Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 03:29 AM EDT

PDB ID	:	3CAD
Title	:	Crystal structure of Natural Killer Cell Receptor, Ly49G
Authors	:	Cho, S.
Deposited on	:	2008-02-19
Resolution	:	2.60 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:

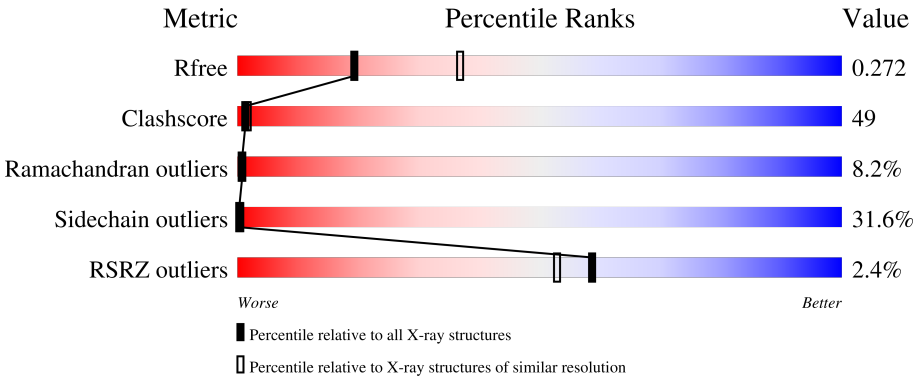
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

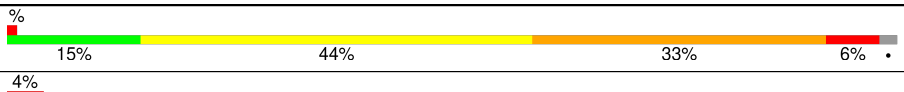
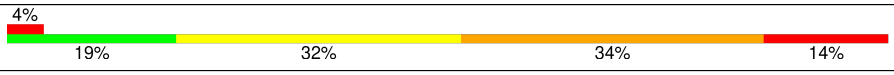
The reported resolution of this entry is 2.60 Å.

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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	125	
1	B	125	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2097 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 Lectin-related NK cell receptor LY49G1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	0	0
			1006	642	167	187	10			
1	B	125	Total	C	N	O	S	0	0	0
			1021	653	169	189	10			

- Molecule 2 is water.

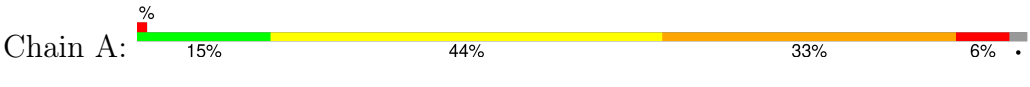
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total	O	0	0
			45	45		
2	B	25	Total	O	0	0
			25	25		

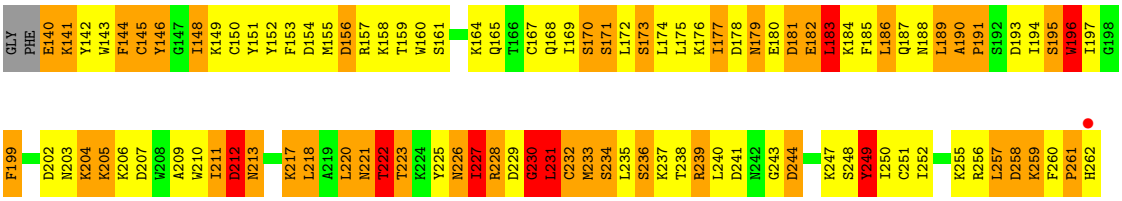
3 Residue-property plots (i)

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: Lectin-related NK cell receptor LY49G1

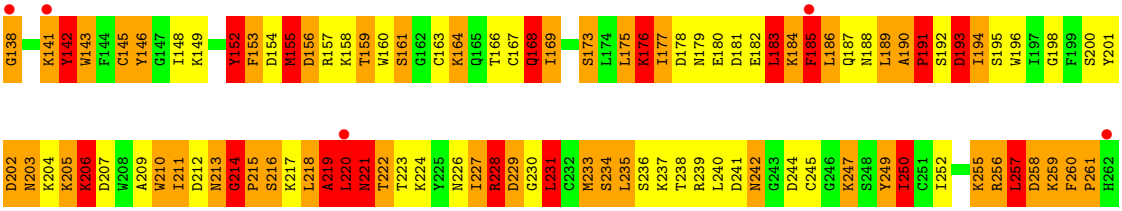
Chain A:





