



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:32 PM UTC

PDB ID : 8ULJ / pdb_00008ulj
Title : Prefusion RSV F bound by neutralizing antibody 2E08
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Deposited on : 2023-10-16
Resolution : 3.00 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

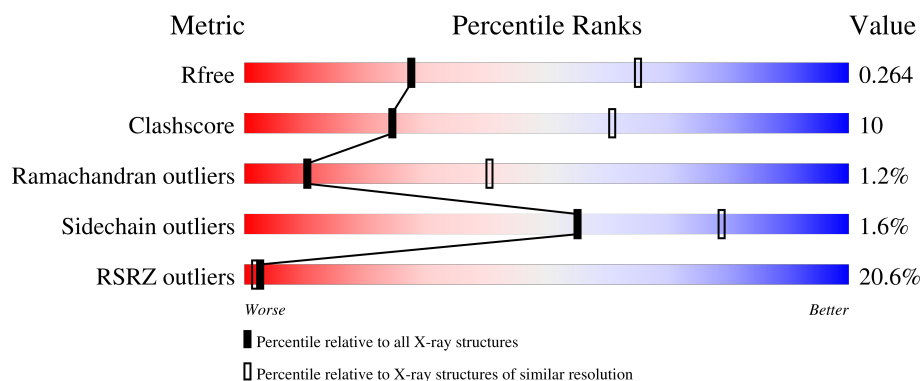
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	A	79	10% 82% 16%
2	L	214	33% 72% 20% 5%
3	H	242	36% 63% 26% 10%
4	B	414	5% 83% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6896 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 Fusion glycoprotein F2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	78	Total	C	N	O	S	0	0	0
			611	384	100	124	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	conflict	UNP P03420

- Molecule 2 is a protein called 2E08 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	209	Total	C	N	O	S	0	1	0
			1516	936	272	304	4			

- Molecule 3 is a protein called 2E08 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	217	Total	C	N	O	S	0	0	0
			1617	1026	267	317	7			

- Molecule 4 is a protein called Fusion glycoprotein F0,Fibritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	408	Total	C	N	O	S	0	0	0
			3152	1997	520	615	20			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	155	CYS	SER	conflict	UNP A0A088S9A7
B	190	PHE	SER	conflict	UNP A0A088S9A7
B	207	LEU	VAL	conflict	UNP A0A088S9A7

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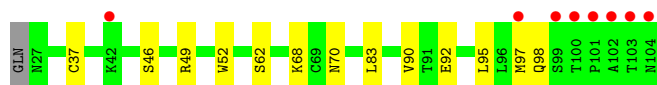
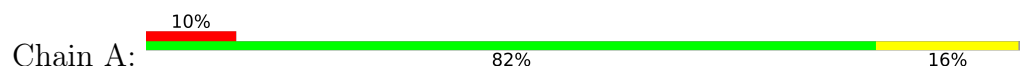
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Chain	Residue	Modelled	Actual	Comment	Reference
B	290	CYS	SER	conflict	UNP A0A088S9A7
B	514	SER	-	linker	UNP A0A088S9A7
B	515	ALA	-	linker	UNP A0A088S9A7
B	516	ILE	-	linker	UNP A0A088S9A7
B	517	GLY	-	linker	UNP A0A088S9A7
B	539	LEU	PHE	conflict	UNP P10104
B	545	GLY	-	expression tag	UNP P10104
B	546	GLY	-	expression tag	UNP P10104
B	547	LEU	-	expression tag	UNP P10104
B	548	VAL	-	expression tag	UNP P10104
B	549	PRO	-	expression tag	UNP P10104
B	550	ARG	-	expression tag	UNP P10104

