Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 06:43 PM EDT

PDB ID	:	3G3B
Title	:	Structure of a lamprey variable lymphocyte receptor mutant in complex with a protein antigen
Authors	:	Deng, L.; Velikovsky, C.A.; Mariuzza, R.A.
Deposited on	:	2009-02-02
Resolution	:	2.40 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:

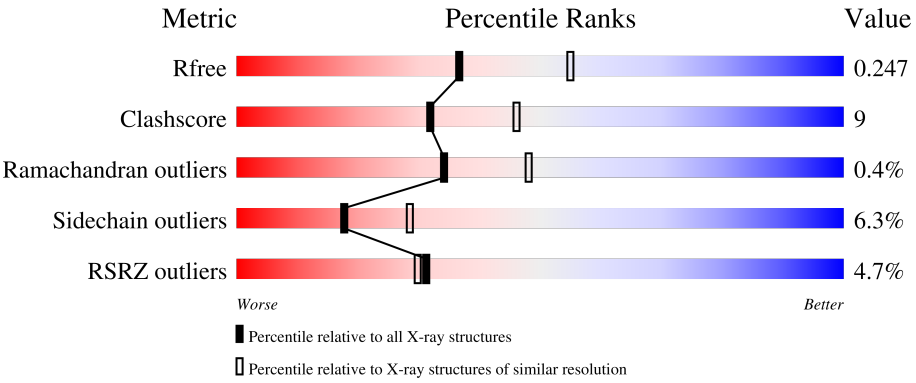
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	170	81% 17%
1	C	170	5% 75% 21%
1	E	170	5% 73% 21% 6%
1	G	170	10% 28% 14% 58%
2	B	129	2% 80% 17%

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Mol	Chain	Length	Quality of chain
2	D	129	2% 81% 14%
2	F	129	2% 73% 21%
2	H	129	4% 77% 18% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8471 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 variable lymphocyte receptor VLRB.2D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1302	816	227	251	8			
1	C	167	Total	C	N	O	S	0	0	0
			1291	809	225	249	8			
1	E	159	Total	C	N	O	S	0	0	0
			1239	781	216	237	5			
1	G	71	Total	C	N	O		0	0	0
			593	386	102	105				

- Molecule 2 is a protein called Lysozyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	127	Total	C	N	O	S	0	0	0
			981	601	188	182	10			
2	D	124	Total	C	N	O	S	0	0	0
			961	591	184	176	10			
2	F	125	Total	C	N	O	S	0	0	0
			969	595	185	179	10			
2	H	123	Total	C	N	O	S	0	0	0
			955	588	183	174	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	29	Total	O	0	0
			29	29		
3	C	39	Total	O	0	0
			39	39		
3	D	27	Total	O	0	0
			27	27		

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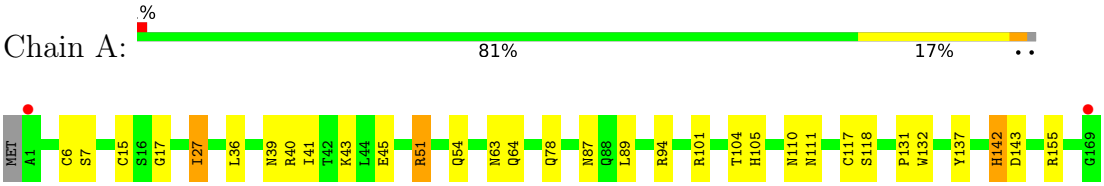
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	11	Total O 11 11	0	0
3	F	19	Total O 19 19	0	0
3	G	2	Total O 2 2	0	0
3	H	20	Total O 20 20	0	0

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.

