:E:69:ILE:HG22	1.95	0.46
2:L:92:ASN:CG	3:Y:77:THR:HG23	2.36	0.46
1:A:4:LEU:HD22	1:A:24:VAL:HG22	1.97	0.46
2:F:66:GLY:HA3	2:F:71:PHE:HA	1.97	0.46
1:A:57[A]:THR:HG22	1:A:58:ASN:N	2.30	0.46
1:H:35:THR:HG23	1:H:49:GLY:O	2.15	0.46
2:N:92:ASN:CG	3:Z:77:THR:HG23	2.35	0.46
1:E:93:ALA:HB1	1:E:100(H):VAL:CG1	2.46	0.46
1:A:16:GLU:O	1:A:82:LEU:HD13	2.16	0.46
1:M:33:TYR:CE2	1:M:102:VAL:HA	2.51	0.46
2:N:33:LEU:HD13	2:N:71:PHE:CD1	2.50	0.46
1:H:184:VAL:HG11	1:H:194:TYR:CE1	2.51	0.45
1:E:203:SER:OG	1:E:205:THR:HG23	2.16	0.45
3:Y:68:LEU:HD21	3:Y:89:LEU:CD1	2.45	0.45
1:M:84:THR:CG2	1:M:85:SER:N	2.79	0.45
1:H:18:LEU:HD11	1:H:109:VAL:HG21	1.99	0.45
1:H:100(D):MET:N	1:H:100(D):MET:HE2	2.32	0.45
1:H:159:LEU:HD21	1:H:182:VAL:HG21	2.00	0.44
1:A:152:VAL:HG11	1:A:180:SER:CB	2.47	0.44
2:F:23:CYS:SG	2:F:33:LEU:HD11	2.57	0.44
1:H:18:LEU:HD11	1:H:109:VAL:HG11	1.97	0.44
3:C:84:MET:O	3:C:88:VAL:HG23	2.18	0.44
1:E:51:MET:HE3	1:E:75:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:VAL:HG23	1:H:79:LEU:HD23	1.99	0.44
2:B:66:GLY:HA3	2:B:71:PHE:HA	2.00	0.44
2:N:33:LEU:HD13	2:N:71:PHE:CB	2.47	0.44
1:A:35:THR:HG21	1:A:100(H):VAL:CG1	2.48	0.44
1:E:38:ARG:HB3	1:E:48:ILE:HD11	1.99	0.44
1:A:79:LEU:O	1:A:82:LEU:HD11	2.18	0.44
1:A:51:MET:HE3	1:A:75:PHE:HB2	2.00	0.43
2:F:29:ILE:HD11	2:F:71:PHE:CE1	2.52	0.43
1:M:111:ARG:NH2	2:N:55:GLU:OE2	2.51	0.43
1:A:33:TYR:HB2	1:A:95:ASP:HB3	2.00	0.43
2:F:136:LEU:HD12	2:F:136:LEU:N	2.34	0.43
2:N:33:LEU:HD23	2:N:33:LEU:C	2.39	0.43
2:N:108:ARG:HH12	2:N:111:ALA:HB2	1.83	0.43
1:E:4:LEU:HD11	1:E:34:TRP:HZ3	1.82	0.43
1:M:33:TYR:HB2	1:M:99:ASP:HB3	2.01	0.43
1:E:128:SER:OG	2:F:214:CYS:SG	2.72	0.43
2:L:54:LEU:HD11	2:L:58:VAL:HG11	2.01	0.43
1:M:16:GLU:O	1:M:86:LEU:HD22	2.18	0.43
3:C:67:LEU:HD23	3:C:88:VAL:HG11	2.01	0.43
2:L:138:ASN:CB	2:L:172:THR:HG21	2.49	0.43
2:N:21:ILE:HG21	2:N:102:THR:HG21	2.00	0.43
3:Y:76:ILE:HD12	3:Y:80[A]:GLN:HB3	1.99	0.42
1:H:47:TRP:CD2	2:L:96:ARG:HG2	2.54	0.42
3:D:64:LEU:O	3:D:68:LEU:HD13	2.20	0.42
1:E:82:LEU:HD23	1:E:111:VAL:HG21	2.00	0.42
1:E:187:SER:HB2	2:L:111:ALA:HB1	2.01	0.42
2:N:8:PRO:O	2:N:102:THR:HG23	2.20	0.42
2:N:175:LEU:HD23	2:N:175:LEU:C	2.39	0.42
1:A:67:VAL:HG22	1:A:79:LEU:CD1	2.42	0.42
