



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:47 AM UTC

PDB ID : 7DR4 / pdb_00007dr4
Title : Complex of anti-human IL-2 antibody and human IL-2
Authors : Kim, M.S.; Kim, J.E.
Deposited on : 2020-12-25
Resolution : 2.49 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

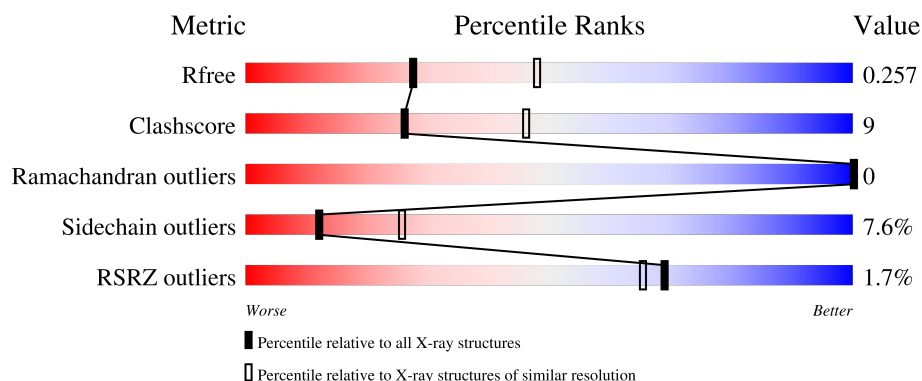
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	224	3% 72% 20% 5%
1	C	224	% 80% 14% .
1	E	224	76% 19% .
1	H	224	2% 80% 17% ..
2	B	214	6% 58% 22% . 16%

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Mol	Chain	Length	Quality of chain
2	D	214	77%21%•
2	F	214	% 75%21%••
2	L	214	72%22%••
3	G	133	2% 74%15%•8%
3	I	133	% 71%20%•8%
3	J	133	77%17%6%
3	K	133	% 64%25%•8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17347 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 anti-human IL-2 antibody, mouse Ig G, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	221	Total	C	N	O	S	0	0	0
			1661	1049	274	331	7			
1	A	212	Total	C	N	O	S	0	0	0
			1599	1013	262	318	6			
1	C	218	Total	C	N	O	S	0	0	0
			1643	1040	271	326	6			
1	E	216	Total	C	N	O	S	0	0	0
			1629	1031	269	323	6			

- Molecule 2 is a protein called anti-human IL-2 antibody, mouse Ig G, kappa chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	1	0
			1654	1030	272	343	9			
2	B	179	Total	C	N	O	S	0	0	0
			1376	864	219	285	8			
2	D	213	Total	C	N	O	S	0	1	0
			1663	1035	273	346	9			
2	F	211	Total	C	N	O	S	0	1	0
			1646	1026	270	341	9			

- Molecule 3 is a protein called Interleukin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	123	Total	C	N	O	S	0	0	0
			1015	656	168	184	7			
3	I	122	Total	C	N	O	S	0	0	0
			1008	652	167	182	7			
3	J	125	Total	C	N	O	S	0	0	0
			1027	662	170	188	7			
3	K	122	Total	C	N	O	S	0	0	0
			1004	646	167	185	6			

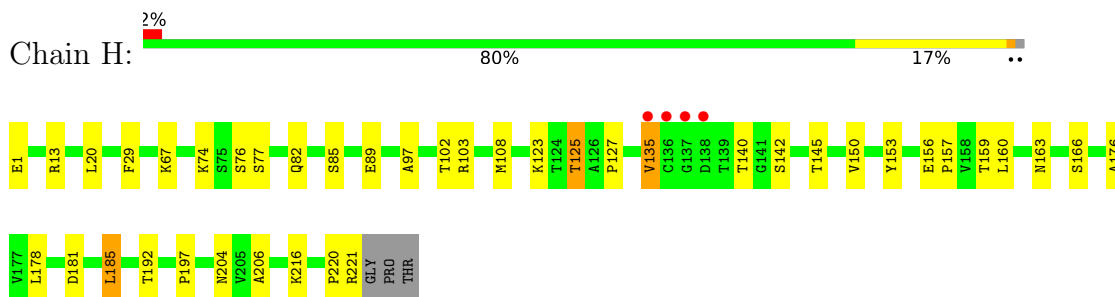
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	27	Total 27	O 27	0	0
4	L	42	Total 42	O 42	0	0
4	A	41	Total 41	O 41	0	0
4	B	52	Total 52	O 52	0	0
4	C	76	Total 76	O 76	0	0
4	D	72	Total 72	O 72	0	0
4	E	13	Total 13	O 13	0	0
4	F	16	Total 16	O 16	0	0
4	G	29	Total 29	O 29	0	0
4	I	8	Total 8	O 8	0	0
4	J	36	Total 36	O 36	0	0
4	K	10	Total 10	O 10	0	0

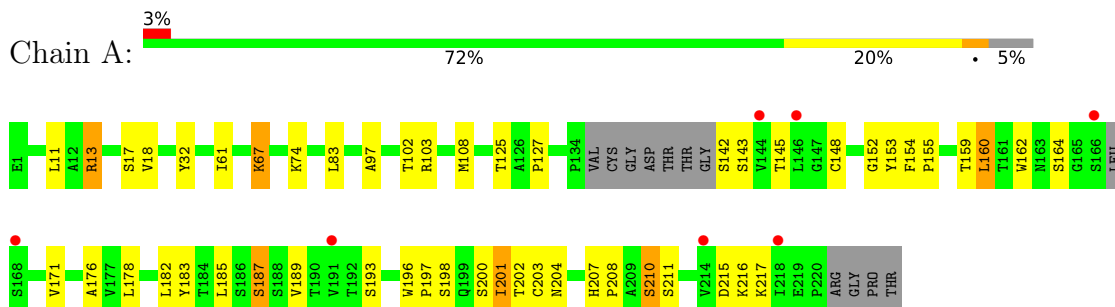
3 Residue-property plots [i](#)

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.