• Molecule 1: Lectin-related NK cell receptor LY49G1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	133.38Å 56.20Å 33.76Å 90.00° 100.29° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 28.88 – 2.39	Depositor EDS
% Data completeness (in resolution range)	90.8 (50.00-2.60) 78.8 (28.88-2.39)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	12.89 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.227 , 0.286 0.268 , 0.272	Depositor DCC
R_{free} test set	363 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å^2)	60.7	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 107.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2097	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.99% 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	1.47	6/1031 (0.6%)	2.10	37/1385 (2.7%)
1	B	1.48	12/1047 (1.1%)	2.15	45/1406 (3.2%)
All	All	1.48	18/2078 (0.9%)	2.13	82/2791 (2.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	23
All	All	0	32

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	GLY	C-N	6.11	1.45	1.34
1	A	199	PHE	C-O	-5.95	1.12	1.23
1	B	212	ASP	C-N	-5.87	1.20	1.34
1	B	260	PHE	CD2-CE2	5.83	1.50	1.39
1	B	190	ALA	C-N	5.65	1.45	1.34
1	B	146	TYR	CB-CG	-5.62	1.43	1.51
1	A	204	LYS	CD-CE	5.49	1.65	1.51
1	B	167	CYS	CB-SG	5.42	1.91	1.82
1	A	196	TRP	CE3-CZ3	5.42	1.47	1.38
1	B	237	LYS	CB-CG	5.42	1.67	1.52
1	B	158	LYS	C-N	5.15	1.45	1.34
1	A	222	THR	CA-CB	5.14	1.66	1.53
1	B	166	THR	N-CA	5.08	1.56	1.46
1	B	168	GLN	C-O	5.08	1.32	1.23
1	B	260	PHE	CE1-CZ	5.07	1.47	1.37
1	A	181	ASP	CB-CG	5.03	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	SER	CA-CB	-5.01	1.45	1.52
1	B	191	PRO	N-CD	5.00	1.54	1.47

