



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:30 PM EDT

PDB ID : 4J4L / pdb_00004j4l
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

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

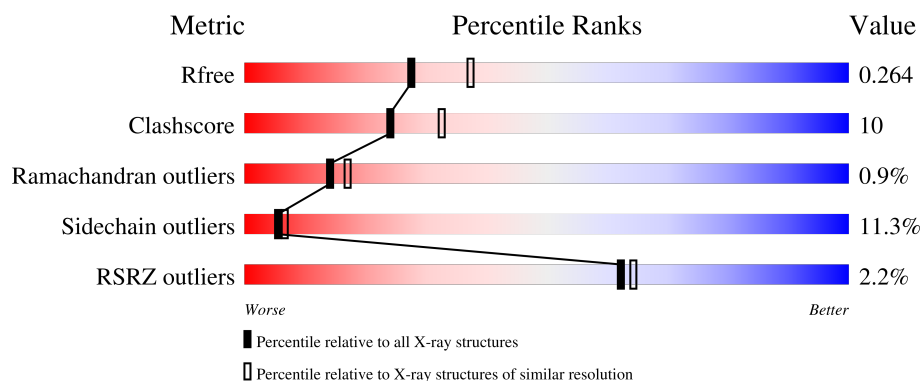
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. 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	267	% 71% 22% ...
1	B	267	3% 64% 22% 7% 6%
2	C	168	4% 69% 21% 8%
2	D	168	% 69% 26% ...

2 Entry composition

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, REPEAT MODULES, 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 A4L9V2
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 A4L9V2
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

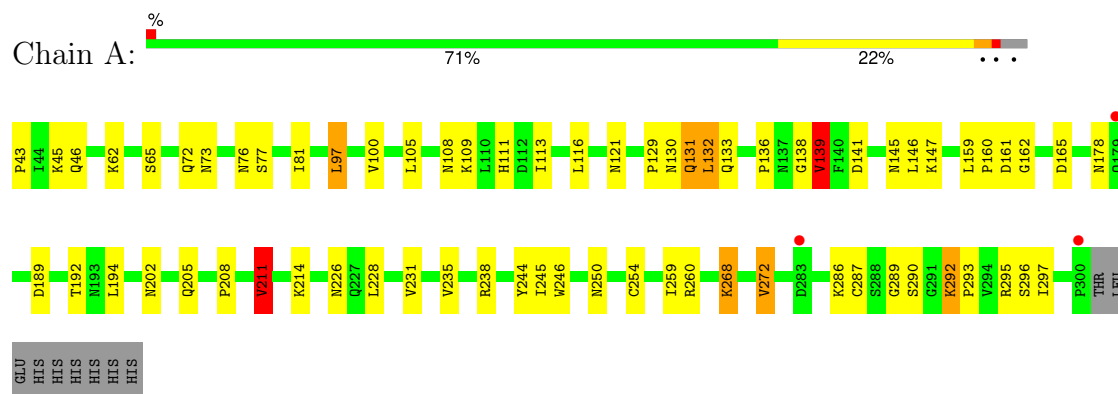
- Molecule 3 is water.

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		

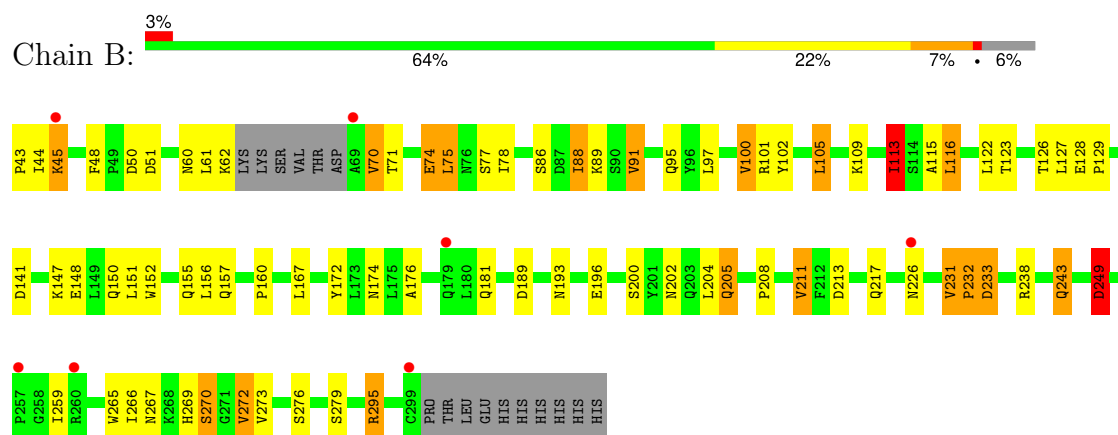
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