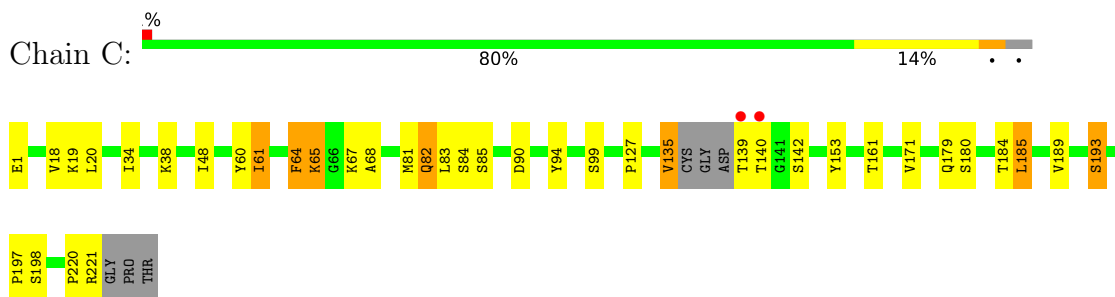
- Molecule 1: anti-human IL-2 antibody, mouse Ig G, heavy chain



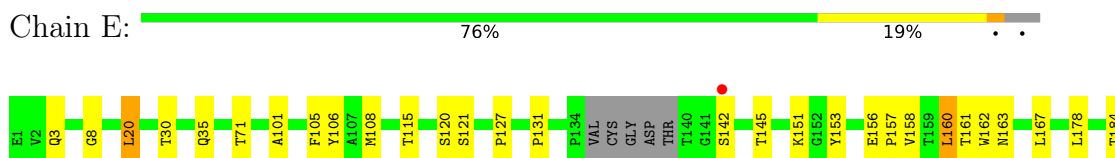
- Molecule 1: anti-human IL-2 antibody, mouse Ig G, heavy chain



- Molecule 1: anti-human IL-2 antibody, mouse Ig G, heavy chain



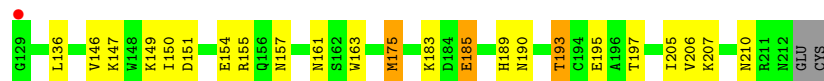
- Molecule 1: anti-human IL-2 antibody, mouse Ig G, heavy chain





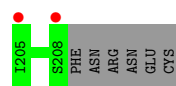
- Molecule 2: anti-human IL-2 antibody, mouse Ig G, kappa chain

Chain L: 72% 22% . .



- Molecule 2: anti-human IL-2 antibody, mouse Ig G, kappa chain

Chain B: 6% 58% 22% 16%



- Molecule 2: anti-human IL-2 antibody, mouse Ig G, kappa chain

Chain D: 77% 21%

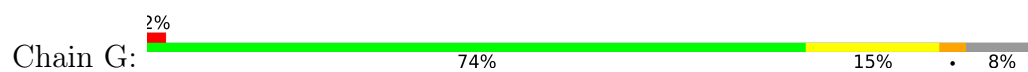


- Molecule 2: anti-human IL-2 antibody, mouse Ig G, kappa chain

Chain F: 75% 21%



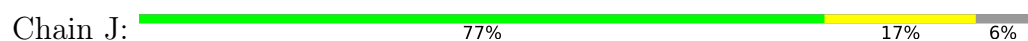
- Molecule 3: Interleukin-2



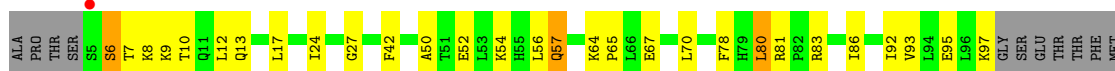
• Molecule 3: Interleukin-2



• Molecule 3: Interleukin-2



• Molecule 3: Interleukin-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.33Å 72.26Å 210.93Å 90.00° 92.71° 90.00°	Depositor
Resolution (Å)	29.79 – 2.49 29.79 – 2.49	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.79-2.49) 95.8 (29.79-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.195 , 0.258 0.192 , 0.257	Depositor DCC
R_{free} test set	1997 reflections (2.38%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17347	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.37	0/1639	0.60	0/2236
1	C	0.44	0/1684	0.69	1/2299 (0.0%)
1	E	0.34	0/1670	0.56	0/2279
1	H	0.32	0/1703	0.56	0/2326
2	B	0.45	0/1403	0.64	1/1906 (0.1%)
2	D	0.46	0/1699	0.69	0/2308
2	F	0.36	0/1682	0.57	0/2285
2	L	0.38	0/1690	0.60	1/2296 (0.0%)
3	G	0.42	0/1031	0.54	0/1388
3	I	0.37	0/1024	0.52	0/1378
3	J	0.44	0/1043	0.61	0/1404
3	K	0.31	0/1019	0.46	0/1373
All	All	0.39	0/17287	0.60	3/23478 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	31	ASP	CA-CB-CG	5.82	118.42	112.60
2	B	31	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	64	PHE	N-CA-C	5.30	119.37	113.01