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	ASP	CB-CG-OD2	13.31	130.28	118.30
1	B	228	ARG	NE-CZ-NH1	12.53	126.56	120.30
1	A	146	TYR	CB-CG-CD1	11.72	128.03	121.00
1	B	231	LEU	CB-CG-CD2	-11.12	92.10	111.00
1	B	221	ASN	C-N-CA	10.96	149.10	121.70
1	B	257	LEU	C-N-CA	10.41	147.73	121.70
1	A	157	ARG	NE-CZ-NH2	10.27	125.44	120.30
1	A	181	ASP	CB-CG-OD1	10.19	127.47	118.30
1	B	212	ASP	C-N-CA	9.76	146.09	121.70
1	A	154	ASP	CB-CG-OD1	-9.63	109.64	118.30
1	B	142	TYR	CA-C-N	-8.93	97.56	117.20
1	A	249	TYR	CB-CG-CD1	-8.25	116.05	121.00
1	A	252	ILE	O-C-N	-7.97	109.94	122.70
1	B	220	LEU	O-C-N	-7.80	110.22	122.70
1	B	193	ASP	CB-CG-OD1	7.79	125.31	118.30
1	B	190	ALA	C-N-CD	7.73	144.62	128.40
1	B	189	LEU	O-C-N	-7.69	110.39	122.70
1	B	216	SER	C-N-CA	7.67	140.87	121.70
1	B	250	ILE	O-C-N	-7.67	110.43	122.70
1	A	152	TYR	CB-CG-CD2	-7.49	116.50	121.00
1	B	241	ASP	CB-CG-OD2	7.31	124.88	118.30
1	A	258	ASP	CB-CG-OD2	7.29	124.86	118.30
1	B	191	PRO	CA-N-CD	-7.26	101.33	111.50
1	A	212	ASP	CB-CG-OD1	-7.22	111.80	118.30
1	A	170	SER	O-C-N	-7.20	111.19	122.70
1	A	205	LYS	CD-CE-NZ	-7.14	95.29	111.70
1	A	218	LEU	CB-CG-CD1	7.07	123.02	111.00
1	B	206	LYS	CA-C-O	7.00	134.81	120.10
1	A	233	MET	CG-SD-CE	6.98	111.37	100.20
1	B	255	LYS	C-N-CA	6.91	138.97	121.70
1	B	183	LEU	CB-CG-CD2	6.91	122.74	111.00
1	A	153	PHE	O-C-N	-6.90	111.67	122.70
1	A	183	LEU	CB-CG-CD2	6.84	122.62	111.00
1	B	169	ILE	CG1-CB-CG2	6.80	126.36	111.40
1	B	153	PHE	CB-CG-CD1	6.76	125.53	120.80
1	A	229	ASP	C-N-CA	-6.66	108.32	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	228	ARG	CD-NE-CZ	6.62	132.87	123.60
1	B	231	LEU	CB-CG-CD1	-6.59	99.80	111.00
1	A	232	CYS	O-C-N	-6.53	112.25	122.70
1	B	176	LYS	CD-CE-NZ	-6.47	96.83	111.70
1	B	189	LEU	CA-C-N	-6.30	103.33	117.20
1	B	141	LYS	N-CA-CB	6.25	121.85	110.60
1	A	190	ALA	C-N-CD	6.24	141.50	128.40
1	B	142	TYR	CA-C-O	6.16	133.04	120.10
1	A	143	TRP	CD1-CG-CD2	6.09	111.17	106.30
1	B	206	LYS	CA-C-N	-6.04	103.91	117.20
1	B	228	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	259	LYS	O-C-N	-5.80	113.42	122.70
1	A	171	SER	CB-CA-C	-5.79	99.09	110.10
1	B	244	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	249	TYR	CB-CG-CD2	5.67	124.40	121.00
1	A	157	ARG	CD-NE-CZ	5.64	131.50	123.60
1	B	215	PRO	C-N-CA	5.63	135.78	121.70
1	B	214	GLY	O-C-N	5.60	131.73	121.10
1	B	230	GLY	O-C-N	-5.54	113.83	122.70
1	A	146	TYR	CG-CD1-CE1	5.53	125.72	121.30
1	A	156	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	B	234	SER	CB-CA-C	-5.50	99.65	110.10
1	A	142	TYR	CB-CG-CD2	5.47	124.28	121.00
1	A	227	ILE	C-N-CA	5.46	135.36	121.70
1	B	175	LEU	C-N-CA	5.41	135.24	121.70
1	B	176	LYS	CB-CA-C	-5.40	99.59	110.40
1	B	177	ILE	CB-CA-C	-5.40	100.79	111.60
1	B	185	PHE	CB-CG-CD2	5.35	124.54	120.80
1	A	218	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	182	GLU	N-CA-C	-5.31	96.66	111.00
1	B	152	TYR	O-C-N	-5.29	114.24	122.70
1	B	222	THR	C-N-CA	5.26	134.85	121.70
1	B	249	TYR	CB-CG-CD1	5.26	124.15	121.00
1	B	192	SER	C-N-CA	5.25	134.84	121.70
1	B	250	ILE	CA-C-N	5.25	128.74	117.20
1	B	156	ASP	CB-CA-C	5.24	120.87	110.40
1	A	225	TYR	N-CA-C	5.21	125.07	111.00
1	A	170	SER	CA-C-O	5.20	131.02	120.10
1	A	202	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	249	TYR	CA-C-N	-5.16	105.85	117.20
1	A	204	LYS	CD-CE-NZ	5.13	123.50	111.70
1	A	157	ARG	NE-CZ-NH1	-5.12	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	202	ASP	C-N-CA	5.11	134.48	121.70
1	A	239	ARG	O-C-N	-5.11	114.52	122.70
1	B	138	GLY	N-CA-C	-5.05	100.47	113.10
1	A	146	TYR	CA-CB-CG	5.01	122.92	113.40