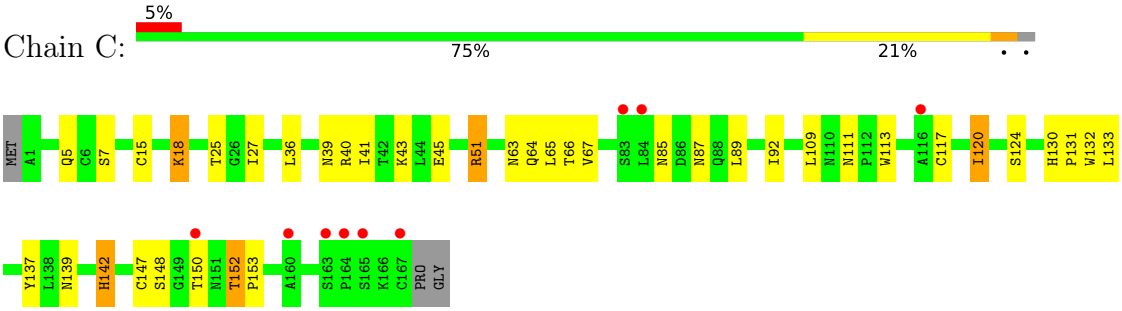
• Molecule 1: variable lymphocyte receptor VLRB.2D

Chain A:



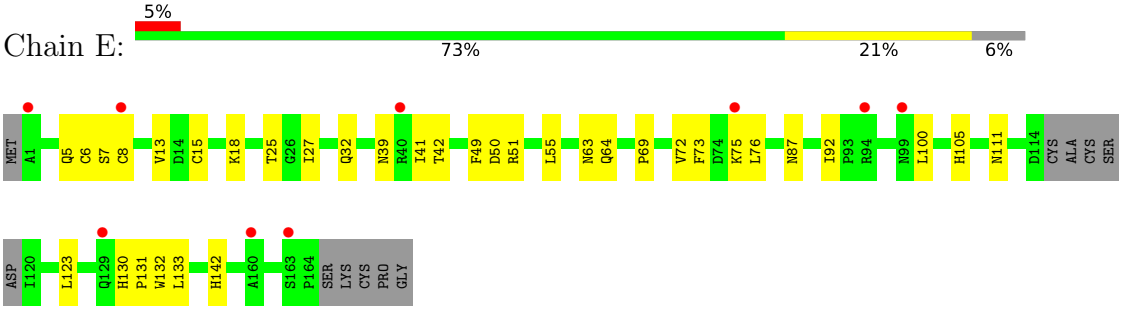
• Molecule 1: variable lymphocyte receptor VLRB.2D

Chain C:



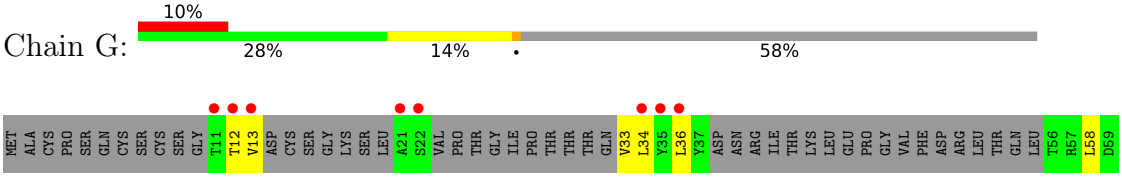
• Molecule 1: variable lymphocyte receptor VLRB.2D

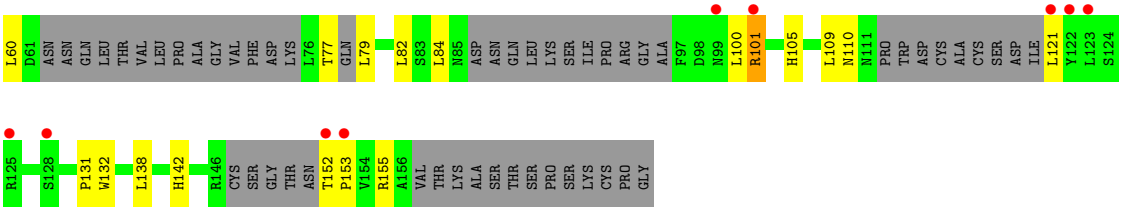
Chain E:



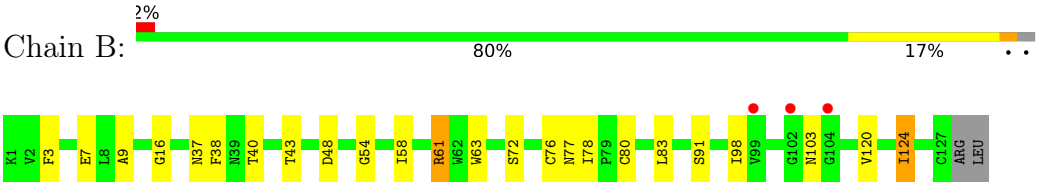
• Molecule 1: variable lymphocyte receptor VLRB.2D

Chain G:

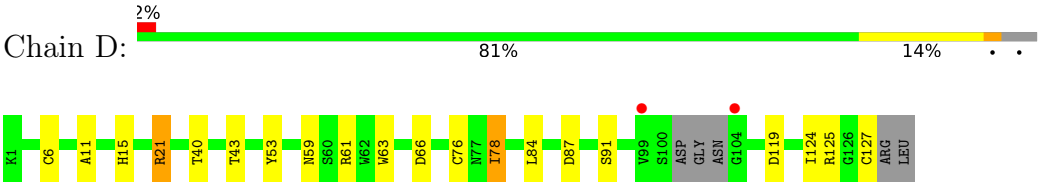




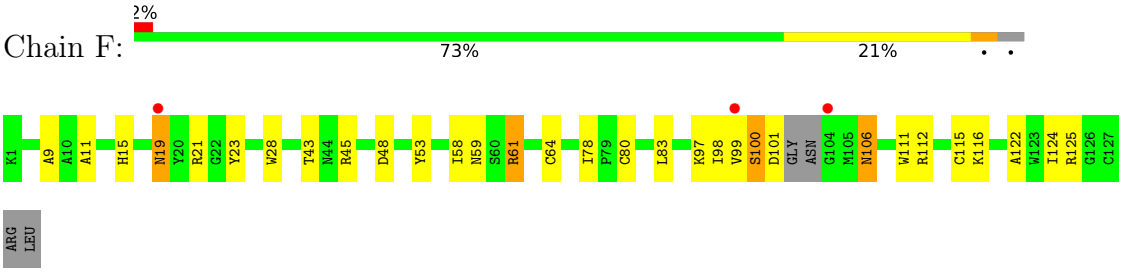
• Molecule 2: Lysozyme C



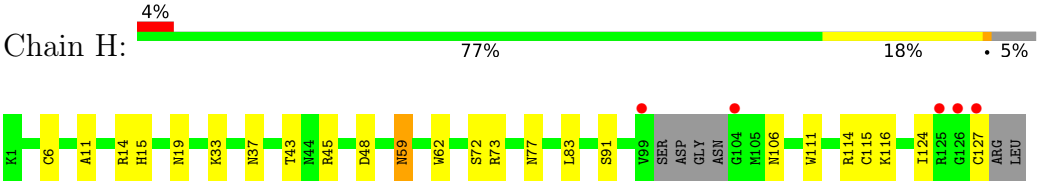
• Molecule 2: Lysozyme C



• Molecule 2: Lysozyme C



• Molecule 2: Lysozyme C



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.87Å 106.24Å 218.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.40) 99.9 (29.95-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.56 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.286 0.243 , 0.247	Depositor DCC
R_{free} test set	2942 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8471	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.74	0/1331	0.79	0/1821
1	C	0.76	0/1319	0.78	0/1804
1	E	0.64	0/1266	0.71	0/1732
1	G	0.68	0/601	0.79	0/812
2	B	0.82	0/1001	0.82	0/1354
2	D	0.88	0/980	0.87	2/1324 (0.2%)
2	F	0.77	0/988	0.82	1/1335 (0.1%)
2	H	0.75	0/974	0.80	1/1316 (0.1%)
All	All	0.76	0/8460	0.80	4/11498 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	45	ARG	NE-CZ-NH2	-5.93	117.34	120.30
2	H	45	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	D	21	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	D	87	ASP	CB-CG-OD1	5.16	122.95	118.30

