



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:47 AM UTC

PDB ID : 5MHR / pdb_00005mhr
Title : T3D reovirus sigma1 complexed with 9BG5 Fab fragments
Authors : Stehle, T.; Dietrich, M.H.
Deposited on : 2016-11-25
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

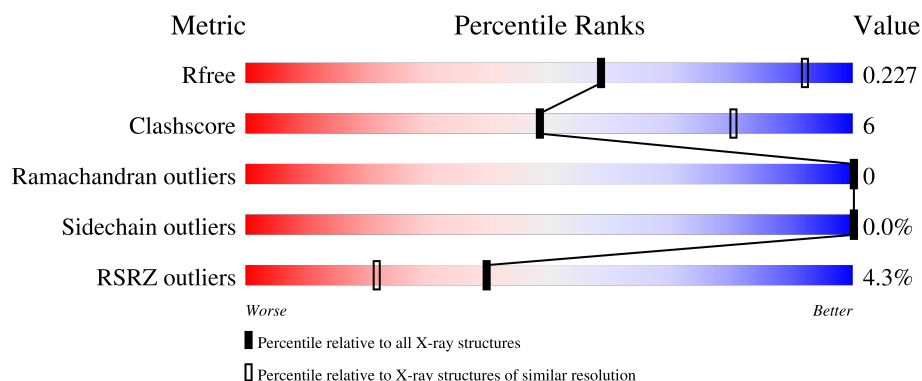
1 Overall quality at a glance

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	165	
1	B	165	
1	C	165	
1	D	165	
1	E	165	

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Mol	Chain	Length	Quality of chain
1	F	165	 % 87% 12% .
2	G	214	 7% 89% 9% .
2	H	214	 8% 84% 12% .
2	J	214	 41% 10% 50%
2	L	214	 43% 7% 50%
2	O	214	 8% 81% 17% .
2	Q	214	 7% 83% 15% .
3	I	219	 11% 84% 13% .
3	K	219	 51% 5% 44%
3	M	219	 % 44% 11% 46%
3	N	219	 2% 84% 14% .
3	P	219	 5% 88% 10% .
3	R	219	 11% 87% 10% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22593 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 Viral attachment protein sigma 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1242	795	209	233	5			
1	B	163	Total	C	N	O	S	0	0	0
			1255	801	211	238	5			
1	C	162	Total	C	N	O	S	0	0	0
			1243	796	210	232	5			
1	D	163	Total	C	N	O	S	0	0	0
			1242	795	208	234	5			
1	E	162	Total	C	N	O	S	0	0	0
			1245	797	210	233	5			
1	F	163	Total	C	N	O	S	0	0	0
			1250	797	211	237	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	GLY	-	expression tag	UNP Q86335
A	292	SER	-	expression tag	UNP Q86335
B	291	GLY	-	expression tag	UNP Q86335
B	292	SER	-	expression tag	UNP Q86335
C	291	GLY	-	expression tag	UNP Q86335
C	292	SER	-	expression tag	UNP Q86335
D	291	GLY	-	expression tag	UNP Q86335
D	292	SER	-	expression tag	UNP Q86335
E	291	GLY	-	expression tag	UNP Q86335
E	292	SER	-	expression tag	UNP Q86335
F	291	GLY	-	expression tag	UNP Q86335
F	292	SER	-	expression tag	UNP Q86335

- Molecule 2 is a protein called 9BG5 Fab light chain,LOC100046793 protein,MAb 110 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	211	Total	C	N	O	S	0	0	0
			1522	954	250	311	7			
2	H	205	Total	C	N	O	S	0	0	0
			1455	913	241	293	8			
2	J	108	Total	C	N	O	S	0	0	0
			793	499	130	159	5			
2	L	107	Total	C	N	O	S	0	0	0
			778	490	124	159	5			
2	O	210	Total	C	N	O	S	0	0	0
			1470	921	245	296	8			
2	Q	210	Total	C	N	O	S	0	0	0
			1422	885	240	289	8			

- Molecule 3 is a protein called 9BG5 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	213	Total	C	N	O	S	0	0	0
			1491	953	240	291	7			
3	K	122	Total	C	N	O	S	0	0	0
			887	569	137	177	4			
3	M	119	Total	C	N	O	S	0	0	0
			853	550	132	168	3			
3	N	214	Total	C	N	O	S	0	0	0
			1544	991	247	300	6			
3	P	213	Total	C	N	O	S	0	0	0
			1474	938	237	293	6			
3	R	213	Total	C	N	O	S	0	0	0
			1427	909	234	278	6			

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: Viral attachment protein sigma 1

Chain A: 



- Molecule 1: Viral attachment protein sigma 1

Chain B: 



- Molecule 1: Viral attachment protein sigma 1

Chain C: 



- Molecule 1: Viral attachment protein sigma 1

Chain D: 



- Molecule 1: Viral attachment protein sigma 1

Chain E: 

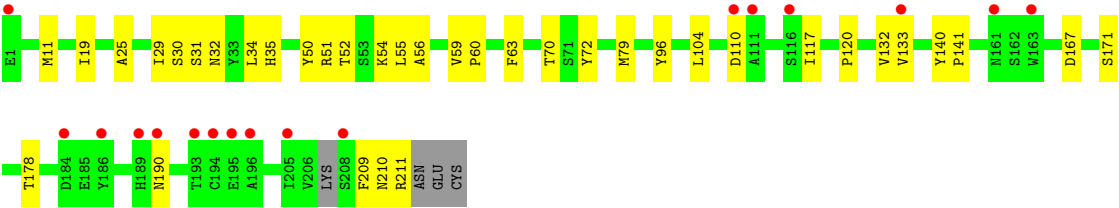
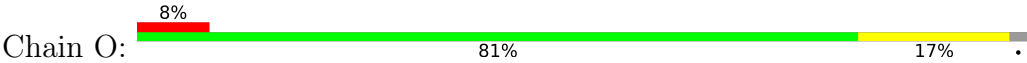