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	CYS	Mainchain
1	A	191	PRO	Mainchain
1	A	193	ASP	Mainchain
1	A	226	ASN	Mainchain
1	A	230	GLY	Mainchain
1	A	231	LEU	Mainchain
1	A	236	SER	Mainchain
1	A	249	TYR	Mainchain
1	A	260	PHE	Mainchain
1	B	138	GLY	Mainchain
1	B	142	TYR	Mainchain
1	B	143	TRP	Mainchain
1	B	145	CYS	Mainchain
1	B	155	MET	Mainchain
1	B	159	THR	Mainchain
1	B	161	SER	Mainchain
1	B	173	SER	Mainchain
1	B	185	PHE	Mainchain
1	B	186	LEU	Mainchain
1	B	189	LEU	Mainchain
1	B	190	ALA	Mainchain
1	B	207	ASP	Mainchain
1	B	210	TRP	Mainchain
1	B	213	ASN	Peptide,Mainchain
1	B	214	GLY	Mainchain
1	B	215	PRO	Mainchain
1	B	219	ALA	Mainchain
1	B	220	LEU	Mainchain
1	B	221	ASN	Mainchain
1	B	227	ILE	Mainchain
1	B	238	THR	Mainchain

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	1006	0	976	112	2
1	B	1021	0	981	89	5
2	A	45	0	0	2	3
2	B	25	0	0	1	0
All	All	2097	0	1957	197	5

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 49.

