Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:40 PM GMT

PDB ID	:	4J4L
Title	:	Modular evolution and design of the protein binding interface
Authors	:	Cheong, H.K.; Kim, H.J.
Deposited on	:	2013-02-07
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

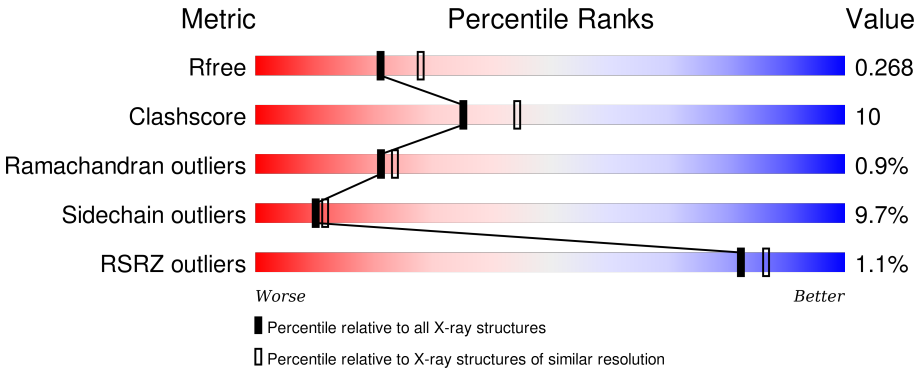
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	267	72% 21%
1	B	267	66% 22% 5% 6%
2	C	168	4% 71% 20% 8%
2	D	168	% 70% 24%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6751 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 Internalin B, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2035	1297	345	389	4			
1	B	251	Total	C	N	O	S	0	0	0
			1982	1264	336	378	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	ALA	ASP	CONFLICT	UNP D2P9A6
A	302	LEU	-	EXPRESSION TAG	UNP Q4G1L3
A	303	GLU	-	EXPRESSION TAG	UNP Q4G1L3
A	304	HIS	-	EXPRESSION TAG	UNP Q4G1L3
A	305	HIS	-	EXPRESSION TAG	UNP Q4G1L3
A	306	HIS	-	EXPRESSION TAG	UNP Q4G1L3
A	307	HIS	-	EXPRESSION TAG	UNP Q4G1L3
A	308	HIS	-	EXPRESSION TAG	UNP Q4G1L3
A	309	HIS	-	EXPRESSION TAG	UNP Q4G1L3
B	59	ALA	ASP	CONFLICT	UNP D2P9A6
B	302	LEU	-	EXPRESSION TAG	UNP Q4G1L3
B	303	GLU	-	EXPRESSION TAG	UNP Q4G1L3
B	304	HIS	-	EXPRESSION TAG	UNP Q4G1L3
B	305	HIS	-	EXPRESSION TAG	UNP Q4G1L3
B	306	HIS	-	EXPRESSION TAG	UNP Q4G1L3
B	307	HIS	-	EXPRESSION TAG	UNP Q4G1L3
B	308	HIS	-	EXPRESSION TAG	UNP Q4G1L3
B	309	HIS	-	EXPRESSION TAG	UNP Q4G1L3

- Molecule 2 is a protein called Interleukin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	155	Total	C	N	O	S	0	0	0
			1246	780	216	241	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	166	Total	C	N	O	S	0	0	0
			1330	832	229	260	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	17	GLY	-	EXPRESSION TAG	UNP P05231
C	18	SER	-	EXPRESSION TAG	UNP P05231
D	17	GLY	-	EXPRESSION TAG	UNP P05231
D	18	SER	-	EXPRESSION TAG	UNP P05231

- Molecule 3 is water.

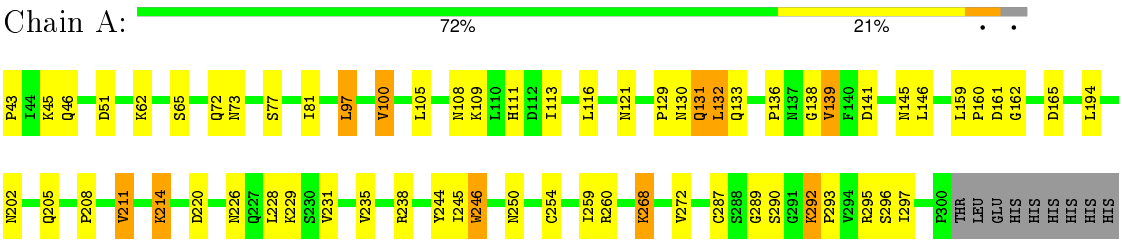
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	28	Total	O	0	0
			28	28		
3	C	37	Total	O	0	0
			37	37		
3	D	32	Total	O	0	0
			32	32		

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 errors 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.

