WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary 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)

The following versions of software and data (see references ⓘ) were used in the production of this report:

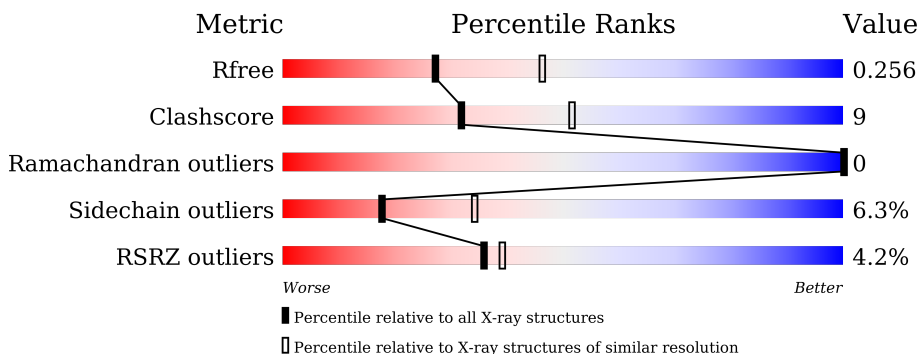|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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	Percentile Ranks	Value
Rfree		0.256
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		6.3%
RSRZ outliers		4.2%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	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 <=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	2% 76% 21%
2	L	214	2% 77% 19%
3	G	133	2% 75% 14% 8%
3	I	133	5% 70% 20% 8%
3	J	133	% 80% 14% 6%
3	K	133	4% 63% 27% 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.

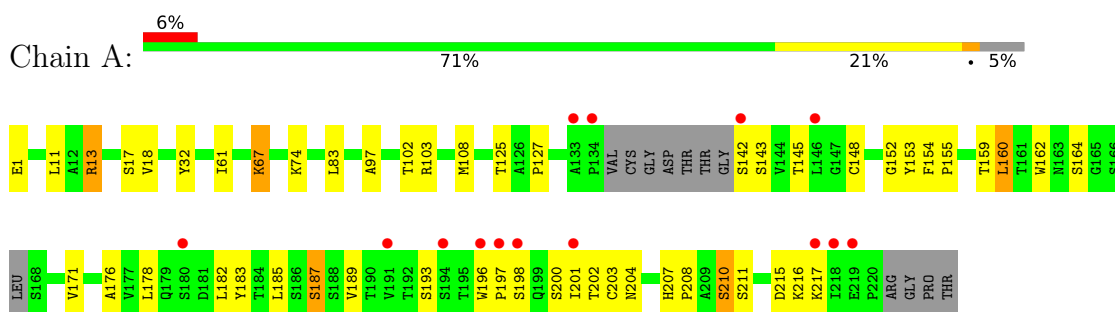| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	27	Total 27	O 27	0	0
4	L	42	Total 42	O 42	0	0
4	A	41	Total 41	O 41	0	0
4	B	52	Total 52	O 52	0	0
4	C	76	Total 76	O 76	0	0
4	D	72	Total 72	O 72	0	0
4	E	13	Total 13	O 13	0	0
4	F	16	Total 16	O 16	0	0
4	G	29	Total 29	O 29	0	0
4	I	8	Total 8	O 8	0	0
4	J	36	Total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

3 Residue-property plots ⓘ

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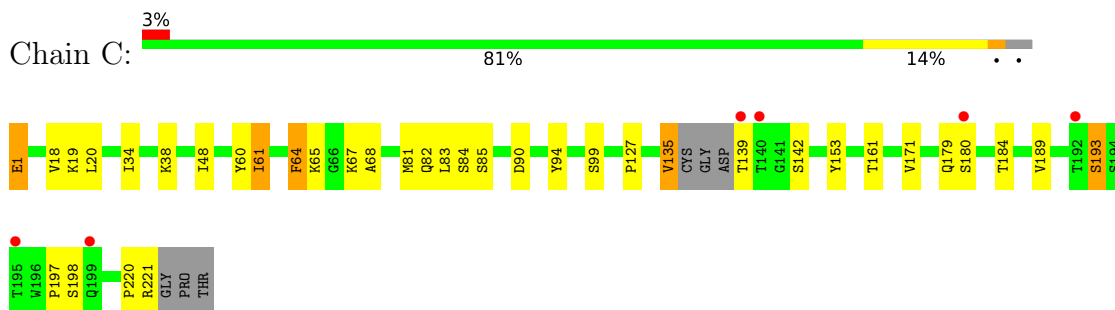
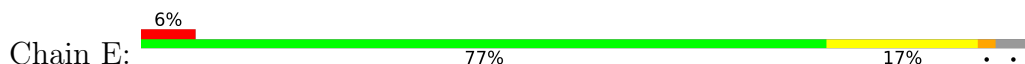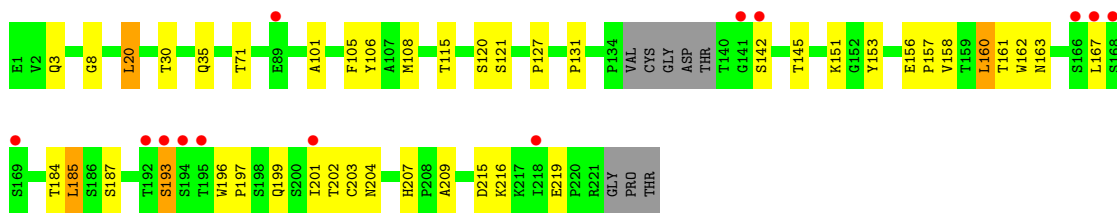• Molecule 1: anti-human IL-2 antibody, mouse Ig G, heavy chain