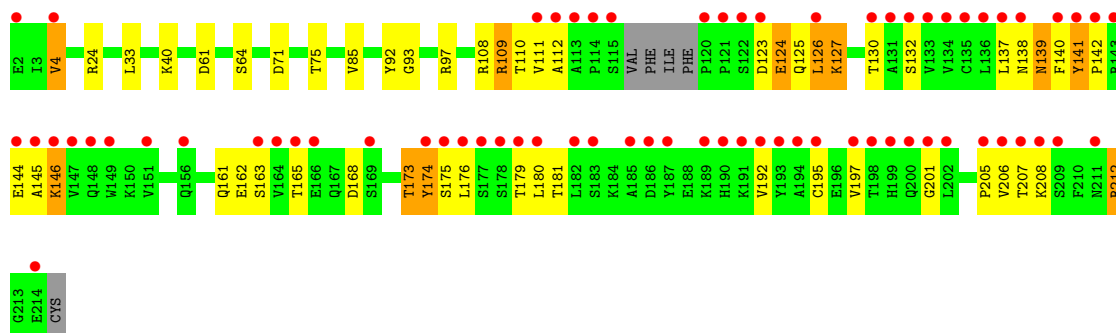
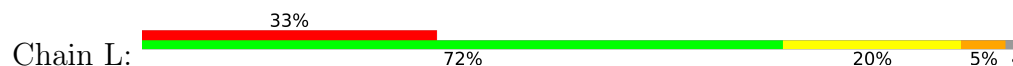
3 Residue-property plots [i](#)

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.

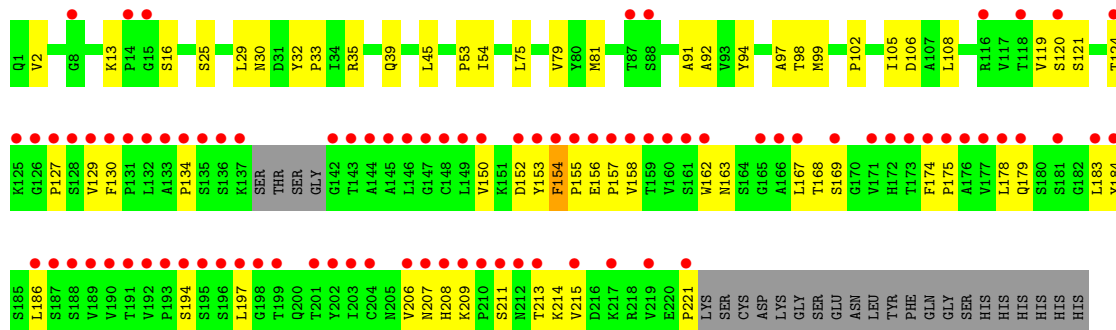
- Molecule 1: Fusion glycoprotein F2



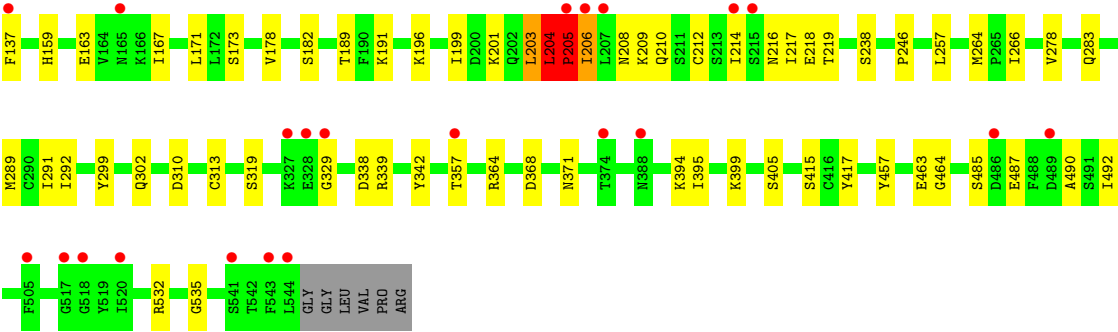
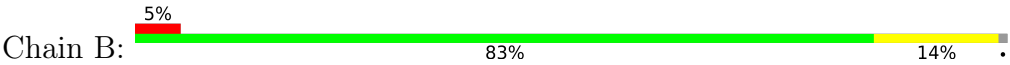
- Molecule 2: 2E08 Fab Light Chain



- Molecule 3: 2E08 Fab Heavy Chain



- Molecule 4: Fusion glycoprotein F0,Fibritin



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.72Å 164.72Å 146.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.39 – 3.00 43.39 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (43.39-3.00) 94.7 (43.39-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.237 , 0.264 0.238 , 0.264	Depositor DCC
R_{free} test set	1982 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6896	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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](#)

