



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2026 – 06:07 PM EDT

PDB ID : 9Z0S / pdb_00009z0s
Title : Fab/epitope complex structure of anti-Tau monoclonal antibody PHF-1
Authors : Pan, R.; Kong, X.P.
Deposited on : 2025-11-03
Resolution : 2.55 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 Phenix2.2
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.2
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

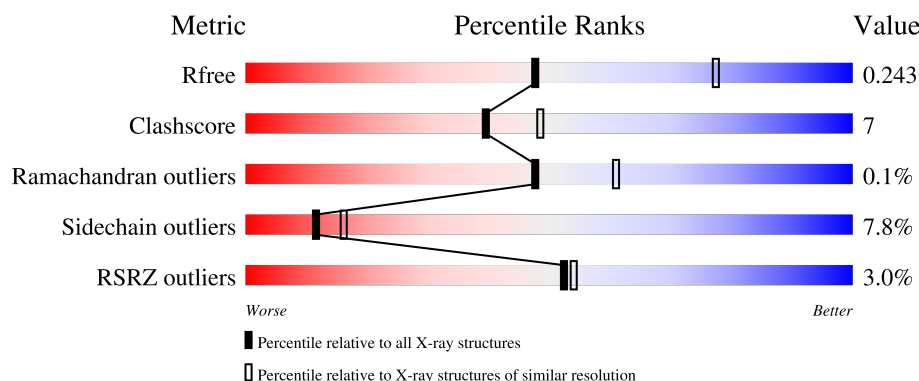
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	219	 80% 17% •
1	D	219	 82% 15% •
1	G	219	 3% 76% 22% •
1	K	219	 75% 24% •
1	L	219	 79% 20% •

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Mol	Chain	Length	Quality of chain
1	O	219	
2	B	223	
2	E	223	
2	H	223	
2	I	223	
2	M	223	
2	Q	223	
3	C	23	
3	F	23	
3	J	23	
3	N	23	
3	P	23	
3	R	23	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21526 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 Light chain of Fab fragment of anti-Tau mAb PHF-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	219	Total	C	N	O	S	0	0	0
			1687	1059	285	337	6			
1	A	219	Total	C	N	O	S	0	0	0
			1687	1059	285	337	6			
1	D	219	Total	C	N	O	S	0	0	0
			1687	1059	285	337	6			
1	G	219	Total	C	N	O	S	0	0	0
			1687	1059	285	337	6			
1	K	219	Total	C	N	O	S	0	0	0
			1687	1059	285	337	6			
1	O	219	Total	C	N	O	S	0	0	0
			1687	1059	285	337	6			

- Molecule 2 is a protein called Heavy chain of Fab fragment of anti-Tau mAb PHF-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1655	1044	276	329	6			
2	B	220	Total	C	N	O	S	0	0	0
			1647	1040	275	326	6			
2	E	220	Total	C	N	O	S	0	0	0
			1647	1040	275	326	6			
2	I	220	Total	C	N	O	S	0	0	0
			1647	1040	275	326	6			
2	M	220	Total	C	N	O	S	0	0	0
			1647	1040	275	326	6			
2	Q	220	Total	C	N	O	S	0	0	0
			1647	1040	275	326	6			

- Molecule 3 is a protein called Microtubule-associated protein tau.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	6	Total	C	N	O	P	0	0	0
			52	33	7	11	1			
3	C	9	Total	C	N	O	P	0	0	0
			76	49	10	16	1			
3	F	9	Total	C	N	O	P	0	0	0
			76	49	10	16	1			
3	J	8	Total	C	N	O	P	0	0	0
			67	44	9	13	1			
3	N	9	Total	C	N	O	P	0	0	0
			76	49	10	16	1			
3	R	6	Total	C	N	O	P	0	0	0
			52	33	7	11	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	88	Total	O	0	0
			88	88		
4	H	96	Total	O	0	0
			96	96		
4	P	9	Total	O	0	0
			9	9		
4	A	119	Total	O	0	0
			119	119		
4	B	90	Total	O	0	0
			90	90		
4	C	8	Total	O	0	0
			8	8		
4	D	88	Total	O	0	0
			88	88		
4	E	116	Total	O	0	0
			116	116		
4	F	15	Total	O	0	0
			15	15		
4	G	105	Total	O	0	0
			105	105		
4	I	79	Total	O	0	0
			79	79		
4	J	9	Total	O	0	0
			9	9		
4	K	91	Total	O	0	0
			91	91		
4	M	92	Total	O	0	0
			92	92		

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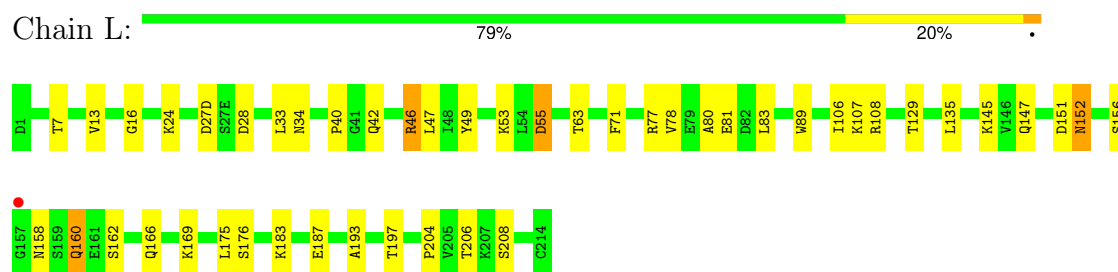
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	N	11	Total 11	O 11	0	0
4	O	50	Total 50	O 50	0	0
4	Q	47	Total 47	O 47	0	0
4	R	2	Total 2	O 2	0	0

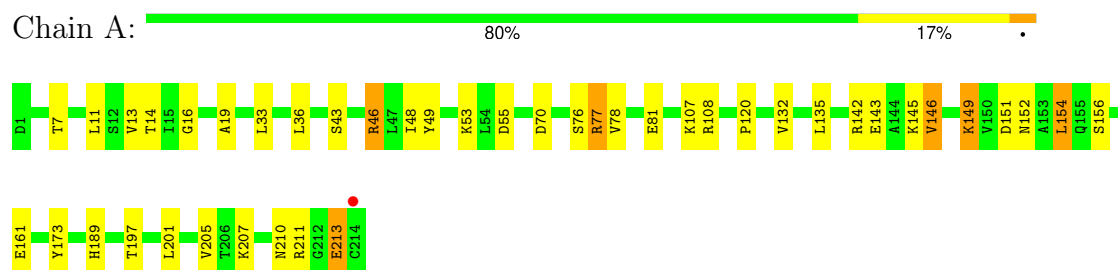
3 Residue-property plots [i](#)

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.

