Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 11:58 PM EDT

PDB ID	:	5WLG
Title	:	Crystal Structure of H-2Db with the GAP501 peptide (SQL)
Authors	:	Gras, S.; Farenc, C.; Josephs, T.; Rossjohn, J.
Deposited on	:	2017-07-26
Resolution	:	2.10 Å(reported)

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

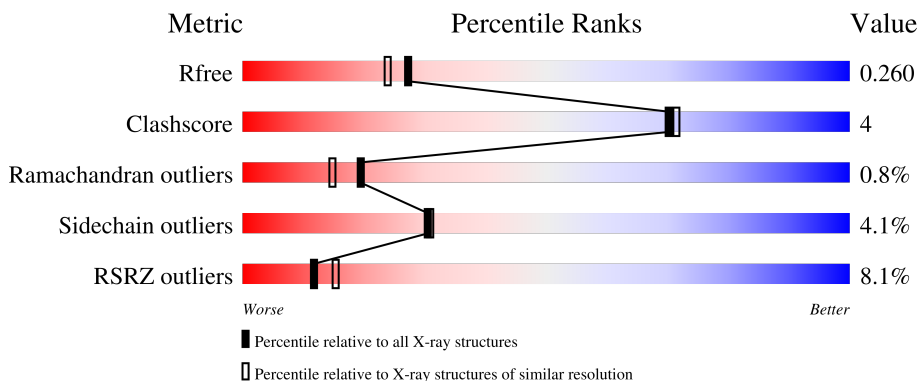|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.10 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		0.260
Clashscore		4
Ramachandran outliers		0.8%
Sidechain outliers		4.1%
RSRZ outliers		8.1%

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	278	2%; 88% / 11%
1	F	278	9%; 85% / 13% ·
2	B	99	%; 94% / 5% ·
2	G	99	11%; 87% / 9% · · ·
3	C	9	100%

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Mol	Chain	Length	Quality of chain
3	H	9	89% 11%
4	D	182	4% 87% 12%
4	I	182	16% 83% 13%
5	E	243	7% 90% 9%
5	J	243	14% 90% 8%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 13901 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total 2290	C 1446	N 406	O 429	S 9	0	1	0
1	F	277	Total 2271	C 1435	N 401	O 426	S 9	0	0	0

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total 810	C 517	N 137	O 149	S 7	0	0	0
2	G	98	Total 810	C 517	N 137	O 149	S 7	0	0	0

- Molecule 3 is a protein called GAP50 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total 74	C 48	N 12	O 14	0	0	0
3	H	9	Total 74	C 48	N 12	O 14	0	0	0

- Molecule 4 is a protein called T cell receptor alpha variable 8D-2,Human nkt tcr alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	182	Total 1431	C 879	N 249	O 293	S 10	0	2	0
4	I	177	Total 1386	C 851	N 242	O 283	S 10	0	2	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	91	VAL	-	linker	UNP A0A075B616
D	92	TYR	-	linker	UNP A0A075B616
D	93	ALA	-	linker	UNP A0A075B616
D	94	GLN	-	linker	UNP A0A075B616
D	95	GLY	-	linker	UNP A0A075B616
D	96	LEU	-	linker	UNP A0A075B616
D	97	THR	-	linker	UNP A0A075B616
D	98	PHE	-	linker	UNP A0A075B616
D	99	GLY	-	linker	UNP A0A075B616
D	100	LEU	-	linker	UNP A0A075B616
D	101	GLY	-	linker	UNP A0A075B616
D	102	THR	-	linker	UNP A0A075B616
D	103	ARG	-	linker	UNP A0A075B616
D	104	VAL	-	linker	UNP A0A075B616
D	105	SER	-	linker	UNP A0A075B616
D	106	VAL	-	linker	UNP A0A075B616
D	107	PHE	-	linker	UNP A0A075B616
D	108	PRO	-	linker	UNP A0A075B616
D	109	ASN	-	linker	UNP A0A075B616
I	92	VAL	-	linker	UNP A0A075B616
I	93	TYR	-	linker	UNP A0A075B616
I	94	ALA	-	linker	UNP A0A075B616
I	95	GLN	-	linker	UNP A0A075B616
I	96	GLY	-	linker	UNP A0A075B616
I	97	LEU	-	linker	UNP A0A075B616
I	98	THR	-	linker	UNP A0A075B616
I	99	PHE	-	linker	UNP A0A075B616
I	100	GLY	-	linker	UNP A0A075B616
I	101	LEU	-	linker	UNP A0A075B616
I	102	GLY	-	linker	UNP A0A075B616
I	103	THR	-	linker	UNP A0A075B616
I	104	ARG	-	linker	UNP A0A075B616
I	105	VAL	-	linker	UNP A0A075B616
I	106	SER	-	linker	UNP A0A075B616
I	107	VAL	-	linker	UNP A0A075B616
I	108	PHE	-	linker	UNP A0A075B616
I	109	PRO	-	linker	UNP A0A075B616
I	110	ASN	-	linker	UNP A0A075B616