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	0.19	0/618	0.38	0/835
2	L	0.36	0/1546	0.59	1/2107 (0.0%)
3	H	0.14	0/1653	0.43	0/2257
4	B	0.18	0/3203	0.38	2/4345 (0.0%)
All	All	0.23	0/7020	0.45	3/9544 (0.0%)

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	L	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	205	PRO	N-CA-C	-7.16	97.71	112.47
2	L	175	SER	N-CA-C	6.37	116.48	108.45
4	B	205	PRO	CA-N-CD	-5.04	104.95	112.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	108	ARG	Sidechain
2	L	109	ARG	Sidechain
2	L	212	ARG	Sidechain

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	611	0	618	13	0
2	L	1516	0	1378	39	0
3	H	1617	0	1601	54	0
4	B	3152	0	3180	46	0
All	All	6896	0	6777	135	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 10.

All (135) 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)
4:B:203:LEU:C	4:B:205:PRO:HD3	2.05	0.81
3:H:32:TYR:HB3	3:H:98:THR:HG21	1.63	0.80
3:H:158:VAL:HG23	3:H:207:ASN:HB3	1.65	0.76
2:L:205:PRO:HB2	2:L:208:LYS:HD2	1.67	0.75
3:H:167:LEU:HD23	3:H:168:THR:H	1.52	0.74
2:L:139:ASN:HA	2:L:174:TYR:H	1.55	0.71
3:H:121:SER:H	3:H:154:PHE:HZ	1.38	0.71
3:H:162:TRP:O	3:H:163:ASN:ND2	2.24	0.70
3:H:129:VAL:HG12	3:H:206:VAL:HG11	1.74	0.68
2:L:111:VAL:HG13	2:L:142:PRO:HG2	1.76	0.68
2:L:146:LYS:H	2:L:197:VAL:HG13	1.59	0.67
3:H:153:TYR:HB2	3:H:184:TYR:HB2	1.77	0.66
2:L:206:VAL:HG22	2:L:207:THR:HG23	1.77	0.65
2:L:4:VAL:HA	2:L:24:ARG:O	1.97	0.65
3:H:98:THR:HG22	3:H:99:MET:H	1.63	0.64
4:B:204:LEU:N	4:B:205:PRO:HD3	2.13	0.64
2:L:137:LEU:HD13	2:L:145:ALA:HB1	1.79	0.63
4:B:137:PHE:CE1	4:B:339:ARG:HD2	2.34	0.63
2:L:165:THR:HG21	2:L:174:TYR:HB3	1.81	0.63
4:B:246:PRO:HB3	4:B:283:GLN:HA	1.81	0.63
3:H:208:HIS:HB3	3:H:213:THR:HG23	1.81	0.62
2:L:40:LYS:HG3	2:L:85:VAL:HG11	1.81	0.62
1:A:62:SER:HB2	4:B:196:LYS:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:194:SER:O	3:H:197:LEU:HB2	2.02	0.60
3:H:35:ARG:NH1	3:H:106:ASP:OD1	2.35	0.59
3:H:168:THR:OG1	3:H:169:SER:N	2.35	0.59
3:H:127:PRO:HB3	3:H:209:LYS:HE2	1.84	0.59
2:L:161:GLN:HE22	3:H:179:GLN:HA	1.67	0.59
3:H:91:ALA:HB2	3:H:119:VAL:H	1.66	0.59
3:H:39:GLN:HB3	3:H:45:LEU:HD23	1.85	0.57
2:L:33:LEU:HD12	2:L:93:GLY:HA2	1.88	0.56
1:A:68:LYS:O	4:B:208:ASN:ND2	2.39	0.56
4:B:310:ASP:OD1	4:B:364:ARG:NH2	2.39	0.56
4:B:171:LEU:HD13	4:B:191:LYS:HB2	1.89	0.55