All (197) 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:179:ASN:O	1:A:218:LEU:HD12	1.23	1.32
1:B:203:ASN:O	1:B:206:LYS:HD2	1.14	1.28
1:A:217:LYS:NZ	1:A:217:LYS:HB2	1.37	1.26
1:A:140:GLU:OE1	1:A:144:PHE:HE1	1.22	1.21
1:B:180:GLU:O	1:B:184:LYS:HG3	1.41	1.16
1:A:230:GLY:HA3	1:A:243:GLY:HA2	1.18	1.12
1:A:231:LEU:HD23	1:B:227:ILE:HD13	1.29	1.12
1:A:140:GLU:OE1	1:A:144:PHE:CE1	2.04	1.08
1:A:148:ILE:H	1:A:148:ILE:HD12	1.16	1.05
1:A:179:ASN:O	1:A:218:LEU:CD1	2.03	1.04
1:B:205:LYS:HE2	1:B:209:ALA:HB2	1.39	1.03
1:A:217:LYS:NZ	1:A:217:LYS:CB	2.24	1.01
1:A:194:ILE:CG2	1:A:234:SER:OG	2.09	1.01
1:B:235:LEU:HD12	1:B:239:ARG:O	1.61	1.01
1:B:203:ASN:O	1:B:206:LYS:CD	2.08	1.00
1:B:196:TRP:HZ2	1:B:247:LYS:O	1.42	1.00
1:B:226:ASN:O	1:B:229:ASP:HB2	1.60	0.98
1:A:217:LYS:HB2	1:A:217:LYS:HZ3	0.95	0.95
1:A:182:GLU:O	1:A:186:LEU:HB2	1.67	0.95
1:B:184:LYS:O	1:B:188:ASN:HB2	1.67	0.94
1:A:217:LYS:HB2	1:A:217:LYS:HZ2	1.32	0.93
1:A:247:LYS:NZ	2:A:32:HOH:O	2.01	0.92
1:B:195:SER:OG	1:B:250:ILE:HG13	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASN:O	1:A:206:LYS:HG3	1.72	0.89
1:B:235:LEU:CD1	1:B:239:ARG:O	2.21	0.88
1:A:231:LEU:CD2	1:B:227:ILE:HD13	2.05	0.87
1:B:180:GLU:O	1:B:184:LYS:CG	2.20	0.87
1:A:217:LYS:CB	1:A:217:LYS:HZ3	1.86	0.86
1:B:202:ASP:O	1:B:206:LYS:HA	1.75	0.86
1:A:194:ILE:HG21	1:A:234:SER:OG	1.74	0.86
1:B:235:LEU:HD13	1:B:240:LEU:HB3	1.55	0.85
1:A:180:GLU:C	1:A:182:GLU:H	1.79	0.85
1:A:203:ASN:C	1:A:206:LYS:H	1.79	0.85
1:A:183:LEU:O	1:A:183:LEU:HD12	1.76	0.84
1:A:148:ILE:HD12	1:A:148:ILE:N	1.90	0.84
1:A:230:GLY:HA3	1:A:243:GLY:CA	2.06	0.84
1:B:193:ASP:O	1:B:236:SER:HA	1.77	0.84
1:A:195:SER:HB3	1:A:250:ILE:HG13	1.58	0.84
1:B:194:ILE:HG12	1:B:249:TYR:CD1	2.14	0.83
1:A:203:ASN:OD1	1:B:226:ASN:ND2	2.12	0.83
1:B:175:LEU:CD2	1:B:177:ILE:HD11	2.09	0.82
1:A:221:ASN:O	1:A:223:THR:N	2.14	0.81
1:A:203:ASN:O	1:A:206:LYS:N	2.15	0.80
1:A:233:MET:HE3	1:A:241:ASP:O	1.81	0.80
1:B:216:SER:C	1:B:218:LEU:H	1.86	0.78
1:A:230:GLY:CA	1:A:243:GLY:HA2	2.10	0.76
1:B:175:LEU:HD23	1:B:177:ILE:HD11	1.67	0.76
1:A:210:TRP:C	1:A:212:ASP:H	1.87	0.76
1:A:180:GLU:O	1:A:184:LYS:N	2.16	0.75
1:A:194:ILE:HG22	1:A:195:SER:N	2.01	0.75
1:A:227:ILE:HG22	1:A:231:LEU:HD11	1.69	0.75
1:A:205:LYS:NZ	1:A:213:ASN:HB3	2.02	0.74
1:B:183:LEU:HD22	1:B:187:GLN:NE2	2.01	0.74
1:A:140:GLU:HB2	1:A:141:LYS:HE3	1.69	0.74
1:A:158:LYS:C	1:A:248:SER:OG	2.26	0.73
1:B:160:TRP:CZ2	1:B:200:SER:HB3	2.24	0.73
1:A:180:GLU:O	1:A:182:GLU:N	2.22	0.72
1:A:255:LYS:HD3	1:A:256:ARG:H	1.52	0.72
1:B:233:MET:HE3	1:B:234:SER:N	2.04	0.72
1:A:177:ILE:HG23	1:A:182:GLU:HG2	1.72	0.71
1:A:185:PHE:O	1:A:188:ASN:HB3	1.91	0.71
1:A:221:ASN:C	1:A:223:THR:H	1.91	0.71
1:B:196:TRP:CZ2	1:B:247:LYS:O	2.35	0.70
1:B:176:LYS:HA	1:B:210:TRP:CZ3	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ILE:O	1:B:216:SER:OG	2.10	0.69
1:A:199:PHE:HD2	1:A:233:MET:HG3	1.56	0.69
1:A:194:ILE:HG22	1:A:195:SER:H	1.56	0.69