- Molecule 1: Viral attachment protein sigma 1

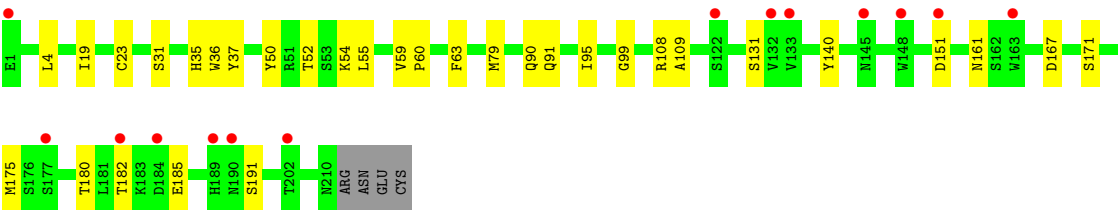
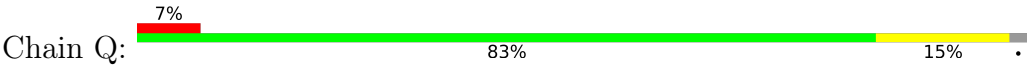


LYS
THR
SER
THR
SER
PRO
PRO
ILE
VAL
LYS
SER
PHE
ASN
ASN
ASN
GLU
CYS

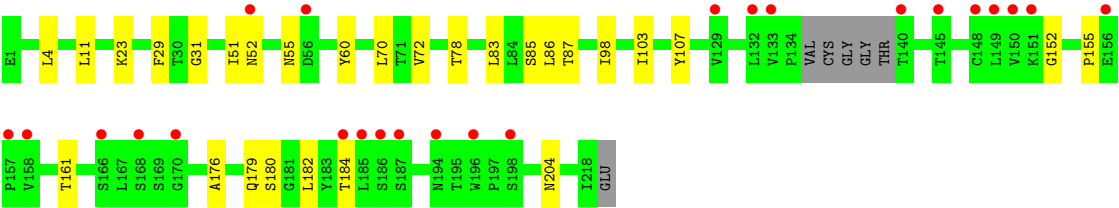
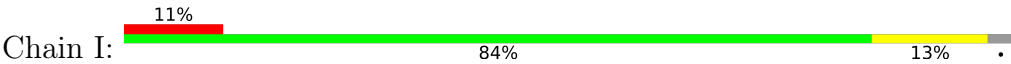
- Molecule 2: 9BG5 Fab light chain,LOC100046793 protein,MAb 110 light chain



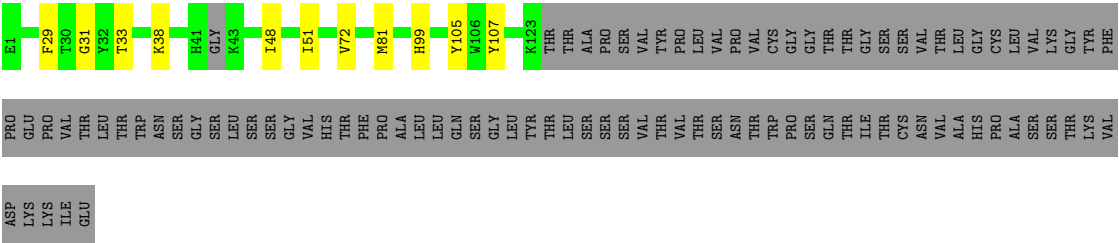
- Molecule 2: 9BG5 Fab light chain,LOC100046793 protein,MAb 110 light chain