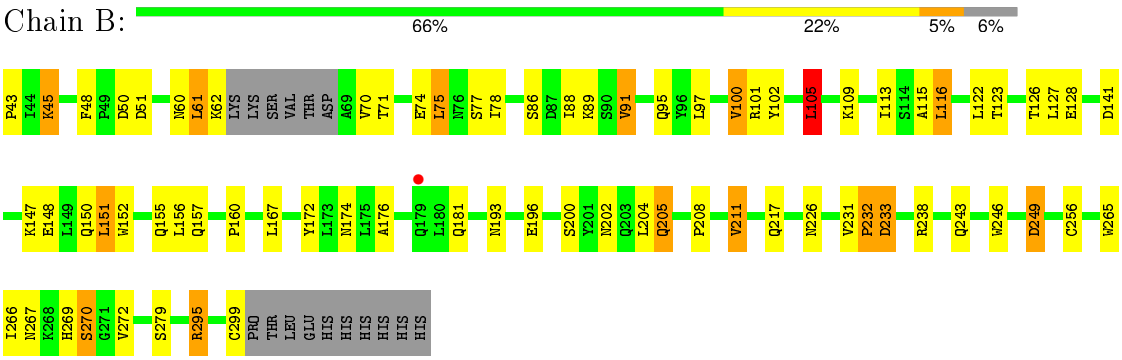
- Molecule 1: Internalin B, Variable lymphocyte receptor B

Chain A:



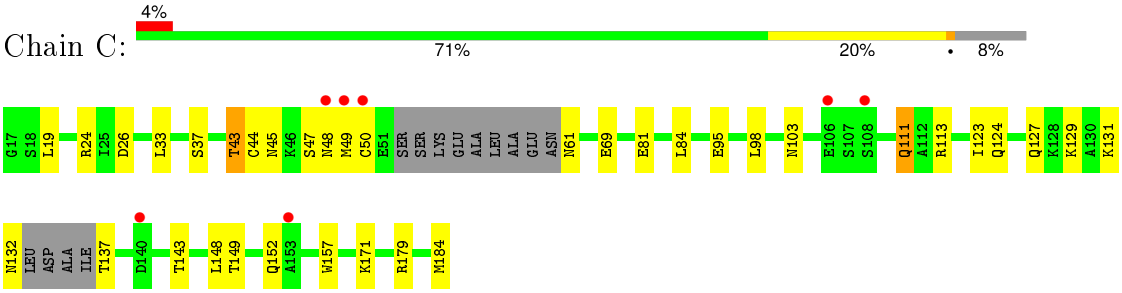
- Molecule 1: Internalin B, Variable lymphocyte receptor B

Chain B:



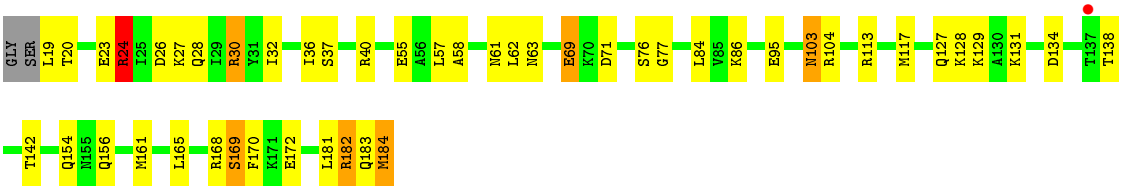
- Molecule 2: Interleukin-6

Chain C:



- Molecule 2: Interleukin-6

Chain D:


GLY SER L19 T20 E23 R24 I25 D26 K27 Q28 I29 R30 Y31 I32 I36 S37 R40 E55 A56 L57 A58 N61 L62 N63 E69 K70 D71 S76 G77 L84 V85 K86 E95 N103 R104 R113 M117 Q127 K128 K129 A130 K131 D134 T137 T138
T142 Q154 N155 Q156 M161 L165 R168 S169 F170 K171 E172 L181 R182 Q183 M184