1:A:210:TRP:C	1:A:212:ASP:N	2.45	0.68
1:B:205:LYS:CE	1:B:209:ALA:HB2	2.19	0.68
1:A:233:MET:CE	1:A:241:ASP:O	2.42	0.68
1:A:141:LYS:HZ1	1:A:144:PHE:HE1	1.41	0.67
1:A:235:LEU:HA	1:A:240:LEU:HG	1.76	0.66
1:B:228:ARG:HB2	1:B:228:ARG:HH11	1.61	0.66
1:B:175:LEU:CD2	1:B:177:ILE:CD1	2.74	0.65
1:B:175:LEU:HD21	1:B:177:ILE:HD11	1.79	0.65
1:B:229:ASP:HB3	1:B:242:ASN:ND2	2.11	0.64
1:B:142:TYR:O	1:B:152:TYR:HA	1.97	0.64
1:B:229:ASP:HB3	1:B:242:ASN:HD21	1.63	0.64
1:A:165:GLN:O	1:A:169:ILE:HG13	1.99	0.62
1:A:151:TYR:HE2	1:A:175:LEU:HD13	1.63	0.62
1:A:199:PHE:CD2	1:A:233:MET:HG3	2.35	0.62
1:A:183:LEU:HD12	1:A:183:LEU:C	2.16	0.61
1:A:205:LYS:HZ2	1:A:213:ASN:HB3	1.64	0.60
1:A:217:LYS:CB	1:A:217:LYS:HZ2	2.00	0.60
1:A:195:SER:O	1:A:234:SER:HA	2.02	0.59
1:A:187:GLN:O	1:A:188:ASN:C	2.39	0.59
1:A:194:ILE:CG2	1:A:195:SER:H	2.16	0.59
1:A:194:ILE:CG2	1:A:195:SER:N	2.65	0.59
1:B:164:LYS:HD2	1:B:211:ILE:CD1	2.33	0.59
1:A:199:PHE:HB3	1:A:233:MET:HG3	1.84	0.58
1:A:180:GLU:C	1:A:182:GLU:N	2.46	0.58
1:B:229:ASP:CB	1:B:242:ASN:HD21	2.16	0.58
1:A:230:GLY:HA3	1:A:244:ASP:H	1.68	0.58
1:B:219:ALA:O	1:B:220:LEU:C	2.42	0.57
1:A:227:ILE:HD12	1:A:228:ARG:N	2.20	0.56
1:A:167:CYS:HB3	1:A:172:LEU:HB2	1.87	0.56
1:A:188:ASN:C	1:A:188:ASN:OD1	2.42	0.56
1:A:160:TRP:CG	1:A:232:CYS:SG	2.99	0.56
1:B:233:MET:HE3	1:B:234:SER:H	1.69	0.56
1:A:203:ASN:O	1:A:206:LYS:CG	2.52	0.56
1:A:159:THR:N	1:A:248:SER:OG	2.39	0.55
1:B:256:ARG:O	1:B:257:LEU:HB2	2.04	0.55
1:B:202:ASP:O	1:B:206:LYS:CA	2.53	0.55
1:A:148:ILE:N	1:A:148:ILE:CD1	2.65	0.55
1:A:213:ASN:OD1	1:A:213:ASN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLU:N	1:B:218:LEU:HD22	2.22	0.54
1:B:157:ARG:HD3	1:B:249:TYR:HA	1.89	0.54
1:B:183:LEU:HD22	1:B:187:GLN:CD	2.28	0.54
1:A:227:ILE:HD11	1:B:203:ASN:OD1	2.08	0.54
1:B:203:ASN:HD22	1:B:204:LYS:H	1.55	0.54
1:A:221:ASN:C	1:A:223:THR:N	2.59	0.53
1:A:184:LYS:HE2	2:A:47:HOH:O	2.08	0.53
1:B:180:GLU:C	1:B:184:LYS:HG3	2.24	0.53
1:B:228:ARG:HH11	1:B:228:ARG:CB	2.22	0.53
1:B:155:MET:CE	1:B:191:PRO:HB2	2.39	0.53
1:A:257:LEU:CD1	1:A:261:PRO:HG3	2.38	0.53
1:B:176:LYS:HE2	2:B:48:HOH:O	2.08	0.53
1:A:205:LYS:HZ1	1:A:213:ASN:HB3	1.71	0.52
1:A:230:GLY:CA	1:A:244:ASP:H	2.22	0.52
1:B:233:MET:HE3	1:B:233:MET:C	2.29	0.52
1:B:177:ILE:HG22	1:B:218:LEU:HD23	1.91	0.52
1:B:233:MET:HE1	1:B:240:LEU:HD13	1.91	0.52
1:A:160:TRP:CD1	1:A:232:CYS:HB3	2.45	0.52
1:B:194:ILE:HG12	1:B:249:TYR:CE1	2.45	0.52
1:B:155:MET:HE1	1:B:191:PRO:HB2	1.91	0.52
1:A:197:ILE:O	1:A:197:ILE:HG13	2.10	0.52
1:A:227:ILE:HG22	1:A:231:LEU:CD1	2.40	0.51
1:A:170:SER:O	1:A:171:SER:CB	2.57	0.51
1:A:230:GLY:HA3	1:A:244:ASP:N	2.25	0.51
1:B:257:LEU:HG	1:B:258:ASP:HB2	1.91	0.51
1:A:228:ARG:O	1:A:228:ARG:HD2	2.10	0.51
1:A:259:LYS:N	1:A:259:LYS:HD3	2.26	0.51
1:B:194:ILE:HD12	1:B:194:ILE:H	1.76	0.50
1:A:149:LYS:HG2	1:A:255:LYS:O	2.11	0.50
1:A:164:LYS:HE2	1:A:211:ILE:CG2	2.42	0.50
1:B:149:LYS:HG2	1:B:255:LYS:O	2.11	0.50
