



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2017 – 05:56 PM EST

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 : unknown
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

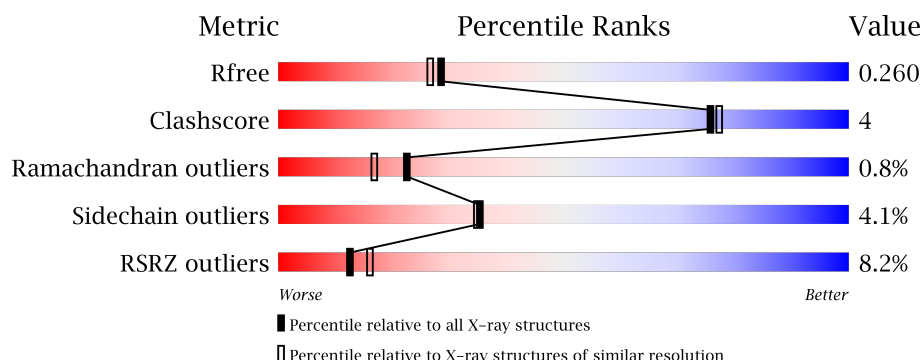
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	278	<div> <div>2%</div> <div>88%</div> <div>11%</div> </div>
1	F	278	<div> <div>9%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
2	B	99	<div> <div>%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>
2	G	99	<div> <div>11%</div> <div>87%</div> <div>9%</div> <div>...</div> </div>
3	C	9	<div> <div>100%</div> </div>

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

2 Entry composition [i](#)

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	C	N	O	S	0	1	0
			2290	1446	406	429	9			
1	F	277	Total	C	N	O	S	0	0	0
			2271	1435	401	426	9			

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

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

- Molecule 3 is a protein called GAP50 peptide, SQL.

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

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

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

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 chimera.

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 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	95	ASP	-	linker	UNP P04213
E	96	TRP	-	linker	UNP P04213
E	97	GLY	-	linker	UNP P04213
E	98	ASP	-	linker	UNP P04213
E	99	THR	-	linker	UNP P04213
E	100	GLY	-	linker	UNP P04213
E	101	GLN	-	linker	UNP P04213
E	102	LEU	-	linker	UNP P04213
E	103	TYR	-	linker	UNP P04213
E	104	PHE	-	linker	UNP P04213
E	105	GLY	-	linker	UNP P04213
E	106	GLU	-	linker	UNP P04213
E	107	GLY	-	linker	UNP P04213
E	108	SER	-	linker	UNP P04213
E	109	LYS	-	linker	UNP P04213
E	110	LEU	-	linker	UNP P04213
E	111	THR	-	linker	UNP P04213
E	112	VAL	-	linker	UNP P04213
E	113	LEU	-	linker	UNP P04213
J	95	ASP	-	linker	UNP P04213
J	96	TRP	-	linker	UNP P04213
J	97	GLY	-	linker	UNP P04213
J	98	ASP	-	linker	UNP P04213
J	99	THR	-	linker	UNP P04213
J	100	GLY	-	linker	UNP P04213
J	101	GLN	-	linker	UNP P04213
J	102	LEU	-	linker	UNP P04213
J	103	TYR	-	linker	UNP P04213
J	104	PHE	-	linker	UNP P04213
J	105	GLY	-	linker	UNP P04213
J	106	GLU	-	linker	UNP P04213
J	107	GLY	-	linker	UNP P04213
J	108	SER	-	linker	UNP P04213
J	109	LYS	-	linker	UNP P04213
J	110	LEU	-	linker	UNP P04213

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Chain	Residue	Modelled	Actual	Comment	Reference
J	111	THR	-	linker	UNP P04213
J	112	VAL	-	linker	UNP P04213
J	113	LEU	-	linker	UNP P04213