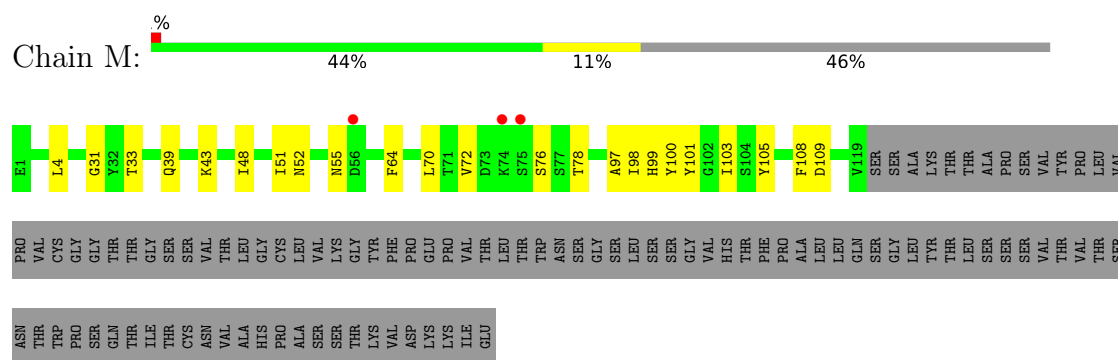
- Molecule 3: 9BG5 Fab heavy chain



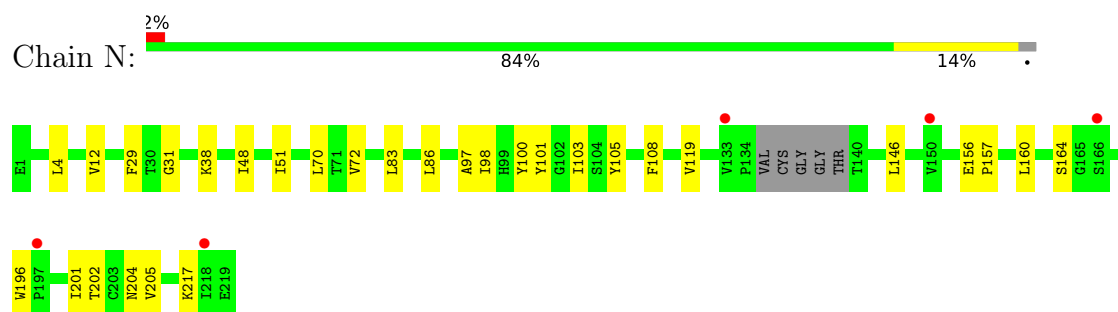
- Molecule 3: 9BG5 Fab heavy chain



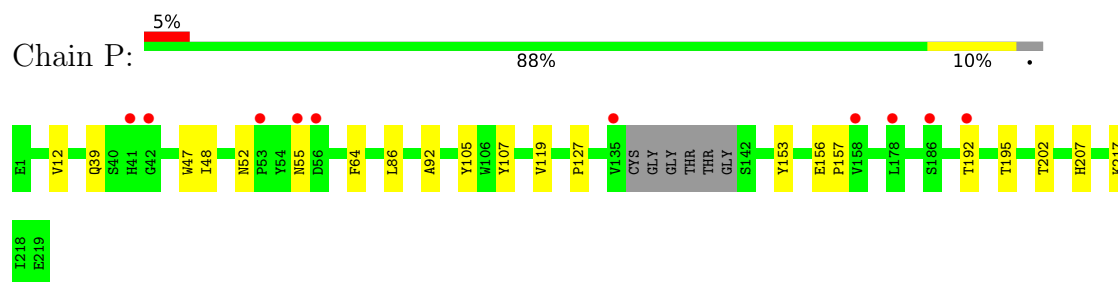
- Molecule 3: 9BG5 Fab heavy chain



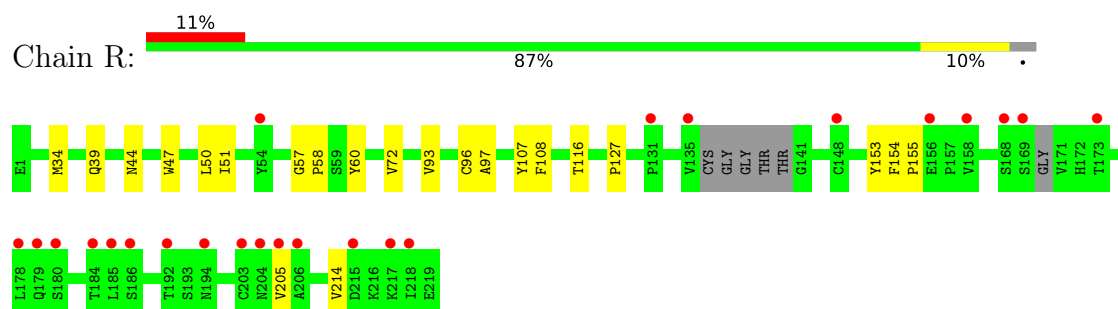
• Molecule 3: 9BG5 Fab heavy chain



• Molecule 3: 9BG5 Fab heavy chain



• Molecule 3: 9BG5 Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.16Å 109.31Å 131.70Å 103.13° 113.56° 103.48°	Depositor
Resolution (Å)	49.05 – 3.00 49.05 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.05-3.00) 98.8 (49.05-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.212 , 0.247 (Not available) , 0.227	Depositor DCC
R_{free} test set	4734 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22593	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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

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	0.21	0/1278	0.45	2/1744 (0.1%)
1	B	0.19	0/1291	0.43	0/1761
1	C	0.21	0/1279	0.45	2/1746 (0.1%)
1	D	0.19	0/1278	0.44	0/1745
1	E	0.21	0/1281	0.44	0/1747
1	F	0.21	0/1286	0.43	0/1756
2	G	0.14	0/1557	0.34	0/2129
2	H	0.17	0/1486	0.35	0/2025
2	J	0.20	0/809	0.42	0/1098
2	L	0.16	0/794	0.37	0/1080
2	O	0.18	0/1501	0.37	0/2055
2	Q	0.15	0/1450	0.37	1/1985 (0.1%)
3	I	0.18	0/1535	0.40	0/2116
3	K	0.15	0/912	0.34	0/1253
3	M	0.16	0/879	0.39	0/1212
3	N	0.19	0/1589	0.38	0/2185
3	P	0.13	0/1518	0.30	0/2099
3	R	0.16	0/1469	0.33	0/2032
All	All	0.18	0/23192	0.39	5/31768 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	108	ARG	CB-CA-C	-5.74	109.97	116.63
1	A	375	LEU	CA-C-N	5.51	123.68	119.66
1	A	375	LEU	C-N-CA	5.51	123.68	119.66
1	C	375	LEU	CA-C-N	5.22	123.47	119.66
1	C	375	LEU	C-N-CA	5.22	123.47	119.66

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	1242	0	1189	10	0
1	B	1255	0	1204	15	0
1	C	1243	0	1192	16	0
1	D	1242	0	1181	14	0
1	E	1245	0	1195	15	0
1	F	1250	0	1190	12	0
2	G	1522	0	1379	12	0
2	H	1455	0	1279	15	0
2	J	793	0	771	13	0
2	L	778	0	748	11	0
2	O	1470	0	1305	27	0
2	Q	1422	0	1224	18	0
3	I	1491	0	1273	19	0
3	K	887	0	766	8	0
3	M	853	0	716	16	0
3	N	1544	0	1380	18	0
3	P	1474	0	1229	15	0
3	R	1427	0	1124	13	0
All	All	22593	0	20345	236	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 6.

