Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 02:00 PM EDT

PDB ID	:	6WMW
Title	:	GFRAL receptor bound with two antibody Fabs (3P10, 25M22)
Authors	:	White, A.; Lakshminarasimhan, D.; Olland, A.; Suto, R.K.
Deposited on	:	2020-04-21
Resolution	:	2.91 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 2.91 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	Percentile Ranks	Value
Rfree		0.288
Clashscore		9
Ramachandran outliers		1.0%
Sidechain outliers		11.2%
RSRZ outliers		2.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
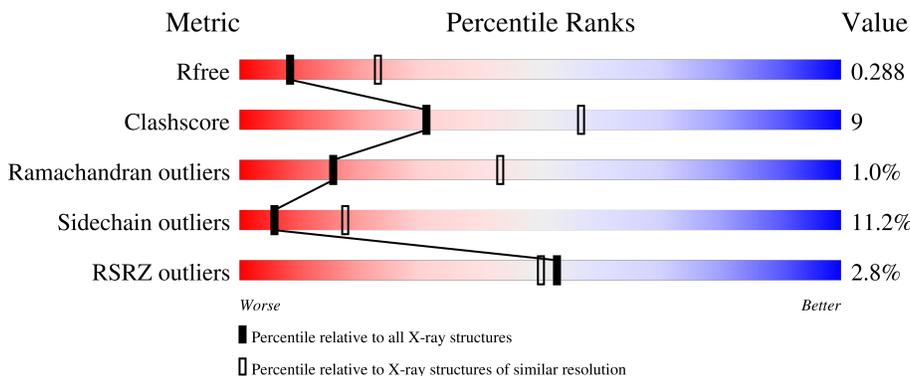
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	B	245	63% 12% · 22%
2	H	225	3% 68% 23% · 6%
3	L	218	2% 67% 29% ·
4	M	232	4% 75% 19% · ·
5	N	241	3% 63% 23% · 10%
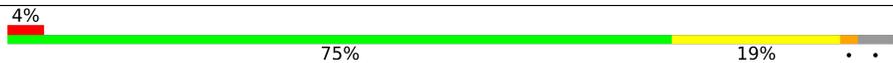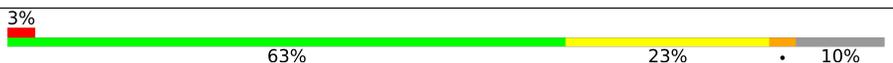
2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8097 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 GDNF family receptor alpha-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	192	Total	C	N	O	S	0	0	0
			1496	921	266	284	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	107	HIS	-	expression tag	UNP Q6UXV0
B	108	HIS	-	expression tag	UNP Q6UXV0
B	109	HIS	-	expression tag	UNP Q6UXV0
B	110	HIS	-	expression tag	UNP Q6UXV0
B	111	HIS	-	expression tag	UNP Q6UXV0
B	112	HIS	-	expression tag	UNP Q6UXV0
B	113	GLY	-	expression tag	UNP Q6UXV0
B	114	GLY	-	expression tag	UNP Q6UXV0

- Molecule 2 is a protein called FAB3P10 heavy chain fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total	C	N	O	S	0	0	0
			1592	1015	258	314	5			

- Molecule 3 is a protein called FAB3P10 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	218	Total	C	N	O	S	0	0	0
			1660	1040	278	334	8			

- Molecule 4 is a protein called FAB25M22 heavy chain fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	222	Total	C	N	O	S	0	0	0
			1671	1060	279	325	7			