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

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

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

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	215	Total	O	0	0
			215	215		
8	B	97	Total	O	0	0
			97	97		
8	C	1	Total	O	0	0
			1	1		
8	D	97	Total	O	0	0
			97	97		
8	E	120	Total	O	0	0
			120	120		
8	F	139	Total	O	0	0
			139	139		
8	G	47	Total	O	0	0
			47	47		
8	H	1	Total	O	0	0
			1	1		
8	I	66	Total	O	0	0
			66	66		

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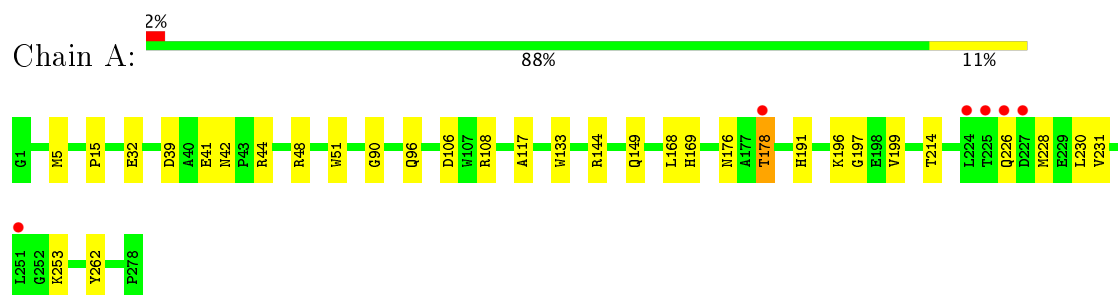
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	107	Total	O	0	0
			107	107		

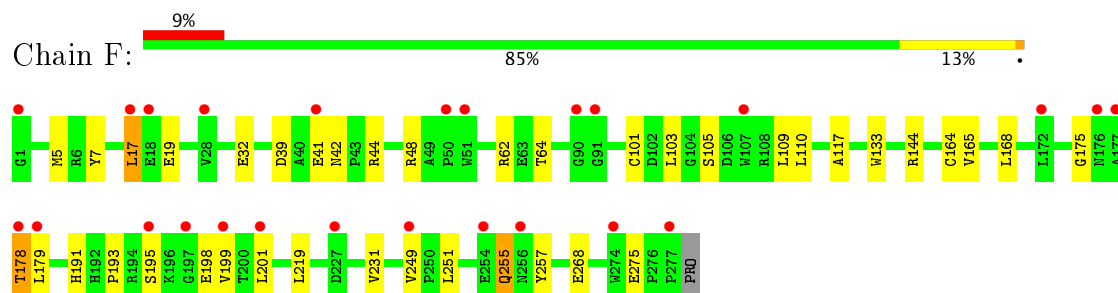
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

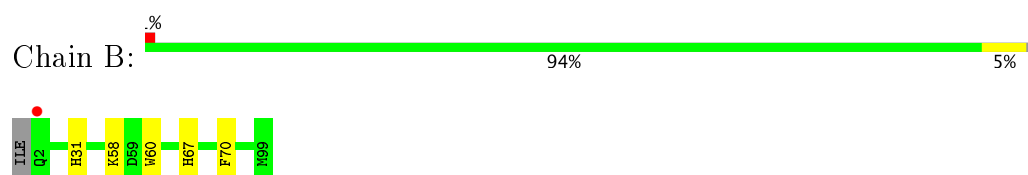
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



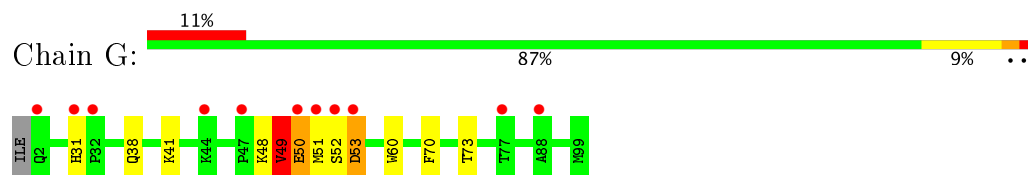
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: GAP50 peptide, SQL




There are no outlier residues recorded for this chain.

