



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:34 AM UTC

PDB ID : 2F5B / pdb_00002f5b
Title : CRYSTAL STRUCTURE OF FAB' FROM THE HIV-1 NEUTRALIZING ANTIBODY 2F5 IN COMPLEX WITH ITS GP41 EPITOPE
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Deposited on : 1999-04-09
Resolution : 2.00 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

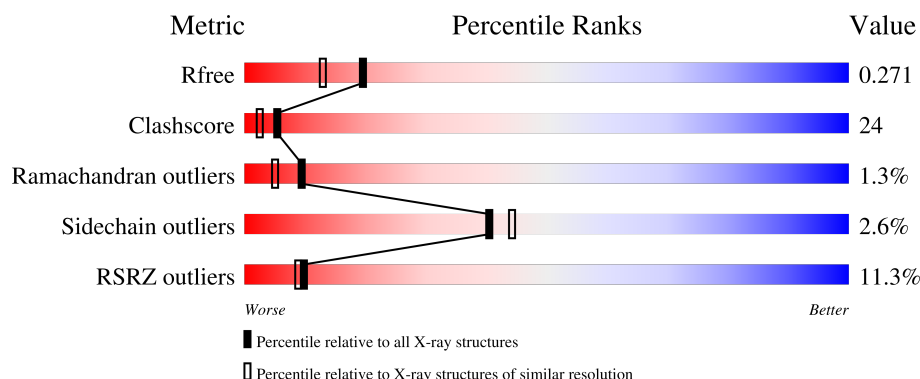
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	L	214	10% 64% 35% .
2	H	235	12% 60% 32% 7% .
3	P	7	14% 71% 29%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3788 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 PROTEIN (ANTIBODY 2F5 (LIGHT CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1644	1025	281	333	5			

- Molecule 2 is a protein called PROTEIN (ANTIBODY 2F5 (HEAVY CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	232	Total	C	N	O	S	0	0	1
			1727	1095	294	331	7			

- Molecule 3 is a protein called PROTEIN (GP41 EPITOPE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	7	Total	C	N	O	0	0	0
			60	38	9	13			

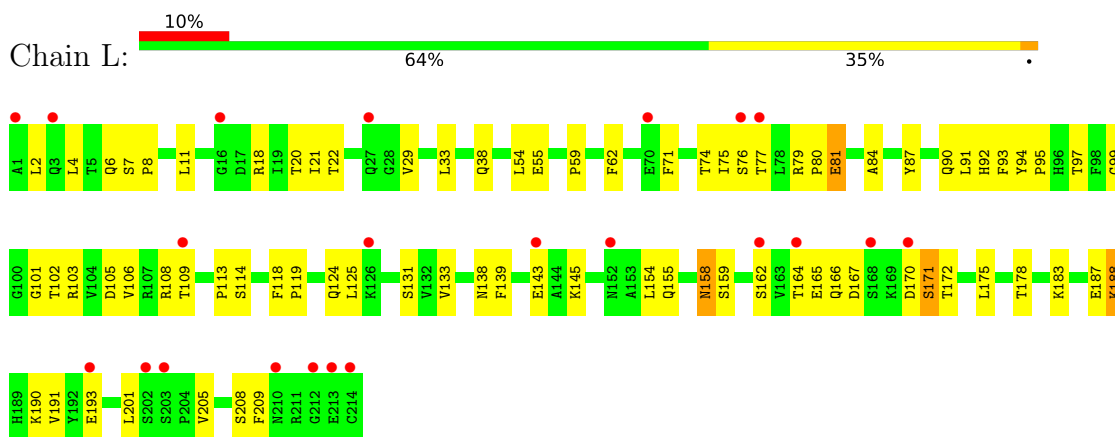
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	166	Total	O	0	0
			166	166		
4	H	184	Total	O	0	0
			184	184		
4	P	7	Total	O	0	0
			7	7		