1:E:33:TYR:HB2	1:E:95:ASP:HB3	2.00	0.42
2:N:54:LEU:HD23	2:N:55:GLU:O	2.20	0.42
1:H:12:VAL:HG21	1:H:18:LEU:HD13	2.02	0.42
2:B:181:LEU:HD23	2:B:186:TYR:HB2	2.01	0.42
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.55	0.41
2:F:130:ALA:O	2:F:181:LEU:HD12	2.19	0.41
2:N:136:LEU:HD12	2:N:136:LEU:N	2.35	0.41
2:N:21:ILE:CG2	2:N:102:THR:HG21	2.49	0.41
1:A:100(B):THR:O	1:A:100(C):ASP:CB	2.68	0.41
1:E:82:LEU:HD23	1:E:111:VAL:CG2	2.51	0.41
2:F:186:TYR:CE2	2:F:211:ARG:HD3	2.56	0.41
2:N:23:CYS:SG	2:N:33:LEU:HD11	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:222:ARG:NH2	1:M:224:GLU:OE2	2.47	0.41
1:E:20:LEU:HD11	1:E:109:VAL:HG21	2.03	0.41
1:H:80:THR:HG23	1:H:81:SER:N	2.35	0.41
1:H:166:PHE:CE1	2:L:164:THR:HG23	2.56	0.41
2:L:48:ILE:HD12	2:L:73:LEU:CD1	2.48	0.41
2:B:49:TYR:O	2:B:91:HIS:CE1	2.74	0.41
1:M:4:LEU:HD21	1:M:34:TRP:CZ3	2.56	0.41
3:Z:74:MET:HE1	3:Z:84:MET:CE	2.51	0.41
1:A:138:LEU:CD1	1:A:211:VAL:HG11	2.45	0.40
2:B:120:PRO:HD3	2:B:132:VAL:HG22	2.02	0.40
1:A:63:LEU:HD23	1:A:67:VAL:HG21	2.03	0.40
1:A:145:TYR:CE1	1:A:150:VAL:HG23	2.55	0.40
1:H:23:VAL:HG22	1:H:74:GLN:HG2	2.03	0.40
1:A:18:LEU:HB2	1:A:82:LEU:HD21	2.03	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	219/230 (95%)	212 (97%)	6 (3%)	1 (0%)	29	48
1	E	216/230 (94%)	206 (95%)	8 (4%)	2 (1%)	17	31
1	H	216/230 (94%)	209 (97%)	7 (3%)	0	100	100
1	M	220/230 (96%)	214 (97%)	6 (3%)	0	100	100
2	B	212/215 (99%)	203 (96%)	8 (4%)	1 (0%)	29	48
2	F	214/215 (100%)	204 (95%)	9 (4%)	1 (0%)	29	48
2	L	213/215 (99%)	209 (98%)	4 (2%)	0	100	100
2	N	212/215 (99%)	207 (98%)	5 (2%)	0	100	100
3	C	33/123 (27%)	32 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	33/123 (27%)	33 (100%)	0	0	100	100
3	Y	35/123 (28%)	34 (97%)	1 (3%)	0	100	100
3	Z	34/123 (28%)	34 (100%)	0	0	100	100
All	All	1857/2272 (82%)	1797 (97%)	55 (3%)	5 (0%)	41	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	16	GLU
1	E	215	SER
1	A	100(C)	ASP
2	F	138	ASN
2	B	138	ASN

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	189/198 (96%)	182 (96%)	7 (4%)	34	60
1	E	189/198 (96%)	184 (97%)	5 (3%)	46	72
1	H	189/198 (96%)	181 (96%)	8 (4%)	30	54
1	M	187/198 (94%)	180 (96%)	7 (4%)	34	60