All (236) 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:G:108:ARG:NH2	2:G:170:ASP:OD1	2.25	0.70
3:N:83:LEU:HB3	3:N:86:LEU:HD21	1.72	0.69
2:J:25:ALA:O	2:J:70:THR:OG1	2.11	0.68
2:Q:31:SER:O	2:Q:52:THR:OG1	2.10	0.68
3:I:11:LEU:HD22	3:I:155:PRO:HG3	1.76	0.68
3:M:51:ILE:HD11	3:M:70:LEU:HB3	1.77	0.66
2:J:19:ILE:HD13	2:J:79:MET:HB2	1.78	0.66
1:A:296:LEU:HD21	1:A:307:ILE:HD12	1.78	0.65
2:O:19:ILE:HD13	2:O:79:MET:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:48:ILE:HD13	3:K:81:MET:HE1	1.78	0.64
2:J:31:SER:O	2:J:52:THR:OG1	2.13	0.64
2:L:31:SER:O	2:L:52:THR:OG1	2.15	0.63
1:D:336:GLN:HG2	3:N:103:ILE:HD13	1.81	0.62
3:K:51:ILE:HG21	3:K:72:VAL:HG21	1.81	0.62
2:O:117:ILE:HD12	2:O:209:PHE:HD1	1.65	0.62
3:R:34:MET:HE1	3:R:96:CYS:HB2	1.82	0.62
3:N:146:LEU:HD13	3:N:201:ILE:HG21	1.80	0.62
2:L:91:GLN:NE2	2:L:95:ILE:O	2.33	0.61
3:P:156:GLU:HG2	3:P:157:PRO:HA	1.81	0.61
3:P:12:VAL:HG21	3:P:86:LEU:HD13	1.82	0.61
3:R:127:PRO:HB3	3:R:153:TYR:HB3	1.83	0.61
2:L:19:ILE:HD13	2:L:79:MET:HB2	1.82	0.61
3:R:93:VAL:HG22	3:R:116:THR:HG22	1.83	0.60
3:M:33:THR:HG22	3:M:52:ASN:HD22	1.66	0.60
1:F:419:GLU:OE2	1:F:427:ARG:NH1	2.32	0.60
3:K:38:LYS:HB2	3:K:48:ILE:HD11	1.83	0.60
2:H:19:ILE:HD13	2:H:79:MET:HB2	1.83	0.59
2:H:51:ARG:HB2	2:H:54:LYS:HD2	1.85	0.59
3:I:152:GLY:HA2	3:I:182:LEU:HD22	1.84	0.59
1:E:338:ASN:ND2	3:M:101:TYR:O	2.36	0.58
1:E:419:GLU:OE1	1:E:427:ARG:NH1	2.27	0.58
2:H:170:ASP:OD1	2:H:172:THR:OG1	2.19	0.57
3:N:51:ILE:HD11	3:N:70:LEU:HB3	1.87	0.57
1:C:417:TRP:CZ2	1:C:429:ARG:HG2	2.40	0.56
2:O:25:ALA:O	2:O:70:THR:HG23	2.04	0.56
3:M:48:ILE:HG23	3:M:64:PHE:CG	2.40	0.56
2:O:11:MET:HE3	2:O:104:LEU:HD13	1.87	0.56
2:J:37:TYR:HE1	2:J:90:GLN:HB3	1.69	0.56
2:O:51:ARG:HB2	2:O:54:LYS:HD2	1.87	0.56
1:C:296:LEU:HD21	1:C:307:ILE:HD12	1.88	0.56
2:O:35:HIS:CD2	3:P:107:TYR:HB3	2.41	0.55
1:D:451:PRO:HG3	1:E:344:VAL:HG21	1.89	0.55
2:G:31:SER:O	2:G:52:THR:OG1	2.21	0.55
2:Q:50:TYR:O	2:Q:54:LYS:HB2	2.06	0.55
1:D:324:VAL:HG13	1:D:368:LEU:HD23	1.89	0.55
2:O:110:ASP:HA	2:O:140:TYR:HB3	1.88	0.55
1:B:414:LYS:HD3	1:B:430:VAL:HG12	1.89	0.55
2:Q:55:LEU:HD23	2:Q:59:VAL:HG23	1.89	0.55
1:C:324:VAL:HG22	1:C:368:LEU:HD22	1.88	0.55
3:M:51:ILE:HD13	3:M:72:VAL:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:29:ILE:HD11	2:G:34:LEU:HD23	1.89	0.54
1:C:338:ASN:HB2	3:I:103:ILE:HG22	1.88	0.54
1:C:419:GLU:OE1	2:J:30:SER:OG	2.20	0.54
3:I:23:LYS:HB2	3:I:78:THR:HG22	1.89	0.54
2:L:29:ILE:HD11	2:L:34:LEU:HD23	1.88	0.54
1:E:321:ILE:HG22	1:E:336:GLN:HE21	1.73	0.54
3:N:156:GLU:OE1	3:N:157:PRO:HA	2.07	0.54
3:I:161:THR:HG23	3:I:204:ASN:HB2	1.90	0.53
2:O:34:LEU:HG	2:O:72:TYR:CD2	2.44	0.53
2:H:31:SER:O	2:H:52:THR:OG1	2.21	0.53
1:A:416:LEU:HA	1:A:429:ARG:O	2.08	0.53
1:D:419:GLU:OE1	2:L:30:SER:OG	2.22	0.52
1:F:414:LYS:HD3	1:F:430:VAL:HG12	1.90	0.52
3:I:4:LEU:HD11	3:I:98:ILE:HG23	1.91	0.52
3:R:97:ALA:HB1	3:R:108:PHE:HB3	1.91	0.52
3:N:164:SER:HA	3:N:204:ASN:HD21	1.74	0.52
2:G:81:ALA:O	2:G:84:VAL:HG23	2.09	0.52
2:Q:35:HIS:CD2	3:R:107:TYR:HB3	2.44	0.52
1:B:419:GLU:OE2	2:H:30:SER:OG	2.23	0.51
3:N:29:PHE:HD2	3:N:31:GLY:H	1.59	0.51
2:Q:19:ILE:HD13	2:Q:79:MET:HB2	1.92	0.51
2:Q:167:ASP:HB3	2:Q:171:SER:N	2.25	0.51
3:P:202:THR:HA	3:P:217:LYS:HA	1.92	0.50
1:C:419:GLU:OE2	1:C:427:ARG:NH1	2.39	0.50
3:I:51:ILE:HD11	3:I:70:LEU:HB3	1.92	0.50
2:J:30:SER:HB3	2:J:33:TYR:HD2	1.76	0.50
1:B:403:LEU:HD13	1:B:438:HIS:CE1	2.46	0.50
2:L:20:ILE:HG12	2:L:75:THR:HG23	1.93	0.50
2:G:32:ASN:HB3	3:N:105:TYR:CD1	2.47	0.50
3:M:33:THR:OG1	3:M:99:HIS:HB2	2.11	0.50
2:Q:167:ASP:HB3	2:Q:171:SER:H	1.76	0.49
2:G:115:VAL:HB	2:G:207:LYS:HG3	1.94	0.49
1:A:451:PRO:HG3	1:B:344:VAL:HG21	1.94	0.49
1:C:414:LYS:HD3	1:C:430:VAL:HG12	1.94	0.49
1:D:414:LYS:HD3	1:D:430:VAL:HG12	1.95	0.49
3:I:29:PHE:HD2	3:I:31:GLY:H	1.60	0.49
3:N:12:VAL:HG23	3:N:119:VAL:HG22	1.94	0.49
3:N:160:LEU:CD1	3:N:205:VAL:HG22	2.43	0.48
1:E:322:GLY:O	1:E:336:GLN:HG3	2.12	0.48
3:N:202:THR:HA	3:N:217:LYS:HA	1.95	0.48
1:F:437:THR:HG23	3:I:85:SER:OG	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:32:ASN:HB3	3:M:105:TYR:CD1	2.49	0.48