1:A:199:PHE:CD1	1:A:209:ALA:C	2.85	0.49
1:B:236:SER:HG	1:B:239:ARG:C	2.16	0.49
1:B:175:LEU:HD21	1:B:177:ILE:CD1	2.41	0.49
1:B:216:SER:C	1:B:218:LEU:N	2.60	0.49
1:A:194:ILE:HG23	1:A:234:SER:OG	2.05	0.49
1:A:180:GLU:O	1:A:184:LYS:HB2	2.12	0.49
1:B:176:LYS:HA	1:B:210:TRP:CE3	2.48	0.49
1:B:255:LYS:HG3	1:B:256:ARG:O	2.13	0.49
1:B:213:ASN:OD1	1:B:214:GLY:N	2.46	0.49
1:B:183:LEU:HD12	1:B:218:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:MET:SD	1:A:191:PRO:HG3	2.54	0.48
1:B:168:GLN:HA	1:B:168:GLN:OE1	2.14	0.47
1:A:170:SER:O	1:A:171:SER:HB2	2.15	0.47
1:B:175:LEU:HD23	1:B:177:ILE:CD1	2.37	0.47
1:B:233:MET:HE3	1:B:233:MET:CA	2.44	0.47
1:A:151:TYR:CE2	1:A:175:LEU:HD13	2.46	0.46
1:B:145:CYS:HB3	1:B:149:LYS:O	2.15	0.46
1:B:185:PHE:CD2	1:B:186:LEU:HD23	2.51	0.46
1:B:233:MET:HA	1:B:242:ASN:HA	1.96	0.46
1:B:240:LEU:C	1:B:240:LEU:HD12	2.36	0.46
1:A:199:PHE:HB3	1:A:233:MET:CG	2.46	0.46
1:B:159:THR:O	1:B:160:TRP:C	2.53	0.46
1:B:198:GLY:O	1:B:210:TRP:HA	2.15	0.45
1:B:227:ILE:HD12	1:B:228:ARG:N	2.32	0.45
1:B:195:SER:OG	1:B:250:ILE:CG1	2.52	0.45
1:A:210:TRP:O	1:A:212:ASP:N	2.50	0.45
1:A:145:CYS:HA	1:A:150:CYS:HA	2.00	0.44
1:B:260:PHE:HA	1:B:261:PRO:HD2	1.58	0.44
1:A:174:LEU:HD12	1:A:174:LEU:HA	1.85	0.44
1:A:189:LEU:HD23	1:A:189:LEU:N	2.32	0.44
1:B:146:TYR:CD2	1:B:146:TYR:C	2.91	0.44
1:A:220:LEU:H	1:A:220:LEU:HD12	1.82	0.44
1:B:179:ASN:OD1	1:B:181:ASP:HB2	2.18	0.44
1:A:183:LEU:O	1:A:187:GLN:HG2	2.17	0.44
1:A:227:ILE:HA	1:A:231:LEU:HD12	2.00	0.43
1:A:185:PHE:HA	1:A:188:ASN:CB	2.48	0.43
1:B:182:GLU:O	1:B:186:LEU:HG	2.19	0.43
1:B:163:CYS:SG	1:B:196:TRP:HD1	2.42	0.43
1:B:194:ILE:CG1	1:B:249:TYR:CD1	2.96	0.43
1:A:151:TYR:CZ	1:A:186:LEU:HD21	2.54	0.42
1:A:247:LYS:HD3	1:A:249:TYR:OH	2.19	0.42
1:B:201:TYR:HB3	1:B:231:LEU:HB3	2.00	0.42
1:B:160:TRP:HB3	1:B:245:CYS:HB3	2.02	0.42
1:A:226:ASN:HB2	1:A:228:ARG:H	1.85	0.42
1:A:167:CYS:HB3	1:A:173:SER:N	2.35	0.41
1:A:197:ILE:HG21	1:A:235:LEU:HD12	2.01	0.41
1:A:258:ASP:HB2	1:A:259:LYS:NZ	2.35	0.41
1:A:199:PHE:CE1	1:A:209:ALA:C	2.94	0.41
1:B:164:LYS:HD2	1:B:211:ILE:HD11	2.00	0.41
1:B:195:SER:CB	1:B:250:ILE:HG13	2.48	0.41
1:A:141:LYS:NZ	1:A:144:PHE:CE1	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LEU:HA	1:B:240:LEU:HA	2.03	0.41
1:B:235:LEU:HD13	1:B:239:ARG:O	2.11	0.41
1:A:183:LEU:HD13	1:A:183:LEU:HA	1.74	0.41
1:B:234:SER:OG	1:B:235:LEU:N	2.54	0.41
1:A:255:LYS:CD	1:A:256:ARG:H	2.30	0.40
1:A:179:ASN:OD1	1:A:180:GLU:N	2.53	0.40
1:B:227:ILE:C	1:B:229:ASP:N	2.69	0.40
1:A:160:TRP:HD1	1:A:196:TRP:CE3	2.39	0.40
1:A:196:TRP:CZ2	1:A:247:LYS:O	2.75	0.40
1:A:227:ILE:HA	1:A:231:LEU:CD1	2.52	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ASP:OD1	2:A:34:HOH:O[4_554]	0.78	1.42
1:B:258:ASP:CG	2:A:34:HOH:O[4_554]	1.14	1.06
1:A:262:HIS:CE1	1:B:141:LYS:NZ[4_545]	1.62	0.58
1:B:258:ASP:OD2	2:A:34:HOH:O[4_554]	1.70	0.50
1:A:262:HIS:ND1	1:B:141:LYS:NZ[4_545]	1.96	0.24