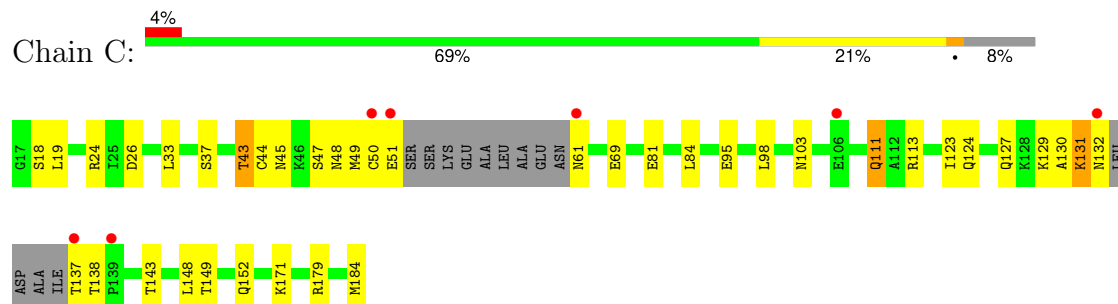
- Molecule 1: Internalin B, REPEAT MODULES, Variable lymphocyte receptor B



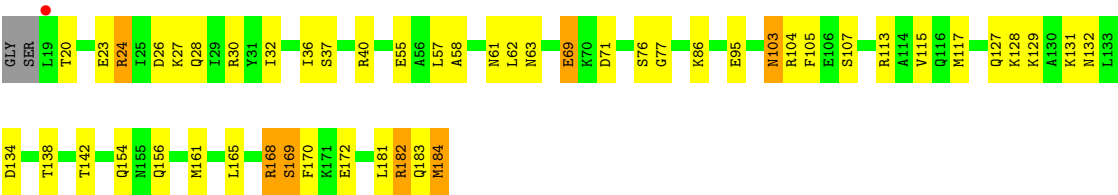
- Molecule 1: Internalin B, REPEAT MODULES, Variable lymphocyte receptor B



- Molecule 2: Interleukin-6



● Molecule 2: Interleukin-6



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 2.29Å)	Xtriage
Refinement program	CNS, REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.268 0.207 , 0.264	Depositor DCC
R_{free} test set	2129 reflections (5.05%)	wwPDB-VP
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 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	1.06	0/2075	1.23	7/2821 (0.2%)
1	B	0.91	1/2020 (0.0%)	1.14	5/2745 (0.2%)
2	C	1.08	0/1259	1.20	4/1687 (0.2%)
2	D	1.01	0/1345	1.18	1/1807 (0.1%)
All	All	1.01	1/6699 (0.0%)	1.19	17/9060 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	273	VAL	CA-C	5.02	1.58	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	VAL	CA-C-N	9.85	132.16	119.84
1	B	231	VAL	C-N-CA	9.85	132.16	119.84
2	C	130	ALA	N-CA-C	8.32	121.94	109.95
1	A	139	VAL	CB-CA-C	-7.25	102.60	111.88
1	A	211	VAL	N-CA-CB	6.54	118.65	110.47
2	C	131	LYS	N-CA-C	6.48	121.34	107.67
1	A	189	ASP	N-CA-C	5.94	117.75	111.28
1	A	178	ASN	CA-C-N	-5.71	110.62	121.54
1	A	178	ASN	C-N-CA	-5.71	110.62	121.54
1	B	113	ILE	CB-CA-C	-5.50	104.38	111.20
2	D	115	VAL	N-CA-C	-5.44	105.08	111.00
1	B	189	ASP	N-CA-C	5.43	117.20	111.28
2	C	18	SER	N-CA-C	-5.41	105.48	112.68
1	B	213	ASP	N-CA-C	5.26	119.32	113.01
1	A	178	ASN	N-CA-C	-5.14	101.76	109.79
2	C	138	THR	N-CA-C	5.14	117.61	110.20
1	A	286	LYS	N-CA-C	5.06	117.69	109.24