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.32Å 134.00Å 148.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.09 – 2.30 61.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.2 (61.09-2.30) 95.2 (61.09-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.268 0.204 , 0.268	Depositor DCC
R_{free} test set	2129 reflections (5.59%)	DCC
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 40123 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6751	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.81	1/2075 (0.0%)	0.90	2/2821 (0.1%)
1	B	0.69	1/2020 (0.0%)	0.84	3/2745 (0.1%)
2	C	0.81	1/1259 (0.1%)	0.89	0/1687
2	D	0.76	0/1345	0.92	6/1807 (0.3%)
All	All	0.77	3/6699 (0.0%)	0.88	11/9060 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	TRP	CD2-CE2	6.02	1.48	1.41
2	C	157	TRP	CD2-CE2	5.96	1.48	1.41
1	B	246	TRP	CD2-CE2	5.13	1.47	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	30	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	B	151	LEU	CA-CB-CG	6.76	130.84	115.30
2	D	24	ARG	NE-CZ-NH1	6.13	123.36	120.30
2	D	84	LEU	CB-CG-CD1	-6.08	100.66	111.00
2	D	30	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	61	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	220	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	105	LEU	CA-CB-CG	5.22	127.30	115.30
2	D	19	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	100	VAL	CG1-CB-CG2	-5.04	102.84	110.90
2	D	24	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2035	0	2058	46	0
1	B	1982	0	2001	45	0
2	C	1246	0	1261	18	0
2	D	1330	0	1348	27	0
3	A	61	0	0	7	0
3	B	28	0	0	3	0
3	C	37	0	0	2	0
3	D	32	0	0	5	0
All	All	6751	0	6668	130	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 10.