4:B:399:LYS:HG3	4:B:485:SER:HB2	1.88	0.55
2:L:124:GLU:HA	2:L:127:LYS:HE3	1.88	0.55
4:B:264:MET:HE2	4:B:266:ILE:HD13	1.88	0.54
2:L:165:THR:HG21	2:L:174:TYR:HD2	1.73	0.54
3:H:156:GLU:HG2	3:H:157:PRO:HD2	1.90	0.54
4:B:167:ILE:HG23	4:B:189:THR:HG21	1.88	0.54
2:L:61:ASP:N	2:L:61:ASP:OD1	2.41	0.53
4:B:338:ASP:OD1	4:B:338:ASP:N	2.35	0.53
2:L:138:ASN:O	2:L:139:ASN:C	2.51	0.53
3:H:35:ARG:HD2	4:B:173:SER:HB3	1.89	0.53
3:H:155:PRO:HD2	3:H:209:LYS:HB3	1.91	0.53
2:L:97:ARG:NE	3:H:106:ASP:OD2	2.42	0.53
2:L:125:GLN:HG2	2:L:130:THR:O	2.09	0.53
4:B:209:LYS:O	4:B:209:LYS:HD2	2.09	0.52
3:H:153:TYR:HE1	3:H:186:LEU:HD22	1.74	0.52
3:H:97:ALA:HB3	3:H:108:LEU:HD13	1.92	0.51
3:H:13:LYS:O	3:H:16:SER:OG	2.29	0.51
2:L:24:ARG:HH21	2:L:71:ASP:HB2	1.76	0.51
1:A:95:LEU:O	1:A:98:GLN:HG2	2.11	0.51
3:H:178:LEU:HA	3:H:184:TYR:HA	1.92	0.51
2:L:125:GLN:HG3	3:H:130:PHE:CE2	2.47	0.50
1:A:90:VAL:HG13	4:B:292:ILE:HD11	1.93	0.50
3:H:120:SER:HB2	3:H:154:PHE:CE2	2.47	0.49
4:B:357:THR:HG21	4:B:371:ASN:HD22	1.77	0.49
3:H:153:TYR:CE1	3:H:186:LEU:HD22	2.48	0.49
2:L:140:PHE:HE2	2:L:142:PRO:O	1.94	0.49
2:L:140:PHE:CZ	2:L:145:ALA:HB2	2.48	0.49
4:B:289:MET:HE2	4:B:299:TYR:HB3	1.94	0.49
4:B:163:GLU:OE2	4:B:182:SER:OG	2.30	0.49
4:B:199:ILE:O	4:B:204:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:195:CYS:O	2:L:208:LYS:NZ	2.31	0.48
3:H:124:THR:HA	3:H:155:PRO:HG3	1.95	0.48
3:H:75:LEU:H	3:H:75:LEU:HD23	1.78	0.48
3:H:167:LEU:HD23	3:H:168:THR:N	2.25	0.48
3:H:174:PHE:HB3	3:H:175:PRO:HD2	1.96	0.48
3:H:153:TYR:CG	3:H:209:LYS:HE3	2.49	0.48
3:H:127:PRO:HD3	3:H:209:LYS:HG2	1.95	0.47
3:H:33:PRO:O	3:H:98:THR:HG23	2.13	0.47
3:H:81:MET:HE1	3:H:94:TYR:CD1	2.49	0.47
4:B:216:ASN:O	4:B:219:THR:HG22	2.15	0.47
3:H:150:VAL:HB	3:H:186:LEU:HD23	1.96	0.47
2:L:141:TYR:HB3	2:L:142:PRO:HD3	1.97	0.46
4:B:487:GLU:HB3	4:B:490:ALA:HB2	1.97	0.46
2:L:64:SER:OG	2:L:75:THR:OG1	2.33	0.46
1:A:49:ARG:HE	4:B:368:ASP:CG	2.24	0.46
4:B:415:SER:HB3	4:B:417:TYR:CE2	2.50	0.46
4:B:171:LEU:HD11	4:B:189:THR:HG22	1.98	0.45
2:L:162:GLU:HB3	2:L:176:LEU:HD11	1.97	0.45
2:L:142:PRO:O	2:L:144:GLU:N	2.50	0.45
3:H:134:PRO:HG3	3:H:221:PRO:HB3	1.97	0.45
4:B:159:HIS:NE2	4:B:291:ILE:HD13	2.31	0.45
3:H:129:VAL:CG1	3:H:206:VAL:HG11	2.45	0.45
2:L:140:PHE:C	2:L:173:THR:HG22	2.42	0.45
4:B:532:ARG:NH2	4:B:535:GLY:O	2.50	0.45