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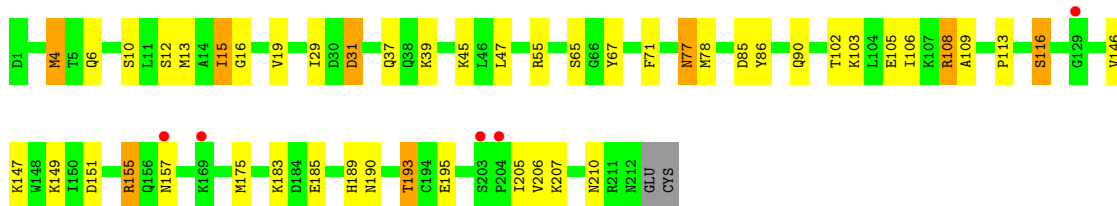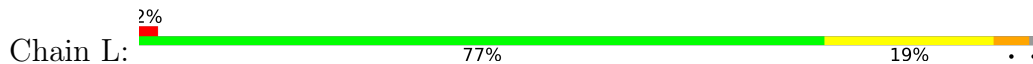

• Molecule 1: anti-human IL-2 antibody, mouse Ig G, heavy chain

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E1 V2 Q3 G8 L20 T30 Q35 T71 E89 A101 F105 Y106 A107 M108 T115 S120 S121 P127 P131 P134 VAL CYS GLY ASP THR T140 G141 S142 T145 K151 G152 Y153 E156 P157 V158 T159 L160 T161 W162 N163 S166 L167 S168

S169 T184 L185 S186 S187 T192 S193 S194 T195 W196 P197 S198 Q199 S200 I201 T202 C203 N204 H207 P208 A209 D215 K216 K217 I218 E219 P220 R221 GLY PRO THR

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

Chain L:

2%
77% 19% ● ●

D1 M4 T5 Q6 S10 L11 S12 A14 I15 G16 V19 I29 D30 D31 Q37 Q38 K39 K45 L46 L47 R55 S65 G66 Y67 F71 N77 M78 D85 Y86 Q90 T102 K103 L104 E105 I106 K107 R108 A109 P113 S116 G129 V146

K147 W148 K149 I150 D151 R155 Q156 N157 K169 M175 K183 D184 E185 H189 N190 T193 C194 E195 S203 P204 I205 V206 K207 N210 R211 N212 GLU CYS

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

Chain B:

12%
60% 20% ● 16%

D1 I2 V3 M4 M13 V19 T20 T25 I29 D30 D31 D32 M33 E50 R55 Y67 F71 V72 M78 C88 L89 Q90 N93 T97 K107 R108 P113 T114 V115 S116 I117 F118 P119 Q124 L125 T126 S127 GLY GLY ALA S131 V132 V133 N137