- Molecule 5 is a protein called T-cell receptor beta chain V region C5,Human nkt tcr beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total 1933	C 1215	N 333	O 378	S 7	0	1	0
5	J	241	Total 1928	C 1212	N 333	O 376	S 7	0	2	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	95	ASP	GLY	conflict	UNP P04213
E	96	TRP	THR	conflict	UNP P04213
E	?	-	GLY	deletion	UNP P04213
E	?	-	ALA	deletion	UNP P04213
E	?	-	LEU	deletion	UNP P04213
E	100	GLY	-	insertion	UNP P04213
E	102	LEU	-	insertion	UNP P04213
E	106	GLU	PRO	conflict	UNP P04213
E	108	SER	THR	conflict	UNP P04213
E	109	LYS	ARG	conflict	UNP P04213
E	111	THR	LEU	conflict	UNP P04213
J	95	ASP	GLY	conflict	UNP P04213
J	96	TRP	THR	conflict	UNP P04213
J	?	-	GLY	deletion	UNP P04213
J	?	-	ALA	deletion	UNP P04213
J	?	-	LEU	deletion	UNP P04213
J	100	GLY	-	insertion	UNP P04213
J	102	LEU	-	insertion	UNP P04213
J	106	GLU	PRO	conflict	UNP P04213
J	108	SER	THR	conflict	UNP P04213
J	109	LYS	ARG	conflict	UNP P04213
J	111	THR	LEU	conflict	UNP P04213