4:B:329:GLY:O	4:B:399:LYS:NZ	2.50	0.45
2:L:165:THR:HG21	2:L:174:TYR:CD2	2.52	0.44
2:L:132:SER:HA	2:L:180:LEU:O	2.17	0.44
3:H:2:VAL:HA	3:H:25:SER:O	2.18	0.44
4:B:206:ILE:HG22	4:B:214:ILE:HB	2.00	0.44
1:A:92:GLU:OE2	4:B:238:SER:OG	2.28	0.44
1:A:46:SER:HB3	4:B:313:CYS:SG	2.58	0.43
2:L:132:SER:OG	2:L:181:THR:HG22	2.18	0.43
2:L:165:THR:CG2	2:L:174:TYR:HB3	2.46	0.43
4:B:405:SER:HB3	4:B:457:TYR:CE2	2.53	0.43
4:B:217:ILE:HG22	4:B:218:GLU:OE2	2.18	0.43
3:H:29:LEU:HG	3:H:53:PRO:HG2	1.99	0.43
4:B:257:LEU:HD23	4:B:278:VAL:HG13	1.99	0.43
3:H:30:ASN:HB3	3:H:54:ILE:HD12	2.00	0.43
1:A:70:ASN:HB3	4:B:210:GLN:O	2.19	0.43
3:H:155:PRO:CD	3:H:209:LYS:HB3	2.48	0.43
2:L:168:ASP:HB2	2:L:173:THR:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:394:LYS:HB3	4:B:394:LYS:HE3	1.67	0.43
1:A:97:MET:HE3	4:B:292:ILE:HG22	2.00	0.43
3:H:129:VAL:HG21	3:H:215:VAL:HG11	2.00	0.43
3:H:152:ASP:HA	3:H:183:LEU:HB3	2.00	0.42
2:L:173:THR:HB	2:L:174:TYR:H	1.56	0.42
4:B:338:ASP:HB2	4:B:342:TYR:OH	2.19	0.42
3:H:29:LEU:HD11	3:H:79:VAL:HG23	2.02	0.42
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.95	0.42
2:L:112:ALA:HB3	2:L:201:GLY:HA3	2.02	0.42
4:B:357:THR:HG21	4:B:371:ASN:ND2	2.35	0.42
3:H:129:VAL:HG11	3:H:215:VAL:HG11	2.01	0.42
4:B:463:GLU:OE1	4:B:464:GLY:N	2.52	0.42
4:B:415:SER:HB3	4:B:417:TYR:HE2	1.85	0.42
3:H:156:GLU:O	3:H:158:VAL:HG13	2.19	0.41
4:B:395:ILE:HD13	4:B:492:ILE:HD13	2.02	0.41
1:A:52:TRP:CE3	4:B:302:GLN:HG2	2.55	0.41
1:A:97:MET:HE1	4:B:289:MET:SD	2.60	0.41
2:L:126:LEU:HD13	2:L:126:LEU:HA	1.94	0.41
3:H:102:PRO:HB2	4:B:178:VAL:HG23	2.02	0.41
2:L:123:ASP:O	2:L:124:GLU:C	2.64	0.41
2:L:163:SER:CB	3:H:175:PRO:HG3	2.51	0.41
4:B:216:ASN:CG	4:B:218:GLU:HG2	2.46	0.41
1:A:37:CYS:SG	4:B:319:SER:HB3	2.61	0.40
2:L:132:SER:HB3	2:L:179:THR:HG23	2.01	0.40
3:H:209:LYS:HA	3:H:209:LYS:HD3	1.60	0.40
2:L:33:LEU:HB3	2:L:92:TYR:CD2	2.56	0.40
3:H:214:LYS:HE3	3:H:214:LYS:HB3	1.98	0.40
3:H:153:TYR:HA	3:H:209:LYS:HD2	2.02	0.40
3:H:39:GLN:O	3:H:92:ALA:HB1	2.22	0.40
3:H:120:SER:HB2	3:H:154:PHE:CZ	2.56	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	76/79 (96%)	73 (96%)	3 (4%)	0	100	100
2	L	206/214 (96%)	181 (88%)	20 (10%)	5 (2%)	4	24
3	H	213/242 (88%)	190 (89%)	20 (9%)	3 (1%)	9	36
4	B	406/414 (98%)	392 (97%)	11 (3%)	3 (1%)	18	53
All	All	901/949 (95%)	836 (93%)	54 (6%)	11 (1%)	10	40