N138 F139 Y140 D143 I144 N145 V146 K147 TRP LYS ILE ASP GLY SER GLU ARG GLN ASN GLY V159 L160 D167 S168 K169 D170 S171 S176 S177 T178 L179 T180 LEU THR LYS ASP GLU TYR GLU ARG HIS ASN SER TYR THR CYS GLU A196 T197 H198 K199 T200 S201 T202 S203 P204 I205 V206
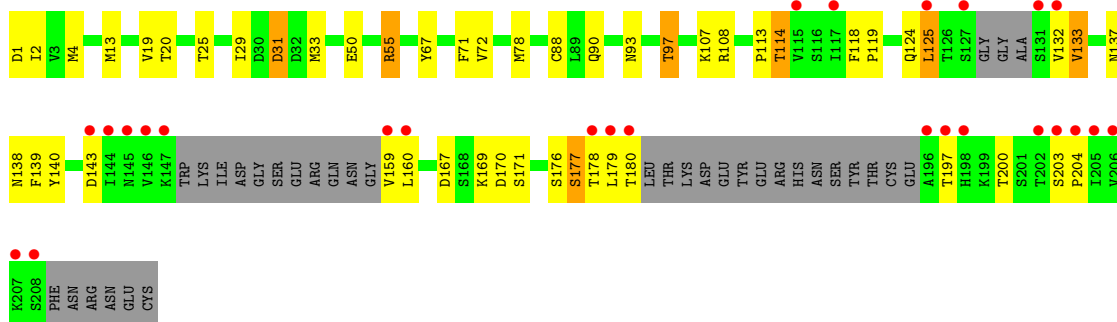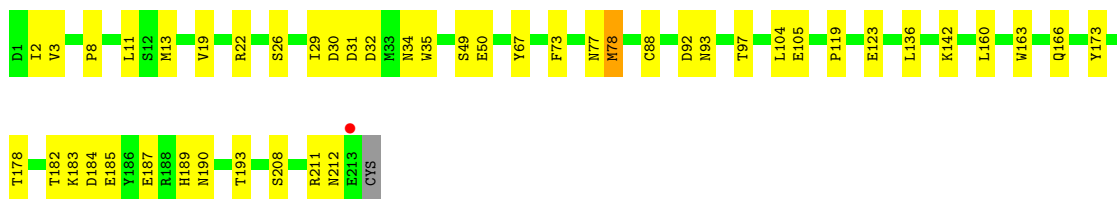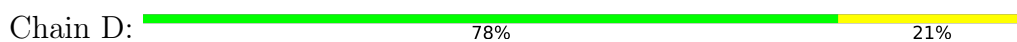
K207 S208 PHE ASN ARG ASN GLU CYS

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

Chain D:

78% 21%

D1 I2 V3 P8 L11 S12 M13 V19 R22 S26 I29 D30 D31 D32 M33 N34 W35 S49 E50 Y67 F73 N77 M78 C88 D92 N93 T97 L104 E105 P119 E123 L136 K142 L160 W163 Q166 Y173

T178 T182 K183 D184 E185 Y186 E187 R188 H189 N190 T193 S208 R211 N212 E213 CYS
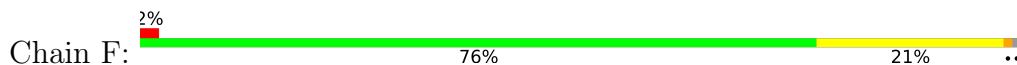
● Molecule 2: anti-human IL-2 antibody, mouse Ig G, kappa chain

Chain F:

2%
76% 21% ●●

D1 I2 V3 M4 L11 V19 R22 T25 S26 T27 D28 I29 D30 D31 D32 W35 N52 P59 S60 R61 F62 Y67 F73 N77 D82 D85 D92 N93 L94 T97 K103 R108 A109 D110 F118 P119 S122 E123 Q124 L125 T126

S131 D151 Q156 T182 K183 D184 E185 Y186 E187 R188 H189 E195 A196 T197 H198 K199 T200 S203 V206 N210 R211 ASN GLU CYS

- Molecule 3: Interleukin-2

Chain G:

2%
75% 14% · 8%

ALA PRO THR SER SER THR K8 Q13 G27 M46 P47 K48 K49 A50 K54 K76 N77 F78 H79 L80 R81 P82 R83 S87 L94 E95 L96 K97 G98 SER GLU THR T102 E106 E110 T111 A112 E116 F117 R120 L132 T133

- Molecule 3: Interleukin-2

Chain I:

5%
70% 20% · 8%

ALA PRO THR SER SER THR K8 E15 L18 G27 Y31 M46 K49 E52 L53 K54 Q57 E60 S75 K76 N77 F78 R81 P82 R83 D84 L85 N90 L94 G98 SER GLU THR F103 M104 C105 D109 E110 T111 T113 I114 V115

E116 F117 I122 T123 F124 I128 I129 S130 T131 L132 T133

- Molecule 3: Interleukin-2

Chain J:

%
80% 14% 6%

ALA PRO THR SER S5 G27 F42 K43 A50 E60 E67 L70 F78 H79 L80 R83 I86 L94 G98 SER GLU THR F103 M104 C105 E106 E110 T111 A112 E116 R120 T131 L132 T133

- Molecule 3: Interleukin-2

Chain K:

4%
63% 27% · 8%

ALA PRO THR SER S5 S6 T7 K8 K9 T10 Q11 L12 Q13 L17 I24 G27 Y31 F42 A50 T51 E52 L53 K54 H55 L56 Q57 K64 P65 L66 E67 L70 F78 H79 L80 R81 P82 R83 I86 I92 V93 L94 E95 L96 K97 GLY SER GLU THR THR

PHE MET C105 E106 D109 T113 I114 V115 E116 F117 L118 N119 R120 C125 T131 L132 T133

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.28 (at 2.51Å)	Xtriage
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	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	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 ⓘ

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.

The worst 5 of 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

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	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 ⓘ

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	203	SER
3	I	85	LEU
2	D	78	MET
3	I	60	GLU
3	K	6	SER

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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	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

The worst 5 of 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

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.