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	1599	0	1555	37	0
1	C	1643	0	1606	24	0
1	E	1629	0	1590	28	0
1	H	1661	0	1619	19	0
2	B	1376	0	1335	51	0
2	D	1663	0	1587	40	0
2	F	1646	0	1575	33	0
2	L	1654	0	1581	34	0
3	G	1015	0	1055	17	0
3	I	1008	0	1048	14	0
3	J	1027	0	1065	11	0
3	K	1004	0	1044	25	0
4	A	41	0	0	1	0
4	B	52	0	0	2	0
4	C	76	0	0	0	0
4	D	72	0	0	5	0
4	E	13	0	0	0	0
4	F	16	0	0	0	0
4	G	29	0	0	0	0
4	H	27	0	0	2	0
4	I	8	0	0	0	0
4	J	36	0	0	0	0
4	K	10	0	0	0	0
4	L	42	0	0	2	0
All	All	17347	0	16660	317	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 (317) 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:B:159:VAL:N	2:B:179:LEU:HD13	1.49	1.25
2:B:159:VAL:CA	2:B:179:LEU:HD13	1.69	1.23
2:D:2:ILE:HD11	2:D:93:ASN:HD21	1.08	1.13
2:F:30:ASP:HB3	2:F:67:TYR:CZ	1.86	1.09
2:B:159:VAL:N	2:B:179:LEU:CD1	2.16	1.07
2:D:30:ASP:HB3	2:D:67:TYR:CZ	1.92	1.04
2:B:159:VAL:HA	2:B:179:LEU:HD13	1.37	1.02
2:B:31:ASP:HB3	2:B:67:TYR:CD2	1.98	0.98
2:B:133:VAL:HG22	2:B:178:THR:CG2	1.97	0.94
2:B:133:VAL:CG2	2:B:178:THR:HG22	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:O	3:J:42:PHE:HA	1.71	0.90
2:B:133:VAL:HG22	2:B:178:THR:HG22	1.54	0.88
2:D:31:ASP:OD1	4:D:301:HOH:O	1.94	0.86
2:B:2:ILE:HD11	2:B:93:ASN:HD21	1.45	0.82
2:B:133:VAL:CG2	2:B:178:THR:CG2	2.59	0.80
1:C:61:ILE:HG22	1:C:64:PHE:HB2	1.63	0.80
3:K:57:GLN:HG2	3:K:97:LYS:HD2	1.65	0.79
2:L:15:ILE:HG23	2:L:106:ILE:HD11	1.63	0.79
2:F:2:ILE:HG13	2:F:93:ASN:HD21	1.47	0.79
2:D:2:ILE:CD1	2:D:93:ASN:HD21	1.94	0.78
2:L:108:ARG:NH1	2:L:109:ALA:O	2.16	0.78
2:B:25:THR:HG21	2:B:29:ILE:HD13	1.65	0.77
2:B:31:ASP:HB3	2:B:67:TYR:HD2	1.50	0.77
2:F:30:ASP:HB3	2:F:67:TYR:OH	1.83	0.77
2:D:2:ILE:HD11	2:D:93:ASN:ND2	1.94	0.76
1:H:135:VAL:HA	1:H:221:ARG:HD2	1.67	0.76
3:G:132:LEU:HD21	3:I:132:LEU:HD21	1.68	0.76
2:F:108:ARG:NH2	2:F:109:ALA:O	2.19	0.75
2:D:30:ASP:HB3	2:D:67:TYR:OH	1.88	0.72
1:E:127:PRO:HB3	1:E:153:TYR:HB3	1.70	0.72
1:A:32:TYR:CE1	1:A:102:THR:HG22	2.26	0.71
2:B:159:VAL:CA	2:B:179:LEU:CD1	2.60	0.71
1:E:156:GLU:HB2	1:E:157:PRO:HA	1.73	0.71
2:B:159:VAL:HA	2:B:179:LEU:CD1	2.18	0.70
2:L:31:ASP:HB3	2:L:67:TYR:CD1	2.26	0.70
3:K:80:LEU:HD12	3:K:81:ARG:H	1.57	0.70
2:D:190:ASN:OD1	2:D:212:ASN:ND2	2.26	0.69
2:L:13:MET:HG3	2:L:19:VAL:HG22	1.74	0.69
2:L:29:ILE:HD11	2:L:71:PHE:CZ	2.27	0.69
2:B:136:LEU:HD13	2:B:175:MET:HE2	1.75	0.69
2:D:3:VAL:HG22	2:D:26:SER:HB3	1.75	0.68
1:A:207:HIS:ND1	1:A:210:SER:OG	2.26	0.68
1:E:167:LEU:N	1:E:167:LEU:HD12	2.08	0.68
2:F:30:ASP:O	2:F:67:TYR:CD1	2.47	0.68
1:C:1:GLU:N	1:C:1:GLU:OE2	2.26	0.67
2:F:30:ASP:HB3	2:F:67:TYR:CE1	2.28	0.67
3:I:113:THR:HG22	3:I:115:VAL:H	1.59	0.67
1:A:204:ASN:ND2	1:A:215:ASP:OD2	2.28	0.66
2:B:4:MET:HE2	2:B:23:CYS:SG	2.35	0.66
2:D:30:ASP:HB3	2:D:67:TYR:CE1	2.31	0.66
2:F:187:GLU:O	2:F:211:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:127:PRO:HB3	1:H:153:TYR:HB3	1.78	0.65
1:C:19:LYS:HG3	1:C:82:GLN:HG2	1.80	0.64
1:E:160:LEU:HD12	1:E:185:LEU:HD21	1.80	0.64
2:L:149:LYS:HB2	2:L:193:THR:HG23	1.80	0.63
2:F:3:VAL:HB	2:F:26:SER:HB3	1.81	0.63
1:H:103:ARG:O	3:K:42:PHE:HA	1.98	0.63
1:E:163:ASN:HB2	1:E:167:LEU:HD13	1.80	0.63
3:K:6:SER:HA	3:K:9:LYS:HB3	1.79	0.63
2:L:161:ASN:HB3	2:L:175:MET:HE2	1.80	0.62
2:B:160:LEU:O	2:B:177:SER:HA	1.99	0.62
1:A:171:VAL:HG22	1:A:189:VAL:HG22	1.81	0.62
1:E:204:ASN:ND2	1:E:215:ASP:OD1	2.30	0.62
1:C:179:GLN:HB2	2:D:160:LEU:HD11	1.82	0.62
1:A:160:LEU:HD13	1:A:187:SER:HB2	1.81	0.62
2:D:29:ILE:HG13	2:D:29:ILE:O	2.00	0.61
3:J:112:ALA:HB1	3:J:116:GLU:HB2	1.82	0.61
2:L:39:LYS:NZ	4:L:304:HOH:O	2.34	0.61
1:C:67:LYS:HE3	1:C:84:SER:O	2.02	0.60
1:H:197:PRO:HG3	1:H:220:PRO:HG3	1.82	0.60
2:L:85:ASP:OD1	2:L:103:LYS:HD2	2.02	0.60
2:B:160:LEU:N	2:B:178:THR:O	2.34	0.60
1:C:38:LYS:HB2	1:C:48:ILE:HD11	1.83	0.60
1:C:67:LYS:HE2	1:C:90:ASP:OD2	2.02	0.60
2:F:110:ASP:OD2	2:F:199:LYS:NZ	2.25	0.59
3:G:48:LYS:HE3	3:G:106:GLU:HB3	1.84	0.59
1:A:196:TRP:HD1	1:A:201:ILE:HD13	1.68	0.58
2:D:193:THR:OG1	2:D:208:SER:HB3	2.03	0.58
2:B:133:VAL:HG23	2:B:178:THR:HG22	1.84	0.58
3:I:27:GLY:HA3	3:I:78:PHE:CZ	2.39	0.58
2:B:90:GLN:HE21	2:B:97:THR:CG2	2.17	0.58
2:F:4:MET:SD	2:F:25:THR:HG22	2.43	0.58
2:F:124:GLN:OE1	2:F:131:SER:N	2.36	0.58
1:A:196:TRP:CD1	1:A:201:ILE:HD13	2.38	0.57
2:D:13:MET:HG3	2:D:19:VAL:HG22	1.86	0.57
2:F:198:HIS:ND1	2:F:200:THR:HB	2.20	0.57
2:B:133:VAL:HA	2:B:178:THR:HG22	1.86	0.56
2:B:159:VAL:N	2:B:179:LEU:HD11	2.18	0.56
3:G:50:ALA:HB3	3:G:120:ARG:NH2	2.20	0.56
2:D:32:ASP:HA	2:D:50:GLU:HB3	1.86	0.56
1:C:48:ILE:HG23	1:C:64:PHE:CD2	2.41	0.56
3:G:112:ALA:HB1	3:G:116:GLU:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:ASP:O	2:D:67:TYR:CD1	2.59	0.55
2:B:2:ILE:O	2:B:97:THR:HG21	2.07	0.55
1:H:102:THR:HB	1:H:103:ARG:HG2	1.89	0.55
1:H:178:LEU:HD11	1:H:181:ASP:HA	1.88	0.55
2:B:2:ILE:HD11	2:B:93:ASN:ND2	2.19	0.55
2:D:77:ASN:HB2	4:D:360:HOH:O	2.07	0.54
2:L:163:TRP:CZ2	2:L:175:MET:HE3	2.42	0.54
2:F:59:PRO:HG2	2:F:62:PHE:CE2	2.42	0.54
1:E:8:GLY:N	3:K:7:THR:OG1	2.39	0.54
1:A:145:THR:HA	1:A:189:VAL:O	2.07	0.54
1:H:145:THR:HG21	2:L:116:SER:OG	2.08	0.54
3:G:27:GLY:HA3	3:G:78:PHE:CZ	2.43	0.54
3:K:56:LEU:HB3	3:K:93:VAL:HG13	1.90	0.53