2	B	183/190 (96%)	178 (97%)	5 (3%)	44	71
2	F	188/190 (99%)	183 (97%)	5 (3%)	44	71
2	L	188/190 (99%)	184 (98%)	4 (2%)	53	78
2	N	186/190 (98%)	178 (96%)	8 (4%)	29	53
3	C	29/104 (28%)	26 (90%)	3 (10%)	7	14
3	D	30/104 (29%)	27 (90%)	3 (10%)	7	15
3	Y	32/104 (31%)	31 (97%)	1 (3%)	40	67
3	Z	29/104 (28%)	27 (93%)	2 (7%)	15	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1619/1968 (82%)	1561 (96%)	58 (4%)	35	61

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	100(E)	ARG
1	A	100(G)	ARG
1	A	129	LYS
1	A	183	THR
1	A	205	THR
1	A	209	LYS
2	B	90	GLN
2	B	96	ARG
2	B	152	ASN
2	B	188	LYS
2	B	214	CYS
3	C	66	GLU
3	C	79	ASP
3	C	83	LEU
3	D	66	GLU
3	D	79	ASP
3	D	83	LEU
1	E	63	LEU
1	E	100(G)	ARG
1	E	178	LEU
1	E	183	THR
1	E	205	THR
2	F	53	HIS
2	F	90	GLN
2	F	96	ARG
2	F	100	GLN
2	F	181	LEU
1	H	28	SER
1	H	63	LEU
1	H	79	LEU
1	H	80	THR
1	H	82	LEU
1	H	99	MET
1	H	100(D)	MET
1	H	100(G)	ARG
2	L	47	LEU

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Mol	Chain	Res	Type
2	L	79	GLN
2	L	154	LEU
2	L	172	THR
1	M	7	SER
1	M	67	ARG
1	M	83	LEU
1	M	84	THR
1	M	86	LEU
1	M	106	THR
1	M	111	ARG
2	N	47	LEU
2	N	50	TYR
2	N	51	THR
2	N	70	ASP
2	N	90	GLN
2	N	162	SER
2	N	174	SER
2	N	188	LYS
3	Y	89	LEU
3	Z	79	ASP
3	Z	90	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	164	HIS
2	F	53	HIS
2	F	137	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, 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	224/230 (97%)	0.78	17 (7%)	13	14	30, 44, 62, 78	0
1	E	223/230 (96%)	0.82	20 (8%)	9	9	29, 43, 59, 66	0
1	H	221/230 (96%)	0.69	14 (6%)	20	21	28, 38, 57, 70	0
1	M	223/230 (96%)	0.67	14 (6%)	20	21	28, 39, 57, 67	0
2	B	214/215 (99%)	0.59	12 (5%)	24	25	29, 39, 49, 61	4 (1%)
2	F	214/215 (99%)	0.70	15 (7%)	16	16	29, 40, 48, 59	5 (2%)
2	L	214/215 (99%)	0.49	5 (2%)	60	63	29, 37, 46, 61	6 (2%)
2	N	214/215 (99%)	0.60	10 (4%)	31	33	28, 37, 47, 59	7 (3%)
3	C	35/123 (28%)	0.64	3 (8%)	10	10	40, 49, 67, 75	0
3	D	35/123 (28%)	0.94	4 (11%)	5	4	39, 51, 73, 81	0
3	Y	36/123 (29%)	1.16	6 (16%)	1	1	39, 49, 69, 75	0
3	Z	36/123 (29%)	0.91	6 (16%)	1	1	35, 45, 60, 72	0
All	All	1889/2272 (83%)	0.69	126 (6%)	17	18	28, 40, 58, 81	22 (1%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	216	CYS	6.4