1:F:437:THR:HG21	3:I:87:THR:CG2	2.43	0.48
2:H:139:PHE:HB2	2:H:198:HIS:CE1	2.49	0.48
2:O:31:SER:O	2:O:52:THR:OG1	2.24	0.48
3:R:154:PHE:CB	3:R:155:PRO:HD3	2.43	0.48
1:C:336:GLN:HG2	3:I:103:ILE:HG12	1.96	0.48
2:H:156:GLN:O	2:H:159:VAL:HG22	2.14	0.47
2:Q:161:ASN:HB3	2:Q:175:MET:HE2	1.96	0.47
2:J:51:ARG:HD2	3:K:105:TYR:CD2	2.50	0.47
1:A:394:TYR:CZ	1:A:451:PRO:HD3	2.49	0.47
3:N:97:ALA:HB1	3:N:108:PHE:HB3	1.97	0.47
3:P:52:ASN:HB3	3:P:55:ASN:HB2	1.96	0.47
1:B:417:TRP:CZ2	1:B:429:ARG:HG2	2.50	0.47
2:O:11:MET:HE1	2:O:19:ILE:HG23	1.95	0.47
2:G:124:GLN:O	2:G:127:SER:OG	2.31	0.47
2:J:35:HIS:CG	3:K:107:TYR:HB3	2.49	0.47
3:P:127:PRO:HD3	3:P:207:HIS:ND1	2.30	0.47
2:O:35:HIS:CG	3:P:107:TYR:HB3	2.50	0.47
2:Q:131:SER:HA	2:Q:180:THR:HA	1.96	0.47
1:D:368:LEU:HD12	1:D:426:LEU:HD23	1.97	0.46
1:E:416:LEU:HD13	1:E:430:VAL:HG22	1.95	0.46
2:H:35:HIS:CD2	3:I:107:TYR:HB3	2.50	0.46
2:H:113:PRO:HB3	2:H:139:PHE:HB3	1.96	0.46
3:I:83:LEU:HB3	3:I:86:LEU:HD21	1.98	0.46
3:P:192:THR:O	3:P:195:THR:OG1	2.34	0.46
1:C:393:THR:O	1:C:393:THR:HG22	2.15	0.46
1:F:341:ILE:HG12	1:F:350:ILE:HD13	1.97	0.46
1:F:417:TRP:CZ2	1:F:429:ARG:HG2	2.51	0.46
1:B:316:ARG:HB3	1:B:343:ILE:HB	1.96	0.46
1:B:416:LEU:HD13	1:B:430:VAL:HG22	1.96	0.46
2:H:164:THR:HG22	2:H:174:SER:H	1.79	0.46
3:N:38:LYS:HB2	3:N:48:ILE:HD11	1.97	0.46
2:O:167:ASP:HB3	2:O:171:SER:N	2.31	0.46
3:M:4:LEU:HD11	3:M:98:ILE:HG23	1.96	0.46
1:F:324:VAL:HG12	1:F:368:LEU:HD22	1.98	0.46
2:Q:182:THR:HG23	2:Q:185:GLU:H	1.79	0.46
1:B:339:SER:OG	1:B:352:LEU:HD23	2.16	0.46
1:D:295:ASN:OD1	1:D:295:ASN:N	2.48	0.46
1:E:419:GLU:OE2	2:O:30:SER:OG	2.22	0.46
2:O:190:ASN:O	2:O:210:ASN:HA	2.16	0.46
1:D:393:THR:HG22	1:D:393:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:LEU:HA	1:D:429:ARG:O	2.15	0.46
2:G:144:ILE:HG12	2:G:198:HIS:HD2	1.80	0.46
2:L:51:ARG:HB2	2:L:54:LYS:HD2	1.98	0.46
2:G:52:THR:O	2:G:65:GLY:HA3	2.17	0.45
1:B:416:LEU:HA	1:B:429:ARG:O	2.16	0.45
2:O:32:ASN:HB3	3:P:105:TYR:CD1	2.52	0.45
3:P:12:VAL:HG23	3:P:119:VAL:HG22	1.98	0.45
1:E:336:GLN:OE1	3:M:31:GLY:HA3	2.16	0.45
2:O:167:ASP:HB3	2:O:171:SER:H	1.81	0.45
1:A:344:VAL:HG21	1:C:451:PRO:HG3	1.99	0.45
1:E:338:ASN:HB2	3:M:103:ILE:HG22	1.99	0.45
3:I:179:GLN:O	3:I:180:SER:C	2.60	0.45
3:M:76:SER:HB2	3:M:78:THR:HG22	1.97	0.45
2:O:120:PRO:HD3	2:O:132:VAL:HG22	1.99	0.45
3:R:58:PRO:HB2	3:R:60:TYR:CE1	2.51	0.45
1:A:401:ILE:HD12	1:A:414:LYS:HG3	1.98	0.45
1:F:394:TYR:CZ	1:F:451:PRO:HD3	2.51	0.45
2:G:37:TYR:HE1	2:G:90:GLN:HB3	1.82	0.45
2:H:167:ASP:HB3	2:H:171:SER:H	1.81	0.45
1:C:394:TYR:CZ	1:C:451:PRO:HD3	2.52	0.44
2:J:91:GLN:OE1	2:J:93:SER:N	2.50	0.44
3:N:4:LEU:HD11	3:N:98:ILE:HG23	1.99	0.44
3:R:57:GLY:HA2	3:R:58:PRO:HD3	1.85	0.44
3:M:39:GLN:HG2	3:M:43:LYS:HA	2.00	0.44
2:O:29:ILE:HD11	2:O:34:LEU:HD23	1.99	0.44
3:P:127:PRO:HB3	3:P:153:TYR:HB3	1.98	0.44
1:A:341:ILE:HG12	1:A:350:ILE:HD13	1.99	0.44
3:N:51:ILE:HD13	3:N:72:VAL:HG23	2.00	0.44
1:D:394:TYR:CZ	1:D:451:PRO:HD3	2.52	0.44
2:Q:35:HIS:CG	3:R:107:TYR:HB3	2.53	0.44
1:C:416:LEU:HA	1:C:429:ARG:O	2.18	0.44
1:D:338:ASN:HB2	3:N:103:ILE:HG22	2.00	0.44
2:Q:23:CYS:HB2	2:Q:36:TRP:CH2	2.52	0.44
2:O:60:PRO:HG2	2:O:63:PHE:CD1	2.52	0.44
3:R:47:TRP:CZ2	3:R:50:LEU:HD23	2.53	0.44
2:J:11:MET:HE3	2:J:11:MET:HB2	1.85	0.44
2:Q:91:GLN:NE2	2:Q:95:ILE:O	2.51	0.44
1:F:416:LEU:HA	1:F:429:ARG:O	2.18	0.43
3:M:52:ASN:HB3	3:M:55:ASN:HB2	2.00	0.43
2:H:29:ILE:HD11	2:H:34:LEU:HD23	2.00	0.43
1:B:385:PRO:O	1:B:453:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:32:ASN:HB3	3:K:105:TYR:CD1	2.53	0.43
1:B:451:PRO:HG3	1:C:344:VAL:HG21	2.00	0.43
3:N:100:TYR:O	3:N:101:TYR:HB2	2.19	0.43
3:R:205:VAL:H	3:R:214:VAL:HG12	1.83	0.43
2:O:133:VAL:HG23	2:O:178:THR:HG22	2.00	0.43
1:E:414:LYS:NZ	1:E:432:GLY:O	2.38	0.43
2:Q:4:LEU:HB2	2:Q:99:GLY:HA2	1.99	0.43
2:O:32:ASN:O	3:P:105:TYR:HB3	2.19	0.43
1:C:416:LEU:HD12	1:C:430:VAL:HG22	2.01	0.42
1:E:414:LYS:HD3	1:E:430:VAL:HG12	2.01	0.42
3:R:39:GLN:HA	3:R:44:ASN:O	2.19	0.42
1:A:319:MET:SD	1:A:321:ILE:HD11	2.60	0.42
1:D:414:LYS:NZ	1:D:432:GLY:O	2.40	0.42
2:G:60:PRO:HG2	2:G:63:PHE:CE1	2.54	0.42
3:P:48:ILE:HG23	3:P:64:PHE:CG	2.54	0.42