All (130) 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:D:154:GLN:NE2	3:D:231:HOH:O	1.99	0.89
1:A:208:PRO:HB2	1:A:211:VAL:HG13	1.54	0.87
1:A:226:ASN:HB2	1:A:250:ASN:HD21	1.47	0.78
2:C:111:GLN:HE21	2:C:111:GLN:H	1.31	0.78
2:C:111:GLN:HE21	2:C:111:GLN:N	1.82	0.77
1:A:145:ASN:OD1	3:A:457:HOH:O	2.03	0.76
1:B:95:GLN:HG3	1:B:115:ALA:HB1	1.69	0.74
1:A:108:ASN:ND2	1:A:130:ASN:HD22	1.85	0.74
1:A:77:SER:OG	3:A:442:HOH:O	2.02	0.74
1:A:290:SER:HB2	1:A:292:LYS:HD3	1.70	0.74
2:C:131:LYS:O	2:C:132:ASN:HB2	1.88	0.73
1:A:287:CYS:SG	1:A:297:ILE:HD11	2.29	0.72
1:A:254:CYS:SG	1:A:297:ILE:HD13	2.30	0.72
1:A:162:GLY:HA2	1:A:165:ASP:OD2	1.90	0.72
2:D:62:LEU:HD12	2:D:165:LEU:HD23	1.72	0.70
2:C:111:GLN:NE2	2:C:111:GLN:H	1.87	0.69
1:A:108:ASN:HD22	1:A:130:ASN:HD22	1.38	0.69
1:A:287:CYS:SG	1:A:297:ILE:CD1	2.81	0.68
3:B:427:HOH:O	2:D:24:ARG:HD2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:LEU:O	2:D:169:SER:HB2	1.95	0.67
1:B:148:GLU:HG2	1:B:172:TYR:HB3	1.75	0.67
1:A:290:SER:CB	1:A:292:LYS:HD3	2.25	0.66
2:D:104:ARG:HH22	2:D:156:GLN:NE2	1.92	0.66
3:A:403:HOH:O	2:C:24:ARG:HD2	1.97	0.65
1:B:101:ARG:HH11	1:B:101:ARG:HG2	1.62	0.65
2:D:40:ARG:NH1	3:D:207:HOH:O	2.31	0.64
2:D:181:LEU:HA	2:D:184:MET:HG3	1.80	0.64
1:B:128:GLU:OE2	2:D:27:LYS:HE2	1.98	0.64
1:A:228:LEU:H	1:A:250:ASN:HD22	1.45	0.63
1:B:48:PHE:HZ	1:B:97:LEU:HD11	1.64	0.62
1:B:266:ILE:O	1:B:270:SER:N	2.34	0.60
1:A:268:LYS:O	1:A:268:LYS:HG2	1.99	0.60
2:D:103:ASN:HD22	2:D:103:ASN:N	2.00	0.60
1:A:43:PRO:HG2	1:A:46:GLN:HG2	1.85	0.59
1:B:113:ILE:O	1:B:116:LEU:HB2	2.03	0.59
1:B:71:THR:HG23	1:B:74:GLU:H	1.69	0.58
1:B:267:ASN:HD21	1:B:295:ARG:HD3	1.69	0.57
2:D:58:ALA:HB3	2:D:61:ASN:ND2	2.20	0.57
1:B:243:GLN:NE2	3:B:404:HOH:O	2.38	0.57
1:B:70:VAL:CG2	1:B:75:LEU:HD13	2.34	0.56
1:A:138:GLY:HA3	1:A:141:ASP:OD1	2.05	0.56
1:B:128:GLU:HG3	1:B:152:TRP:HB2	1.87	0.56
1:A:73:ASN:HB2	2:D:69:GLU:OE1	2.06	0.55
1:B:78:ILE:HD12	1:B:97:LEU:HD21	1.88	0.55
1:B:91:VAL:HG11	1:B:105:LEU:HD11	1.88	0.55
1:B:101:ARG:NH1	1:B:101:ARG:HG2	2.22	0.55
2:D:183:GLN:NE2	3:D:203:HOH:O	2.40	0.54
1:A:121:ASN:HB2	3:A:455:HOH:O	2.06	0.54
1:A:228:LEU:H	1:A:250:ASN:ND2	2.06	0.54
1:B:70:VAL:HG21	1:B:75:LEU:HD13	1.89	0.54
1:B:126:THR:HG21	2:D:23:GLU:HG2	1.90	0.54
2:D:26:ASP:OD2	2:D:182:ARG:HD3	2.09	0.54
1:B:150:GLN:HE22	2:D:24:ARG:HB2	1.73	0.53
1:B:249:ASP:OD2	2:D:117:MET:HG3	2.09	0.52
1:A:72:GLN:HE22	2:D:77:GLY:HA3	1.74	0.52
1:A:81:ILE:HD11	1:A:97:LEU:HD23	1.91	0.51
3:A:439:HOH:O	2:C:113:ARG:HG2	2.09	0.51
1:B:267:ASN:ND2	1:B:295:ARG:HD3	2.25	0.51
1:B:43:PRO:HB2	1:B:45:LYS:HG2	1.92	0.51
1:B:256:CYS:HG	1:B:299:CYS:HG	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:131:LYS:O	2:C:132:ASN:CB	2.60	0.50
1:A:231:VAL:HB	1:A:235:VAL:HG11	1.93	0.50
1:B:78:ILE:HD12	1:B:97:LEU:CD2	2.41	0.50
1:B:176:ALA:HA	1:B:200:SER:O	2.12	0.49
1:A:226:ASN:CB	1:A:250:ASN:HD21	2.23	0.49
2:D:168:ARG:HD2	2:D:172:GLU:OE2	2.11	0.49
1:B:100:VAL:HG22	1:B:122:LEU:HD13	1.95	0.49
1:A:136:PRO:HG2	1:A:139:VAL:HG13	1.95	0.48
1:A:290:SER:OG	1:A:292:LYS:HG2	2.12	0.48