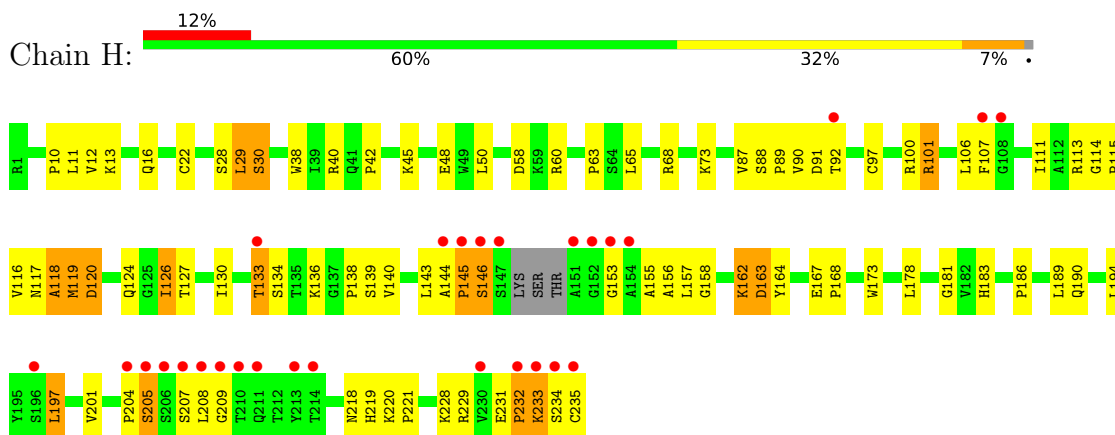
3 Residue-property plots

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.

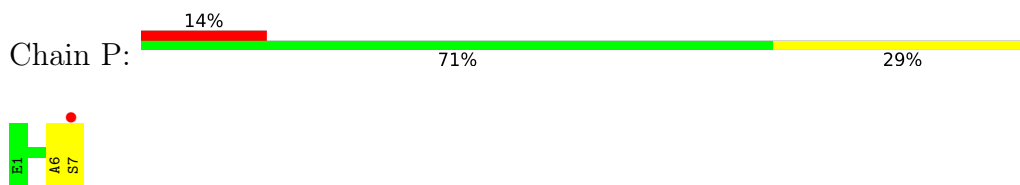
- Molecule 1: PROTEIN (ANTIBODY 2F5 (LIGHT CHAIN))



- Molecule 2: PROTEIN (ANTIBODY 2F5 (HEAVY CHAIN))



- Molecule 3: PROTEIN (GP41 EPI TOPE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.00Å 65.00Å 175.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.7 (20.00-2.00) 86.2 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 1.90Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.232 , 0.258 (Not available) , 0.271	Depositor DCC
R_{free} test set	2288 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3788	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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	L	0.34	0/1681	0.87	3/2284 (0.1%)
2	H	0.42	1/1769 (0.1%)	0.96	12/2418 (0.5%)
3	P	0.43	0/61	0.72	0/80
All	All	0.38	1/3511 (0.0%)	0.91	15/4782 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	146	SER	C-N	-5.72	1.25	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	162	LYS	N-CA-C	7.49	121.64	109.59
2	H	144	ALA	CA-C-N	6.99	128.57	119.84
2	H	144	ALA	C-N-CA	6.99	128.57	119.84
1	L	97	THR	N-CA-C	6.92	119.77	110.35
2	H	120	ASP	N-CA-C	6.85	121.38	112.89
2	H	119	MET	N-CA-C	-6.66	96.20	107.99
1	L	171	SER	N-CA-C	-6.19	105.68	113.23
2	H	30	SER	N-CA-C	-6.06	104.31	113.89
1	L	114	SER	N-CA-C	-5.82	99.79	109.46
2	H	167	GLU	N-CA-C	-5.77	101.73	110.39
2	H	139	SER	N-CA-C	-5.65	99.97	109.07
2	H	133	THR	N-CA-C	5.26	117.86	110.23
2	H	97	CYS	N-CA-C	-5.26	101.58	109.95
2	H	58	ASP	N-CA-C	-5.16	102.64	110.28
2	H	163	ASP	N-CA-C	5.08	118.14	111.28

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	L	1644	0	1588	91	0
2	H	1727	0	1740	81	0
3	P	60	0	56	1	0
4	H	184	0	0	3	0
4	L	166	0	0	7	0
4	P	7	0	0	0	0
All	All	3788	0	3384	163	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 24.