- Molecule 3: GAP50 peptide, SQL

Chain H: 




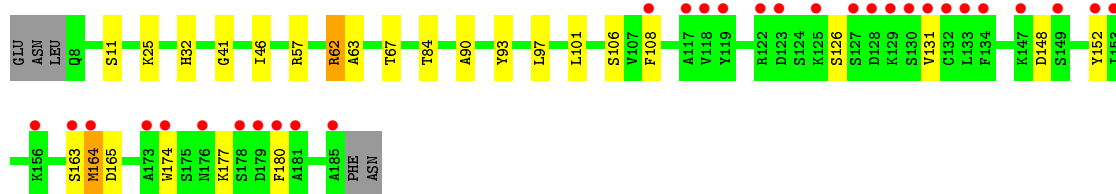
- Molecule 4: T cell receptor alpha variable 8D-2,Human nkt tcr alpha chain chimera

Chain D: 



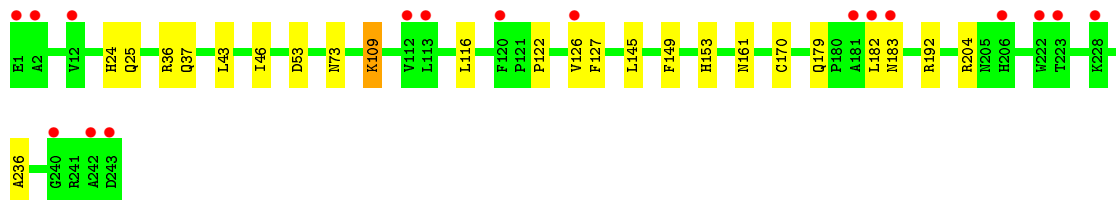
- Molecule 4: T cell receptor alpha variable 8D-2,Human nkt tcr alpha chain chimera

Chain I: 

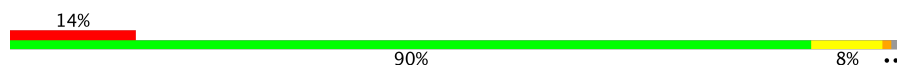


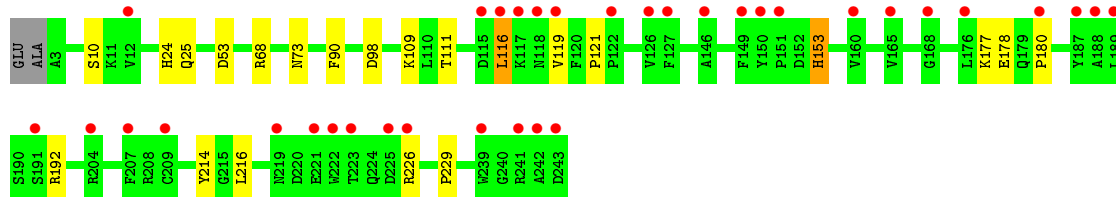
- Molecule 5: T-cell receptor beta chain V region C5,Human nkt tcr beta chain chimera

Chain E: 



- Molecule 5: T-cell receptor beta chain V region C5,Human nkt tcr beta chain chimera

Chain J: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.73 Å 70.21 Å 116.49 Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.10 Å)	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 (5.17%)	DCC
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	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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

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:101:CYS:CB	1:F:164:CYS:HG	2.26	0.43
1:F:62:ARG:HD2	4:I:93:TYR:O	2.19	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%)	25	20
1	F	275/278 (99%)	261 (95%)	11 (4%)	3 (1%)	17	11
2	B	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
2	G	96/99 (97%)	91 (95%)	3 (3%)	2 (2%)	8	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%)	11	5
4	I	177/182 (97%)	169 (96%)	6 (3%)	2 (1%)	17	11
5	E	242/243 (100%)	236 (98%)	5 (2%)	1 (0%)	38	35
5	J	241/243 (99%)	233 (97%)	8 (3%)	0	100	100
All	All	1600/1622 (99%)	1532 (96%)	55 (3%)	13 (1%)	22	17