1:A:18:VAL:HG12	1:A:83:LEU:HB2	1.90	0.53
2:B:13:MET:HG3	2:B:19:VAL:HG22	1.90	0.53
1:A:196:TRP:CG	1:A:197:PRO:HA	2.43	0.53
2:F:29:ILE:O	2:F:29:ILE:HG13	2.09	0.53
2:B:2:ILE:HG13	4:B:343:HOH:O	2.09	0.53
2:L:113:PRO:HG2	2:L:205:ILE:HD12	1.90	0.53
3:G:102:THR:O	3:G:102:THR:OG1	2.23	0.53
1:A:148:CYS:HB2	1:A:162:TRP:CH2	2.44	0.52
2:B:90:GLN:HE21	2:B:97:THR:HG22	1.74	0.52
3:K:67:GLU:HB2	3:K:86:ILE:HG13	1.92	0.52
1:A:142:SER:N	1:A:193:SER:HG	2.07	0.52
1:E:3:GLN:NE2	3:K:131:THR:O	2.43	0.52
2:B:180:THR:O	2:B:180:THR:HG22	2.09	0.52
1:E:167:LEU:N	1:E:167:LEU:CD1	2.73	0.51
3:I:46:MET:HE1	3:I:117:PHE:HA	1.92	0.51
1:E:151:LYS:HG3	1:E:184:THR:HG22	1.92	0.51
2:L:4:MET:SD	2:L:4:MET:N	2.83	0.51
3:K:24:ILE:HD13	3:K:70:LEU:HD21	1.93	0.51
2:F:59:PRO:HG2	2:F:62:PHE:HE2	1.76	0.51
2:F:32:ASP:HB2	2:F:92:ASP:HB2	1.93	0.51
2:L:155:ARG:NH2	2:L:185:GLU:OE1	2.44	0.50
1:C:197:PRO:HB3	1:C:220:PRO:HG3	1.93	0.50
2:D:22:ARG:HH11	2:D:22:ARG:HB2	1.76	0.50
2:D:78:MET:HE3	2:D:106:ILE:HD13	1.93	0.50
3:K:17:LEU:HD22	3:K:125:CYS:SG	2.51	0.50
2:D:8:PRO:HG3	2:D:11:LEU:HD13	1.94	0.50
3:K:113:THR:HG23	3:K:116:GLU:H	1.77	0.50
1:A:127:PRO:HB3	1:A:153:TYR:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:MET:SD	1:E:108:MET:N	2.84	0.50
1:C:161:THR:HG21	3:J:94:LEU:HD13	1.94	0.49
2:B:13:MET:HB2	2:B:78:MET:HG3	1.94	0.49
3:J:27:GLY:HA3	3:J:78:PHE:CZ	2.48	0.49
2:B:133:VAL:HG23	2:B:178:THR:CG2	2.42	0.49
1:A:176:ALA:HA	1:A:185:LEU:HB3	1.94	0.49
2:B:133:VAL:CG2	2:B:178:THR:HG21	2.42	0.49
2:F:30:ASP:O	2:F:67:TYR:CG	2.66	0.49
3:K:13:GLN:NE2	3:K:95:GLU:OE1	2.46	0.49
2:B:108:ARG:NE	2:B:170:ASP:O	2.46	0.49
1:E:20:LEU:HG	1:E:115:THR:HG21	1.95	0.49
2:F:195:GLU:HG2	2:F:206:VAL:HG22	1.94	0.49
3:K:50:ALA:HB3	3:K:120:ARG:NH2	2.28	0.49
2:D:13:MET:HB2	2:D:78:MET:HE2	1.94	0.49
3:I:112:ALA:HB1	3:I:116:GLU:HB2	1.95	0.48
3:J:70:LEU:HD22	3:J:80:LEU:HD21	1.94	0.48
3:I:46:MET:HA	3:I:46:MET:HE2	1.94	0.48
3:J:50:ALA:HB3	3:J:120:ARG:NH2	2.27	0.48
1:H:150:VAL:HB	1:H:185:LEU:CD1	2.43	0.48
1:H:185:LEU:HD12	1:H:185:LEU:H	1.79	0.48
1:A:32:TYR:CZ	1:A:102:THR:HG22	2.49	0.48
2:L:147:LYS:HE2	2:L:149:LYS:HE3	1.95	0.48
2:F:25:THR:HG21	2:F:29:ILE:HD13	1.95	0.48
2:L:108:ARG:O	4:L:301:HOH:O	2.19	0.48
1:E:196:TRP:CG	1:E:197:PRO:HA	2.49	0.48
2:L:13:MET:HB2	2:L:78:MET:HG3	1.96	0.48
1:A:32:TYR:CD1	1:A:102:THR:HG22	2.48	0.48
1:E:131:PRO:HD3	1:E:216:LYS:HD2	1.96	0.47
3:K:113:THR:CG2	3:K:116:GLU:H	2.27	0.47
2:F:30:ASP:O	2:F:67:TYR:HA	2.15	0.47
3:K:27:GLY:HA3	3:K:78:PHE:CZ	2.50	0.47
1:C:64:PHE:CE2	1:C:68:ALA:HB2	2.49	0.47
2:B:197:THR:HG22	2:B:204:PRO:HB3	1.96	0.47
1:E:142:SER:O	1:E:193:SER:HB2	2.14	0.47
1:E:161:THR:OG1	1:E:204:ASN:OD1	2.33	0.47
3:I:52:GLU:OE1	3:I:54:LYS:HE2	2.14	0.47
2:L:16:GLY:HA2	2:L:77:ASN:HB2	1.96	0.47
2:L:151:ASP:OD2	2:L:189:HIS:ND1	2.47	0.47
2:B:33:MET:SD	2:B:88:CYS:HB2	2.55	0.47
2:B:107:LYS:HA	2:B:140:TYR:OH	2.14	0.47
2:D:189:HIS:O	2:D:211:ARG:NH2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ALA:HB2	1:A:185:LEU:HD23	1.97	0.47
3:G:46:MET:HE1	3:G:117:PHE:HD2	1.81	0.46
1:E:160:LEU:HD13	1:E:187:SER:HB2	1.98	0.46
3:J:80:LEU:HD12	3:J:80:LEU:HA	1.81	0.46
1:A:13:ARG:HE	1:A:13:ARG:HB3	1.21	0.46
2:B:108:ARG:HD2	2:B:171:SER:O	2.16	0.46
1:A:74:LYS:HG3	4:A:324:HOH:O	2.15	0.46
2:B:4:MET:HE1	2:B:25:THR:CG2	2.46	0.46
2:D:34:ASN:OD1	2:D:49:SER:HA	2.16	0.46
2:F:122:SER:O	2:F:126:THR:HG23	2.15	0.46
2:D:30:ASP:O	2:D:67:TYR:HA	2.16	0.45
2:D:163:TRP:HD1	4:D:352:HOH:O	2.00	0.45
1:H:156:GLU:OE1	1:H:176:ALA:HB3	2.17	0.45
2:B:133:VAL:HG22	2:B:178:THR:HG21	1.92	0.45
1:C:142:SER:O	1:C:193:SER:HB3	2.15	0.45
3:G:97:LYS:O	3:G:97:LYS:HG2	2.16	0.45
3:K:64:LYS:HB2	3:K:65:PRO:HD3	1.96	0.45
2:D:123:GLU:HG2	4:D:353:HOH:O	2.16	0.45
1:E:151:LYS:HA	1:E:184:THR:HG22	1.99	0.45
3:K:13:GLN:HB3	3:K:92:ILE:HG23	1.98	0.45
2:D:35:TRP:CE2	2:D:73:PHE:HB2	2.51	0.45
1:C:48:ILE:HD13	1:C:48:ILE:HG21	1.72	0.45
1:C:127:PRO:HB3	1:C:153:TYR:HB3	1.98	0.45
2:B:159:VAL:HG22	2:B:179:LEU:HD22	1.98	0.45
2:B:167:ASP:OD1	2:B:169:LYS:HG2	2.16	0.45
1:H:76:SER:HA	1:A:164:SER:HB3	1.98	0.45
1:A:202:THR:OG1	1:A:217:LYS:HG2	2.17	0.45
2:L:29:ILE:HD13	2:L:33:MET:HE2	1.99	0.45
1:E:162:TRP:CZ3	1:E:203:CYS:HB3	2.52	0.45
1:E:196:TRP:CD1	1:E:197:PRO:HA	2.51	0.45
2:L:6:GLN:NE2	2:L:86:TYR:O	2.43	0.44
2:L:29:ILE:CD1	2:L:33:MET:HE2	2.48	0.44
1:C:68:ALA:HA	1:C:82:GLN:O	2.17	0.44
1:H:29:PHE:CD2	1:H:77:SER:HA	2.53	0.44
1:H:123:LYS:O	1:H:125:THR:HG22	2.17	0.44
2:B:29:ILE:HD11	2:B:71:PHE:CE2	2.52	0.44
2:D:163:TRP:CD1	4:D:352:HOH:O	2.69	0.44
2:L:29:ILE:HD11	2:L:71:PHE:CE2	2.53	0.44
1:C:64:PHE:CE2	1:C:68:ALA:CB	3.00	0.44
2:F:118:PHE:HA	2:F:119:PRO:HD3	1.81	0.44
2:L:31:ASP:OD1	3:I:81:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:VAL:HG22	2:D:119:PRO:HD3	1.99	0.44
3:G:27:GLY:HA3	3:G:78:PHE:CE2	2.52	0.44
1:A:200:SER:O	1:A:201:ILE:HD12	2.18	0.44
1:H:163:ASN:O	1:H:166:SER:HB3	2.17	0.44
2:L:29:ILE:CG1	2:L:71:PHE:CZ	3.00	0.44
2:F:2:ILE:HG13	2:F:93:ASN:ND2	2.24	0.44
1:C:185:LEU:C	1:C:185:LEU:HD12	2.42	0.44
3:K:52:GLU:HB2	3:K:54:LYS:HG2	2.00	0.44
1:A:97:ALA:HB1	1:A:108:MET:HB3	1.99	0.44
1:A:207:HIS:CE1	1:A:210:SER:HG	2.35	0.44
1:E:162:TRP:CH2	1:E:203:CYS:HB3	2.53	0.44