• Molecule 5 is a protein called FAB25M22 light chain.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	N	216	1678	1062	275	337	4	0	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: GDNF family receptor alpha-like
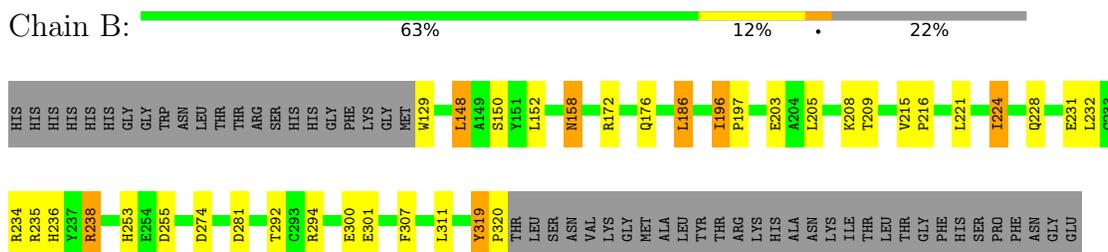
• Molecule 2: FAB3P10 heavy chain fragment
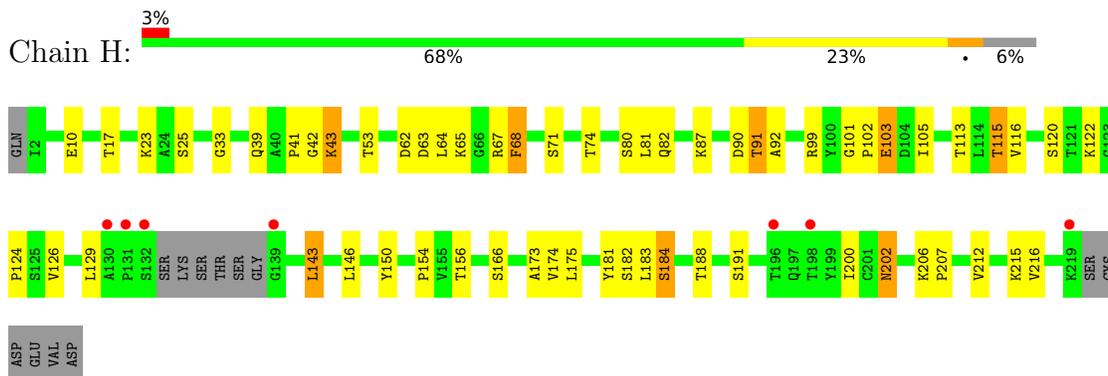
• Molecule 3: FAB3P10 light chain
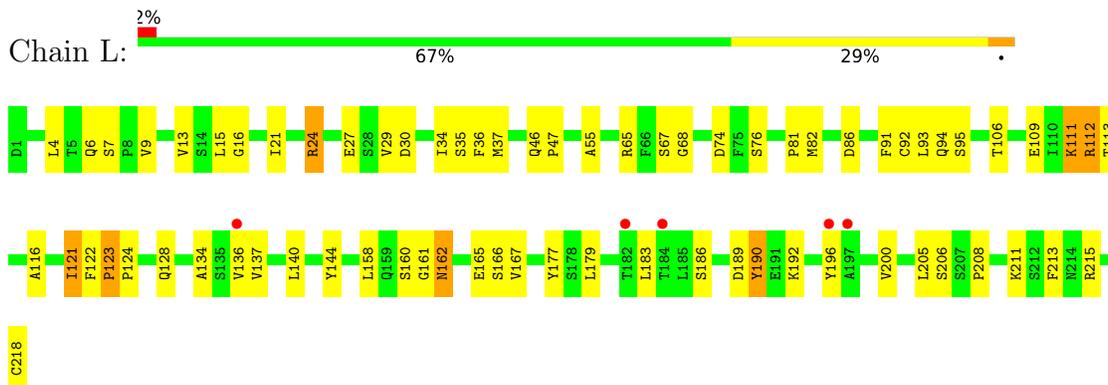
• Molecule 4: FAB25M22 heavy chain fragment

Chain M:

4%

75%　19%

Q1 D10 L11 V12 K13 P14 G15 S21 W36 M37 P41 W47 I48 G49 K65 T71 S77 M81 Q82 L83 T87 S88 R98 L104 R105 R106 T107 M112 S120 V123 S124 S125 A126 S127 P131 P135 L136 A137 P138 S139 SER LYS SER