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 ⓘ

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%)	38	38
1	F	235/236 (100%)	222 (94%)	13 (6%)	25	22
2	B	92/93 (99%)	90 (98%)	2 (2%)	57	62
2	G	92/93 (99%)	85 (92%)	7 (8%)	15	11
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%)	33	32
4	I	158/161 (98%)	152 (96%)	6 (4%)	38	38
5	E	210/209 (100%)	202 (96%)	8 (4%)	38	38
5	J	210/209 (100%)	203 (97%)	7 (3%)	43	45
All	All	1413/1414 (100%)	1354 (96%)	59 (4%)	35	33

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

Some 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 carbohydrates 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(Å ²)	Q<0.9
1	A	278/278 (100%)	0.11	6 (2%) 62 67	18, 32, 70, 102	4 (1%)
1	F	277/278 (99%)	0.67	25 (9%) 10 13	28, 49, 92, 132	5 (1%)
2	B	98/99 (98%)	-0.15	1 (1%) 82 85	21, 36, 63, 87	1 (1%)
2	G	98/99 (98%)	0.79	11 (11%) 6 7	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%)	0.01	0 100 100	27, 30, 40, 41	0
4	D	182/182 (100%)	0.34	7 (3%) 41 48	27, 47, 99, 119	0
4	I	177/182 (97%)	0.90	30 (16%) 2 2	30, 58, 127, 158	6 (3%)
5	E	243/243 (100%)	0.57	17 (6%) 17 22	21, 52, 81, 120	0
5	J	241/243 (99%)	0.84	35 (14%) 3 4	28, 58, 114, 138	2 (0%)
All	All	1612/1622 (99%)	0.52	132 (8%) 12 16	18, 48, 97, 158	19 (1%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	17	LEU	20.1
4	I	174	TRP	6.9
4	I	125	LYS	6.3
1	F	197	GLY	6.2
5	E	243	ASP	6.2
5	J	119	VAL	5.7
1	F	1	GLY	5.6
4	D	143	SER	4.9
5	J	243	ASP	4.9
5	J	221	GLU	4.8
5	J	225	ASP	4.8
2	B	2	GLN	4.7
4	I	164	MET	4.3

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

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

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Mol	Chain	Res	Type	RSRZ
1	F	90	GLY	2.3
5	E	206	HIS	2.3
1	F	172	LEU	2.3
4	I	134	PHE	2.3
5	E	113	LEU	2.3
4	I	108	PHE	2.3
4	I	173	ALA	2.3
1	F	249	VAL	2.3
4	D	173	TRP	2.3
5	E	240	GLY	2.3
4	I	156	LYS	2.2
5	J	115	ASP	2.2
2	G	77	THR	2.2
2	G	2	GLN	2.2
5	J	188	ALA	2.2
5	J	160	VAL	2.2
5	J	168	GLY	2.1
2	G	47	PRO	2.1
4	I	131	VAL	2.1
5	E	112	VAL	2.1
5	J	191	SER	2.1
5	E	183	ASN	2.1
1	F	199	VAL	2.1
4	D	178	ASP	2.1
5	J	226	ARG	2.1
4	I	185	ALA	2.1
4	I	123	ASP	2.1
1	F	227	ASP	2.1
5	E	242	ALA	2.1
5	J	146	ALA	2.1
5	E	222	TRP	2.1
1	F	50	PRO	2.0
2	G	31	HIS	2.0
1	F	91	GLY	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
6	NA	G	101	1/1	0.90	0.14	-0.80	66,66,66,66	0
6	NA	I	201	1/1	0.84	0.17	-2.04	61,61,61,61	0
7	CL	A	302	1/1	0.85	0.13	-	67,67,67,67	0
6	NA	A	301	1/1	0.96	0.11	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.