All (163) 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:H:92:THR:HG22	2:H:130:ILE:H	1.18	1.05
1:L:90:GLN:HE22	1:L:93:PHE:H	0.96	0.94
1:L:90:GLN:NE2	1:L:92:HIS:H	1.72	0.88
1:L:90:GLN:NE2	1:L:93:PHE:H	1.72	0.86
2:H:87:VAL:HB	2:H:130:ILE:HD13	1.60	0.83
2:H:91:ASP:HB2	2:H:130:ILE:HD12	1.58	0.83
1:L:90:GLN:HE21	1:L:92:HIS:H	1.24	0.82
2:H:91:ASP:HB2	2:H:130:ILE:CD1	2.09	0.82
2:H:118:ALA:O	2:H:119:MET:HE2	1.81	0.80
1:L:118:PHE:HB2	1:L:133:VAL:HG22	1.63	0.80
2:H:42:PRO:HG2	2:H:45:LYS:HB2	1.68	0.76
2:H:40:ARG:HD2	2:H:50:LEU:HD21	1.66	0.76
2:H:40:ARG:HD3	2:H:48:GLU:OE1	1.86	0.74
1:L:162:SER:HB3	2:H:186:PRO:HG2	1.70	0.74
2:H:89:PRO:O	2:H:92:THR:HG23	1.88	0.74
1:L:95:PRO:HG3	2:H:63:PRO:CD	2.18	0.73
1:L:118:PHE:HB2	1:L:133:VAL:CG2	2.19	0.73
1:L:91:LEU:HD21	2:H:119:MET:HE3	1.73	0.71
2:H:101:ARG:HD3	2:H:120:ASP:OD2	1.92	0.70
1:L:90:GLN:NE2	1:L:92:HIS:N	2.39	0.70
1:L:188:LYS:HB2	1:L:188:LYS:NZ	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:133:THR:HG21	2:H:194:LEU:HD23	1.74	0.68
1:L:106:VAL:H	1:L:166:GLN:HE22	1.42	0.67
2:H:92:THR:HG22	2:H:130:ILE:N	2.02	0.67
1:L:79:ARG:HB3	1:L:81:GLU:OE2	1.96	0.66
2:H:118:ALA:C	2:H:119:MET:HE2	2.20	0.66
1:L:81:GLU:H	1:L:81:GLU:CD	2.04	0.66
1:L:95:PRO:HG3	2:H:63:PRO:HD3	1.78	0.66
1:L:20:THR:HG22	1:L:74:THR:HG22	1.77	0.65
1:L:90:GLN:HE22	1:L:93:PHE:N	1.81	0.65
2:H:113:ARG:O	2:H:116:VAL:HG22	1.95	0.65
1:L:155:GLN:HB3	1:L:158:ASN:HD21	1.62	0.64
2:H:126:ILE:C	2:H:126:ILE:HD13	2.23	0.63
2:H:106:LEU:HG	2:H:107:PHE:HD2	1.63	0.63
1:L:190:LYS:HG3	1:L:191:VAL:HG23	1.82	0.62
2:H:87:VAL:HB	2:H:130:ILE:CD1	2.29	0.62
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.81	0.62
1:L:133:VAL:HG21	2:H:143:LEU:HD22	1.81	0.62
1:L:118:PHE:HD2	1:L:133:VAL:HG23	1.63	0.61
2:H:204:PRO:O	2:H:205:SER:CB	2.48	0.61
1:L:2:LEU:HD11	1:L:29:VAL:CG1	2.31	0.61
2:H:114:GLY:N	2:H:115:PRO:HD2	2.16	0.60
1:L:18:ARG:HB2	1:L:18:ARG:NH1	2.16	0.60
2:H:106:LEU:HB2	2:H:111:ILE:HD13	1.83	0.60
1:L:91:LEU:CD2	2:H:119:MET:HE3	2.32	0.60
2:H:197:LEU:C	2:H:197:LEU:HD12	2.26	0.60
1:L:6:GLN:HE21	1:L:99:GLY:HA3	1.66	0.59
1:L:188:LYS:HB2	1:L:188:LYS:HZ2	1.67	0.59
1:L:201:LEU:HD13	1:L:205:VAL:HG12	1.85	0.59
2:H:126:ILE:HD13	2:H:127:THR:N	2.17	0.59
2:H:220:LYS:HB2	2:H:221:PRO:HD3	1.85	0.58
2:H:233:LYS:N	2:H:233:LYS:HD3	2.18	0.58
2:H:145:PRO:HB3	2:H:156:ALA:O	2.03	0.58
1:L:6:GLN:OE1	1:L:102:THR:HG23	2.04	0.58
2:H:136:LYS:HE2	4:H:413:HOH:O	2.03	0.58
1:L:54:LEU:HD13	1:L:54:LEU:C	2.29	0.57