3:K:131:THR:HG22	3:K:132:LEU:HD23	2.00	0.44
3:J:23:MET:HE1	3:J:85:LEU:HD22	2.00	0.44
3:J:67:GLU:HG3	3:J:86:ILE:HG13	1.98	0.44
2:D:22:ARG:HB2	2:D:22:ARG:NH1	2.33	0.43
1:E:105:PHE:CD2	2:F:94:LEU:HD11	2.52	0.43
1:A:103:ARG:O	3:J:43:LYS:N	2.49	0.43
2:B:118:PHE:HA	2:B:119:PRO:HD3	1.86	0.43
2:B:125:LEU:HD13	2:B:125:LEU:HA	1.75	0.43
3:G:13:GLN:NE2	3:G:95:GLU:OE1	2.51	0.43
3:G:94:LEU:HD23	3:G:94:LEU:HA	1.84	0.43
2:L:190:ASN:O	2:L:210:ASN:HA	2.19	0.43
2:D:136:LEU:N	2:D:136:LEU:HD12	2.34	0.43
2:F:11:LEU:HD12	2:F:11:LEU:HA	1.79	0.43
3:I:90:ASN:O	3:I:94:LEU:HG	2.18	0.43
1:A:202:THR:HA	1:A:216:LYS:O	2.19	0.43
2:F:2:ILE:HD13	2:F:27:THR:OG1	2.19	0.43
2:F:182:THR:OG1	2:F:185:GLU:HG3	2.19	0.43
3:I:83:ARG:NH2	3:K:83:ARG:HD3	2.34	0.43
3:K:8:LYS:O	3:K:12:LEU:HB2	2.19	0.43
3:K:70:LEU:HD23	3:K:70:LEU:HA	1.83	0.43
2:L:19:VAL:CG2	2:L:78:MET:HG2	2.49	0.43
1:A:32:TYR:CE1	1:A:102:THR:CG2	3.00	0.43
2:B:55:ARG:HD3	4:B:304:HOH:O	2.18	0.43
2:D:105:GLU:HB3	2:D:166:GLN:OE1	2.19	0.43
2:D:4:MET:HB3	2:D:4:MET:HE3	1.76	0.42
1:E:151:LYS:HG3	1:E:184:THR:CG2	2.49	0.42
3:I:18:LEU:HD11	3:I:122:ILE:HG23	2.01	0.42
3:I:110:GLU:HG3	3:I:111:THR:O	2.18	0.42
2:L:85:ASP:HA	2:L:102:THR:O	2.19	0.42
2:B:4:MET:HE1	2:B:25:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:46:MET:HE1	3:G:117:PHE:CD2	2.54	0.42
1:A:154:PHE:HA	1:A:155:PRO:HA	1.83	0.42
2:D:182:THR:OG1	2:D:185:GLU:HG2	2.19	0.42
2:B:160:LEU:HB2	2:B:178:THR:O	2.19	0.42
3:K:113:THR:HG23	3:K:115:VAL:N	2.35	0.42
2:L:12:SER:HA	2:L:105:GLU:O	2.19	0.42
2:L:55:ARG:HD2	2:L:55:ARG:HA	1.75	0.42
1:A:208:PRO:O	1:A:211:SER:OG	2.28	0.42
2:B:113:PRO:HB3	2:B:139:PHE:HB3	2.00	0.42
2:D:13:MET:HE3	2:D:13:MET:HB3	1.90	0.42
1:A:67:LYS:HB2	1:A:67:LYS:HE2	1.76	0.42
1:C:48:ILE:HG23	1:C:64:PHE:CE2	2.55	0.42
1:C:81:MET:HE1	1:C:94:TYR:CD2	2.54	0.42
2:F:11:LEU:HD23	2:F:19:VAL:HG13	2.02	0.42
2:F:151:ASP:OD2	2:F:189:HIS:ND1	2.47	0.42
1:E:127:PRO:CB	1:E:153:TYR:HB3	2.47	0.41
2:F:183:LYS:O	2:F:187:GLU:HG2	2.20	0.41
3:G:48:LYS:CE	3:G:106:GLU:HB3	2.50	0.41
1:A:178:LEU:HB2	1:A:183:TYR:CE1	2.55	0.41
2:B:137:ASN:HB3	2:B:138:ASN:OD1	2.20	0.41
1:C:18:VAL:HG12	1:C:83:LEU:HB2	2.02	0.41
1:C:221:ARG:HD3	1:C:221:ARG:HA	1.72	0.41
2:D:8:PRO:CG	2:D:11:LEU:HD13	2.50	0.41
1:H:67:LYS:HE2	1:H:67:LYS:HB2	1.79	0.41
1:H:185:LEU:HA	4:H:309:HOH:O	2.19	0.41
2:L:146:VAL:HA	2:L:195:GLU:O	2.21	0.41
2:F:35:TRP:CE2	2:F:73:PHE:HB2	2.55	0.41
2:B:114:THR:HG23	2:B:137:ASN:O	2.21	0.41
3:G:83:ARG:HH21	3:J:83:ARG:H	1.68	0.41
1:H:156:GLU:OE2	1:H:157:PRO:HA	2.21	0.41
2:F:61:ARG:NH2	2:F:82:ASP:OD1	2.48	0.41
1:C:171:VAL:HG22	1:C:189:VAL:HG23	2.01	0.41
1:E:35:GLN:HG3	1:E:108:MET:CG	2.50	0.41
3:K:80:LEU:HD12	3:K:81:ARG:N	2.32	0.41
1:H:159:THR:HB	1:H:206:ALA:HB3	2.02	0.41
2:L:207:LYS:HA	2:L:207:LYS:HD3	1.72	0.41
4:H:313:HOH:O	2:L:45:LYS:HA	2.20	0.41
2:D:2:ILE:HD13	2:D:2:ILE:HG21	1.72	0.41
2:L:37:GLN:HB2	2:L:47:LEU:HD11	2.03	0.41
1:A:162:TRP:CZ3	1:A:203:CYS:HB3	2.55	0.41
2:B:20:THR:HG23	2:B:72:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:ASP:HB2	2:D:92:ASP:HB2	2.01	0.41
3:G:8:LYS:HD3	3:G:8:LYS:HA	1.53	0.41
3:I:124:PHE:O	3:I:128:ILE:HG12	2.21	0.41
2:D:142:LYS:HB3	2:D:173:TYR:CD2	2.56	0.41
2:D:183:LYS:O	2:D:187:GLU:HG2	2.20	0.41
1:E:163:ASN:HD21	1:E:201:ILE:HG12	1.86	0.41
2:D:4:MET:HE2	2:D:99:GLY:N	2.37	0.40
1:A:32:TYR:CZ	1:A:102:THR:CG2	3.05	0.40
1:A:152:GLY:HA2	1:A:182:LEU:HB3	2.02	0.40
2:F:85:ASP:OD1	2:F:103:LYS:HG3	2.20	0.40
1:A:178:LEU:HD13	1:A:183:TYR:CE1	2.56	0.40
3:K:24:ILE:HG22	3:K:118:LEU:HD11	2.04	0.40
1:A:171:VAL:HG22	1:A:189:VAL:HG13	2.03	0.40
1:E:101:ALA:HB3	1:E:106:TYR:CE2	2.57	0.40
1:E:207:HIS:CE1	1:E:209:ALA:HB3	2.56	0.40
3:I:85:LEU:HD23	3:I:85:LEU:HA	1.94	0.40
1:H:97:ALA:HB1	1:H:108:MET:HB3	2.04	0.40
2:B:50:GLU:OE1	3:G:81:ARG:NH2	2.33	0.40
1:C:60:TYR:CD1	1:C:65:LYS:HG2	2.56	0.40
3:G:46:MET:CE	3:G:117:PHE:HD2	2.35	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	206/224 (92%)	202 (98%)	4 (2%)	0	100	100
1	C	214/224 (96%)	211 (99%)	3 (1%)	0	100	100
1	E	212/224 (95%)	208 (98%)	4 (2%)	0	100	100
1	H	219/224 (98%)	210 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	171/214 (80%)	164 (96%)	7 (4%)	0	100	100
2	D	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
2	F	210/214 (98%)	205 (98%)	5 (2%)	0	100	100
2	L	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
3	G	119/133 (90%)	118 (99%)	1 (1%)	0	100	100
3	I	118/133 (89%)	114 (97%)	4 (3%)	0	100	100
3	J	121/133 (91%)	120 (99%)	1 (1%)	0	100	100
3	K	118/133 (89%)	115 (98%)	3 (2%)	0	100	100
All	All	2131/2284 (93%)	2081 (98%)	50 (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	177/186 (95%)	164 (93%)	13 (7%)	13	27
1	C	182/186 (98%)	167 (92%)	15 (8%)	10	23
1	E	180/186 (97%)	164 (91%)	16 (9%)	9	20
1	H	184/186 (99%)	168 (91%)	16 (9%)	9	21
2	B	163/193 (84%)	146 (90%)	17 (10%)	7	14
2	D	193/193 (100%)	184 (95%)	9 (5%)	23	47
2	F	191/193 (99%)	181 (95%)	10 (5%)	21	42
2	L	192/193 (100%)	169 (88%)	23 (12%)	5	10
3	G	117/126 (93%)	108 (92%)	9 (8%)	12	25
3	I	116/126 (92%)	108 (93%)	8 (7%)	14	30
3	J	119/126 (94%)	113 (95%)	6 (5%)	22	44
3	K	117/126 (93%)	112 (96%)	5 (4%)	26	51
All	All	1931/2020 (96%)	1784 (92%)	147 (8%)	12	26