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	1302	0	1288	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1291	0	1278	29	0
1	E	1239	0	1234	23	0
1	G	593	0	583	14	0
2	B	981	0	937	15	0
2	D	961	0	923	10	0
2	F	969	0	927	25	0
2	H	955	0	918	9	0
3	A	33	0	0	2	0
3	B	29	0	0	3	0
3	C	39	0	0	3	0
3	D	27	0	0	0	0
3	E	11	0	0	0	0
3	F	19	0	0	1	0
3	G	2	0	0	0	0
3	H	20	0	0	3	0
All	All	8471	0	8088	140	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 (140) 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)
1:A:6:CYS:HG	1:A:15:CYS:HG	1.08	1.00
1:G:58:LEU:HD21	1:G:60:LEU:HD11	1.51	0.90
1:A:39:ASN:HB2	1:A:63:ASN:HD21	1.36	0.89
1:E:39:ASN:HB2	1:E:63:ASN:HD21	1.40	0.87
1:G:77:THR:HB	1:G:101:ARG:HD2	1.63	0.81
2:B:61:ARG:HH11	2:B:61:ARG:HG2	1.46	0.79
1:A:104:THR:OG1	1:A:105:HIS:HD2	1.65	0.78
2:H:59:ASN:CG	3:H:141:HOH:O	2.21	0.78
2:F:21:ARG:HH21	2:F:100:SER:HA	1.51	0.76
2:F:61:ARG:CG	2:F:61:ARG:HH11	1.98	0.75
1:C:39:ASN:HB2	1:C:63:ASN:HD21	1.55	0.72
1:C:40:ARG:HA	1:C:64:GLN:HE22	1.57	0.69
2:B:61:ARG:HH11	2:B:61:ARG:CG	2.07	0.68
1:A:110:ASN:ND2	1:A:137:TYR:OH	2.27	0.67
1:A:39:ASN:HB2	1:A:63:ASN:ND2	2.09	0.67
2:D:6:CYS:HG	2:D:127:CYS:HG	0.67	0.66
1:C:18:LYS:H	1:C:39:ASN:ND2	1.93	0.66
1:E:63:ASN:HB2	1:E:87:ASN:HD21	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LEU:H	1:C:111:ASN:HD22	1.42	0.65
2:B:63:TRP:O	2:B:76:CYS:HB2	1.97	0.65
1:E:42:THR:HG22	1:E:64:GLN:HB2	1.77	0.65
1:A:87:ASN:HB2	1:A:111:ASN:HD21	1.62	0.63
2:B:3:PHE:CD2	2:B:7:GLU:HG2	2.33	0.62
3:A:181:HOH:O	2:B:61:ARG:HD2	2.00	0.62
2:F:21:ARG:NH2	2:F:100:SER:HA	2.14	0.62
1:A:104:THR:OG1	1:A:105:HIS:CD2	2.50	0.61
1:C:43:LYS:HE2	1:C:45:GLU:OE2	2.01	0.61
1:C:18:LYS:H	1:C:39:ASN:HD21	1.48	0.61
1:E:87:ASN:HB2	1:E:111:ASN:HD21	1.66	0.60
1:A:17:GLY:O	2:D:21:ARG:NH2	2.34	0.60
1:C:27:ILE:O	1:C:51:ARG:NH2	2.35	0.59
1:C:139:ASN:HB3	3:C:185:HOH:O	2.01	0.59
1:C:15:CYS:HB2	1:C:36:LEU:HD23	1.85	0.59
1:A:89:LEU:H	1:A:111:ASN:HD22	1.50	0.58
1:G:79:LEU:HD21	1:G:82:LEU:HD13	1.86	0.58
2:F:61:ARG:HH11	2:F:61:ARG:HG3	1.69	0.57
1:C:63:ASN:HB2	1:C:87:ASN:HD21	1.68	0.57
1:C:147:CYS:HB2	1:C:150:THR:OG1	2.05	0.57
1:E:105:HIS:HE1	3:F:137:HOH:O	1.87	0.57
1:A:27:ILE:O	1:A:51:ARG:NH2	2.38	0.57
2:D:59:ASN:OD1	2:D:61:ARG:HB3	2.04	0.56
2:H:62:TRP:O	2:H:73:ARG:O	2.22	0.56
1:C:130:HIS:HB3	1:C:133:LEU:HD12	1.88	0.55