1:B:265:TRP:O	1:B:269:HIS:N	2.45	0.48
1:B:50:ASP:OD1	1:B:50:ASP:C	2.51	0.48
1:A:113:ILE:HB	1:A:116:LEU:HD12	1.94	0.48
1:B:74:GLU:O	1:B:77:SER:HB2	2.14	0.48
1:B:231:VAL:HA	1:B:232:PRO:HD3	1.68	0.48
3:A:413:HOH:O	2:C:19:LEU:HG	2.14	0.48
1:B:102:TYR:CD1	1:B:102:TYR:C	2.87	0.48
1:B:123:THR:CG2	1:B:147:LYS:HE2	2.45	0.47
1:A:132:LEU:HD22	1:A:133:GLN:H	1.79	0.47
2:D:36:ILE:HD11	2:D:170:PHE:CD2	2.50	0.47
1:A:129:PRO:HB2	1:A:132:LEU:HB2	1.96	0.47
2:C:123:ILE:O	2:C:127:GLN:HG3	2.14	0.47
1:B:50:ASP:OD1	1:B:51:ASP:N	2.49	0.46
2:C:84:LEU:HD22	2:C:184:MET:HE1	1.98	0.46
2:C:26:ASP:HB3	3:C:203:HOH:O	2.15	0.46
1:B:196:GLU:HG3	3:B:405:HOH:O	2.15	0.46
2:D:57:LEU:HG	2:D:161:MET:HB3	1.97	0.46
1:A:130:ASN:C	1:A:131:GLN:HE21	2.19	0.45
2:C:129:LYS:HE3	2:C:184:MET:HE1	1.98	0.45
1:A:131:GLN:N	1:A:131:GLN:HE21	2.14	0.45
2:C:148:LEU:O	2:C:152:GLN:HG3	2.16	0.45
1:B:202:ASN:HB2	1:B:226:ASN:OD1	2.15	0.45
1:A:290:SER:HB2	1:A:292:LYS:CD	2.46	0.44
1:A:202:ASN:HB2	1:A:226:ASN:OD1	2.18	0.44
1:B:62:LYS:HD3	1:B:62:LYS:HA	1.82	0.44
2:D:28:GLN:O	2:D:32:ILE:HG13	2.18	0.44
2:C:179:ARG:NH1	3:C:226:HOH:O	2.43	0.44
2:C:47:SER:HB2	2:C:49:MET:SD	2.58	0.44
1:B:113:ILE:HD12	1:B:127:LEU:HD21	1.99	0.43
1:A:111:HIS:CD2	1:A:132:LEU:HA	2.54	0.43
1:A:290:SER:OG	1:A:292:LYS:HD3	2.18	0.43
2:C:43:THR:CG2	2:C:44:CYS:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD22	1:A:133:GLN:N	2.34	0.43
1:A:111:HIS:HD2	1:A:132:LEU:HA	1.82	0.42
2:D:71:ASP:CG	2:D:86:LYS:HD3	2.39	0.42
1:A:100:VAL:HG13	1:A:100:VAL:O	2.19	0.42
1:B:193:ASN:HA	1:B:217:GLN:NE2	2.34	0.42
1:B:86:SER:OG	1:B:88:ILE:HD12	2.19	0.42
1:A:244:TYR:HB3	1:A:246:TRP:CZ3	2.54	0.42
1:A:259:ILE:HG13	1:A:259:ILE:O	2.20	0.42
1:A:245:ILE:HG22	1:A:272:VAL:HG23	2.02	0.42
1:B:181:GLN:O	1:B:204:LEU:HA	2.20	0.42
2:D:95:GLU:HG2	3:D:209:HOH:O	2.19	0.42
1:A:138:GLY:CA	1:A:141:ASP:OD1	2.68	0.41
2:C:33:LEU:HD23	2:C:33:LEU:HA	1.78	0.41
1:A:293:PRO:O	1:A:296:SER:OG	2.25	0.41
1:B:113:ILE:HB	1:B:116:LEU:HD22	2.02	0.41
1:A:136:PRO:O	1:A:139:VAL:HG22	2.20	0.41
2:D:129:LYS:HE2	2:D:129:LYS:HB3	1.64	0.41
1:A:259:ILE:O	1:A:260:ARG:C	2.58	0.41
1:B:150:GLN:HG2	1:B:174:ASN:HB3	2.03	0.41
1:A:159:LEU:HA	1:A:160:PRO:HD3	1.91	0.41
2:D:103:ASN:N	2:D:103:ASN:ND2	2.68	0.40
1:B:269:HIS:HB3	1:B:272:VAL:HG13	2.04	0.40
1:B:208:PRO:O	1:B:211:VAL:HG22	2.21	0.40
2:C:95:GLU:O	2:C:98:LEU:HB2	2.20	0.40
2:D:127:GLN:NE2	3:D:218:HOH:O	2.52	0.40
1:B:205:GLN:HG2	1:B:205:GLN:H	1.68	0.40
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.97	0.40
1:A:214:LYS:HG2	3:A:424:HOH:O	2.21	0.40
2:D:128:LYS:HD3	2:D:128:LYS:HA	1.77	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	256/267 (96%)	241 (94%)	14 (6%)	1 (0%)	39 48
1	B	247/267 (92%)	224 (91%)	18 (7%)	5 (2%)	9 7
2	C	149/168 (89%)	146 (98%)	3 (2%)	0	100 100
2	D	164/168 (98%)	156 (95%)	7 (4%)	1 (1%)	30 36
All	All	816/870 (94%)	767 (94%)	42 (5%)	7 (1%)	21 24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	GLY
1	B	160	PRO
1	B	233	ASP
1	B	270	SER
2	D	131	LYS
1	B	232	PRO
1	B	249	ASP