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLU
1	H	13	ARG
1	H	20	LEU
1	H	74	LYS
1	H	82	GLN
1	H	85	SER
1	H	89	GLU
1	H	125	THR
1	H	135	VAL
1	H	140	THR
1	H	142	SER
1	H	160	LEU
1	H	185	LEU
1	H	192	THR
1	H	204	ASN
1	H	216	LYS
2	L	4	MET
2	L	10	SER
2	L	15	ILE
2	L	31	ASP
2	L	65[A]	SER
2	L	65[B]	SER
2	L	76	GLU
2	L	77	ASN
2	L	78	MET
2	L	107	LYS
2	L	108	ARG
2	L	116	SER
2	L	123	GLU
2	L	136	LEU
2	L	150	ILE
2	L	154	GLU
2	L	157	ASN
2	L	175	MET
2	L	183	LYS
2	L	185	GLU
2	L	193	THR
2	L	197	THR
2	L	206	VAL
1	A	11	LEU
1	A	13	ARG
1	A	17	SER

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Mol	Chain	Res	Type
1	A	61	ILE
1	A	67	LYS
1	A	125	THR
1	A	143	SER
1	A	159	THR
1	A	160	LEU
1	A	187	SER
1	A	198	SER
1	A	201	ILE
1	A	210	SER
2	B	1	ASP
2	B	31	ASP
2	B	78	MET
2	B	81	GLU
2	B	97	THR
2	B	114	THR
2	B	124	GLN
2	B	125	LEU
2	B	126	THR
2	B	132	VAL
2	B	133	VAL
2	B	136	LEU
2	B	143	ASP
2	B	176	SER
2	B	177	SER
2	B	200	THR
2	B	203	SER
1	C	20	LEU
1	C	34	ILE
1	C	61	ILE
1	C	65	LYS
1	C	82	GLN
1	C	85	SER
1	C	99	SER
1	C	135	VAL
1	C	139	THR
1	C	140	THR
1	C	180	SER
1	C	184	THR
1	C	185	LEU
1	C	193	SER
1	C	198	SER