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Na 1	0	0
6	G	1	Total 1	Na 1	0	0
6	I	1	Total 1	Na 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Cl 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	215	Total 215	O 215	0	0
8	B	97	Total 97	O 97	0	0
8	C	1	Total 1	O 1	0	0
8	D	97	Total 97	O 97	0	0
8	E	120	Total 120	O 120	0	0
8	F	139	Total 139	O 139	0	0
8	G	47	Total 47	O 47	0	0
8	H	1	Total 1	O 1	0	0
8	I	66	Total 66	O 66	0	0
8	J	107	Total 107	O 107	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: H-2 class I histocompatibility antigen, D-B alpha chain
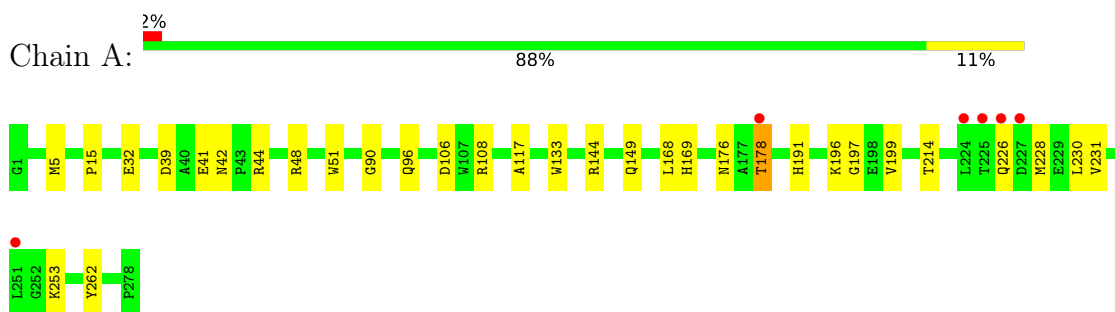
• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain
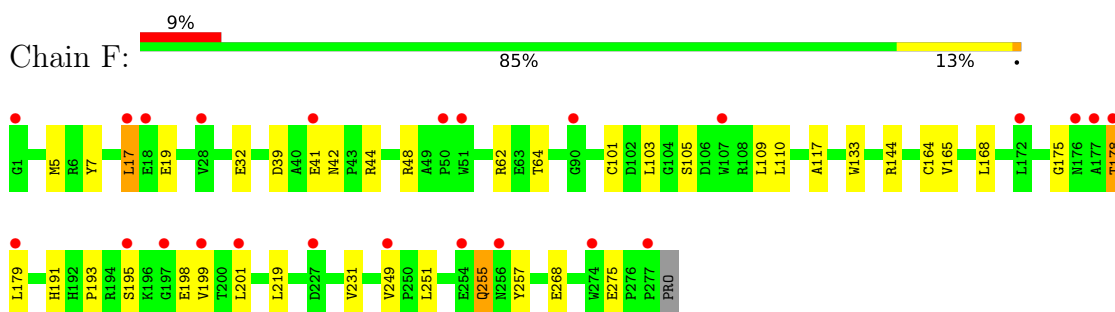
• Molecule 2: Beta-2-microglobulin
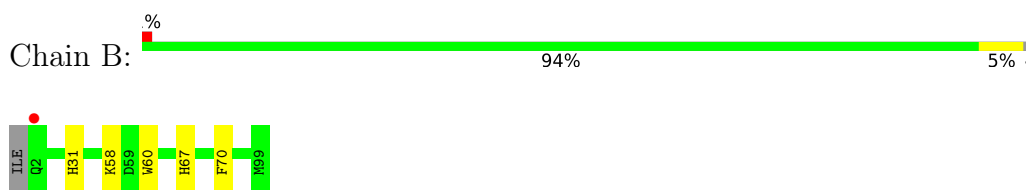
• Molecule 2: Beta-2-microglobulin
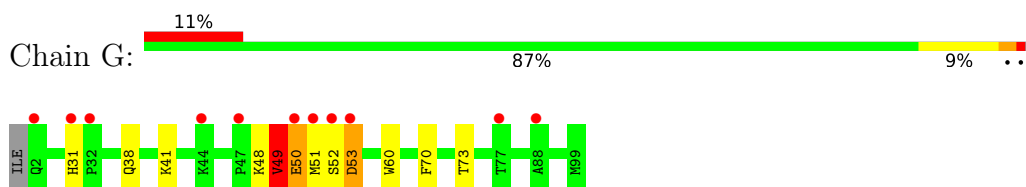
• Molecule 3: GAP50 peptide

Chain C:

100%

There are no outlier residues recorded for this chain.

• Molecule 3: GAP50 peptide

Chain H:

89% 11%

• Molecule 4: T cell receptor alpha variable 8D-2,Human nkt tcr alpha chain

Chain D:

4%

87% 12%
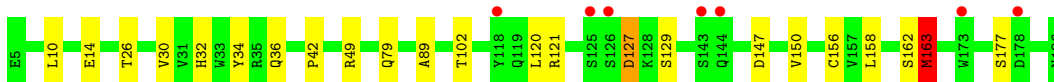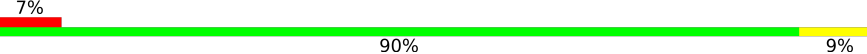
• Molecule 4: T cell receptor alpha variable 8D-2,Human nkt tcr alpha chain

Chain I:

16%

83% 13%
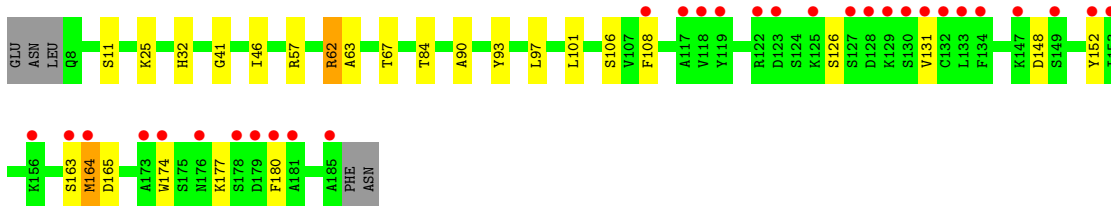
• Molecule 5: T-cell receptor beta chain V region C5,Human nkt tcr beta chain