1	E	216	CYS	6.2
1	A	191	THR	6.2
3	Y	88	VAL	5.2
3	Y	92	ALA	5.0
1	H	190	GLY	4.7
1	A	9	PRO	4.1
1	E	160	THR	4.1
2	N	19	VAL	3.7
3	C	91	PHE	3.7
1	A	12	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	63	LEU	3.6
3	Z	89	LEU	3.6
1	M	66	SER	3.5
1	A	216	CYS	3.5
1	A	84	ALA	3.5
2	N	12	SER	3.4
1	M	28	SER	3.3
3	D	64	LEU	3.3
1	A	27	GLY	3.3
1	M	162	VAL	3.3
2	N	144	ALA	3.3
1	A	26	GLY	3.3
1	E	1	GLN	3.2
3	Y	62	ASN	3.2
1	E	67	VAL	3.1
1	E	107	ILE	3.1
1	E	191	THR	3.1
2	B	19	VAL	3.1
1	E	100(D)	MET	3.0
2	F	129	THR	3.0
2	N	214	CYS	3.0
1	A	2	VAL	2.9
1	E	4	LEU	2.9
3	C	95	ALA	2.9
3	Y	79	ASP	2.9
1	A	131	THR	2.8
2	F	127	SER	2.8
2	F	128	GLY	2.8
1	E	14	PRO	2.8
1	H	96	ALA	2.8
1	E	9	PRO	2.8
2	L	212	GLY	2.8
2	N	140	TYR	2.8
3	D	94	GLU	2.8
2	B	129	THR	2.8
3	Z	65	SER	2.8
2	N	190	LYS	2.7
1	A	215	SER	2.7
2	F	43	ALA	2.7
2	N	60	SER	2.6
3	Z	93	ALA	2.6
2	F	214	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	98	PHE	2.6
2	B	66	GLY	2.6
2	B	127	SER	2.6
1	E	159	LEU	2.6
1	H	132	SER	2.6
1	M	19	SER	2.5
1	M	125	SER	2.5
2	F	163	VAL	2.5
2	F	112	ALA	2.5
2	N	52	SER	2.5
3	C	89	LEU	2.5
2	B	5	SER	2.5
1	E	48	ILE	2.5
1	H	18	LEU	2.4
3	Z	91	PHE	2.4
1	H	91	TYR	2.4
1	A	23	VAL	2.4
1	A	28	SER	2.4
2	B	182	SER	2.4
1	H	27	GLY	2.4
1	H	65	SER	2.4
1	M	202	GLY	2.3
2	F	77	SER	2.3
2	F	130	ALA	2.3
2	N	128	GLY	2.3
2	B	11	LEU	2.3
1	A	132	SER	2.3
3	Y	69	SER	2.3
1	M	92	ALA	2.3
2	N	13	ALA	2.3
2	L	125	LEU	2.3
1	M	7	SER	2.2
1	M	200	SER	2.2
2	L	184	ALA	2.2
2	F	22	THR	2.2
1	A	108	LEU	2.2
1	M	127	SER	2.2
1	M	228	CYS	2.2
3	Y	95	ALA	2.2
3	Z	92	ALA	2.2
3	D	68	LEU	2.2
3	Z	64	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	33	TYR	2.2
2	F	60	SER	2.2
2	F	205	VAL	2.2
2	F	52	SER	2.2
2	B	106	ILE	2.2
1	H	42	GLY	2.2
1	E	172	SER	2.2
1	E	215	SER	2.2
1	M	84	THR	2.1
2	B	214	CYS	2.1
1	E	72(A)	ALA	2.1
3	D	92	ALA	2.1
2	B	27	GLN	2.1
2	L	187	GLU	2.1
1	A	10	GLY	2.1
1	A	1	GLN	2.1
2	L	208	SER	2.1
1	M	27	GLY	2.1
1	H	134	GLY	2.1
2	F	181	LEU	2.1
1	E	41	PRO	2.0
1	M	62	PRO	2.0
1	A	89	VAL	2.0
2	B	104	VAL	2.0
1	E	31	SER	2.0
1	E	129	LYS	2.0
1	E	177	SER	2.0
1	H	70	SER	2.0
2	B	67	SER	2.0
1	H	62	SER	2.0
1	H	215	SER	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.