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Mol	Chain	Res	Type
2	D	3	VAL
2	D	4	MET
2	D	50	GLU
2	D	78	MET
2	D	88	CYS
2	D	97	THR
2	D	169	LYS
2	D	178	THR
2	D	184	ASP
1	E	20	LEU
1	E	30	THR
1	E	71	THR
1	E	120	SER
1	E	121	SER
1	E	145	THR
1	E	158	VAL
1	E	160	LEU
1	E	178	LEU
1	E	185	LEU
1	E	193	SER
1	E	199	GLN
1	E	202	THR
1	E	214	VAL
1	E	217	LYS
1	E	219	GLU
2	F	11	LEU
2	F	22	ARG
2	F	27	THR
2	F	77	ASN
2	F	97	THR
2	F	106	ILE
2	F	114	THR
2	F	122	SER
2	F	184	ASP
2	F	200	THR
3	G	8	LYS
3	G	54	LYS
3	G	80	LEU
3	G	87	SER
3	G	91	VAL
3	G	97	LYS
3	G	102	THR

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Mol	Chain	Res	Type
3	G	106	GLU
3	G	110	GLU
3	I	15	GLU
3	I	46	MET
3	I	49	LYS
3	I	57	GLN
3	I	60	GLU
3	I	85	LEU
3	I	130	SER
3	I	133	THR
3	J	49	LYS
3	J	60	GLU
3	J	72	LEU
3	J	106	GLU
3	J	110	GLU
3	J	131	THR
3	K	6	SER
3	K	10	THR
3	K	57	GLN
3	K	80	LEU
3	K	131	THR