Chain E:

7%

90% 9%
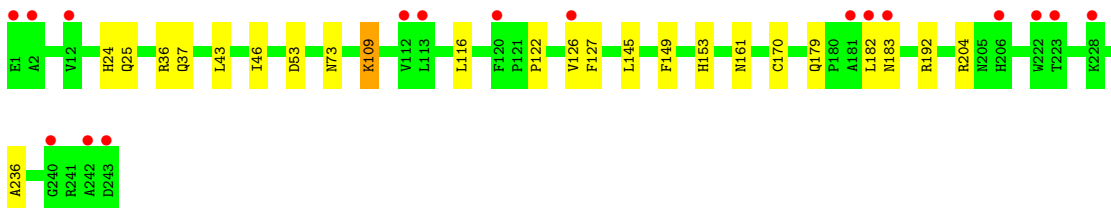
• Molecule 5: T-cell receptor beta chain V region C5,Human nkt tcr beta chain

Chain J:

14%

90% 8%
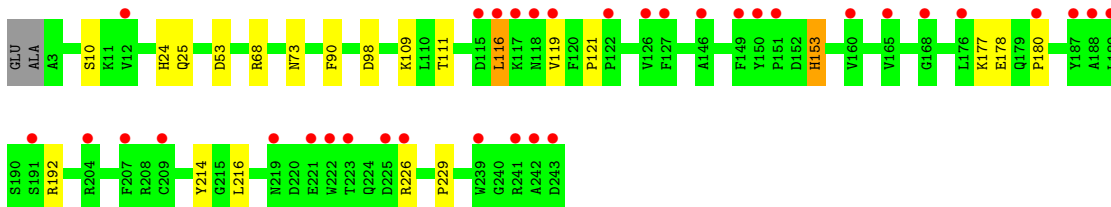
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	115.73Å 70.21Å 116.49Å 90.00° 108.28° 90.00°	Depositor
Resolution (Å)	47.05 – 2.10 47.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.05-2.10) 99.9 (47.05-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.218 , 0.249 0.227 , 0.260	Depositor DCC
R_{free} test set	5105 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 51.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13901	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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 ⓘ

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

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	0.41	0/2359	0.69	0/3204
1	F	0.40	0/2339	0.71	0/3178
2	B	0.42	0/836	0.65	0/1133
2	G	0.42	0/836	0.69	0/1133
3	C	0.47	0/74	0.77	0/97
3	H	0.51	0/74	0.93	0/97
4	D	0.41	0/1454	0.71	0/1967
4	I	0.38	0/1408	0.69	0/1906
5	E	0.38	0/1986	0.67	0/2705
5	J	0.38	0/1981	0.65	0/2698
All	All	0.40	0/13347	0.69	0/18118

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	2290	0	2162	17	0
1	F	2271	0	2145	20	0
2	B	810	0	783	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	810	0	783	8	0
3	C	74	0	81	0	0
3	H	74	0	81	2	0
4	D	1431	0	1368	11	0
4	I	1386	0	1330	14	0
5	E	1933	0	1817	12	0
5	J	1928	0	1812	13	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
7	A	1	0	0	0	0
8	A	215	0	0	1	0
8	B	97	0	0	2	0
8	C	1	0	0	0	0
8	D	97	0	0	0	0
8	E	120	0	0	0	0
8	F	139	0	0	1	0
8	G	47	0	0	1	0
8	H	1	0	0	0	0
8	I	66	0	0	0	0
8	J	107	0	0	0	0
All	All	13901	0	12362	89	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 4.