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	4	VAL
3	H	154	PHE
3	H	211	SER
4	B	205	PRO
2	L	139	ASN
2	L	174	TYR
4	B	201	LYS
4	B	204	LEU
2	L	146	LYS
2	L	141	TYR
3	H	105	ILE

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	70/71 (99%)	70 (100%)	0	100	100
2	L	149/185 (80%)	141 (95%)	8 (5%)	20	53
3	H	181/206 (88%)	181 (100%)	0	100	100
4	B	369/373 (99%)	365 (99%)	4 (1%)	65	83
All	All	769/835 (92%)	757 (98%)	12 (2%)	55	79

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	109	ARG
2	L	110	THR
2	L	124	GLU
2	L	126	LEU
2	L	127	LYS
2	L	173	THR
2	L	192	VAL
2	L	212	ARG
4	B	203	LEU
4	B	204	LEU
4	B	206	ILE
4	B	212	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	161	GLN
3	H	65	GLN
4	B	165	ASN
4	B	262	ASN
4	B	283	GLN
4	B	371	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

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	78/79 (98%)	0.55	8 (10%) 12 6	44, 68, 140, 151	0
2	L	209/214 (97%)	1.54	70 (33%) 1 1	44, 89, 166, 195	1 (0%)
3	H	217/242 (89%)	2.11	88 (40%) 0 1	45, 102, 183, 200	0
4	B	408/414 (98%)	0.27	22 (5%) 31 16	40, 63, 119, 177	0
All	All	912/949 (96%)	1.02	188 (20%) 2 2	40, 74, 171, 200	1 (0%)