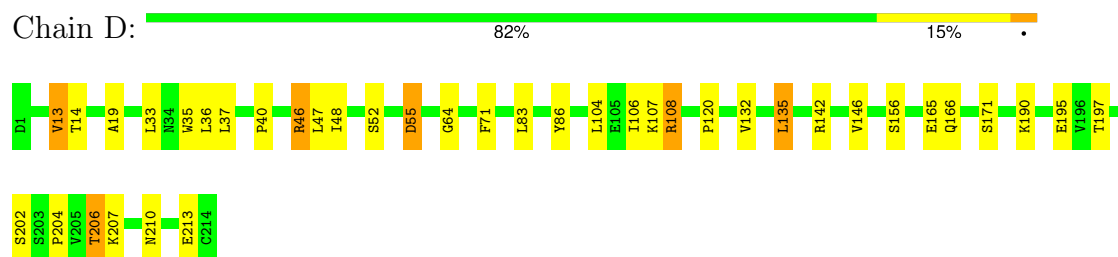
- Molecule 1: Light chain of Fab fragment of anti-Tau mAb PHF-1



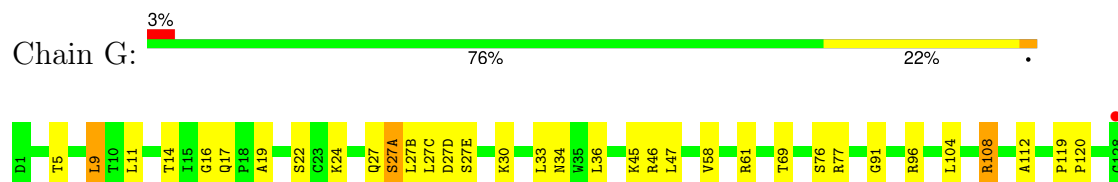
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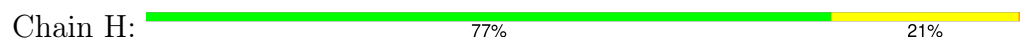
- Molecule 1: Light chain of Fab fragment of anti-Tau mAb PHF-1



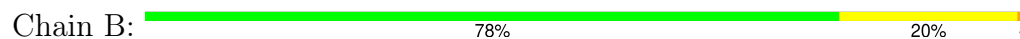
- Molecule 1: Light chain of Fab fragment of anti-Tau mAb PHF-1



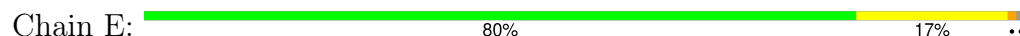
- Molecule 2: Heavy chain of Fab fragment of anti-Tau mAb PHF-1

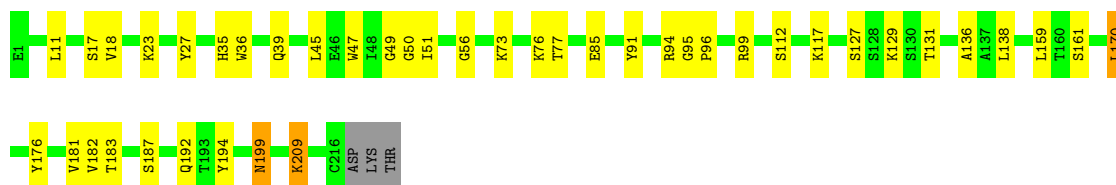


- Molecule 2: Heavy chain of Fab fragment of anti-Tau mAb PHF-1

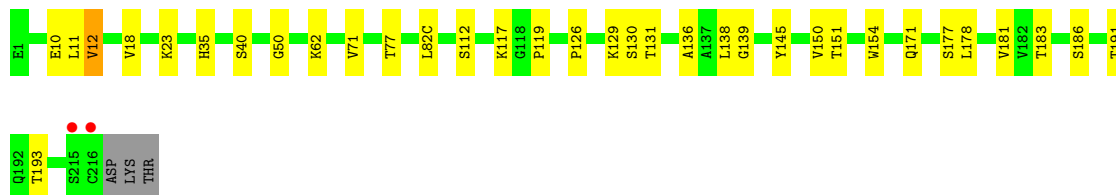
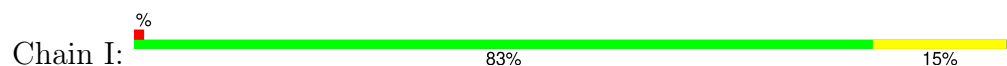


- Molecule 2: Heavy chain of Fab fragment of anti-Tau mAb PHF-1

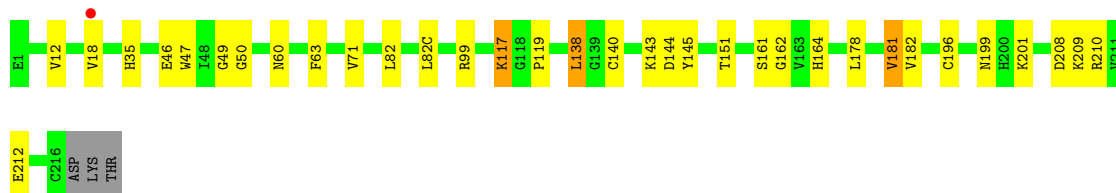
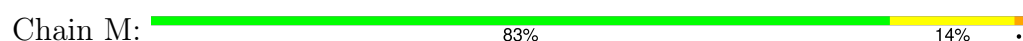




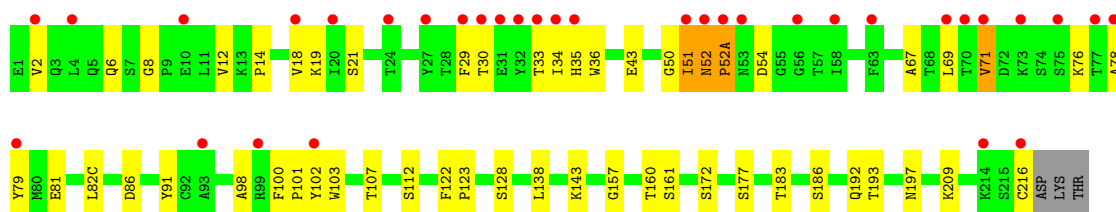
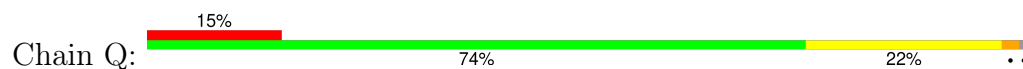
- Molecule 2: Heavy chain of Fab fragment of anti-Tau mAb PHF-1



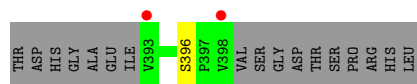
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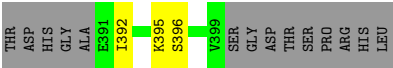


- Molecule 3: Microtubule-associated protein tau

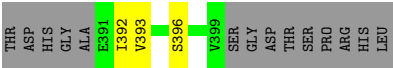


- Molecule 3: Microtubule-associated protein tau

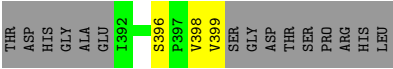




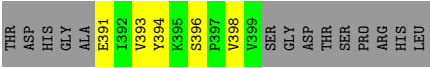
● Molecule 3: Microtubule-associated protein tau