All (89) 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:G:48:LYS:HA	2:G:49:VAL:HG12	1.18	1.10
2:G:48:LYS:HA	2:G:49:VAL:CG1	2.00	0.91
1:A:196:LYS:HB3	1:A:197:GLY:HA3	1.54	0.90
1:F:103:LEU:HD11	1:F:165:VAL:HG22	1.52	0.90
1:A:196:LYS:CB	1:A:197:GLY:HA3	2.07	0.83
1:F:193:PRO:HA	1:F:199:VAL:HG23	1.66	0.76
1:F:103:LEU:HD13	1:F:168:LEU:HD23	1.69	0.75
4:D:36:GLN:HE22	5:E:37:GLN:HE22	1.35	0.74
1:F:32:GLU:OE2	1:F:48:ARG:HD2	1.91	0.70
5:E:24:HIS:HD2	5:E:73:ASN:HD21	1.39	0.68
1:A:32:GLU:OE2	1:A:48:ARG:HD2	1.96	0.66
1:F:175:GLY:O	1:F:179:LEU:HD12	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:HD2	8:A:492:HOH:O	1.99	0.63
4:D:158:LEU:HB3	5:E:170[B]:CYS:HB2	1.81	0.63
5:E:36:ARG:HB2	5:E:46:ILE:HD11	1.81	0.62
4:I:90:ALA:HB1	4:I:97:LEU:HD22	1.82	0.62
4:D:30:VAL:HG12	4:D:49[B]:ARG:HG2	1.82	0.62
2:B:31:HIS:HD2	8:B:170:HOH:O	1.81	0.62
2:B:67:HIS:HD2	8:B:181:HOH:O	1.84	0.59
4:I:97:LEU:HG	5:J:98:ASP:HB3	1.85	0.58
5:J:24:HIS:HD2	5:J:73:ASN:HD21	1.49	0.58
1:F:103:LEU:HD21	1:F:165:VAL:HG13	1.86	0.58
1:A:228:MET:HE3	1:A:230:LEU:HD13	1.86	0.57
5:E:24:HIS:HD2	5:E:73:ASN:ND2	2.04	0.56
4:D:162:SER:O	4:D:163:MET:HB2	2.06	0.56
1:A:196:LYS:CB	1:A:197:GLY:CA	2.82	0.55
5:E:179:GLN:HB3	5:E:182:LEU:HD13	1.88	0.54
2:G:49:VAL:O	2:G:49:VAL:HG13	2.07	0.54
1:F:103:LEU:CD1	1:F:165:VAL:HG22	2.34	0.54
4:D:42:PRO:HG2	5:E:43:LEU:HD11	1.90	0.54
1:A:15:PRO:HB3	1:A:90:GLY:HA2	1.90	0.53
1:F:201:LEU:HD22	1:F:249:VAL:HG21	1.89	0.53
1:A:191:HIS:NE2	1:A:199:VAL:HG21	2.24	0.53
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.44	0.52
2:G:50:GLU:O	2:G:50:GLU:HG3	2.08	0.52
5:J:153:HIS:HB3	5:J:214:TYR:HB2	1.92	0.52
1:A:191:HIS:CE1	1:A:199:VAL:HG21	2.45	0.51
4:I:46:ILE:HG21	4:I:63:ALA:CB	2.40	0.51
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.92	0.51
5:E:122:PRO:HB3	5:E:149:PHE:HB3	1.91	0.51
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.92	0.51
1:F:44:ARG:HG3	1:F:64:THR:OG1	2.11	0.50
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.47	0.50
5:J:24:HIS:HD2	5:J:73:ASN:ND2	2.09	0.50
1:F:7:TYR:CD2	3:H:2:GLN:HG3	2.48	0.49
5:J:177:LYS:HD3	5:J:180:PRO:HA	1.96	0.48
2:G:48:LYS:HA	2:G:49:VAL:CB	2.44	0.48
1:A:106:ASP:OD2	1:A:108[A]:ARG:HD3	2.14	0.48
1:F:5:MET:HB2	1:F:168:LEU:HD13	1.95	0.47