1:D:298:TYR:CD1	1:D:299:PRO:HA	2.54	0.42
3:P:39:GLN:O	3:P:92:ALA:HB1	2.19	0.42
1:A:416:LEU:HD12	1:A:430:VAL:HG22	2.01	0.42
1:A:417:TRP:CZ2	1:A:429:ARG:HG2	2.55	0.42
3:I:152:GLY:CA	3:I:182:LEU:HD22	2.48	0.42
3:K:33:THR:OG1	3:K:99:HIS:HB2	2.19	0.42
3:I:51:ILE:HD13	3:I:72:VAL:HG23	2.01	0.42
1:E:417:TRP:CZ2	1:E:429:ARG:HG2	2.55	0.42
3:I:52:ASN:HB3	3:I:55:ASN:HB3	2.02	0.42
3:M:97:ALA:HB1	3:M:108:PHE:HB3	2.00	0.42
2:Q:60:PRO:HG2	2:Q:63:PHE:CD1	2.54	0.42
1:E:324:VAL:HG22	1:E:368:LEU:HD22	2.01	0.42
2:H:106:ILE:O	2:H:166:GLN:NE2	2.52	0.42
2:O:96:TYR:HD2	3:P:47:TRP:CD1	2.38	0.42
2:L:34:LEU:HG	2:L:72:TYR:CG	2.54	0.42
1:E:385:PRO:O	1:E:453:SER:HB2	2.20	0.41
1:F:293:SER:HB2	1:F:294:PRO:HD3	2.01	0.41
2:O:210:ASN:O	2:O:211:ARG:NE	2.49	0.41
3:R:51:ILE:HG21	3:R:72:VAL:HG21	2.02	0.41
1:D:316:ARG:HB3	1:D:343:ILE:HB	2.02	0.41
2:G:144:ILE:HG12	2:G:198:HIS:CD2	2.56	0.41
2:Q:37:TYR:HE1	2:Q:90:GLN:HB3	1.85	0.41
1:B:358:PHE:HA	1:B:440:ASN:HA	2.01	0.41
1:E:394:TYR:CZ	1:E:451:PRO:HD3	2.56	0.41
3:M:48:ILE:HG23	3:M:64:PHE:CB	2.49	0.41
2:Q:151:ASP:N	2:Q:191:SER:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:50:TYR:O	2:O:54:LYS:HB2	2.21	0.41
2:O:56:ALA:O	2:O:59:VAL:HG22	2.20	0.41
2:J:3:VAL:HG22	2:J:26:SER:HB3	2.02	0.41
2:L:34:LEU:HD22	2:L:34:LEU:HA	1.94	0.41
1:C:385:PRO:O	1:C:453:SER:HB2	2.20	0.41
1:F:442:LYS:HE3	1:F:442:LYS:HB3	1.89	0.41
3:I:176:ALA:HA	3:I:184:THR:O	2.21	0.41
3:N:146:LEU:HD11	3:N:196:TRP:CG	2.56	0.41
3:K:29:PHE:HD2	3:K:31:GLY:H	1.67	0.41
2:O:55:LEU:HD11	2:O:63:PHE:O	2.21	0.41
2:O:140:TYR:CD1	2:O:141:PRO:HA	2.56	0.41
1:B:369:ASN:OD1	1:B:371:VAL:HG22	2.21	0.40
1:B:394:TYR:CE1	1:B:450:TYR:HA	2.56	0.40
2:H:37:TYR:HE1	2:H:90:GLN:HB3	1.86	0.40
3:M:100:TYR:HB3	3:M:109:ASP:OD2	2.22	0.40
1:B:347:TYR:OH	1:C:344:VAL:HB	2.22	0.40
3:I:60:TYR:HE1	3:I:70:LEU:HD13	1.87	0.40
2:J:29:ILE:HD11	2:J:34:LEU:HD23	2.03	0.40
2:Q:109:ALA:O	2:Q:140:TYR:HB3	2.21	0.40
1:F:358:PHE:HA	1:F:440:ASN:HA	2.03	0.40
2:H:198:HIS:CD2	2:H:199:LYS:H	2.40	0.40
2:L:50:TYR:O	2:L:54:LYS:HB2	2.22	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	A	160/165 (97%)	157 (98%)	3 (2%)	0	100	100
1	B	161/165 (98%)	158 (98%)	3 (2%)	0	100	100
1	C	160/165 (97%)	156 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	161/165 (98%)	157 (98%)	4 (2%)	0	100	100
1	E	160/165 (97%)	157 (98%)	3 (2%)	0	100	100
1	F	161/165 (98%)	157 (98%)	4 (2%)	0	100	100
2	G	209/214 (98%)	206 (99%)	3 (1%)	0	100	100
2	H	197/214 (92%)	193 (98%)	4 (2%)	0	100	100
2	J	106/214 (50%)	103 (97%)	3 (3%)	0	100	100
2	L	105/214 (49%)	102 (97%)	3 (3%)	0	100	100
2	O	206/214 (96%)	201 (98%)	5 (2%)	0	100	100
2	Q	208/214 (97%)	202 (97%)	6 (3%)	0	100	100
3	I	209/219 (95%)	204 (98%)	5 (2%)	0	100	100
3	K	118/219 (54%)	116 (98%)	2 (2%)	0	100	100
3	M	117/219 (53%)	113 (97%)	4 (3%)	0	100	100
3	N	210/219 (96%)	208 (99%)	2 (1%)	0	100	100
3	P	209/219 (95%)	204 (98%)	5 (2%)	0	100	100
3	R	207/219 (94%)	202 (98%)	5 (2%)	0	100	100
All	All	3064/3588 (85%)	2996 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	134/138 (97%)	134 (100%)	0	100	100
1	B	137/138 (99%)	137 (100%)	0	100	100
1	C	134/138 (97%)	134 (100%)	0	100	100
1	D	133/138 (96%)	133 (100%)	0	100	100
1	E	134/138 (97%)	134 (100%)	0	100	100
1	F	135/138 (98%)	135 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	156/187 (83%)	156 (100%)	0	100	100
2	H	140/187 (75%)	140 (100%)	0	100	100
2	J	85/187 (46%)	84 (99%)	1 (1%)	63	82
2	L	84/187 (45%)	84 (100%)	0	100	100
2	O	143/187 (76%)	143 (100%)	0	100	100
2	Q	131/187 (70%)	131 (100%)	0	100	100
3	I	136/188 (72%)	136 (100%)	0	100	100
3	K	85/188 (45%)	85 (100%)	0	100	100
3	M	76/188 (40%)	76 (100%)	0	100	100
3	N	151/188 (80%)	151 (100%)	0	100	100
3	P	135/188 (72%)	135 (100%)	0	100	100
3	R	114/188 (61%)	114 (100%)	0	100	100
All	All	2243/3078 (73%)	2242 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	82	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	312	ASN
1	A	397	GLN
1	B	332	ASN
1	B	422	GLN
1	C	295	ASN
1	C	397	GLN
1	E	336	GLN
1	F	388	HIS
1	F	397	GLN
2	G	137	ASN
2	H	38	GLN
3	K	63	ASN
2	L	38	GLN
2	O	38	GLN

