



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 06:27 PM JST

PDB ID : 7DR4
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 : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

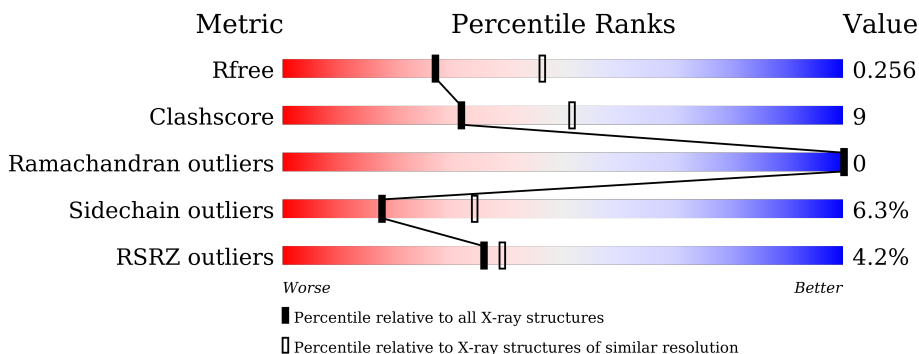
1 Overall quality at a glance

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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	 6% 71% 21% • 5%
1	C	224	 3% 81% 14% • •
1	E	224	 6% 77% 17% • •
1	H	224	 3% 81% 17% • •
2	B	214	 12% 60% 20% • 16%
2	D	214	 78% 21%

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Mol	Chain	Length	Quality of chain
2	F	214	<p>2% 76% 21% ..</p>
2	L	214	<p>2% 77% 19% ..</p>
3	G	133	<p>2% 75% 14% • 8%</p>
3	I	133	<p>5% 70% 20% • 8%</p>
3	J	133	<p>1% 80% 14% 6%</p>
3	K	133	<p>4% 63% 27% • 8%</p>

2 Entry composition [i](#)

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

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

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

- Molecule 3 is a protein called Interleukin-2.

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

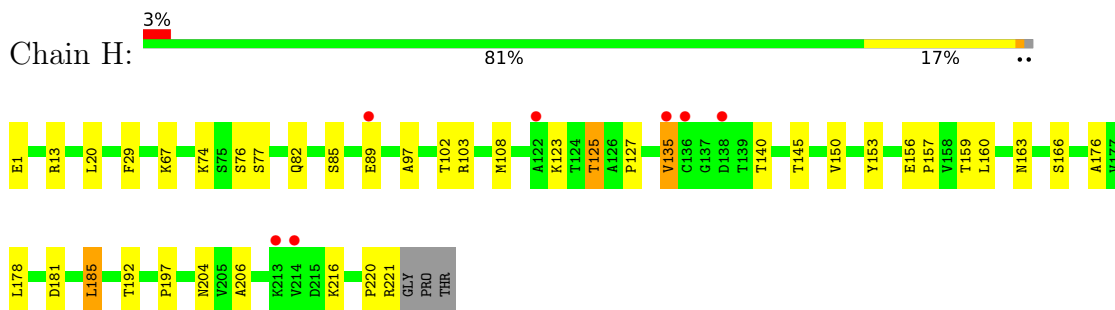
- Molecule 4 is water.

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

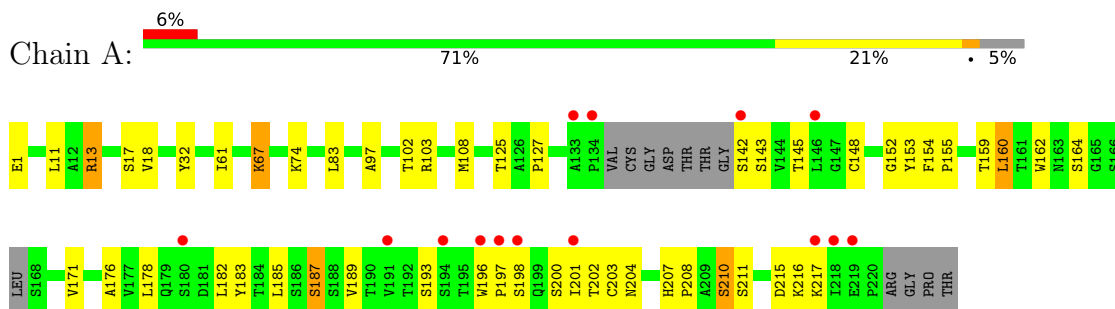
3 Residue-property plots [i](#)

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.