2:H:100:ARG:CD	2:H:119:MET:HE1	2.35	0.57
1:L:170:ASP:O	1:L:171:SER:HB2	2.06	0.56
1:L:105:ASP:HB2	1:L:166:GLN:NE2	2.22	0.55
2:H:13:LYS:H	2:H:16:GLN:NE2	2.03	0.55
1:L:183:LYS:O	1:L:187:GLU:HG2	2.07	0.55
2:H:145:PRO:HG2	2:H:232:PRO:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:154:LEU:HD11	4:L:359:HOH:O	2.08	0.53
2:H:10:PRO:C	2:H:11:LEU:HD12	2.32	0.53
2:H:106:LEU:HG	2:H:107:PHE:CD2	2.43	0.53
1:L:59:PRO:HG2	1:L:62:PHE:CE1	2.43	0.53
1:L:167:ASP:HB3	1:L:170:ASP:HB2	1.90	0.53
1:L:75:ILE:HD12	1:L:75:ILE:N	2.24	0.53
1:L:7:SER:O	1:L:22:THR:HG22	2.09	0.52
1:L:54:LEU:HD13	1:L:55:GLU:O	2.09	0.52
1:L:94:TYR:CZ	2:H:60:ARG:HG3	2.45	0.52
2:H:204:PRO:O	2:H:205:SER:HB3	2.10	0.52
1:L:11:LEU:HD23	1:L:11:LEU:C	2.35	0.52
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.44	0.52
1:L:164:THR:HG22	1:L:165:GLU:N	2.25	0.52
2:H:40:ARG:HB3	2:H:50:LEU:HD11	1.92	0.52
2:H:133:THR:HG21	2:H:194:LEU:CD2	2.39	0.52
2:H:138:PRO:HB3	2:H:164:TYR:HB3	1.92	0.51
1:L:29:VAL:HG11	1:L:90:GLN:CG	2.41	0.51
1:L:143:GLU:H	1:L:143:GLU:CD	2.18	0.51
2:H:100:ARG:HD2	2:H:119:MET:HE1	1.92	0.51
2:H:157:LEU:C	2:H:157:LEU:HD12	2.35	0.51
2:H:100:ARG:CG	2:H:119:MET:HE1	2.41	0.50
1:L:193:GLU:HG2	1:L:208:SER:HB3	1.93	0.50
2:H:229:ARG:NH1	2:H:231:GLU:OE1	2.44	0.50
1:L:74:THR:HG23	4:L:245:HOH:O	2.10	0.50
1:L:170:ASP:HB3	1:L:172:THR:HG23	1.94	0.49
2:H:146:SER:HA	2:H:233:LYS:NZ	2.27	0.49
1:L:103:ARG:HD3	4:L:361:HOH:O	2.12	0.49
2:H:140:VAL:O	2:H:228:LYS:HE3	2.12	0.49
1:L:4:LEU:HD11	1:L:90:GLN:HB2	1.94	0.49
2:H:232:PRO:O	2:H:233:LYS:HB3	2.12	0.49
1:L:2:LEU:C	1:L:2:LEU:HD23	2.38	0.48
1:L:138:ASN:OD1	2:H:183:HIS:HE1	1.96	0.48
1:L:21:ILE:HG23	1:L:102:THR:HG21	1.95	0.48
2:H:158:GLY:HA2	2:H:173:TRP:CH2	2.48	0.48
3:P:6:ALA:O	3:P:7:SER:HB2	2.14	0.48
1:L:59:PRO:HG2	1:L:62:PHE:HE1	1.78	0.48
1:L:18:ARG:CB	1:L:18:ARG:HH11	2.26	0.48
1:L:108:ARG:HH21	1:L:109:THR:HG23	1.78	0.48
2:H:133:THR:HG22	2:H:134:SER:O	2.13	0.48
1:L:79:ARG:HB3	1:L:80:PRO:HD2	1.95	0.47
1:L:119:PRO:HB3	1:L:209:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:GLN:O	1:L:84:ALA:HB1	2.14	0.47
1:L:193:GLU:HG2	1:L:208:SER:CB	2.44	0.47
4:L:305:HOH:O	2:H:183:HIS:HD2	1.96	0.47
1:L:6:GLN:NE2	1:L:101:GLY:H	2.12	0.47
1:L:54:LEU:HD12	4:L:249:HOH:O	2.14	0.47
1:L:125:LEU:O	1:L:183:LYS:HD2	2.15	0.47
1:L:190:LYS:HG3	1:L:191:VAL:N	2.30	0.47
2:H:234:SER:O	2:H:235:CYS:HB3	2.15	0.47
1:L:18:ARG:HB2	1:L:18:ARG:HH11	1.80	0.47
1:L:164:THR:HG23	4:L:285:HOH:O	2.14	0.46