● Molecule 3: Microtubule-associated protein tau



● Molecule 3: Microtubule-associated protein tau



● Molecule 3: Microtubule-associated protein tau



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.00Å 120.50Å 142.40Å 90.00° 106.86° 90.00°	Depositor
Resolution (Å)	35.40 – 2.55 35.40 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.40-2.55) 99.9 (35.40-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.183 , 0.245 0.183 , 0.243	Depositor DCC
R_{free} test set	6073 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21526	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.80% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP

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	0.42	0/1722	0.64	0/2336
1	D	0.39	0/1722	0.61	0/2336
1	G	0.45	1/1722 (0.1%)	0.64	1/2336 (0.0%)
1	K	0.39	0/1722	0.58	0/2336
1	L	0.38	0/1722	0.58	0/2336
1	O	0.35	0/1722	0.54	0/2336
2	B	0.39	0/1688	0.59	0/2298
2	E	0.40	0/1688	0.61	0/2298
2	H	0.38	0/1696	0.60	0/2309
2	I	0.39	0/1688	0.59	0/2298
2	M	0.41	0/1688	0.58	0/2298
2	Q	0.33	0/1688	0.53	0/2298
3	C	0.40	0/66	0.55	0/87
3	F	0.26	0/66	0.45	0/87
3	J	0.43	0/57	0.52	0/75
3	N	0.30	0/66	0.45	0/87
3	P	0.35	0/42	0.49	0/54
3	R	0.25	0/42	0.46	0/54
All	All	0.39	1/20807 (0.0%)	0.59	1/28259 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	58	VAL	CA-C	-5.81	1.48	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	58	VAL	CA-C-O	5.33	122.29	119.15