T143 S144 G145 A148 A149 L150 L153 Y157 P161 V162 T163 A180 G186 L190 V196 P197 S198 S199 S200 T203 Q204 T205 Y206 I207 C208 K213 P214 V223 E224 P225 LYS SER CYS ASP GLU VAL ASP
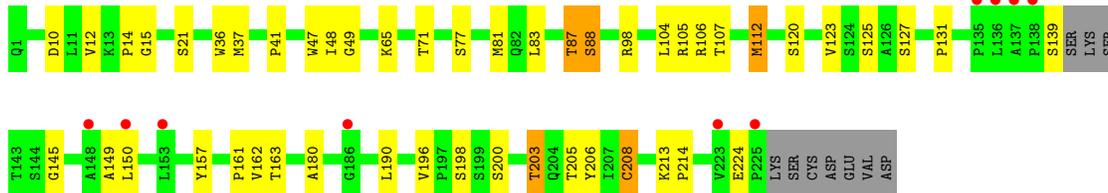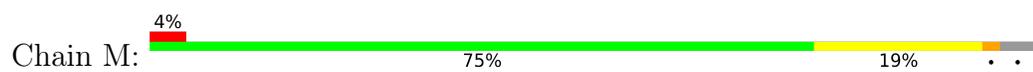
• Molecule 5: FAB25M22 light chain

Chain N:

3%

63%　23%　10%

MET ASP MET ARG VAL PRO ALA GLN LEU LEU GLY LEU LEU LEU LEU TRP LEU ARG GLY ALA ARG CYS D23 T27 Q28 L33 N36 Q40 A41 S42 I43 S44 S50 N53 S54 D55 L60 D61 W62 Y63 L64 Q65 K66 L74 I75 S83 R88 S94 G95

T96 D97 F98 E108 D109 F116 Q117 S118 Y123 T124 F125 T129 K134 R135 S141 V142 F143 I144 F145 P146 P147 S148 D149 G155 T156 A157 S158 V159 V160 C161 L162 L163 E170 W175 N185 E192 Q193 D197 S198 T199 L202 S203 L206 T207 L208 S209

K210 A211 D212 Y213 E214 Y219 A220 T224 H225 Q226 G227 L228 P231 V232 T233 F236 N237 R238 GLY GLU CYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.50Å 116.05Å 227.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.70 – 2.91 47.65 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.70-2.91) 99.3 (47.65-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.222 , 0.290 0.225 , 0.288	Depositor DCC
R_{free} test set	1591 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	64.6	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 29.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8097	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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	B	0.44	0/1523	0.67	0/2060
2	H	0.45	0/1633	0.69	0/2230
3	L	0.50	0/1698	0.70	0/2303
4	M	0.43	0/1713	0.67	0/2331
5	N	0.43	0/1715	0.65	0/2329
All	All	0.45	0/8282	0.68	0/11253