1:L:2:LEU:HD11	1:L:29:VAL:HG12	1.98	0.46
2:H:218:ASN:HD22	2:H:219:HIS:N	2.13	0.46
1:L:118:PHE:CD2	1:L:133:VAL:HG23	2.47	0.46
1:L:164:THR:HG22	1:L:165:GLU:O	2.16	0.46
1:L:21:ILE:HD13	1:L:102:THR:OG1	2.16	0.46
2:H:100:ARG:HG3	2:H:119:MET:HE1	1.98	0.46
1:L:29:VAL:HG11	1:L:90:GLN:HG3	1.98	0.45
1:L:7:SER:HB2	1:L:22:THR:CG2	2.47	0.45
2:H:145:PRO:HD3	2:H:157:LEU:HB3	1.98	0.45
2:H:65:LEU:HD22	2:H:65:LEU:N	2.31	0.45
1:L:6:GLN:HE22	1:L:87:TYR:HA	1.81	0.45
2:H:88:SER:OG	2:H:90:VAL:HG22	2.16	0.45
1:L:2:LEU:HD12	1:L:93:PHE:CD2	2.52	0.45
2:H:163:ASP:HB3	2:H:194:LEU:HD13	1.99	0.44
1:L:29:VAL:HG11	1:L:90:GLN:HG2	2.00	0.44
1:L:133:VAL:CG2	2:H:143:LEU:HD22	2.47	0.44
2:H:178:LEU:C	2:H:178:LEU:HD23	2.43	0.44
2:H:133:THR:HG23	4:H:399:HOH:O	2.18	0.44
1:L:188:LYS:NZ	1:L:188:LYS:CB	2.80	0.44
2:H:117:ASN:O	2:H:118:ALA:HB2	2.18	0.44
2:H:155:ALA:CB	2:H:208:LEU:HD11	2.48	0.44
1:L:90:GLN:NE2	1:L:93:PHE:N	2.53	0.43
1:L:105:ASP:HB2	1:L:166:GLN:HE22	1.84	0.43
2:H:181:GLY:O	2:H:201:VAL:HA	2.19	0.43
1:L:76:SER:O	1:L:77:THR:HB	2.18	0.43
1:L:201:LEU:CD1	1:L:205:VAL:HG12	2.48	0.43
2:H:12:VAL:O	2:H:130:ILE:HA	2.18	0.42
2:H:207:SER:C	2:H:209:GLY:N	2.76	0.42
1:L:158:ASN:ND2	1:L:158:ASN:H	2.18	0.42
2:H:197:LEU:C	2:H:197:LEU:CD1	2.93	0.42
2:H:28:SER:C	2:H:30:SER:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:233:LYS:O	2:H:234:SER:HB2	2.19	0.42
2:H:162:LYS:NZ	2:H:190:GLN:OE1	2.53	0.42
1:L:164:THR:CG2	1:L:165:GLU:N	2.82	0.42
1:L:54:LEU:HD13	1:L:55:GLU:N	2.34	0.42
2:H:231:GLU:O	2:H:232:PRO:O	2.37	0.42
1:L:103:ARG:HD2	4:L:365:HOH:O	2.20	0.41
1:L:124:GLN:NE2	1:L:131:SER:H	2.18	0.41
2:H:145:PRO:HD3	2:H:157:LEU:CB	2.51	0.41
1:L:159:SER:HA	1:L:178:THR:O	2.20	0.41
1:L:8:PRO:O	1:L:102:THR:HG22	2.21	0.41
1:L:119:PRO:HB3	1:L:209:PHE:CZ	2.56	0.41
2:H:124:GLN:HG2	4:H:322:HOH:O	2.21	0.41
1:L:175:LEU:HD23	1:L:175:LEU:C	2.46	0.41
2:H:126:ILE:O	2:H:126:ILE:HG23	2.21	0.41
1:L:95:PRO:HG3	2:H:63:PRO:HD2	1.99	0.40
2:H:22:CYS:HB2	2:H:38:TRP:CZ2	2.56	0.40
2:H:29:LEU:HG	2:H:73:LYS:HD2	2.02	0.40
2:H:145:PRO:HB2	2:H:146:SER:H	1.65	0.40
2:H:68:ARG:NH2	2:H:91:ASP:OD2	2.42	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	L	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
2	H	228/235 (97%)	216 (95%)	6 (3%)	6 (3%)	4	1
3	P	5/7 (71%)	5 (100%)	0	0	100	100
All	All	445/456 (98%)	425 (96%)	14 (3%)	6 (1%)	9	5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	145	PRO
2	H	232	PRO
2	H	205	SER
2	H	118	ALA
2	H	233	LYS
2	H	153	GLY