5:J:119:VAL:HG12	5:J:229:PRO:HB2	1.96	0.47
1:F:198:GLU:HB2	1:F:249:VAL:O	2.15	0.47
8:F:333:HOH:O	3:H:2:GLN:HG2	2.14	0.46
4:I:177:LYS:HB2	4:I:180:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:46:ILE:HG21	4:I:63:ALA:HB3	1.98	0.46
4:I:57:ARG:HG2	4:I:62:ARG:HG3	1.97	0.46
1:F:255:GLN:H	1:F:255:GLN:HG3	1.53	0.46
4:D:120:LEU:HB3	5:E:127:PHE:HB3	1.97	0.46
4:I:131:VAL:HG12	4:I:174:TRP:HB3	1.97	0.46
4:D:32:HIS:HD2	4:D:34:TYR:OH	1.97	0.45
2:G:31:HIS:HD2	8:G:244:HOH:O	1.98	0.45
5:J:121:PRO:HD3	5:J:229:PRO:HB3	1.98	0.45
4:D:14:GLU:HG3	4:D:79:GLN:HA	1.99	0.45
4:D:32:HIS:HB2	4:D:89:ALA:HB3	1.98	0.45
5:J:116:LEU:HG	5:J:216:LEU:HD21	1.99	0.45
1:F:191:HIS:CE1	1:F:199:VAL:HG21	2.52	0.44
1:A:196:LYS:HB2	1:A:197:GLY:HA3	1.94	0.44
4:I:11:SER:HB3	4:I:108:PHE:HE2	1.82	0.44
4:D:10:LEU:HD12	4:D:102:THR:HG21	1.99	0.43
4:I:152:TYR:HE1	5:J:178:GLU:HA	1.82	0.43
5:J:10:SER:OG	5:J:153:HIS:HD2	2.02	0.43
1:F:62:ARG:HD2	4:I:93:TYR:O	2.19	0.43
1:F:101:CYS:CB	1:F:164:CYS:HG	2.26	0.43
1:F:219:LEU:HD13	1:F:257:TYR:CZ	2.54	0.43
5:J:111:THR:OG1	5:J:153:HIS:HE1	2.02	0.43
4:I:32:HIS:HB2	4:I:90:ALA:HB3	2.02	0.42
1:A:133:TRP:HB2	1:A:144:ARG:HG3	2.01	0.42
5:E:24:HIS:CD2	5:E:73:ASN:HD21	2.28	0.42
1:F:133:TRP:HB2	1:F:144:ARG:HG3	2.02	0.41
4:I:41:GLY:HA2	5:J:90:PHE:CE1	2.55	0.41
5:E:109:LYS:HD3	5:E:153:HIS:CD2	2.54	0.41
4:D:147:ASP:HB3	4:D:150:VAL:HB	2.02	0.41
2:G:52:SER:O	2:G:53:ASP:HB2	2.21	0.41
1:F:101:CYS:HB2	1:F:109:LEU:CD1	2.50	0.41
5:J:68:ARG:HD2	5:J:73:ASN:O	2.21	0.41
4:I:163:SER:HA	4:I:164:MET:HA	1.77	0.41
1:A:51:TRP:HD1	1:A:178:THR:HG21	1.85	0.40
4:I:84:THR:HG23	4:I:106:SER:HA	2.03	0.40
1:A:214:THR:HB	1:A:262:TYR:HB2	2.03	0.40
5:E:126:VAL:HG23	5:E:236:ALA:HB3	2.02	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	277/278 (100%)	262 (95%)	13 (5%)	2 (1%)	22	18
1	F	275/278 (99%)	261 (95%)	11 (4%)	3 (1%)	14	9
2	B	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
2	G	96/99 (97%)	91 (95%)	3 (3%)	2 (2%)	7	3
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	182/182 (100%)	174 (96%)	5 (3%)	3 (2%)	9	5
4	I	177/182 (97%)	169 (96%)	6 (3%)	2 (1%)	14	9
5	E	242/243 (100%)	236 (98%)	5 (2%)	1 (0%)	34	32
5	J	241/243 (99%)	233 (97%)	8 (3%)	0	100	100
All	All	1600/1622 (99%)	1532 (96%)	55 (3%)	13 (1%)	19	15