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	112	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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1496	0	1434	22	0
2	H	1592	0	1548	33	0
3	L	1660	0	1596	39	0
4	M	1671	0	1642	24	0
5	N	1678	0	1633	36	0
All	All	8097	0	7853	145	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (145) 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:M:104:LEU:O	4:M:105:ARG:HD3	1.69	0.92
4:M:87:THR:O	4:M:123:VAL:HG21	1.77	0.83
2:H:67:ARG:NH1	2:H:90:ASP:OD2	2.13	0.81
5:N:214:GLU:HG2	5:N:238:ARG:HH11	1.50	0.76
5:N:214:GLU:HG2	5:N:238:ARG:NH1	2.01	0.76
1:B:232:LEU:O	1:B:236:HIS:ND1	2.18	0.76
2:H:87:LYS:O	2:H:116:VAL:HG11	1.86	0.75
5:N:135:ARG:NH1	5:N:197:ASP:O	2.20	0.73
3:L:30:ASP:OD1	3:L:35:SER:OG	2.04	0.72
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.72	0.70
3:L:21:ILE:HD12	3:L:106:THR:HG21	1.74	0.69
1:B:224:ILE:HD12	1:B:311:LEU:HD11	1.75	0.69
4:M:48:ILE:HG21	4:M:81:MET:HE2	1.76	0.68
2:H:91:THR:HG23	2:H:115:THR:HA	1.77	0.67
2:H:129:LEU:HD23	3:L:122:PHE:CG	2.30	0.66
5:N:94:SER:O	5:N:96:THR:N	2.29	0.65
1:B:319:TYR:HB3	1:B:320:PRO:CD	2.27	0.64
2:H:143:LEU:HD13	2:H:216:VAL:HG11	1.79	0.64
3:L:121:ILE:HG21	3:L:211:LYS:O	1.97	0.64
5:N:88:ARG:NH1	5:N:109:ASP:OD2	2.30	0.64
3:L:65:ARG:NH2	3:L:86:ASP:OD1	2.29	0.64
5:N:33:LEU:HD21	5:N:41:ALA:HB1	1.80	0.64
1:B:224:ILE:HD13	1:B:307:PHE:CD1	2.34	0.63
4:M:208:CYS:O	4:M:208:CYS:SG	2.56	0.63
4:M:98:ARG:O	4:M:112:MET:HA	2.00	0.62
1:B:203:GLU:OE2	4:M:106:ARG:HD3	2.01	0.60
4:M:36:TRP:HB3	4:M:81:MET:HE1	1.82	0.60
2:H:99:ARG:O	2:H:101:GLY:HA2	2.01	0.60
1:B:319:TYR:CB	1:B:320:PRO:CD	2.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:131:PRO:HB3	4:M:157:TYR:HB3	1.85	0.58
3:L:123:PRO:HB3	3:L:213:PHE:CE2	2.38	0.58
1:B:221:LEU:HD11	1:B:300:GLU:HB3	1.86	0.58
3:L:165:GLU:HB2	3:L:179:LEU:HD11	1.86	0.57
5:N:60:LEU:HD22	5:N:98:PHE:CG	2.39	0.57
4:M:104:LEU:O	4:M:105:ARG:CD	2.50	0.56
5:N:88:ARG:HH12	5:N:109:ASP:CG	2.08	0.56
2:H:43:LYS:O	2:H:43:LYS:HG3	2.06	0.56
1:B:319:TYR:CB	1:B:320:PRO:HD2	2.36	0.56
4:M:12:VAL:O	4:M:123:VAL:HA	2.07	0.55
2:H:200:ILE:HG13	2:H:215:LYS:HA	1.89	0.55
1:B:234:ARG:NH1	1:B:238:ARG:HH21	2.03	0.55
3:L:121:ILE:HG13	3:L:122:PHE:N	2.21	0.55
5:N:145:PHE:O	5:N:159:VAL:HG22	2.06	0.55
2:H:183:LEU:C	2:H:183:LEU:HD12	2.27	0.54
2:H:64:LEU:HG	2:H:68:PHE:CE1	2.43	0.54