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	162/165 (98%)	-0.45	0 100 100	29, 43, 81, 116	0
1	B	163/165 (98%)	-0.40	1 (0%) 85 69	29, 44, 82, 117	0
1	C	162/165 (98%)	-0.45	0 100 100	26, 43, 78, 130	0
1	D	163/165 (98%)	-0.36	1 (0%) 85 69	29, 46, 92, 134	0
1	E	162/165 (98%)	-0.34	2 (1%) 76 55	32, 48, 97, 136	0
1	F	163/165 (98%)	-0.23	1 (0%) 85 69	35, 56, 98, 134	0
2	G	211/214 (98%)	0.33	16 (7%) 20 10	40, 75, 131, 156	0
2	H	205/214 (95%)	0.34	17 (8%) 17 9	35, 71, 141, 170	0
2	J	108/214 (50%)	-0.40	0 100 100	36, 49, 77, 101	0
2	L	107/214 (50%)	-0.40	0 100 100	36, 49, 73, 81	0
2	O	210/214 (98%)	0.42	17 (8%) 18 9	43, 77, 154, 197	0
2	Q	210/214 (98%)	0.38	14 (6%) 24 12	34, 79, 163, 181	0
3	I	213/219 (97%)	0.49	24 (11%) 10 6	32, 73, 142, 175	0
3	K	122/219 (55%)	0.18	0 100 100	41, 78, 115, 128	0
3	M	119/219 (54%)	0.30	3 (2%) 58 35	45, 84, 114, 139	0
3	N	214/219 (97%)	0.17	5 (2%) 61 38	39, 74, 120, 145	0
3	P	213/219 (97%)	0.49	10 (4%) 36 19	51, 107, 142, 167	0
3	R	213/219 (97%)	0.73	24 (11%) 10 6	40, 101, 166, 182	0
All	All	3120/3588 (86%)	0.10	135 (4%) 40 21	26, 63, 140, 197	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	150	VAL	6.5
3	R	186	SER	4.4
2	H	131	SER	4.2