2:D:76:CYS:HB2	2:D:78:ILE:HD11	1.87	0.55
1:E:131:PRO:HD2	1:E:132:TRP:CZ3	2.42	0.55
1:G:105:HIS:CE1	2:H:48:ASP:HB3	2.41	0.55
1:C:40:ARG:CA	1:C:64:GLN:HE22	2.19	0.55
1:C:65:LEU:H	1:C:87:ASN:HD22	1.53	0.55
1:E:18:LYS:H	1:E:39:ASN:HD21	1.53	0.55
2:F:21:ARG:HH21	2:F:100:SER:CA	2.19	0.55
2:F:58:ILE:HB	2:F:83:LEU:HD23	1.88	0.55
1:C:5:GLN:O	1:C:18:LYS:HD3	2.07	0.55
1:G:131:PRO:HD2	1:G:132:TRP:CE3	2.42	0.54
2:F:61:ARG:HH11	2:F:61:ARG:HG2	1.73	0.54
1:A:63:ASN:HB2	1:A:87:ASN:HD21	1.72	0.54
1:A:142:HIS:HB3	3:A:198:HOH:O	2.07	0.53
1:G:131:PRO:HD2	1:G:132:TRP:CZ3	2.43	0.53
2:F:64:CYS:HB3	2:F:78:ILE:CD1	2.40	0.52
1:C:142:HIS:ND1	3:C:181:HOH:O	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:LYS:H	1:E:39:ASN:ND2	2.08	0.51
1:A:41:ILE:H	1:A:63:ASN:HD22	1.59	0.51
2:F:9:ALA:HB1	2:F:124:ILE:CD1	2.40	0.51
2:B:80:CYS:O	2:B:83:LEU:HB2	2.11	0.50
1:A:40:ARG:HG2	1:A:64:GLN:OE1	2.11	0.50
1:C:137:TYR:HB3	2:D:63:TRP:HZ2	1.77	0.50
1:E:5:GLN:O	1:E:18:LYS:HD3	2.12	0.50
1:C:150:THR:HB	1:C:152:THR:HG23	1.94	0.50
2:D:119:ASP:OD1	2:D:125:ARG:NH2	2.45	0.50
2:B:3:PHE:HD2	2:B:7:GLU:HG2	1.78	0.49
2:H:33:LYS:HE3	2:H:37:ASN:OD1	2.11	0.49
1:C:87:ASN:HB2	1:C:111:ASN:HD21	1.77	0.49
2:F:19:ASN:N	2:F:23:TYR:O	2.45	0.49
2:H:11:ALA:O	2:H:15:HIS:HD2	1.95	0.49
1:E:8:CYS:SG	1:E:13:VAL:HG22	2.52	0.49
1:G:34:LEU:HD21	1:G:36:LEU:HD11	1.95	0.49
2:H:59:ASN:CB	3:H:141:HOH:O	2.61	0.48
1:E:69:PRO:HG2	1:E:72:VAL:HB	1.95	0.48
1:A:143:ASP:OD1	1:A:155:ARG:HD3	2.13	0.48
2:B:9:ALA:HB1	2:B:124:ILE:HD12	1.95	0.48
2:B:58:ILE:HD12	2:B:98:ILE:CD1	2.43	0.48
1:A:43:LYS:NZ	1:A:45:GLU:OE2	2.42	0.47
2:B:37:ASN:O	2:B:38:PHE:HB2	2.15	0.46
1:A:105:HIS:CE1	2:B:48:ASP:HB3	2.51	0.46
1:E:92:ILE:HG13	1:E:123:LEU:HD13	1.97	0.46
1:G:152:THR:HB	1:G:153:PRO:HD2	1.96	0.46
1:C:41:ILE:H	1:C:63:ASN:ND2	2.14	0.45
1:G:13:VAL:O	1:G:13:VAL:HG12	2.16	0.45
1:A:15:CYS:HB2	1:A:36:LEU:HD23	1.98	0.45
1:C:131:PRO:HD2	1:C:132:TRP:CZ3	2.51	0.45
1:E:39:ASN:CB	1:E:63:ASN:HD21	2.22	0.45
1:G:58:LEU:HD21	1:G:60:LEU:CD1	2.35	0.45
2:F:111:TRP:CD1	2:F:115:CYS:HB2	2.51	0.45
1:E:76:LEU:O	1:E:100:LEU:HD23	2.18	0.44
1:E:73:PHE:HB3	1:E:100:LEU:HD21	1.98	0.44
2:B:16:GLY:HA2	3:B:131:HOH:O	2.18	0.44
1:C:111:ASN:HB2	1:C:113:TRP:CE2	2.53	0.44
2:F:11:ALA:O	2:F:15:HIS:HD2	2.00	0.44
1:C:120:ILE:HD12	1:C:120:ILE:HA	1.88	0.44