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	1687	0	1663	25	0
1	D	1687	0	1663	22	0
1	G	1687	0	1663	23	0
1	K	1687	0	1663	24	0
1	L	1687	0	1663	25	0
1	O	1687	0	1663	41	0
2	B	1647	0	1624	25	0
2	E	1647	0	1624	22	0
2	H	1655	0	1628	30	0
2	I	1647	0	1624	14	0
2	M	1647	0	1624	15	0
2	Q	1647	0	1624	31	0
3	C	76	0	76	0	0
3	F	76	0	75	1	0
3	J	67	0	69	0	0
3	N	76	0	75	1	0
3	P	52	0	49	0	0
3	R	52	0	49	0	0
4	A	119	0	0	2	0
4	B	90	0	0	3	0
4	C	8	0	0	0	0
4	D	88	0	0	1	0
4	E	116	0	0	1	0
4	F	15	0	0	0	0
4	G	105	0	0	3	0
4	H	96	0	0	1	0
4	I	79	0	0	1	0
4	J	9	0	0	0	0
4	K	91	0	0	7	0
4	L	88	0	0	1	0
4	M	92	0	0	0	0
4	N	11	0	0	1	0
4	O	50	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	9	0	0	0	0
4	Q	47	0	0	2	0
4	R	2	0	0	0	0
All	All	21526	0	20119	273	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (273) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ARG:HD2	1:D:55:ASP:OD2	1.76	0.85
2:B:11:LEU:HD11	2:B:112:SER:HB3	1.61	0.81
1:L:46:ARG:HH21	2:H:99:ARG:HB3	1.51	0.76
2:I:11:LEU:HD11	2:I:112:SER:HB3	1.72	0.71
2:M:210:ARG:HD3	2:M:212:GLU:OE2	1.89	0.71
1:L:46:ARG:HD2	1:L:55:ASP:OD2	1.92	0.70
1:G:112:ALA:O	4:G:301:HOH:O	2.10	0.70
1:O:27(A):SER:HB3	4:O:311:HOH:O	1.90	0.70
1:K:83:LEU:HD11	1:K:166:GLN:HB3	1.74	0.69
1:L:197:THR:HG22	1:L:204:PRO:HG3	1.75	0.68
1:A:146:VAL:HG13	1:A:161:GLU:OE2	1.92	0.68
2:I:12:VAL:HG21	2:I:82(C):LEU:HD12	1.76	0.68
1:A:156:SER:C	4:A:301:HOH:O	2.38	0.66
1:A:11:LEU:HD21	1:A:19:ALA:HB1	1.76	0.66
1:A:13:VAL:HG21	1:A:78:VAL:HG21	1.78	0.66
1:G:209:PHE:HB3	2:I:129:LYS:HG2	1.77	0.65
1:D:197:THR:HG22	1:D:204:PRO:HG3	1.77	0.65
1:O:45:LYS:HA	1:O:46:ARG:NH1	2.11	0.65
2:E:76:LYS:HD3	1:G:9:LEU:HD21	1.79	0.65
1:L:40:PRO:O	4:L:301:HOH:O	2.15	0.65
1:A:151:ASP:O	1:A:152:ASN:HB2	1.95	0.64
2:H:129:LYS:NZ	4:H:301:HOH:O	2.30	0.63
2:B:12:VAL:HG21	2:B:82(C):LEU:HD13	1.79	0.63
1:O:46:ARG:HH11	1:O:46:ARG:H	1.45	0.63
4:O:303:HOH:O	2:Q:209:LYS:HD2	2.00	0.62
1:K:195:GLU:HG3	1:K:206:THR:HG22	1.82	0.61
1:G:146:VAL:HG22	1:G:161:GLU:OE2	2.01	0.60
1:K:1:ASP:OD2	4:K:301:HOH:O	2.16	0.60
1:K:214:CYS:HB2	4:K:319:HOH:O	2.01	0.60
2:H:210:ARG:HD3	2:H:212:GLU:OE2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:160:GLN:HG3	2:H:169:VAL:HG21	1.84	0.60
1:G:16:GLY:O	1:G:77:ARG:HG3	2.02	0.59
2:Q:123:PRO:O	4:Q:301:HOH:O	2.16	0.59
2:H:213:PRO:HB2	2:B:195:ILE:HD12	1.85	0.58
1:A:46:ARG:HG3	1:A:55:ASP:OD2	2.04	0.58
2:I:193:THR:HA	4:I:304:HOH:O	2.02	0.58
1:D:46:ARG:HH21	2:E:99:ARG:HB3	1.69	0.58
1:O:46:ARG:H	1:O:46:ARG:HD2	1.68	0.58
2:H:4:LEU:HD22	2:H:24:THR:HG22	1.85	0.58
1:O:46:ARG:H	1:O:46:ARG:CD	2.18	0.57
1:A:197:THR:HG23	4:A:324:HOH:O	2.04	0.57
2:Q:19:LYS:HD3	2:Q:79:TYR:CD2	2.40	0.57
2:I:35:HIS:CE1	2:I:50:GLY:HA3	2.39	0.57
2:B:4:LEU:HD22	2:B:24:THR:HG22	1.87	0.57
2:I:119:PRO:HB3	2:I:145:TYR:HB3	1.87	0.56
2:H:123:PRO:HD3	2:H:209:LYS:HE2	1.86	0.56
1:O:52:SER:HB3	1:O:64:GLY:O	2.05	0.56
2:Q:67:ALA:HA	2:Q:81:GLU:O	2.05	0.56
2:E:192:GLN:HG2	2:E:194:TYR:CZ	2.40	0.56
1:O:116:PHE:HD2	1:O:135:LEU:HD13	1.69	0.56
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.42	0.55
1:G:161:GLU:HG3	4:G:324:HOH:O	2.07	0.55
1:G:151:ASP:OD2	1:G:189:HIS:HB3	2.07	0.55
1:O:89:TRP:CZ2	2:Q:100:PHE:HB2	2.42	0.54
1:A:149:LYS:HG2	1:A:154:LEU:HD13	1.89	0.54
2:E:117:LYS:NZ	4:E:302:HOH:O	2.41	0.54
2:H:170:LEU:HD21	1:G:108:ARG:C	2.33	0.54
1:K:161:GLU:HG3	4:K:327:HOH:O	2.07	0.54
1:G:210:ASN:HB2	1:G:213:GLU:HG2	1.89	0.53
2:Q:2:VAL:HB	2:Q:102:TYR:CE1	2.43	0.53
1:D:40:PRO:HG3	1:D:165:GLU:HG2	1.89	0.53
1:O:40:PRO:HB3	1:O:165:GLU:HG2	1.91	0.53
1:G:191:VAL:HG12	4:G:341:HOH:O	2.08	0.53
1:D:135:LEU:HD11	2:E:181:VAL:HG11	1.91	0.53
2:Q:52(A):PRO:HA	2:Q:71:VAL:HG11	1.90	0.53
1:L:183:LYS:HE2	1:L:187:GLU:OE2	2.09	0.53
1:O:27(D):ASP:OD2	1:O:28:ASP:OD2	2.26	0.53
2:M:119:PRO:HB3	2:M:145:TYR:HB3	1.91	0.52
1:O:146:VAL:HG13	1:O:161:GLU:OE2	2.08	0.52
2:E:11:LEU:HD11	2:E:112:SER:HB3	1.91	0.52
2:B:19:LYS:HE2	2:B:81:GLU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.45	0.52
1:L:46:ARG:NH2	2:H:99:ARG:HB3	2.22	0.52
2:B:69:LEU:HB3	4:B:306:HOH:O	2.09	0.52
1:D:52:SER:HB3	1:D:64:GLY:O	2.10	0.51
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.93	0.51
1:A:49:TYR:OH	1:A:53:LYS:HE2	2.09	0.51
1:D:142:ARG:NH1	4:D:302:HOH:O	2.44	0.51
1:O:91:GLY:HA2	1:O:96:ARG:HD2	1.92	0.51
2:E:39:GLN:HB2	2:E:45:LEU:HD23	1.92	0.51
2:H:190:GLY:HA3	2:B:159:LEU:HD13	1.92	0.50
2:I:131:THR:HG22	2:I:136:ALA:HB2	1.93	0.50
1:D:108:ARG:HG3	1:D:171:SER:HB2	1.93	0.50
1:O:11:LEU:HD21	1:O:19:ALA:HB1	1.94	0.50
1:O:80:ALA:HA	1:O:106:ILE:CD1	2.42	0.50
1:A:16:GLY:O	1:A:77:ARG:HG3	2.11	0.50
3:N:394:TYR:HA	4:N:502:HOH:O	2.10	0.50
1:K:70:ASP:OD2	4:K:303:HOH:O	2.20	0.50
1:O:16:GLY:O	1:O:77:ARG:HG3	2.12	0.50
2:H:121:VAL:HB	2:H:207:VAL:HG11	1.93	0.50
1:G:11:LEU:HD21	1:G:19:ALA:HB1	1.94	0.50
1:L:83:LEU:HD13	1:L:166:GLN:HB3	1.94	0.49