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	L	187/187 (100%)	183 (98%)	4 (2%)	47	52
2	H	199/203 (98%)	193 (97%)	6 (3%)	36	38
3	P	6/6 (100%)	6 (100%)	0	100	100
All	All	392/396 (99%)	382 (97%)	10 (3%)	40	44

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	81	GLU
1	L	145	LYS
1	L	158	ASN
1	L	188	LYS
2	H	29	LEU
2	H	101	ARG
2	H	126	ILE
2	H	168	PRO
2	H	189	LEU
2	H	197	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	38	GLN

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Mol	Chain	Res	Type
1	L	90	GLN
1	L	124	GLN
1	L	138	ASN
1	L	155	GLN
1	L	158	ASN
1	L	166	GLN
1	L	199	GLN
2	H	16	GLN
2	H	41	GLN
2	H	78	ASN
2	H	79	GLN
2	H	183	HIS
2	H	218	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	L	214/214 (100%)	0.68	22 (10%)	12 11	21, 33, 43, 52	0
2	H	232/235 (98%)	0.66	28 (12%)	8 8	20, 30, 51, 63	0
3	P	7/7 (100%)	0.14	1 (14%)	6 5	23, 25, 30, 34	0
All	All	453/456 (99%)	0.66	51 (11%)	10 9	20, 31, 47, 63	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	235	CYS	9.3
2	H	145	PRO	5.9
2	H	208	LEU	5.2
2	H	133	THR	5.1
2	H	233	LYS	5.0
2	H	152	GLY	4.8
2	H	154	ALA	4.6
2	H	232	PRO	4.5
2	H	146	SER	4.3
2	H	206	SER	4.1
2	H	234	SER	4.1
2	H	151	ALA	3.9
2	H	209	GLY	3.8
1	L	202	SER	3.8
1	L	214	CYS	3.8
1	L	168	SER	3.7
2	H	147	SER	3.7
2	H	153	GLY	3.3
3	P	7	SER	3.3
2	H	196	SER	3.2
1	L	193	GLU	3.2
2	H	204	PRO	3.2
1	L	170	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	210	ASN	2.9
2	H	108	GLY	2.9
2	H	92	THR	2.9
2	H	205	SER	2.7
1	L	1	ALA	2.7
2	H	144	ALA	2.7
1	L	212	GLY	2.6
2	H	210	THR	2.6
1	L	76	SER	2.6
1	L	27	GLN	2.5
2	H	230	VAL	2.4
1	L	203	SER	2.4
1	L	162	SER	2.3
2	H	207	SER	2.3
1	L	213	GLU	2.3
1	L	3	GLN	2.3
2	H	211	GLN	2.3
1	L	152	ASN	2.2
1	L	126	LYS	2.2
1	L	70	GLU	2.2
1	L	164	THR	2.2
2	H	107	PHE	2.1
2	H	214	THR	2.1
1	L	16	GLY	2.1
2	H	213	TYR	2.1
1	L	143	GLU	2.0
1	L	77	THR	2.0
1	L	109	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.