2:F:21:ARG:HE	2:F:100:SER:HA	1.82	0.44
1:E:6:CYS:HG	1:E:15:CYS:CB	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:CYS:SG	2:H:127:CYS:SG	3.16	0.43
2:B:72:SER:HB2	3:B:150:HOH:O	2.17	0.43
1:E:105:HIS:CE1	2:F:48:ASP:HB3	2.54	0.43
2:F:64:CYS:CB	2:F:78:ILE:CD1	2.96	0.43
1:G:138:LEU:HA	3:H:141:HOH:O	2.18	0.43
1:C:65:LEU:H	1:C:87:ASN:ND2	2.16	0.43
2:F:53:TYR:CD2	2:F:80:CYS:HB3	2.54	0.43
1:C:85:ASN:HB3	1:C:109:LEU:HD23	2.01	0.43
1:A:105:HIS:HE1	3:B:135:HOH:O	2.02	0.43
2:F:19:ASN:HA	2:F:23:TYR:O	2.19	0.43
1:E:32:GLN:HA	1:E:55:LEU:HA	2.00	0.42
2:D:53:TYR:OH	2:D:66:ASP:OD2	2.31	0.42
1:E:51:ARG:H	1:E:51:ARG:HG2	1.68	0.42
2:F:106:ASN:HD21	2:F:116:LYS:NZ	2.17	0.42
1:C:39:ASN:CB	1:C:63:ASN:HD21	2.29	0.42
1:C:92:ILE:O	3:C:207:HOH:O	2.20	0.42
2:D:11:ALA:O	2:D:15:HIS:HD2	2.03	0.42
1:G:109:LEU:H	1:G:109:LEU:HD23	1.84	0.42
1:G:79:LEU:HD23	1:G:100:LEU:HD22	2.02	0.42
1:A:54:GLN:NE2	1:A:78:GLN:OE1	2.53	0.42
1:E:49:PHE:O	1:E:51:ARG:N	2.53	0.42
1:E:130:HIS:HB3	1:E:133:LEU:HD12	2.02	0.42
2:B:40:THR:O	2:B:54:GLY:HA2	2.20	0.42
1:C:152:THR:HA	1:C:153:PRO:HD3	1.84	0.42
2:F:28:TRP:CH2	2:F:99:VAL:HG21	2.55	0.42
2:B:61:ARG:CG	2:B:61:ARG:NH1	2.76	0.41
2:F:122:ALA:HA	2:F:125:ARG:HG3	2.02	0.41
2:F:9:ALA:HB1	2:F:124:ILE:HD13	2.02	0.41
1:C:137:TYR:HB3	2:D:63:TRP:CZ2	2.55	0.41
2:F:64:CYS:CB	2:F:78:ILE:HD12	2.50	0.41
2:F:61:ARG:CG	2:F:61:ARG:NH1	2.70	0.41
2:H:111:TRP:CD1	2:H:115:CYS:HB2	2.55	0.41
1:E:41:ILE:H	1:E:63:ASN:ND2	2.19	0.41
1:E:75:LYS:N	1:E:75:LYS:HD2	2.35	0.40
2:F:106:ASN:O	2:F:112:ARG:NH1	2.48	0.40
1:G:12:THR:HG23	1:G:33:VAL:HB	2.02	0.40
2:D:40:THR:O	2:D:84:LEU:HA	2.21	0.40
2:F:58:ILE:HD12	2:F:98:ILE:CD1	2.51	0.40
2:H:111:TRP:CZ2	2:H:116:LYS:HB2	2.56	0.40
1:A:131:PRO:HD2	1:A:132:TRP:CZ3	2.57	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	167/170 (98%)	158 (95%)	9 (5%)	0	100	100
1	C	165/170 (97%)	152 (92%)	13 (8%)	0	100	100
1	E	155/170 (91%)	143 (92%)	11 (7%)	1 (1%)	25	36
1	G	53/170 (31%)	43 (81%)	8 (15%)	2 (4%)	3	2
2	B	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
2	D	120/129 (93%)	113 (94%)	7 (6%)	0	100	100
2	F	121/129 (94%)	117 (97%)	3 (2%)	1 (1%)	19	29
2	H	119/129 (92%)	118 (99%)	1 (1%)	0	100	100
All	All	1025/1196 (86%)	963 (94%)	58 (6%)	4 (0%)	34	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	50	ASP
2	F	100	SER
1	G	84	LEU
1	G	155	ARG