2:H:33:GLY:HA2	2:H:53:THR:HG23	1.88	0.54
2:H:42:GLY:O	2:H:43:LYS:HG2	2.07	0.54
2:H:129:LEU:HD23	3:L:122:PHE:CD2	2.42	0.54
5:N:159:VAL:HG12	5:N:206:LEU:HB3	1.90	0.54
3:L:123:PRO:HB3	3:L:213:PHE:CZ	2.44	0.53
3:L:162:ASN:OD1	3:L:162:ASN:N	2.41	0.53
3:L:140:LEU:HD21	3:L:200:VAL:HG13	1.91	0.53
4:M:81:MET:SD	4:M:83:LEU:HD21	2.49	0.53
1:B:231:GLU:O	1:B:235:ARG:HG3	2.08	0.53
3:L:16:GLY:HA2	3:L:81:PRO:HB2	1.91	0.53
3:L:29:VAL:HG12	3:L:29:VAL:O	2.10	0.52
5:N:53:ASN:HB3	5:N:55:ASP:OD1	2.10	0.52
1:B:186:LEU:HD21	1:B:205:LEU:HD22	1.91	0.52
3:L:37:MET:SD	3:L:92:CYS:HB2	2.49	0.52
3:L:65:ARG:HD3	3:L:81:PRO:O	2.10	0.51
4:M:180:ALA:HA	4:M:190:LEU:HB3	1.93	0.51
1:B:172:ARG:CD	1:B:232:LEU:HD21	2.41	0.51
2:H:206:LYS:N	2:H:207:PRO:CD	2.74	0.51
4:M:112:MET:HG3	5:N:63:TYR:OH	2.10	0.50
4:M:149:ALA:HB3	5:N:143:PHE:CE2	2.46	0.50
1:B:196:ILE:N	1:B:197:PRO:HD2	2.26	0.50
4:M:213:LYS:N	4:M:214:PRO:CD	2.74	0.50
2:H:71:SER:OG	2:H:80:SER:HB2	2.11	0.50
5:N:118:SER:HA	5:N:123:TYR:CD1	2.47	0.49
5:N:147:PRO:HD3	5:N:159:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:LEU:HB3	3:L:122:PHE:CD2	2.49	0.48
5:N:155:GLY:O	5:N:210:LYS:HB2	2.14	0.48
5:N:62:TRP:HB2	5:N:75:ILE:HB	1.96	0.48
3:L:136:VAL:N	3:L:183:LEU:O	2.45	0.47
5:N:163:LEU:HD12	5:N:163:LEU:N	2.29	0.47
5:N:66:LYS:HD3	5:N:108:GLU:O	2.15	0.47
1:B:292:THR:HB	1:B:294:ARG:H	1.80	0.47
3:L:186:SER:OG	3:L:189:ASP:HB2	2.14	0.47
4:M:88:SER:HA	4:M:123:VAL:CG2	2.45	0.47
3:L:121:ILE:HD11	3:L:213:PHE:CD1	2.50	0.47
1:B:319:TYR:HB3	1:B:320:PRO:HD3	1.96	0.46
3:L:4:LEU:HA	3:L:24:ARG:O	2.15	0.46
3:L:196:TYR:HB2	3:L:213:PHE:CE1	2.51	0.46
1:B:172:ARG:HD3	1:B:232:LEU:HD21	1.97	0.46
5:N:64:LEU:HD12	5:N:65:GLN:N	2.31	0.46
5:N:161:CYS:HB2	5:N:175:TRP:CH2	2.51	0.46
2:H:173:ALA:HA	2:H:183:LEU:HB3	1.98	0.46
3:L:36:PHE:O	3:L:94:GLN:HA	2.16	0.46
1:B:319:TYR:HB3	1:B:320:PRO:HD2	1.95	0.45
2:H:39:GLN:O	2:H:92:ALA:HB1	2.16	0.45
3:L:55:ALA:O	3:L:68:GLY:HA3	2.15	0.45
2:H:202:ASN:H	2:H:202:ASN:HD22	1.65	0.45
1:B:292:THR:HG22	3:L:34:ILE:HD13	1.99	0.45
5:N:146:PRO:HA	5:N:159:VAL:HG23	1.98	0.45
4:M:47:TRP:CZ2	4:M:49:GLY:HA2	2.52	0.45
5:N:192:GLU:O	5:N:193:GLN:C	2.54	0.45
3:L:128:GLN:CB	3:L:134:ALA:HB2	2.46	0.45
5:N:135:ARG:NH1	5:N:199:THR:HG23	2.32	0.44
5:N:163:LEU:HD13	5:N:202:LEU:HB3	1.98	0.44
2:H:102:PRO:HB2	2:H:103:GLU:HG2	2.00	0.44
2:H:212:VAL:O	2:H:212:VAL:HG13	2.18	0.44
3:L:196:TYR:CB	3:L:213:PHE:CE1	3.01	0.44