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	132	LEU	10.2
2	L	136	LEU	10.0
3	H	149	LEU	9.2
3	H	190	VAL	8.5
3	H	135	SER	8.4
3	H	188	SER	8.3
2	L	145	ALA	8.1
3	H	173	THR	8.0
3	H	146	LEU	8.0
2	L	209	SER	6.9
3	H	150	VAL	6.8
1	A	104	ASN	6.3
2	L	120	PRO	6.3
2	L	134	VAL	6.3
2	L	164[A]	VAL	6.0
3	H	157	PRO	5.9
3	H	207	ASN	5.6
3	H	134	PRO	5.5
3	H	137	LYS	5.5
3	H	147	GLY	5.4
2	L	147	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
2	L	197	VAL	5.4
3	H	145	ALA	5.4
3	H	131	PRO	5.4
3	H	193	PRO	5.4
2	L	175	SER	5.3
3	H	176	ALA	5.3
3	H	195	SER	5.3
3	H	191	THR	5.3
2	L	146	LYS	5.2
3	H	172	HIS	5.2
2	L	132	SER	5.1
1	A	100	THR	5.0
3	H	154	PHE	5.0
3	H	129	VAL	5.0
3	H	187	SER	5.0
3	H	189	VAL	5.0
1	A	103	THR	4.9
2	L	135	CYS	4.9
2	L	123	ASP	4.9
2	L	115	SER	4.9
2	L	177	SER	4.9
3	H	174	PHE	4.9
3	H	133	ALA	4.9
3	H	148	CYS	4.8
3	H	136	SER	4.8
1	A	101	PRO	4.8
2	L	148	GLN	4.7
3	H	210	PRO	4.7
2	L	122	SER	4.7
2	L	200	GLN	4.6
2	L	163	SER	4.6
2	L	137	LEU	4.5
2	L	114	PRO	4.4
3	H	178	LEU	4.4
2	L	192	VAL	4.4
3	H	125	LYS	4.3
3	H	167	LEU	4.3
2	L	180	LEU	4.2
3	H	221	PRO	4.2
3	H	171	VAL	4.2
3	H	211	SER	4.2
1	A	102	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	L	151	VAL	4.1
3	H	175	PRO	4.1
2	L	207	THR	4.0
3	H	192	VAL	4.0
3	H	199	THR	4.0
2	L	133	VAL	4.0
3	H	153	TYR	3.9
3	H	213	THR	3.9
2	L	178	SER	3.9
4	B	137	PHE	3.9
3	H	219	VAL	3.9
2	L	112	ALA	3.9
2	L	176	LEU	3.9
3	H	203	ILE	3.8
4	B	329	GLY	3.6
2	L	121	PRO	3.6
3	H	88	SER	3.6
2	L	143	ARG	3.6
2	L	144	GLU	3.6
2	L	169	SER	3.6
2	L	142	PRO	3.5
2	L	206	VAL	3.5
3	H	186	LEU	3.5
4	B	207	LEU	3.5
3	H	202	TYR	3.5
3	H	206	VAL	3.5
2	L	214	GLU	3.4
2	L	130	THR	3.4
2	L	201	GLY	3.4
3	H	196	SER	3.4
3	H	143	THR	3.4
2	L	211	ASN	3.3
2	L	183	SER	3.3
3	H	128	SER	3.3
3	H	166	ALA	3.3
2	L	190	HIS	3.3
2	L	194	ALA	3.3
3	H	184	TYR	3.3
3	H	194	SER	3.3
3	H	144	ALA	3.2
2	L	141	TYR	3.2
3	H	217	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
4	B	357	THR	3.2
2	L	111	VAL	3.2
2	L	198	THR	3.2
4	B	214	ILE	3.1
2	L	131	ALA	3.1
3	H	142	GLY	3.1
3	H	179	GLN	3.1
3	H	156	GLU	3.1
3	H	201	THR	3.0
3	H	155	PRO	3.0
3	H	197	LEU	3.0
3	H	160	VAL	3.0
1	A	99	SER	3.0
4	B	165	ASN	3.0
4	B	486	ASP	3.0
2	L	199	HIS	3.0
2	L	2	GLU	2.9
4	B	328	GLU	2.9
2	L	193	TYR	2.9
2	L	187	TYR	2.9
4	B	520	ILE	2.9
3	H	198	GLY	2.9
2	L	179	THR	2.8
3	H	161	SER	2.8
2	L	186	ASP	2.8
4	B	327	LYS	2.8
3	H	118	THR	2.8
2	L	174	TYR	2.8
2	L	140	PHE	2.7
2	L	208	LYS	2.7
3	H	152	ASP	2.7
3	H	169	SER	2.7
3	H	181	SER	2.7
3	H	126	GLY	2.7
3	H	162	TRP	2.7
3	H	159	THR	2.7
3	H	120	SER	2.6
3	H	177	VAL	2.6
3	H	204	CYS	2.6
2	L	138	ASN	2.6
4	B	518	GLY	2.5
2	L	113	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	195	CYS	2.5
2	L	149	TRP	2.5
3	H	130	PHE	2.5
2	L	202	LEU	2.5
3	H	87	THR	2.4
4	B	505	PHE	2.4
3	H	127	PRO	2.4
4	B	205	PRO	2.4
3	H	158	VAL	2.4
3	H	215	VAL	2.4
2	L	126	LEU	2.4
2	L	205	PRO	2.3
2	L	182	LEU	2.3
4	B	543	PHE	2.3
3	H	15	GLY	2.3
4	B	489	ASP	2.3
4	B	206	ILE	2.3
4	B	215	SER	2.3
4	B	517	GLY	2.3
1	A	97	MET	2.3
2	L	166	GLU	2.2
2	L	185	ALA	2.2
4	B	544	LEU	2.2
2	L	191	LYS	2.2
3	H	116	ARG	2.2
3	H	14	PRO	2.2
4	B	541	SER	2.2
3	H	208	HIS	2.2
3	H	212	ASN	2.1
1	A	42	LYS	2.1
2	L	156	GLN	2.1
2	L	189	LYS	2.1
4	B	388	ASN	2.1
3	H	183	LEU	2.1
3	H	124	THR	2.1
3	H	165	GLY	2.1
2	L	165	THR	2.0
3	H	8	GLY	2.0
3	H	209	LYS	2.0
2	L	4	VAL	2.0
4	B	374	THR	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 oligosaccharides 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.