2:E:131:THR:HG22	2:E:136:ALA:HB2	1.94	0.49
2:I:171:GLN:NE2	2:I:177:SER:HB2	2.27	0.49
2:B:85:GLU:O	4:B:301:HOH:O	2.19	0.49
2:M:47:TRP:CZ2	2:M:49:GLY:HA2	2.47	0.49
1:A:142:ARG:HG3	1:A:173:TYR:CE1	2.48	0.49
1:G:120:PRO:HG3	1:G:130:ALA:HB1	1.94	0.49
1:D:210:ASN:O	1:D:213:GLU:HB3	2.13	0.49
1:O:210:ASN:HB2	1:O:213:GLU:HG3	1.94	0.49
2:B:27:TYR:CE2	2:B:94:ARG:HD2	2.47	0.49
1:O:94:PHE:HD1	1:O:95:PRO:HA	1.77	0.49
1:D:33:LEU:HD22	1:D:71:PHE:CD1	2.48	0.48
2:Q:12:VAL:HG11	2:Q:18:VAL:HB	1.95	0.48
1:D:14:THR:HA	1:D:107:LYS:HB2	1.96	0.48
1:K:15:ILE:HD11	1:K:80:ALA:HB2	1.94	0.48
2:M:117:LYS:HD2	2:M:144:ASP:O	2.13	0.48
1:L:193:ALA:HB2	1:L:208:SER:HB3	1.95	0.48
2:B:28:THR:HB	2:B:31:GLU:HG3	1.94	0.48
2:Q:35:HIS:NE2	2:Q:50:GLY:HA3	2.28	0.48
2:Q:82(C):LEU:HA	2:Q:86:ASP:OD2	2.14	0.48
1:O:30:LYS:HD2	1:O:32:TYR:OH	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:125:LEU:HD22	1:O:183:LYS:HG3	1.96	0.48
1:G:76:SER:O	1:G:77:ARG:HD2	2.14	0.48
1:O:32:TYR:CD1	2:Q:98:ALA:HB1	2.49	0.48
1:O:187:GLU:HA	1:O:211:ARG:NE	2.29	0.48
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.96	0.47
2:B:30:THR:HB	2:B:53:ASN:OD1	2.14	0.47
2:E:170:LEU:HD13	2:E:176:TYR:CE1	2.49	0.47
1:A:46:ARG:HH21	2:B:99:ARG:HB3	1.79	0.47
1:O:27(C):LEU:HB3	4:O:311:HOH:O	2.12	0.47
1:A:76:SER:O	1:A:77:ARG:HD3	2.14	0.47
2:M:164:HIS:HB2	2:M:181:VAL:HG12	1.96	0.47
2:Q:36:TRP:CD1	2:Q:69:LEU:HD22	2.50	0.47
1:D:37:LEU:HD13	1:D:86:TYR:CZ	2.49	0.47
1:A:46:ARG:HD2	1:A:55:ASP:OD2	2.15	0.47
2:I:18:VAL:HG12	2:I:82(C):LEU:HD11	1.96	0.47
2:Q:35:HIS:CE1	2:Q:50:GLY:HA3	2.49	0.47
2:H:11:LEU:HB2	2:H:147:PRO:HG3	1.97	0.47
1:A:142:ARG:HG3	1:A:173:TYR:CD1	2.49	0.47
1:D:33:LEU:HD22	1:D:71:PHE:CG	2.50	0.47
1:G:36:LEU:HD23	1:G:46:ARG:HA	1.96	0.47
1:O:34:ASN:HB2	1:O:89:TRP:CE2	2.50	0.47
2:Q:157:GLY:HA3	4:Q:303:HOH:O	2.14	0.47
2:E:159:LEU:HD21	2:E:182:VAL:HG21	1.96	0.47
1:D:83:LEU:HD13	1:D:166:GLN:HB3	1.97	0.47
1:L:49:TYR:CE2	1:L:53:LYS:HD3	2.49	0.46
2:E:23:LYS:HG2	2:E:77:THR:OG1	2.15	0.46
1:G:24:LYS:HA	1:G:69:THR:O	2.15	0.46
2:M:12:VAL:HG11	2:M:18:VAL:HB	1.98	0.46
2:B:27:TYR:CZ	2:B:94:ARG:HD2	2.51	0.46
1:L:169:LYS:HA	1:L:169:LYS:HD3	1.66	0.46
1:L:160:GLN:OE1	2:H:171:GLN:HG2	2.16	0.46
2:H:119:PRO:HD2	2:H:205:THR:HG21	1.97	0.46
1:D:120:PRO:HD3	1:D:132:VAL:HG22	1.98	0.46
1:O:108:ARG:HD2	1:O:170:ASP:O	2.16	0.46
2:E:27:TYR:CE2	2:E:94:ARG:HD2	2.51	0.46
2:E:127:SER:O	2:E:131:THR:HG23	2.15	0.46
1:G:14:THR:HB	1:G:17:GLN:HG2	1.98	0.46
1:G:91:GLY:HA2	1:G:96:ARG:HD2	1.98	0.46
2:B:198:VAL:O	2:B:206:LYS:HD2	2.16	0.46
1:O:2:VAL:HG13	1:O:27:GLN:HG2	1.98	0.46
1:L:34:ASN:HB2	1:L:89:TRP:NE1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:145:LYS:HB3	1:L:197:THR:OG1	2.16	0.46
2:M:196:CYS:O	2:M:208:ASP:HA	2.16	0.46
1:L:107:LYS:HG2	2:Q:172:SER:HA	1.98	0.45
1:L:162:SER:HB2	2:H:169:VAL:HG13	1.97	0.45
1:A:210:ASN:O	1:A:213:GLU:HG2	2.16	0.45
1:L:151:ASP:O	3:F:392:ILE:HG13	2.16	0.45
2:H:9:PRO:HD2	2:H:201:LYS:HD2	1.99	0.45
2:B:108:LEU:HD23	2:B:149:PRO:HD3	1.98	0.45
1:D:36:LEU:HD23	1:D:46:ARG:HA	1.97	0.45
1:G:119:PRO:HB3	1:G:209:PHE:CZ	2.51	0.45
1:O:46:ARG:HH11	1:O:46:ARG:N	2.12	0.45
1:A:36:LEU:HD23	1:A:46:ARG:HA	1.99	0.45
1:A:189:HIS:O	1:A:211:ARG:HD3	2.17	0.45
2:I:126:PRO:HA	2:I:130:SER:OG	2.16	0.45
2:Q:34:ILE:HG21	2:Q:78:ALA:HB3	1.99	0.45
2:H:12:VAL:HG21	2:H:82(C):LEU:CD1	2.47	0.45
2:M:60:ASN:HB3	2:M:63:PHE:HD2	1.81	0.45
1:O:34:ASN:O	1:O:88:CYS:HA	2.16	0.45
1:L:27(D):ASP:HB3	1:L:28:ASP:OD1	2.17	0.44
1:A:143:GLU:H	1:A:143:GLU:CD	2.25	0.44
2:M:138:LEU:HD22	2:M:182:VAL:HG12	2.00	0.44
1:O:46:ARG:HD2	1:O:46:ARG:N	2.30	0.44
1:L:175:LEU:HD23	1:L:176:SER:N	2.32	0.44
2:H:108:LEU:HD23	2:H:149:PRO:HD3	2.00	0.44
1:D:35:TRP:HB2	1:D:48:ILE:HB	1.99	0.44
1:D:83:LEU:HD21	1:D:106:ILE:HG13	2.00	0.44
2:H:35:HIS:CE1	2:H:50:GLY:HA3	2.52	0.44
1:D:13:VAL:HG11	1:D:19:ALA:HB2	1.99	0.44
1:K:191:VAL:HG12	4:K:341:HOH:O	2.17	0.44
2:I:145:TYR:CE1	2:I:150:VAL:HG13	2.52	0.44
1:O:79:GLU:HB3	1:O:81:GLU:OE2	2.17	0.44
1:K:173:TYR:OH	4:K:302:HOH:O	2.17	0.44
1:L:40:PRO:O	1:L:42:GLN:HG3	2.18	0.44
2:H:95:GLY:HA2	2:H:96:PRO:C	2.42	0.44
1:K:188:LYS:HE3	4:K:381:HOH:O	2.18	0.44
2:M:143:LYS:HG2	2:M:144:ASP:CG	2.43	0.44
1:O:142:ARG:HG3	1:O:173:TYR:CD2	2.52	0.44
2:Q:82(C):LEU:HD23	2:Q:86:ASP:OD2	2.17	0.44
1:K:34:ASN:HB2	1:K:89:TRP:CE2	2.53	0.43
2:H:210:ARG:HG2	2:H:212:GLU:HG3	2.00	0.43
1:O:116:PHE:CD2	1:O:135:LEU:HD13	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:190:GLY:HA2	2:B:155:ASN:HD22	1.83	0.43
2:E:51:ILE:HA	2:E:56:GLY:O	2.19	0.43
1:O:36:LEU:HD11	2:Q:103:TRP:CZ2	2.54	0.43
2:Q:143:LYS:HG3	2:Q:177:SER:OG	2.19	0.43
2:E:35:HIS:CE1	2:E:50:GLY:HA3	2.54	0.43
2:E:36:TRP:HA	2:E:91:TYR:O	2.18	0.43
1:O:108:ARG:HG3	1:O:171:SER:HB2	2.01	0.43
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.99	0.43
1:D:195:GLU:HG3	1:D:206:THR:HG22	2.00	0.43