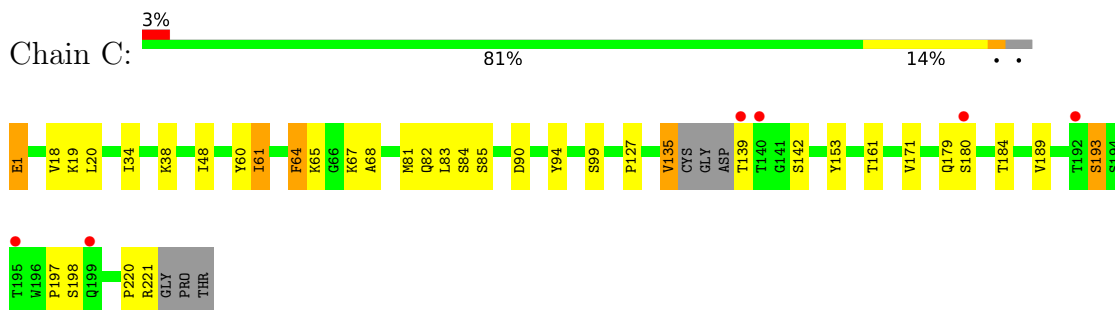
- Molecule 1: anti-human IL-2 antibody, mouse Ig G, heavy chain



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

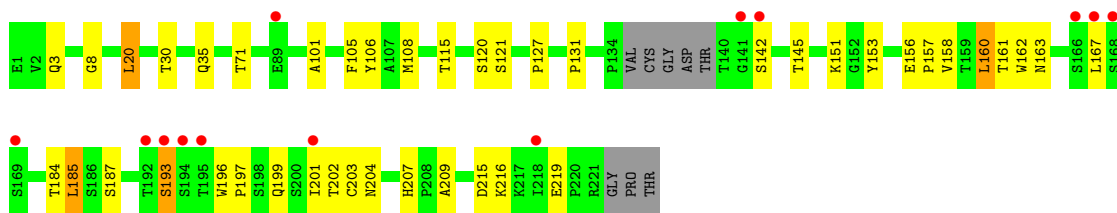


- Molecule 1: anti-human IL-2 antibody, mouse Ig G, heavy chain

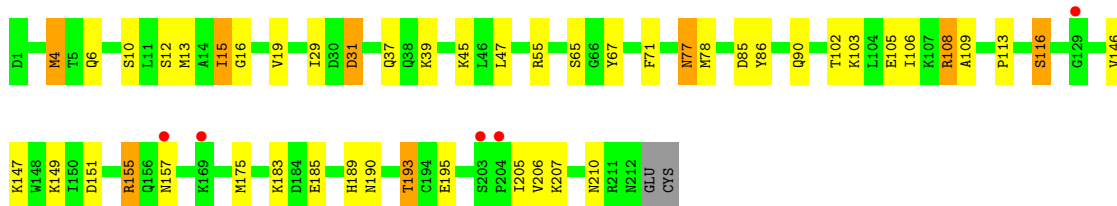
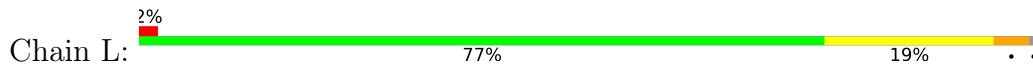