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

Mol	Chain	Res	Type
1	H	5	GLN
1	H	43	GLN
1	H	163	ASN
2	L	137	ASN
1	C	43	GLN
1	C	172	HIS
2	D	77	ASN
2	D	93	ASN
2	D	137	ASN
2	D	138	ASN
2	D	190	ASN
2	D	212	ASN
1	E	5	GLN
2	F	93	ASN
3	J	74	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	212/224 (94%)	0.17	7 (3%) 49 45	10, 33, 81, 90	0
1	C	218/224 (97%)	-0.30	2 (0%) 81 78	8, 20, 51, 86	0
1	E	216/224 (96%)	0.08	1 (0%) 87 85	19, 43, 71, 86	0
1	H	221/224 (98%)	-0.05	4 (1%) 67 64	21, 37, 58, 90	0
2	B	179/214 (83%)	0.16	13 (7%) 21 19	9, 30, 84, 93	0
2	D	213/214 (99%)	-0.35	1 (0%) 87 85	9, 21, 41, 94	1 (0%)
2	F	211/214 (98%)	0.07	3 (1%) 73 70	14, 40, 66, 80	1 (0%)
2	L	212/214 (99%)	-0.05	1 (0%) 87 85	11, 33, 58, 70	1 (0%)
3	G	123/133 (92%)	-0.24	2 (1%) 70 67	11, 27, 51, 72	0
3	I	122/133 (91%)	-0.00	1 (0%) 82 80	21, 35, 62, 76	0
3	J	125/133 (93%)	-0.35	0 100 100	12, 22, 45, 64	0
3	K	122/133 (91%)	0.08	1 (0%) 82 80	20, 44, 65, 82	0
All	All	2174/2284 (95%)	-0.06	36 (1%) 69 65	8, 33, 69, 94	3 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	135	VAL	3.5
1	H	137	GLY	3.2
2	B	205	ILE	3.2
1	A	168	SER	3.1
2	B	180	THR	3.1
2	B	31	ASP	3.1
2	F	4	MET	3.0
2	D	4	MET	2.9
1	E	142	SER	2.8
2	F	29	ILE	2.7
1	A	144	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	139	THR	2.7
2	B	208	SER	2.6
1	H	138	ASP	2.5
1	A	191	VAL	2.5
2	B	127	SER	2.5
1	A	146	LEU	2.5
2	B	117	ILE	2.4
2	B	160	LEU	2.4
2	F	30	ASP	2.4
2	B	159	VAL	2.4
3	I	103	PHE	2.4
2	B	115	VAL	2.4
2	B	196	ALA	2.4
3	G	133	THR	2.3
1	A	214	VAL	2.3
3	K	5	SER	2.3
3	G	102	THR	2.2
1	A	218	ILE	2.2
2	B	118	PHE	2.2
2	L	129	GLY	2.2
2	B	131	SER	2.1
1	H	136	CYS	2.1
1	C	140	THR	2.0
2	B	204	PRO	2.0
1	A	166	SER	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.