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	233/242 (96%)	212 (91%)	21 (9%)	12 14
1	B	226/242 (93%)	205 (91%)	21 (9%)	11 13
2	C	142/152 (93%)	127 (89%)	15 (11%)	8 9
2	D	151/152 (99%)	135 (89%)	16 (11%)	8 9
All	All	752/788 (95%)	679 (90%)	73 (10%)	10 12

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	51	ASP
1	A	62	LYS
1	A	65	SER

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Mol	Chain	Res	Type
1	A	97	LEU
1	A	105	LEU
1	A	109	LYS
1	A	131	GLN
1	A	132	LEU
1	A	139	VAL
1	A	146	LEU
1	A	161	ASP
1	A	194	LEU
1	A	205	GLN
1	A	211	VAL
1	A	214	LYS
1	A	229	LYS
1	A	238	ARG
1	A	268	LYS
1	A	292	LYS
1	A	295	ARG
1	B	45	LYS
1	B	60	ASN
1	B	61	LEU
1	B	75	LEU
1	B	89	LYS
1	B	91	VAL
1	B	100	VAL
1	B	105	LEU
1	B	109	LYS
1	B	116	LEU
1	B	141	ASP
1	B	151	LEU
1	B	155	GLN
1	B	157	GLN
1	B	167	LEU
1	B	205	GLN
1	B	211	VAL
1	B	233	ASP
1	B	238	ARG
1	B	279	SER
1	B	295	ARG
2	C	37	SER
2	C	43	THR
2	C	45	ASN
2	C	48	ASN

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Mol	Chain	Res	Type
2	C	50	CYS
2	C	61	ASN
2	C	69	GLU
2	C	81	GLU
2	C	103	ASN
2	C	111	GLN
2	C	124	GLN
2	C	137	THR
2	C	143	THR
2	C	149	THR
2	C	171	LYS
2	D	20	THR
2	D	24	ARG
2	D	30	ARG
2	D	37	SER
2	D	55	GLU
2	D	63	ASN
2	D	69	GLU
2	D	76	SER
2	D	103	ASN
2	D	113	ARG
2	D	134	ASP
2	D	138	THR
2	D	142	THR
2	D	169	SER
2	D	182	ARG
2	D	184	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	76	ASN
1	A	85	ASN
1	A	92	GLN
1	A	99	ASN
1	A	108	ASN
1	A	131	GLN
1	A	154	ASN
1	A	193	ASN
1	A	203	GLN
1	A	205	GLN

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Mol	Chain	Res	Type
1	A	225	GLN
1	A	227	GLN
1	A	250	ASN
1	B	85	ASN
1	B	150	GLN
1	B	169	ASN
1	B	193	ASN
1	B	203	GLN
1	B	217	GLN
1	B	227	GLN
1	B	243	GLN
1	B	267	ASN
1	B	269	HIS
2	C	28	GLN
2	C	75	GLN
2	C	103	ASN
2	C	111	GLN
2	D	28	GLN
2	D	45	ASN
2	D	102	GLN
2	D	103	ASN
2	D	127	GLN
2	D	132	ASN
2	D	156	GLN

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

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, 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	258/267 (96%)	-0.19	0 100 100	11, 27, 45, 65	0
1	B	251/267 (94%)	-0.02	1 (0%) 93 95	17, 40, 64, 82	0
2	C	155/168 (92%)	0.08	7 (4%) 37 46	11, 29, 58, 83	1 (0%)
2	D	166/168 (98%)	-0.12	1 (0%) 90 93	14, 29, 57, 76	1 (0%)
All	All	830/870 (95%)	-0.08	9 (1%) 82 86	11, 31, 58, 83	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	50	CYS	4.0
2	C	153	ALA	2.8
2	C	106	GLU	2.7
2	C	48	ASN	2.6
2	C	140	ASP	2.5
2	C	49	MET	2.5
2	C	108	SER	2.4
1	B	179	GLN	2.1
2	D	137	THR	2.1

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 carbohydrates 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.