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	2035	0	2058	46	0
1	B	1982	0	2001	46	0
2	C	1246	0	1261	18	0
2	D	1330	0	1348	28	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	132	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 (132) 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:A:108:ASN:ND2	1:A:130:ASN:HD22	1.85	0.74
1:B:95:GLN:HG3	1:B:115:ALA:HB1	1.69	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:162:GLY:HA2	1:A:165:ASP:OD2	1.90	0.72
1:A:254:CYS:SG	1:A:297:ILE:HD13	2.30	0.72
2:D:62:LEU:HD12	2:D:165:LEU:HD23	1.72	0.70
2:C:111:GLN:H	2:C:111:GLN:NE2	1.87	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:84:LEU:HD22	2:C:184:MET:HE1	1.78	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
2:C:129:LYS:HE3	2:C:184:MET:HE2	1.88	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:HG2	1:B:101:ARG:NH1	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:50:ASP:C	1:B:50:ASP:OD1	2.51	0.53
1:B:102:TYR:C	1:B:102:TYR:CD1	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ASP:OD2	2:D:117:MET:HG3	2.09	0.52
1:A:293:PRO:O	1:A:296:SER:OG	2.25	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:A:130:ASN:C	1:A:131:GLN:HE21	2.19	0.50
1:A:231:VAL:HB	1:A:235:VAL:HG11	1.93	0.50
2:C:131:LYS:O	2:C:132:ASN:CB	2.60	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: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
3:A:413:HOH:O	2:C:19:LEU:HG	2.14	0.48
1:B:231:VAL:HA	1:B:232:PRO:HD3	1.68	0.48
1:B:123:THR:CG2	1:B:147:LYS:HE2	2.45	0.47
2:D:71:ASP:CG	2:D:86:LYS:HD3	2.39	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
1:B:196:GLU:HG3	3:B:405:HOH:O	2.15	0.46
2:C:26:ASP:HB3	3:C:203:HOH:O	2.15	0.46
2:D:57:LEU:HG	2:D:161:MET:HB3	1.97	0.46
1:A:259:ILE:O	1:A:260:ARG:C	2.58	0.46
1:A:131:GLN:HE21	1:A:131:GLN:N	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:C:47:SER:HB2	2:C:49:MET:SD	2.58	0.44
2:C:179:ARG:NH1	3:C:226:HOH:O	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:GLN:O	2:D:32:ILE:HG13	2.18	0.44
1:A:111:HIS:CD2	1:A:132:LEU:HA	2.54	0.43
1:B:113:ILE:HD12	1:B:127:LEU:HD21	1.99	0.43
2:D:105:PHE:C	2:D:107:SER:H	2.27	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
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
1:B:71:THR:HG22	1:B:74:GLU:CD	2.44	0.42
1:B:86:SER:OG	1:B:88:ILE:HD12	2.19	0.42
1:B:193:ASN:HA	1:B:217:GLN:NE2	2.34	0.42
1:A:100:VAL:O	1:A:100:VAL:HG13	2.19	0.42
1:A:244:TYR:HB3	1:A:246:TRP:CZ3	2.54	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: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
1:A:259:ILE:O	1:A:259:ILE:HG13	2.20	0.41
2:D:129:LYS:HE2	2:D:129:LYS:HB3	1.64	0.41
1:B:127:LEU:C	1:B:129:PRO:HD3	2.46	0.41
1:B:150:GLN:HG2	1:B:174:ASN:HB3	2.03	0.41
2:D:132:ASN:C	2:D:134:ASP:H	2.29	0.41
1:A:159:LEU:HA	1:A:160:PRO:HD3	1.91	0.41
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.97	0.40
1:B:205:GLN:H	1:B:205:GLN:HG2	1.68	0.40
1:B:208:PRO:O	1:B:211:VAL:HG22	2.21	0.40
1:B:269:HIS:HB3	1:B:272:VAL:HG13	2.04	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: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