- Molecule 1: anti-human IL-2 antibody, mouse Ig G, heavy chain

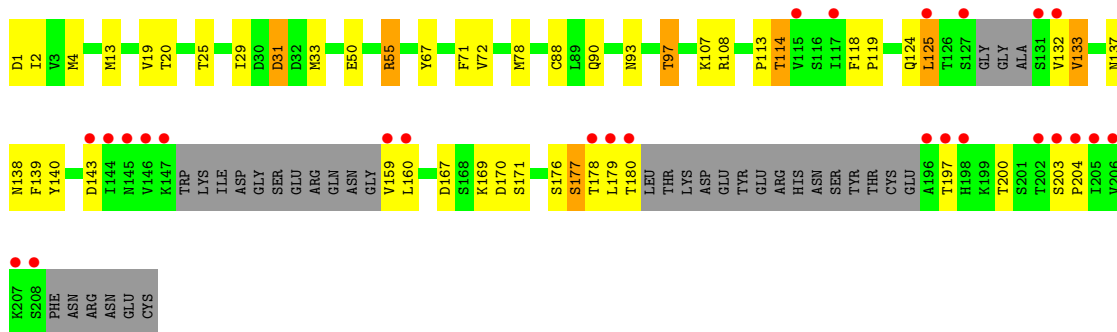




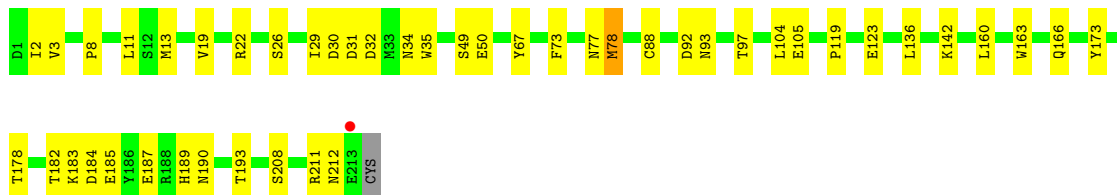
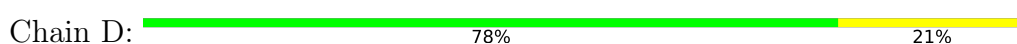
• Molecule 2: anti-human IL-2 antibody, mouse Ig G, kappa chain



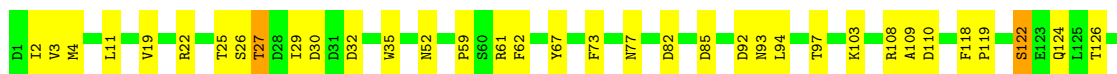
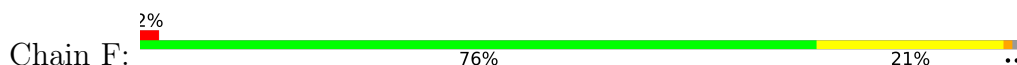
• Molecule 2: anti-human IL-2 antibody, mouse Ig G, kappa chain

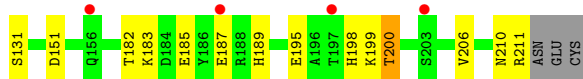


• Molecule 2: anti-human IL-2 antibody, mouse Ig G, kappa chain

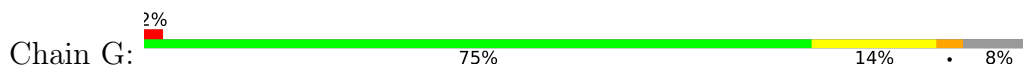


• Molecule 2: anti-human IL-2 antibody, mouse Ig G, kappa chain

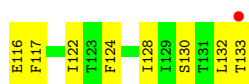




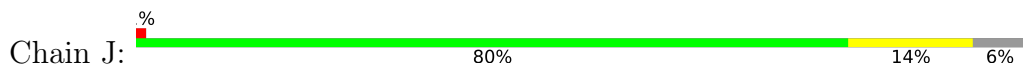
- Molecule 3: Interleukin-2



- 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) 95.9 (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)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.195 , 0.258 0.191 , 0.256	Depositor DCC
R_{free} test set	1994 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtrriage
Anisotropy	0.174	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/1639	0.63	0/2236
1	C	0.46	0/1684	0.66	0/2299
1	E	0.39	0/1670	0.61	0/2279
1	H	0.41	0/1703	0.61	0/2326
2	B	0.48	0/1403	0.59	0/1906
2	D	0.52	0/1699	0.65	0/2308
2	F	0.41	0/1682	0.56	0/2285
2	L	0.44	0/1690	0.62	0/2296
3	G	0.48	0/1031	0.57	0/1388
3	I	0.42	0/1024	0.54	0/1378
3	J	0.50	0/1043	0.60	0/1404
3	K	0.38	0/1019	0.50	0/1373
All	All	0.44	0/17287	0.60	0/23478