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	163	MET
1	F	178	THR
2	G	53	ASP
1	A	176	ASN
2	G	49	VAL
4	I	165	ASP
1	F	195	SER
1	A	226	GLN
4	D	26	THR
4	D	127	ASP
5	E	161	ASN
1	F	17	LEU
4	I	126	SER

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	237/236 (100%)	228 (96%)	9 (4%)	33	34
1	F	235/236 (100%)	222 (94%)	13 (6%)	21	19
2	B	92/93 (99%)	90 (98%)	2 (2%)	52	57
2	G	92/93 (99%)	85 (92%)	7 (8%)	13	10
3	C	8/8 (100%)	8 (100%)	0	100	100
3	H	8/8 (100%)	8 (100%)	0	100	100
4	D	163/161 (101%)	156 (96%)	7 (4%)	29	29
4	I	158/161 (98%)	152 (96%)	6 (4%)	33	34
5	E	210/209 (100%)	202 (96%)	8 (4%)	33	34
5	J	210/209 (100%)	203 (97%)	7 (3%)	38	40
All	All	1413/1414 (100%)	1354 (96%)	59 (4%)	30	30

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	41	GLU
1	A	42	ASN
1	A	44	ARG
1	A	149	GLN
1	A	169	HIS
1	A	178	THR
1	A	231	VAL
1	A	253	LYS
2	B	58	LYS
2	B	70	PHE
4	D	121	ARG
4	D	127	ASP
4	D	129	SER
4	D	156[A]	CYS
4	D	156[B]	CYS

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Mol	Chain	Res	Type
4	D	163	MET
4	D	177	SER
5	E	25	GLN
5	E	53	ASP
5	E	109	LYS
5	E	116	LEU
5	E	145	LEU
5	E	183	ASN
5	E	192	ARG
5	E	204	ARG
1	F	17	LEU
1	F	19	GLU
1	F	39	ASP
1	F	41	GLU
1	F	42	ASN
1	F	105	SER
1	F	110	LEU
1	F	178	THR
1	F	231	VAL
1	F	251	LEU
1	F	255	GLN
1	F	268	GLU
1	F	275	GLU
2	G	38	GLN
2	G	41	LYS
2	G	49	VAL
2	G	50	GLU
2	G	51	MET
2	G	70	PHE
2	G	73	THR
4	I	25	LYS
4	I	62	ARG
4	I	67	THR
4	I	101	LEU
4	I	148	ASP
4	I	164	MET
5	J	25	GLN
5	J	53	ASP
5	J	109	LYS
5	J	116	LEU
5	J	153	HIS
5	J	192	ARG

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Mol	Chain	Res	Type
5	J	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	174	ASN
1	A	176	ASN
2	B	29	GLN
2	B	31	HIS
2	B	38	GLN
4	D	32	HIS
5	E	24	HIS
5	E	37	GLN
5	E	73	ASN
5	E	183	ASN
1	F	65	GLN
1	F	220	ASN
1	F	256	ASN
2	G	29	GLN
2	G	31	HIS
5	J	24	HIS
5	J	73	ASN
5	J	153	HIS
5	J	166	HIS

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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	278/278 (100%)	0.11	6 (2%)	62	66	18, 32, 70, 102	4 (1%)
1	F	277/278 (99%)	0.67	24 (8%)	10	13	28, 49, 92, 132	5 (1%)
2	B	98/99 (98%)	-0.15	1 (1%)	82	85	20, 36, 63, 87	1 (1%)
2	G	98/99 (98%)	0.79	11 (11%)	5	6	36, 57, 89, 102	1 (1%)
3	C	9/9 (100%)	-0.18	0	100	100	19, 21, 29, 30	0
3	H	9/9 (100%)	0.02	0	100	100	27, 30, 40, 41	0
4	D	182/182 (100%)	0.34	7 (3%)	40	46	27, 47, 99, 119	0
4	I	177/182 (97%)	0.90	30 (16%)	1	2	30, 58, 127, 158	6 (3%)
5	E	243/243 (100%)	0.57	17 (6%)	16	20	21, 52, 81, 120	0
5	J	241/243 (99%)	0.84	35 (14%)	2	3	28, 58, 114, 138	2 (0%)
All	All	1612/1622 (99%)	0.52	131 (8%)	12	15	18, 48, 97, 158	19 (1%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	17	LEU	20.2
4	I	174	TRP	6.9
4	I	125	LYS	6.4
1	F	197	GLY	6.3
5	E	243	ASP	6.3
1	F	1	GLY	5.6
5	J	119	VAL	5.6
5	J	243	ASP	4.9
4	D	143	SER	4.9
5	J	221	GLU	4.8
5	J	225	ASP	4.8
2	B	2	GLN	4.6
4	I	164	MET	4.3