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	256/267 (96%)	241 (94%)	14 (6%)	1 (0%)	30	38
1	B	247/267 (92%)	224 (91%)	18 (7%)	5 (2%)	6	5
2	C	149/168 (89%)	146 (98%)	3 (2%)	0	100	100
2	D	164/168 (98%)	156 (95%)	7 (4%)	1 (1%)	21	27
All	All	816/870 (94%)	767 (94%)	42 (5%)	7 (1%)	14	17

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

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%)	211 (91%)	22 (9%)	8	11
1	B	226/242 (93%)	195 (86%)	31 (14%)	3	4
2	C	142/152 (93%)	126 (89%)	16 (11%)	5	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	151/152 (99%)	135 (89%)	16 (11%)	6	8
All	All	752/788 (95%)	667 (89%)	85 (11%)	5	7

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	62	LYS
1	A	65	SER
1	A	76	ASN
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	147	LYS
1	A	161	ASP
1	A	192	THR
1	A	194	LEU
1	A	205	GLN
1	A	211	VAL
1	A	238	ARG
1	A	268	LYS
1	A	272	VAL
1	A	292	LYS
1	A	295	ARG
1	B	44	ILE
1	B	45	LYS
1	B	60	ASN
1	B	61	LEU
1	B	70	VAL
1	B	74	GLU
1	B	75	LEU
1	B	88	ILE
1	B	89	LYS
1	B	91	VAL
1	B	100	VAL
1	B	105	LEU
1	B	109	LYS
1	B	113	ILE

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Mol	Chain	Res	Type
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	243	GLN
1	B	249	ASP
1	B	259	ILE
1	B	272	VAL
1	B	276	SER
1	B	279	SER
1	B	295	ARG
2	C	37	SER
2	C	43	THR
2	C	45	ASN
2	C	48	ASN
2	C	50	CYS
2	C	51	GLU
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

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Mol	Chain	Res	Type
2	D	113	ARG
2	D	138	THR
2	D	142	THR
2	D	168	ARG
2	D	169	SER
2	D	182	ARG
2	D	184	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	73	ASN
1	A	76	ASN
1	A	92	GLN
1	A	99	ASN
1	A	108	ASN
1	A	111	HIS
1	A	131	GLN
1	A	154	ASN
1	A	169	ASN
1	A	203	GLN
1	A	205	GLN
1	A	217	GLN
1	A	227	GLN
1	A	250	ASN
1	B	80	GLN
1	B	85	ASN
1	B	145	ASN
1	B	150	GLN
1	B	155	GLN
1	B	169	ASN
1	B	203	GLN
1	B	217	GLN
1	B	227	GLN
1	B	243	GLN
1	B	267	ASN
2	C	28	GLN
2	C	103	ASN
2	C	111	GLN
2	D	28	GLN
2	D	45	ASN

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Mol	Chain	Res	Type
2	D	103	ASN
2	D	127	GLN
2	D	132	ASN
2	D	156	GLN
2	D	159	GLN

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 oligosaccharides 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, 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	258/267 (96%)	-0.12	3 (1%) 76 77	11, 27, 45, 65	0
1	B	251/267 (94%)	0.39	7 (2%) 55 57	17, 40, 64, 82	0
2	C	155/168 (92%)	0.09	7 (4%) 38 40	9, 29, 58, 83	1 (0%)
2	D	166/168 (98%)	-0.06	1 (0%) 85 86	13, 29, 57, 76	1 (0%)
All	All	830/870 (95%)	0.09	18 (2%) 62 64	9, 31, 58, 83	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	257	PRO	4.2
1	B	45	LYS	3.7
1	A	300	PRO	3.5
1	B	299	CYS	3.1
2	C	132	ASN	3.1
2	C	137	THR	3.0
2	C	50	CYS	2.9
1	B	179	GLN	2.6
1	B	69	ALA	2.5
2	C	139	PRO	2.5
1	B	226	ASN	2.4
1	A	283	ASP	2.3
1	A	179	GLN	2.3
1	B	260	ARG	2.3
2	D	19	LEU	2.1
2	C	51	GLU	2.1
2	C	106	GLU	2.1
2	C	61	ASN	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 oligosaccharides 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.