1:G:61:ARG:HD2	1:G:77:ARG:O	2.19	0.43
2:B:29:PHE:HB2	2:B:76:LYS:HE3	2.00	0.43
1:D:207:LYS:HA	1:D:207:LYS:HD3	1.85	0.43
1:K:72:THR:HG22	1:K:74:LYS:HG3	2.01	0.43
2:B:131:THR:HG22	2:B:136:ALA:HB2	2.01	0.42
2:M:199:ASN:ND2	2:M:201:LYS:HG2	2.34	0.42
1:L:13:VAL:HG11	1:L:78:VAL:HG21	2.01	0.42
2:B:38:LYS:HB2	2:B:48:ILE:HD11	2.01	0.42
1:O:36:LEU:O	1:O:86:TYR:HA	2.19	0.42
1:O:197:THR:HG22	1:O:204:PRO:HG3	2.01	0.42
2:H:12:VAL:HG21	2:H:82(C):LEU:HD12	2.01	0.42
2:B:39:GLN:HB2	2:B:45:LEU:HD23	2.01	0.42
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.54	0.42
1:A:120:PRO:HD3	1:A:132:VAL:HG22	2.00	0.42
2:B:178:LEU:HA	4:B:309:HOH:O	2.18	0.42
2:E:131:THR:HG22	2:E:136:ALA:CB	2.49	0.42
2:I:82(C):LEU:HA	2:I:82(C):LEU:HD23	1.74	0.42
1:O:89:TRP:CH2	2:Q:100:PHE:HB2	2.54	0.42
1:D:213:GLU:OE2	2:E:129:LYS:HE2	2.20	0.42
2:Q:6:GLN:OE1	2:Q:91:TYR:HA	2.20	0.42
1:K:201:LEU:HD13	1:K:205:VAL:HG23	2.02	0.42
1:O:25:SER:O	1:O:69:THR:HB	2.20	0.42
1:K:89:TRP:HB3	1:K:98:PHE:CD2	2.55	0.42
2:M:35:HIS:CE1	2:M:50:GLY:HA3	2.54	0.42
1:A:201:LEU:HD13	1:A:205:VAL:HG23	2.02	0.41
2:B:35:HIS:CE1	2:B:50:GLY:HA3	2.55	0.41
1:G:154:LEU:HG	1:G:155:GLN:N	2.25	0.41
2:H:51:ILE:HG13	2:H:57:THR:HG22	2.02	0.41
2:B:96:PRO:HB2	2:B:99:ARG:HD2	2.02	0.41
2:Q:8:GLY:O	2:Q:107:THR:HG23	2.19	0.41
2:Q:12:VAL:HG21	2:Q:82(C):LEU:HD13	2.01	0.41
1:K:31:THR:O	1:K:50:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:TYR:CZ	2:H:94:ARG:HD2	2.55	0.41
1:K:27:GLN:HG2	1:K:27(A):SER:H	1.85	0.41
1:K:34:ASN:O	1:K:88:CYS:HA	2.21	0.41
1:K:35:TRP:HA	1:K:87:TYR:O	2.20	0.41
1:K:46:ARG:NH1	2:M:99:ARG:HB3	2.35	0.41
1:K:191:VAL:HG22	1:K:210:ASN:OD1	2.19	0.41
1:O:35:TRP:CZ3	1:O:88:CYS:HB3	2.55	0.41
2:M:82:LEU:HB3	2:M:82(C):LEU:HD21	2.03	0.41
2:Q:19:LYS:HD3	2:Q:79:TYR:HD2	1.83	0.41
2:Q:51:ILE:HG13	2:Q:52:ASN:N	2.34	0.41
1:L:16:GLY:O	1:L:77:ARG:HG2	2.21	0.41
1:A:48:ILE:HG23	1:A:53:LYS:O	2.21	0.41
1:L:80:ALA:HA	1:L:106:ILE:CD1	2.51	0.41
2:H:195:ILE:HA	2:H:209:LYS:O	2.21	0.41
1:A:149:LYS:HD3	1:A:154:LEU:HD22	2.03	0.41
1:G:148:TRP:HB2	1:G:155:GLN:HB2	2.03	0.41
2:I:139:GLY:HA2	2:I:154:TRP:CZ2	2.56	0.41
2:Q:14:PRO:HD3	2:Q:112:SER:C	2.44	0.41
1:A:46:ARG:NH2	2:B:99:ARG:HB3	2.35	0.41
1:K:14:THR:OG1	1:K:107:LYS:HE3	2.21	0.41
1:O:124:GLN:HG3	2:Q:122:PHE:CZ	2.55	0.41
2:Q:6:GLN:HE21	2:Q:6:GLN:HB3	1.68	0.41
1:K:61:ARG:HD2	1:K:77:ARG:O	2.21	0.41
1:K:120:PRO:HD3	1:K:132:VAL:HG22	2.02	0.41
1:G:33:LEU:HG	1:G:34:ASN:N	2.34	0.40
1:L:151:ASP:O	1:L:152:ASN:CB	2.69	0.40
2:E:209:LYS:HA	2:E:209:LYS:HD3	1.91	0.40
1:O:76:SER:O	1:O:77:ARG:HD2	2.21	0.40
1:K:37:LEU:HD13	1:K:86:TYR:CZ	2.57	0.40
2:E:95:GLY:HA2	2:E:96:PRO:C	2.46	0.40
2:E:199:ASN:HD21	1:G:27(A):SER:H	1.69	0.40
2:I:23:LYS:HG2	2:I:77:THR:OG1	2.21	0.40
1:O:46:ARG:HG2	2:Q:101:PRO:HA	2.01	0.40
2:Q:29:PHE:CD2	2:Q:76:LYS:HA	2.56	0.40
2:H:11:LEU:HD11	2:H:112:SER:HB3	2.02	0.40
1:A:14:THR:HA	1:A:107:LYS:HB2	2.03	0.40
2:M:162:GLY:O	2:M:182:VAL:HA	2.21	0.40
2:Q:192:GLN:HG2	2:Q:193:THR:H	1.86	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	217/219 (99%)	211 (97%)	5 (2%)	1 (0%)	24	34
1	D	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
1	G	217/219 (99%)	212 (98%)	5 (2%)	0	100	100
1	K	217/219 (99%)	210 (97%)	7 (3%)	0	100	100
1	L	217/219 (99%)	210 (97%)	5 (2%)	2 (1%)	14	20
1	O	217/219 (99%)	203 (94%)	14 (6%)	0	100	100
2	B	218/223 (98%)	213 (98%)	5 (2%)	0	100	100
2	E	218/223 (98%)	215 (99%)	3 (1%)	0	100	100
2	H	219/223 (98%)	211 (96%)	8 (4%)	0	100	100
2	I	218/223 (98%)	210 (96%)	8 (4%)	0	100	100
2	M	218/223 (98%)	211 (97%)	7 (3%)	0	100	100
2	Q	218/223 (98%)	207 (95%)	11 (5%)	0	100	100
3	C	6/23 (26%)	6 (100%)	0	0	100	100
3	F	6/23 (26%)	6 (100%)	0	0	100	100
3	J	5/23 (22%)	5 (100%)	0	0	100	100
3	N	6/23 (26%)	6 (100%)	0	0	100	100
3	P	3/23 (13%)	3 (100%)	0	0	100	100
3	R	3/23 (13%)	3 (100%)	0	0	100	100
All	All	2640/2790 (95%)	2553 (97%)	84 (3%)	3 (0%)	48	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	GLU
1	L	152	ASN
1	L	158	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/194 (100%)	180 (93%)	14 (7%)	13	18
1	D	194/194 (100%)	182 (94%)	12 (6%)	16	24
1	G	194/194 (100%)	171 (88%)	23 (12%)	5	5
1	K	194/194 (100%)	176 (91%)	18 (9%)	8	10
1	L	194/194 (100%)	180 (93%)	14 (7%)	13	18
1	O	194/194 (100%)	179 (92%)	15 (8%)	12	17
2	B	188/191 (98%)	176 (94%)	12 (6%)	16	23
2	E	188/191 (98%)	177 (94%)	11 (6%)	18	27
2	H	189/191 (99%)	176 (93%)	13 (7%)	14	20
2	I	188/191 (98%)	175 (93%)	13 (7%)	14	20
2	M	188/191 (98%)	178 (95%)	10 (5%)	20	31
2	Q	188/191 (98%)	171 (91%)	17 (9%)	9	11
3	C	8/19 (42%)	6 (75%)	2 (25%)	0	0
3	F	8/19 (42%)	7 (88%)	1 (12%)	4	4
3	J	7/19 (37%)	5 (71%)	2 (29%)	0	0
3	N	8/19 (42%)	5 (62%)	3 (38%)	0	0
3	P	5/19 (26%)	5 (100%)	0	100	100
3	R	5/19 (26%)	4 (80%)	1 (20%)	1	1
All	All	2334/2424 (96%)	2153 (92%)	181 (8%)	11	16