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Mol	Chain	Res	Type	RSRZ
5	J	127	PHE	4.2
2	G	50	GLU	4.2
5	J	241	ARG	4.2
1	F	195	SER	4.1
1	A	224	LEU	4.1
4	D	126	SER	4.0
1	F	277	PRO	4.0
1	A	226	GLN	4.0
1	F	179	LEU	4.0
4	I	127	SER	4.0
4	I	180	PHE	3.9
1	A	227	ASP	3.9
4	I	153	ILE	3.9
5	E	120	PHE	3.8
2	G	51	MET	3.8
5	E	223	THR	3.8
5	J	116	LEU	3.8
1	A	178	THR	3.7
1	F	177	ALA	3.7
4	I	178	SER	3.7
5	E	1	GLU	3.6
4	I	133	LEU	3.6
1	F	51	TRP	3.6
5	J	149	PHE	3.6
1	F	41	GLU	3.6
1	F	274	TRP	3.5
1	F	107	TRP	3.5
1	A	225	THR	3.5
5	J	204	ARG	3.5
5	J	118	ASN	3.4
4	I	118	VAL	3.4
5	J	222	TRP	3.4
5	E	2	ALA	3.3
5	J	187	TYR	3.3
4	I	132	CYS	3.3
4	D	125	SER	3.2
4	I	130	SER	3.1
2	G	44	LYS	3.1
4	D	144	GLN	3.1
4	I	129	LYS	3.0
5	J	207	PHE	3.0
5	E	126	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
4	I	128	ASP	2.9
5	J	176	LEU	2.9
1	F	176	ASN	2.9
4	I	176	ASN	2.9
4	I	179	ASP	2.9
5	J	219	ASN	2.8
1	F	178	THR	2.8
1	F	18	GLU	2.8
5	J	12	VAL	2.8
4	I	163	SER	2.8
4	I	122	ARG	2.7
5	J	223	THR	2.7
5	J	165	VAL	2.7
4	I	149	SER	2.7
5	J	239	TRP	2.6
5	J	189	LEU	2.6
2	G	52	SER	2.6
2	G	53	ASP	2.6
5	E	181	ALA	2.6
1	F	256	ASN	2.6
5	J	122	PRO	2.6
5	J	151	PRO	2.6
4	I	147	LYS	2.5
5	E	182	LEU	2.5
4	I	117	ALA	2.5
1	A	251	LEU	2.5
5	E	228	LYS	2.5
5	J	126	VAL	2.5
4	I	152	TYR	2.5
1	F	254	GLU	2.5
5	J	150	TYR	2.5
4	D	118	TYR	2.4
5	E	12	VAL	2.4
4	I	119	TYR	2.4
2	G	32	PRO	2.4
1	F	201	LEU	2.4
5	J	117	LYS	2.4
5	J	180	PRO	2.4
5	J	242	ALA	2.4
2	G	88	ALA	2.4
1	F	28	VAL	2.3
4	I	134	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	90	GLY	2.3
5	E	206	HIS	2.3
4	I	181	ALA	2.3
5	E	240	GLY	2.3
4	I	108	PHE	2.3
4	I	173	ALA	2.3
1	F	172	LEU	2.3
1	F	249	VAL	2.3
4	D	173	TRP	2.3
5	E	113	LEU	2.2
2	G	77	THR	2.2
5	J	115	ASP	2.2
4	I	156	LYS	2.2
5	J	188	ALA	2.2
5	J	191	SER	2.2
2	G	2	GLN	2.1
5	E	112	VAL	2.1
5	J	160	VAL	2.1
5	J	168	GLY	2.1
5	E	183	ASN	2.1
4	D	178	ASP	2.1
4	I	131	VAL	2.1
2	G	47	PRO	2.1
4	I	123	ASP	2.1
1	F	199	VAL	2.1
4	I	185	ALA	2.1
5	J	146	ALA	2.1
5	E	222	TRP	2.1
5	J	226	ARG	2.1
2	G	31	HIS	2.1
1	F	227	ASP	2.0
1	F	50	PRO	2.0
5	E	242	ALA	2.0
5	J	209	CYS	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
6	NA	I	201	1/1	0.84	0.17	61,61,61,61	0
7	CL	A	302	1/1	0.85	0.13	67,67,67,67	0
6	NA	G	101	1/1	0.90	0.14	66,66,66,66	0
6	NA	A	301	1/1	0.96	0.11	45,45,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.