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	23	0
1	E	1629	0	1590	28	0
1	H	1661	0	1619	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1376	0	1335	47	0
2	D	1663	0	1587	35	0
2	F	1646	0	1575	33	0
2	L	1654	0	1581	31	0
3	G	1015	0	1055	15	0
3	I	1008	0	1048	13	0
3	J	1027	0	1065	10	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	4	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	300	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 (300) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:160:LEU:O	2:B:177:SER:HA	1.99	0.62
3:I:46:MET:HE1	3:I:117:PHE:HA	1.81	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
3:G:102:THR:O	3:G:102:THR:OG1	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:142:SER:N	1:A:193:SER:HG	2.07	0.52
1:E:167:LEU:N	1:E:167:LEU:CD1	2.73	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
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
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:L:4:MET:HE1	2:L:90:GLN:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:A:176:ALA:HB2	1:A:185:LEU:HD23	1.97	0.47
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:207:HIS:CE1	1:A:210:SER:HG	2.37	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
1:C:81:MET:HE1	1:C:94:TYR:CD2	2.54	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:78:MET:HE2	2:D:104:LEU:HD11	2.01	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
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
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
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	177/186 (95%)	164 (93%)	13 (7%)	14	27
1	C	182/186 (98%)	169 (93%)	13 (7%)	14	28
1	E	180/186 (97%)	167 (93%)	13 (7%)	14	28
1	H	184/186 (99%)	169 (92%)	15 (8%)	11	22
2	B	163/193 (84%)	148 (91%)	15 (9%)	9	18
2	D	193/193 (100%)	188 (97%)	5 (3%)	46	72
2	F	191/193 (99%)	183 (96%)	8 (4%)	30	54
2	L	192/193 (100%)	177 (92%)	15 (8%)	12	24
3	G	117/126 (93%)	109 (93%)	8 (7%)	16	30
3	I	116/126 (92%)	107 (92%)	9 (8%)	12	24
3	J	119/126 (94%)	115 (97%)	4 (3%)	37	63
3	K	117/126 (93%)	113 (97%)	4 (3%)	37	63
All	All	1931/2020 (96%)	1809 (94%)	122 (6%)	18	34

All (122) 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	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	77	ASN

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Mol	Chain	Res	Type
2	L	108	ARG
2	L	116	SER
2	L	155	ARG
2	L	157	ASN
2	L	175	MET
2	L	183	LYS
2	L	193	THR
2	L	206	VAL
1	A	1	GLU
1	A	11	LEU
1	A	13	ARG
1	A	17	SER
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	210	SER
2	B	1	ASP
2	B	4	MET
2	B	31	ASP
2	B	55	ARG
2	B	97	THR
2	B	114	THR
2	B	124	GLN
2	B	125	LEU
2	B	132	VAL
2	B	133	VAL
2	B	143	ASP
2	B	176	SER
2	B	177	SER
2	B	200	THR
2	B	203	SER
1	C	1	GLU
1	C	20	LEU
1	C	34	ILE
1	C	61	ILE
1	C	64	PHE
1	C	85	SER

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Mol	Chain	Res	Type
1	C	99	SER
1	C	135	VAL
1	C	139	THR
1	C	180	SER
1	C	184	THR
1	C	193	SER
1	C	198	SER
2	D	78	MET
2	D	88	CYS
2	D	97	THR
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	185	LEU
1	E	193	SER
1	E	199	GLN
1	E	202	THR
1	E	219	GLU
2	F	22	ARG
2	F	27	THR
2	F	52	ASN
2	F	77	ASN
2	F	97	THR
2	F	122	SER
2	F	200	THR
2	F	210	ASN
3	G	8	LYS
3	G	54	LYS
3	G	80	LEU
3	G	87	SER
3	G	97	LYS
3	G	102	THR
3	G	106	GLU
3	G	110	GLU
3	I	15	GLU