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	THR
1	L	24	LYS
1	L	46	ARG
1	L	47	LEU
1	L	55	ASP
1	L	63	THR

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Mol	Chain	Res	Type
1	L	81	GLU
1	L	108	ARG
1	L	129	THR
1	L	135	LEU
1	L	147	GLN
1	L	156	SER
1	L	160	GLN
1	L	206	THR
2	H	12	VAL
2	H	71	VAL
2	H	85	GLU
2	H	116	THR
2	H	129	LYS
2	H	135	THR
2	H	138	LEU
2	H	178	LEU
2	H	181	VAL
2	H	183	THR
2	H	186	SER
2	H	209	LYS
2	H	215	SER
1	A	7	THR
1	A	33	LEU
1	A	43	SER
1	A	46	ARG
1	A	70	ASP
1	A	77	ARG
1	A	81	GLU
1	A	108	ARG
1	A	135	LEU
1	A	145	LYS
1	A	146	VAL
1	A	149	LYS
1	A	154	LEU
1	A	207	LYS
2	B	46	GLU
2	B	61	GLN
2	B	85	GLU
2	B	138	LEU
2	B	147	PRO
2	B	151	THR
2	B	159	LEU

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Mol	Chain	Res	Type
2	B	178	LEU
2	B	181	VAL
2	B	183	THR
2	B	209	LYS
2	B	210	ARG
3	C	392	ILE
3	C	395	LYS
1	D	13	VAL
1	D	46	ARG
1	D	47	LEU
1	D	55	ASP
1	D	104	LEU
1	D	108	ARG
1	D	135	LEU
1	D	146	VAL
1	D	156	SER
1	D	190	LYS
1	D	202	SER
1	D	206	THR
2	E	17	SER
2	E	18	VAL
2	E	73	LYS
2	E	85	GLU
2	E	138	LEU
2	E	161	SER
2	E	170	LEU
2	E	183	THR
2	E	187	SER
2	E	199	ASN
2	E	209	LYS
3	F	393	VAL
1	G	5	THR
1	G	9	LEU
1	G	22	SER
1	G	27	GLN
1	G	27(A)	SER
1	G	27(B)	LEU
1	G	27(C)	LEU
1	G	27(D)	ASP
1	G	27(E)	SER
1	G	30	LYS
1	G	45	LYS

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Mol	Chain	Res	Type
1	G	47	LEU
1	G	104	LEU
1	G	108	ARG
1	G	135	LEU
1	G	147	GLN
1	G	154	LEU
1	G	156	SER
1	G	188	LYS
1	G	190	LYS
1	G	197	THR
1	G	213	GLU
1	G	214	CYS
2	I	10	GLU
2	I	12	VAL
2	I	40	SER
2	I	62	LYS
2	I	71	VAL
2	I	117	LYS
2	I	138	LEU
2	I	151	THR
2	I	178	LEU
2	I	181	VAL
2	I	183	THR
2	I	186	SER
2	I	191	THR
3	J	398	VAL
3	J	399	VAL
1	K	9	LEU
1	K	13	VAL
1	K	15	ILE
1	K	33	LEU
1	K	47	LEU
1	K	54	LEU
1	K	55	ASP
1	K	81	GLU
1	K	104	LEU
1	K	108	ARG
1	K	127	SER
1	K	135	LEU
1	K	143	GLU
1	K	146	VAL
1	K	154	LEU

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Mol	Chain	Res	Type
1	K	187	GLU
1	K	190	LYS
1	K	197	THR
2	M	46	GLU
2	M	71	VAL
2	M	117	LYS
2	M	138	LEU
2	M	140	CYS
2	M	151	THR
2	M	161	SER
2	M	178	LEU
2	M	181	VAL
2	M	209	LYS
3	N	391	GLU
3	N	393	VAL
3	N	398	VAL
1	O	7	THR
1	O	10	THR
1	O	15	ILE
1	O	46	ARG
1	O	47	LEU
1	O	49	TYR
1	O	81	GLU
1	O	104	LEU
1	O	108	ARG
1	O	135	LEU
1	O	146	VAL
1	O	147	GLN
1	O	160	GLN
1	O	207	LYS
1	O	214	CYS
2	Q	21	SER
2	Q	30	THR
2	Q	33	THR
2	Q	43	GLU
2	Q	51	ILE
2	Q	52	ASN
2	Q	52(A)	PRO
2	Q	54	ASP
2	Q	71	VAL
2	Q	128	SER
2	Q	138	LEU