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	152/153 (99%)	144 (95%)	8 (5%)	22	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	151/153 (99%)	139 (92%)	12 (8%)	12 19
1	E	144/153 (94%)	140 (97%)	4 (3%)	43 63
1	G	67/153 (44%)	63 (94%)	4 (6%)	19 31
2	B	103/105 (98%)	95 (92%)	8 (8%)	12 19
2	D	101/105 (96%)	97 (96%)	4 (4%)	31 49
2	F	102/105 (97%)	95 (93%)	7 (7%)	15 25
2	H	100/105 (95%)	89 (89%)	11 (11%)	6 8
All	All	920/1032 (89%)	862 (94%)	58 (6%)	18 28

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	27	ILE
1	A	51	ARG
1	A	94	ARG
1	A	101	ARG
1	A	117	CYS
1	A	118	SER
1	A	142	HIS
2	B	43	THR
2	B	61	ARG
2	B	77	ASN
2	B	78	ILE
2	B	91	SER
2	B	103	ASN
2	B	120	VAL
2	B	124	ILE
1	C	7	SER
1	C	18	LYS
1	C	25	THR
1	C	51	ARG
1	C	66	THR
1	C	67	VAL
1	C	117	CYS
1	C	120	ILE
1	C	124	SER
1	C	142	HIS
1	C	148	SER
1	C	152	THR