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Mol	Chain	Res	Type
3	I	49	LYS
3	I	54	LYS
3	I	57	GLN
3	I	60	GLU
3	I	85	LEU
3	I	105	CYS
3	I	130	SER
3	I	133	THR
3	J	60	GLU
3	J	106	GLU
3	J	110	GLU
3	J	131	THR
3	K	6	SER
3	K	10	THR
3	K	80	LEU
3	K	109	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	93	ASN
2	D	190	ASN
2	D	212	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 monosaccharides 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	212/224 (94%)	0.28	14 (6%) 18 19	10, 33, 81, 90	0
1	C	218/224 (97%)	-0.19	6 (2%) 53 56	8, 20, 51, 86	0
1	E	216/224 (96%)	0.20	13 (6%) 21 22	19, 43, 71, 86	0
1	H	221/224 (98%)	0.07	7 (3%) 47 51	21, 37, 58, 90	0
2	B	179/214 (83%)	0.49	26 (14%) 2 2	9, 30, 84, 93	0
2	D	213/214 (99%)	-0.27	1 (0%) 91 91	9, 21, 41, 94	0
2	F	211/214 (98%)	0.10	4 (1%) 66 69	20, 40, 66, 80	0
2	L	212/214 (99%)	0.04	5 (2%) 59 62	15, 33, 58, 70	0
3	G	123/133 (92%)	-0.23	3 (2%) 59 62	11, 27, 51, 72	0
3	I	122/133 (91%)	-0.08	6 (4%) 29 31	21, 35, 62, 76	0
3	J	125/133 (93%)	-0.26	1 (0%) 86 87	12, 22, 45, 64	0
3	K	122/133 (91%)	0.08	5 (4%) 37 40	20, 44, 65, 82	0
All	All	2174/2284 (95%)	0.03	91 (4%) 36 39	8, 33, 69, 94	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	180	THR	5.0
1	E	167	LEU	4.9
2	B	159	VAL	4.6
1	A	180	SER	4.6
1	A	146	LEU	4.4
2	B	202	THR	4.4
3	J	104	MET	4.4
2	B	146	VAL	4.2
2	B	206	VAL	4.2
1	C	140	THR	4.2
2	B	179	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	219	GLU	3.8
2	B	203	SER	3.7
1	E	142	SER	3.7
1	E	201	ILE	3.6
1	A	198	SER	3.6
1	E	166	SER	3.6
3	I	31	TYR	3.5
1	A	194	SER	3.4
2	D	213	GLU	3.3
1	A	197	PRO	3.3
2	B	204	PRO	3.3
3	K	5	SER	3.3
2	B	160	LEU	3.3
2	B	205	ILE	3.3
1	H	136	CYS	3.2
2	B	117	ILE	3.2
1	A	201	ILE	3.2
3	G	102	THR	3.1
2	B	127	SER	3.0
2	B	196	ALA	3.0
2	B	144	ILE	3.0
2	F	203	SER	2.9
2	L	203	SER	2.9
2	B	131	SER	2.9
1	E	192	THR	2.9
3	G	133	THR	2.9
1	H	135	VAL	2.9
2	B	197	THR	2.9
3	I	110	GLU	2.8
2	B	115	VAL	2.8
2	B	125	LEU	2.7
1	E	89	GLU	2.7
3	K	31	TYR	2.7
2	L	204	PRO	2.7
3	I	109	ASP	2.7
1	E	195	THR	2.6
1	C	139	THR	2.6
1	E	168	SER	2.5
1	H	213	LYS	2.5
1	H	138	ASP	2.5
1	E	169	SER	2.5
2	B	198	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	141	GLY	2.5
3	K	133	THR	2.5
2	B	132	VAL	2.4
3	I	76	LYS	2.4
1	E	193	SER	2.4
1	A	217	LYS	2.4
1	A	142	SER	2.4
2	B	208	SER	2.4
2	B	143	ASP	2.4
2	B	147	LYS	2.3
1	C	192	THR	2.3
1	E	194	SER	2.3
2	L	169	LYS	2.3
3	I	133	THR	2.3
2	B	207	LYS	2.3
3	K	7	THR	2.3
3	I	75	SER	2.3
2	L	129	GLY	2.2
1	E	218	ILE	2.2
1	H	214	VAL	2.2
1	A	196	TRP	2.2
3	K	106	GLU	2.2
2	B	178	THR	2.2
1	A	134	PRO	2.2
2	F	197	THR	2.1
1	H	122	ALA	2.1
1	C	199	GLN	2.1
1	C	180	SER	2.1
1	A	218	ILE	2.1
1	A	133	ALA	2.1
1	C	195	THR	2.1
1	H	89	GLU	2.1
2	B	145	ASN	2.1
2	F	187	GLU	2.1
1	A	191	VAL	2.0
2	L	157	ASN	2.0
3	G	76	LYS	2.0
2	F	156	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.