4:M:196:VAL:HG11	4:M:206:TYR:CZ	2.53	0.44
2:H:175:LEU:HD13	2:H:181:TYR:CE1	2.53	0.44
4:M:190:LEU:N	4:M:190:LEU:HD23	2.33	0.44
5:N:36:ASN:OD1	5:N:134:LYS:HB3	2.18	0.44
5:N:28:GLN:HA	5:N:44:SER:O	2.18	0.43
5:N:214:GLU:CG	5:N:238:ARG:HH11	2.25	0.43
5:N:224:THR:HG23	5:N:231:PRO:HG3	2.00	0.43
1:B:301:GLU:HG3	2:H:102:PRO:HG3	1.99	0.43
3:L:167:VAL:HG22	3:L:179:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:161:CYS:HB2	5:N:175:TRP:CZ2	2.53	0.43
2:H:129:LEU:HD21	3:L:137:VAL:HG21	2.01	0.43
1:B:224:ILE:O	1:B:228:GLN:HG2	2.19	0.43
2:H:202:ASN:HD22	2:H:202:ASN:N	2.16	0.43
5:N:116:PHE:HB2	5:N:125:PHE:CD1	2.54	0.43
3:L:116:ALA:HB1	3:L:205:LEU:HG	2.01	0.43
4:M:200:SER:HA	4:M:203:THR:HG23	2.01	0.43
3:L:109:GLU:OE1	3:L:177:TYR:OH	2.34	0.42
3:L:111:LYS:HA	3:L:144:TYR:OH	2.19	0.42
5:N:202:LEU:HD23	5:N:203:SER:N	2.34	0.42
3:L:15:LEU:HD12	3:L:15:LEU:H	1.84	0.42
2:H:183:LEU:HD12	2:H:184:SER:N	2.34	0.42
1:B:148:LEU:HD22	1:B:152:LEU:CD1	2.49	0.42
2:H:174:VAL:HG22	2:H:182:SER:O	2.20	0.42
5:N:50:SER:HA	5:N:95:GLY:O	2.19	0.42
3:L:112:ARG:HH11	3:L:112:ARG:HG2	1.85	0.42
4:M:12:VAL:HG23	4:M:123:VAL:HG12	2.02	0.42
4:M:47:TRP:CH2	4:M:49:GLY:HA2	2.55	0.42
4:M:14:PRO:HA	4:M:15:GLY:HA2	1.75	0.42
2:H:202:ASN:N	2:H:202:ASN:ND2	2.68	0.42
5:N:43:ILE:HG12	5:N:129:THR:HG21	2.03	0.41
5:N:55:ASP:OD1	5:N:55:ASP:N	2.53	0.41
3:L:6:GLN:HE22	3:L:91:PHE:HA	1.85	0.41
3:L:124:PRO:HD3	3:L:136:VAL:HG22	2.03	0.41
3:L:46:GLN:HB3	3:L:47:PRO:HD2	2.02	0.41
2:H:63:ASP:N	2:H:63:ASP:OD1	2.53	0.41
1:B:215:VAL:HA	1:B:216:PRO:HA	1.81	0.41
2:H:124:PRO:CB	2:H:150:TYR:HB3	2.48	0.41
3:L:13:VAL:CG1	3:L:82:MET:HG3	2.51	0.41
2:H:91:THR:CG2	2:H:115:THR:HA	2.49	0.40
3:L:190:TYR:HD1	3:L:196:TYR:HH	1.69	0.40
5:N:64:LEU:HB2	5:N:74:LEU:HD11	2.03	0.40
2:H:41:PRO:C	2:H:43:LYS:H	2.23	0.40
4:M:36:TRP:CB	4:M:81:MET:CE	2.99	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	B	190/245 (78%)	177 (93%)	10 (5%)	3 (2%)	9	31
2	H	208/225 (92%)	166 (80%)	42 (20%)	0	100	100
3	L	216/218 (99%)	189 (88%)	24 (11%)	3 (1%)	11	34
4	M	218/232 (94%)	191 (88%)	25 (12%)	2 (1%)	17	46
5	N	214/241 (89%)	192 (90%)	20 (9%)	2 (1%)	17	46
All	All	1046/1161 (90%)	915 (88%)	121 (12%)	10 (1%)	15	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	319	TYR
5	N	95	GLY
5	N	141	SER
1	B	158	ASN
3	L	208	PRO
3	L	161	GLY
1	B	255	ASP
4	M	41	PRO
3	L	123	PRO
4	M	145	GLY