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Mol	Chain	Res	Type
2	Q	160	THR
2	Q	161	SER
2	Q	183	THR
2	Q	186	SER
2	Q	197	ASN
2	Q	216	CYS
3	R	393	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	138	ASN
2	B	164	HIS
1	D	138	ASN
2	E	3	GLN
2	E	164	HIS
2	E	199	ASN
2	M	164	HIS
1	O	27	GLN
1	O	138	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SEP	J	396	3	8,9,10	1.51	1 (12%)	7,12,14	1.51	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SEP	R	396	3	8,9,10	1.73	1 (12%)	7,12,14	1.70	1 (14%)
3	SEP	F	396	3	8,9,10	1.58	1 (12%)	7,12,14	1.44	1 (14%)
3	SEP	P	396	3	8,9,10	1.76	2 (25%)	7,12,14	1.33	1 (14%)
3	SEP	N	396	3	8,9,10	1.51	1 (12%)	7,12,14	1.27	1 (14%)
3	SEP	C	396	3	8,9,10	1.47	1 (12%)	7,12,14	1.39	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SEP	J	396	3	-	1/6/8/10	-
3	SEP	R	396	3	-	0/6/8/10	-
3	SEP	F	396	3	-	0/6/8/10	-
3	SEP	P	396	3	-	0/6/8/10	-
3	SEP	N	396	3	-	0/6/8/10	-
3	SEP	C	396	3	-	3/6/8/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	396	SEP	P-O1P	3.85	1.62	1.50
3	R	396	SEP	P-O1P	3.73	1.62	1.50
3	F	396	SEP	P-O1P	3.48	1.61	1.50
3	N	396	SEP	P-O1P	3.35	1.60	1.50
3	J	396	SEP	P-O1P	3.33	1.60	1.50
3	C	396	SEP	P-O1P	2.91	1.59	1.50
3	P	396	SEP	P-O2P	2.01	1.62	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	396	SEP	OG-CB-CA	3.86	111.90	108.14
3	C	396	SEP	OG-CB-CA	2.56	110.63	108.14
3	J	396	SEP	OG-P-O1P	2.47	113.13	106.44
3	P	396	SEP	OG-P-O1P	2.41	112.95	106.44
3	N	396	SEP	OG-CB-CA	2.15	110.24	108.14
3	F	396	SEP	OG-CB-CA	2.07	110.16	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	396	SEP	CB-OG-P-O1P
3	C	396	SEP	CB-OG-P-O2P
3	J	396	SEP	CB-OG-P-O1P
3	C	396	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	219/219 (100%)	-0.32	1 (0%) 87 89	21, 31, 45, 71	0
1	D	219/219 (100%)	-0.32	0 100 100	22, 34, 47, 63	0
1	G	219/219 (100%)	-0.19	6 (2%) 56 57	20, 32, 63, 94	0
1	K	219/219 (100%)	-0.12	1 (0%) 87 89	23, 37, 52, 79	0
1	L	219/219 (100%)	-0.15	1 (0%) 87 89	23, 38, 52, 63	0
1	O	219/219 (100%)	0.62	25 (11%) 10 9	23, 54, 89, 102	0
2	B	220/223 (98%)	-0.26	1 (0%) 87 89	21, 33, 52, 71	0
2	E	220/223 (98%)	-0.38	0 100 100	20, 30, 48, 61	0
2	H	221/223 (99%)	-0.19	1 (0%) 87 89	21, 36, 54, 66	0
2	I	220/223 (98%)	-0.18	2 (0%) 81 83	23, 35, 57, 97	0
2	M	220/223 (98%)	-0.22	1 (0%) 87 89	23, 34, 53, 83	0
2	Q	220/223 (98%)	0.83	34 (15%) 5 4	26, 56, 90, 95	0
3	C	8/23 (34%)	0.18	0 100 100	35, 43, 55, 76	0
3	F	8/23 (34%)	0.27	0 100 100	36, 44, 61, 71	0
3	J	7/23 (30%)	0.27	0 100 100	30, 38, 48, 49	0
3	N	8/23 (34%)	-0.02	0 100 100	33, 40, 54, 69	0
3	P	5/23 (21%)	1.32	2 (40%) 1 0	48, 52, 57, 60	0
3	R	5/23 (21%)	2.78	4 (80%) 0 0	88, 88, 89, 91	0
All	All	2676/2790 (95%)	-0.06	79 (2%) 52 54	20, 36, 76, 102	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	77	THR	4.3
3	R	397	PRO	4.0
2	Q	78	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	184	ALA	3.7
2	Q	4	LEU	3.6
1	O	94	PHE	3.5
2	Q	30	THR	3.4
1	O	93	HIS	3.3
1	A	214	CYS	3.3
2	Q	32	TYR	3.3
2	Q	2	VAL	3.3
1	O	54	LEU	3.2
2	Q	216	CYS	3.2
2	Q	33	THR	3.2
1	O	49	TYR	3.2
2	Q	79	TYR	3.2
2	I	216	CYS	3.2
2	Q	18	VAL	3.1
3	R	393	VAL	3.1
3	P	398	VAL	3.1
2	Q	34	ILE	3.0
1	O	89	TRP	3.0
2	Q	51	ILE	2.9
2	Q	214	LYS	2.9
1	G	154	LEU	2.9
2	Q	102	TYR	2.9
2	H	42	GLY	2.9
3	R	394	TYR	2.8
1	O	97	THR	2.8
1	O	2	VAL	2.7
2	Q	69	LEU	2.7
2	Q	35	HIS	2.7
1	O	62	PHE	2.6
2	Q	29	PHE	2.6
1	O	214	CYS	2.6
1	O	50	LEU	2.6
2	Q	70	THR	2.6
2	Q	53	ASN	2.6
1	O	27(B)	LEU	2.6
3	R	398	VAL	2.6
2	Q	24	THR	2.6
2	Q	93	ALA	2.5
2	I	215	SER	2.5
2	Q	20	ILE	2.4
1	O	32	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	214	CYS	2.4
2	Q	27	TYR	2.4
2	M	18	VAL	2.4
2	Q	10	GLU	2.4
2	Q	73	LYS	2.4
2	Q	52	ASN	2.3
1	O	92	THR	2.3
1	O	27(E)	SER	2.3
2	Q	58	ILE	2.3
1	L	157	GLY	2.3
1	O	64	GLY	2.2
1	O	27(C)	LEU	2.2
2	Q	63	PHE	2.2
1	G	128	GLY	2.2
2	Q	75	SER	2.2
1	G	211	ARG	2.2
1	O	58	VAL	2.2
1	O	59	PRO	2.2
1	O	18	PRO	2.1
2	Q	56	GLY	2.1
2	Q	31	GLU	2.1
2	Q	99	ARG	2.1
1	O	75	ILE	2.1
1	K	214	CYS	2.1
2	Q	71	VAL	2.1
3	P	393	VAL	2.1
1	O	11	LEU	2.1
1	O	16	GLY	2.1
1	G	188	LYS	2.1
1	O	46	ARG	2.0
2	B	18	VAL	2.0
1	O	33	LEU	2.0
1	O	4	MET	2.0
2	Q	52(A)	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SEP	R	396	10/11	0.74	0.13	78,92,99,99	0
3	SEP	P	396	10/11	0.92	0.10	39,49,54,55	0
3	SEP	F	396	10/11	0.96	0.07	29,35,37,39	0
3	SEP	J	396	10/11	0.98	0.05	24,27,35,36	0
3	SEP	N	396	10/11	0.98	0.06	27,30,32,34	0
3	SEP	C	396	10/11	0.98	0.06	27,35,39,40	0

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.