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Mol	Chain	Res	Type
2	D	43	THR
2	D	78	ILE
2	D	91	SER
2	D	124	ILE
1	E	7	SER
1	E	25	THR
1	E	27	ILE
1	E	142	HIS
2	F	19	ASN
2	F	43	THR
2	F	59	ASN
2	F	61	ARG
2	F	97	LYS
2	F	101	ASP
2	F	106	ASN
1	G	101	ARG
1	G	110	ASN
1	G	121	LEU
1	G	142	HIS
2	H	14	ARG
2	H	19	ASN
2	H	43	THR
2	H	59	ASN
2	H	72	SER
2	H	77	ASN
2	H	83	LEU
2	H	91	SER
2	H	106	ASN
2	H	114	ARG
2	H	124	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	54	GLN
1	A	63	ASN
1	A	78	GLN
1	A	87	ASN
1	A	105	HIS
1	A	110	ASN
1	A	111	ASN

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Mol	Chain	Res	Type
2	B	57	GLN
2	B	106	ASN
2	B	113	ASN
1	C	39	ASN
1	C	63	ASN
1	C	64	GLN
1	C	87	ASN
1	C	111	ASN
2	D	15	HIS
2	D	57	GLN
2	D	106	ASN
2	D	113	ASN
1	E	39	ASN
1	E	63	ASN
1	E	78	GLN
1	E	87	ASN
1	E	105	HIS
1	E	111	ASN
2	F	15	HIS
2	F	106	ASN
2	F	113	ASN
1	G	105	HIS
1	G	110	ASN
1	G	111	ASN
1	G	142	HIS
2	H	15	HIS
2	H	57	GLN
2	H	77	ASN
2	H	106	ASN
2	H	113	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

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, 95^{th} 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	169/170 (99%)	-0.08	2 (1%)	79	77	26, 44, 58, 71	0
1	C	167/170 (98%)	-0.01	9 (5%)	25	24	28, 43, 62, 79	0
1	E	159/170 (93%)	0.28	9 (5%)	23	22	40, 57, 74, 88	0
1	G	71/170 (41%)	1.26	17 (23%)	0	0	39, 60, 82, 97	0
2	B	127/129 (98%)	-0.11	3 (2%)	59	57	24, 37, 51, 62	4 (3%)
2	D	124/129 (96%)	-0.33	2 (1%)	72	70	25, 34, 46, 60	4 (3%)
2	F	125/129 (96%)	-0.08	3 (2%)	59	57	30, 39, 53, 60	4 (3%)
2	H	123/129 (95%)	-0.01	5 (4%)	37	36	30, 41, 57, 73	4 (3%)
All	All	1065/1196 (89%)	0.05	50 (4%)	31	30	24, 43, 68, 97	16 (1%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	104	GLY	8.7
2	F	104	GLY	7.8
2	D	104	GLY	7.2
1	G	99	ASN	5.8
2	B	99	VAL	5.7
2	H	99	VAL	5.5
1	A	1	ALA	5.0
1	G	35	TYR	4.9
2	H	127	CYS	4.6
1	G	121	LEU	4.4
1	G	123	LEU	4.3
1	E	1	ALA	4.3
2	D	99	VAL	4.1
2	H	125	ARG	3.8
2	B	104	GLY	3.7
1	G	122	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	13	VAL	3.6
1	E	8	CYS	3.6
1	G	152	THR	3.6
1	C	164	PRO	3.5
1	G	34	LEU	3.4
1	G	11	THR	3.4
2	F	99	VAL	3.4
1	E	99	ASN	3.3
1	E	160	ALA	3.3
1	E	163	SER	3.2
1	G	36	LEU	3.2
1	G	153	PRO	3.0
1	G	128	SER	3.0
1	G	12	THR	2.9
1	C	167	CYS	2.9
1	E	40	ARG	2.7
1	C	163	SER	2.6
1	G	125	ARG	2.6
1	C	160	ALA	2.6
2	B	102	GLY	2.6
1	G	21	ALA	2.5
1	A	169	GLY	2.4
1	C	150	THR	2.4
1	C	165	SER	2.4
1	G	101	ARG	2.3
2	H	126	GLY	2.2
1	G	22	SER	2.2
1	E	75	LYS	2.2
1	E	94	ARG	2.1
1	C	84	LEU	2.1
1	E	129	GLN	2.1
1	C	116	ALA	2.1
2	F	19	ASN	2.1
1	C	83	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.