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	B	173/217 (80%)	159 (92%)	14 (8%)	11	32
2	H	176/191 (92%)	148 (84%)	28 (16%)	2	7
3	L	187/189 (99%)	166 (89%)	21 (11%)	6	17
4	M	185/196 (94%)	162 (88%)	23 (12%)	4	13
5	N	193/214 (90%)	177 (92%)	16 (8%)	11	30
All	All	914/1007 (91%)	812 (89%)	102 (11%)	6	17

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	129	TRP
1	B	148	LEU
1	B	150	SER
1	B	158	ASN
1	B	176	GLN
1	B	186	LEU
1	B	196	ILE
1	B	208	LYS
1	B	209	THR
1	B	224	ILE
1	B	238	ARG
1	B	253	HIS
1	B	274	ASP
1	B	281	ASP
2	H	10	GLU
2	H	17	THR
2	H	23	LYS
2	H	25	SER
2	H	43	LYS
2	H	62	ASP
2	H	65	LYS
2	H	68	PHE
2	H	74	THR
2	H	81	LEU
2	H	82	GLN
2	H	91	THR
2	H	103	GLU
2	H	105	ILE
2	H	113	THR
2	H	115	THR
2	H	120	SER

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Mol	Chain	Res	Type
2	H	122	LYS
2	H	126	VAL
2	H	143	LEU
2	H	146	LEU
2	H	154	PRO
2	H	156	THR
2	H	166	SER
2	H	184	SER
2	H	188	THR
2	H	191	SER
2	H	202	ASN
3	L	7	SER
3	L	9	VAL
3	L	24	ARG
3	L	27	GLU
3	L	67	SER
3	L	74	ASP
3	L	76	SER
3	L	93	LEU
3	L	95	SER
3	L	111	LYS
3	L	113	THR
3	L	121	ILE
3	L	158	LEU
3	L	160	SER
3	L	162	ASN
3	L	166	SER
3	L	190	TYR
3	L	192	LYS
3	L	206	SER
3	L	215	ARG
3	L	218	CYS
4	M	10	ASP
4	M	21	SER
4	M	37	MET
4	M	65	LYS
4	M	71	THR
4	M	77	SER
4	M	87	THR
4	M	88	SER
4	M	107	THR
4	M	112	MET

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Mol	Chain	Res	Type
4	M	120	SER
4	M	125	SER
4	M	127	SER
4	M	139	SER
4	M	150	LEU
4	M	161	PRO
4	M	162	VAL
4	M	163	THR
4	M	198	SER
4	M	203	THR
4	M	205	THR
4	M	208	CYS
4	M	224	GLU
5	N	23	ASP
5	N	27	THR
5	N	40	GLN
5	N	83	SER
5	N	98	PHE
5	N	135	ARG
5	N	141	SER
5	N	159	VAL
5	N	170	GLU
5	N	185	ASN
5	N	207	THR
5	N	212	ASP
5	N	224	THR
5	N	226	GLN
5	N	233	THR
5	N	238	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	B	192/245 (78%)	-0.16	0	100	100	35, 59, 94, 137	0
2	H	212/225 (94%)	0.10	7 (3%)	46	42	37, 82, 134, 151	0
3	L	218/218 (100%)	-0.03	5 (2%)	60	59	30, 60, 128, 160	0
4	M	222/232 (95%)	-0.04	10 (4%)	33	30	39, 74, 124, 143	0
5	N	216/241 (89%)	0.07	8 (3%)	41	38	42, 83, 157, 179	0
All	All	1060/1161 (91%)	-0.01	30 (2%)	53	50	30, 71, 135, 179	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	130	ALA	5.2
4	M	137	ALA	4.1
2	H	219	LYS	4.0
4	M	150	LEU	3.9
2	H	131	PRO	3.9
5	N	236	PHE	3.7
4	M	186	GLY	3.5
2	H	139	GLY	3.4
4	M	138	PRO	3.3
5	N	208	LEU	3.1
3	L	197	ALA	3.0
5	N	149	ASP	3.0
2	H	196	THR	2.9
4	M	223	VAL	2.9
5	N	175	TRP	2.9
5	N	219	TYR	2.9
2	H	132	SER	2.8
2	H	198	THR	2.6
5	N	220	ALA	2.6
4	M	148	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	L	196	TYR	2.5
4	M	225	PRO	2.4
3	L	184	THR	2.3
3	L	182	THR	2.3
3	L	136	VAL	2.2
4	M	136	LEU	2.1
4	M	153	LEU	2.1
5	N	157	ALA	2.1
4	M	135	PRO	2.1
5	N	228	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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.