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Mol	Chain	Res	Type	RSRZ
2	Q	163	TRP	4.1
3	M	75	SER	4.0
3	P	41	HIS	3.9
2	H	180	THR	3.9
2	H	143	ASP	3.8
2	O	208	SER	3.6
3	I	186	SER	3.6
2	H	128	GLY	3.6
3	R	148	CYS	3.6
3	R	215	ASP	3.6
3	I	132	LEU	3.5
2	O	184	ASP	3.5
3	R	168	SER	3.5
3	P	135	VAL	3.4
3	I	168	SER	3.3
3	I	157	PRO	3.3
3	I	151	LYS	3.3
3	R	206	ALA	3.2
3	I	185	LEU	3.2
2	O	205	ILE	3.2
2	Q	122	SER	3.2
2	G	178	THR	3.2
3	P	55	ASN	3.2
3	R	169	SER	3.1
3	R	135	VAL	3.0
3	R	204	ASN	3.0
2	G	203	SER	3.0
3	P	56	ASP	3.0
2	G	122	SER	2.9
3	I	145	THR	2.9
2	O	110	ASP	2.9
3	R	178	LEU	2.9
2	G	134	CYS	2.9
2	O	163	TRP	2.9
2	G	200	THR	2.9
2	O	1	GLU	2.9
2	G	131	SER	2.8
3	I	166	SER	2.8
3	P	53	PRO	2.8
2	H	126	THR	2.8
2	Q	132	VAL	2.8
3	P	186	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	R	185	LEU	2.7
3	R	173	THR	2.7
2	Q	148	TRP	2.7
3	N	150	VAL	2.7
2	G	184	ASP	2.7
3	R	217	LYS	2.6
3	R	203	CYS	2.6
3	I	56	ASP	2.6
2	Q	184	ASP	2.6
2	Q	151	ASP	2.5
2	H	195	GLU	2.5
2	G	127	SER	2.5
2	H	122	SER	2.5
2	H	127	SER	2.5
3	R	179	GLN	2.5
3	R	180	SER	2.5
3	I	194	ASN	2.5
2	O	186	TYR	2.5
3	I	149	LEU	2.5
3	R	218	ILE	2.5
2	Q	145	ASN	2.5
3	R	192	THR	2.5
3	M	74	LYS	2.5
2	H	138	ASN	2.4
2	O	193	THR	2.4
2	Q	182	THR	2.4
3	I	196	TRP	2.4
3	I	187	SER	2.4
2	O	189	HIS	2.4
2	H	187	GLU	2.4
2	G	117	ILE	2.4
3	R	156	GLU	2.4
2	G	146	VAL	2.4
3	R	131	PRO	2.4
2	H	184	ASP	2.4
2	H	203	SER	2.4
1	D	455	THR	2.3
3	I	140	THR	2.3
3	M	56	ASP	2.3
3	I	129	VAL	2.3
3	I	133	VAL	2.3
3	N	133	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	R	158	VAL	2.3
3	P	192	THR	2.3
2	G	190	ASN	2.3
3	N	218	ILE	2.3
2	H	130	ALA	2.3
2	Q	1	GLU	2.3
1	E	305	GLY	2.3
2	Q	177	SER	2.3
3	N	166	SER	2.3
2	O	161	ASN	2.3
2	Q	189	HIS	2.2
2	O	116	SER	2.2
3	I	148	CYS	2.2
1	F	305	GLY	2.2
3	I	184	THR	2.2
3	R	54	TYR	2.2
2	G	115	VAL	2.2
2	O	194	CYS	2.2
2	G	109	ALA	2.2
3	P	42	GLY	2.2
3	I	158	VAL	2.2
3	R	194	ASN	2.2
3	P	178	LEU	2.2
2	H	163	TRP	2.2
2	Q	202	THR	2.2
3	R	184	THR	2.2
2	O	133	VAL	2.2
2	H	162	SER	2.2
2	O	111	ALA	2.2
2	O	190	ASN	2.2
2	Q	190	ASN	2.2
1	E	294	PRO	2.2
3	N	197	PRO	2.2
3	R	205	VAL	2.1
1	B	410	GLN	2.1
2	O	196	ALA	2.1
2	O	195	GLU	2.1
3	I	198	SER	2.1
3	I	156	GLU	2.1
3	I	170	GLY	2.1
2	G	145	ASN	2.1
2	G	197	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	P	158	VAL	2.0
3	I	52	ASN	2.0
2	G	156	GLN	2.0
2	H	1	GLU	2.0
2	H	185	GLU	2.0
2	Q	133	VAL	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.