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	121/125 (97%)	88 (73%)	23 (19%)	10 (8%)	1	1
1	B	123/125 (98%)	86 (70%)	27 (22%)	10 (8%)	1	1
All	All	244/250 (98%)	174 (71%)	50 (20%)	20 (8%)	1	1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	181	ASP
1	A	222	THR
1	A	231	LEU
1	A	244	ASP
1	B	191	PRO
1	B	217	LYS
1	B	222	THR
1	B	257	LEU
1	B	258	ASP
1	B	261	PRO
1	A	230	GLY
1	A	261	PRO
1	B	184	LYS
1	B	219	ALA
1	A	190	ALA
1	B	155	MET
1	B	193	ASP
1	A	211	ILE
1	A	227	ILE

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	112/113 (99%)	77 (69%)	35 (31%)	0	0
1	B	113/113 (100%)	77 (68%)	36 (32%)	0	0
All	All	225/226 (100%)	154 (68%)	71 (32%)	0	0

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	GLU
1	A	141	LYS
1	A	144	PHE
1	A	146	TYR

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Mol	Chain	Res	Type
1	A	148	ILE
1	A	156	ASP
1	A	161	SER
1	A	168	GLN
1	A	176	LYS
1	A	177	ILE
1	A	178	ASP
1	A	183	LEU
1	A	186	LEU
1	A	189	LEU
1	A	195	SER
1	A	196	TRP
1	A	204	LYS
1	A	207	ASP
1	A	212	ASP
1	A	213	ASN
1	A	217	LYS
1	A	220	LEU
1	A	221	ASN
1	A	222	THR
1	A	223	THR
1	A	228	ARG
1	A	234	SER
1	A	236	SER
1	A	237	LYS
1	A	238	THR
1	A	239	ARG
1	A	249	TYR
1	A	251	CYS
1	A	257	LEU
1	A	259	LYS
1	B	143	TRP
1	B	148	ILE
1	B	152	TYR
1	B	153	PHE
1	B	154	ASP
1	B	156	ASP
1	B	161	SER
1	B	164	LYS
1	B	168	GLN
1	B	169	ILE
1	B	173	SER

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Mol	Chain	Res	Type
1	B	176	LYS
1	B	178	ASP
1	B	183	LEU
1	B	191	PRO
1	B	194	ILE
1	B	203	ASN
1	B	205	LYS
1	B	206	LYS
1	B	211	ILE
1	B	218	LEU
1	B	220	LEU
1	B	221	ASN
1	B	223	THR
1	B	224	LYS
1	B	228	ARG
1	B	229	ASP
1	B	231	LEU
1	B	233	MET
1	B	235	LEU
1	B	242	ASN
1	B	247	LYS
1	B	250	ILE
1	B	252	ILE
1	B	256	ARG
1	B	259	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	187	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 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	123/125 (98%)	-0.09	1 (0%)	86	84	37, 54, 74, 82	0
1	B	125/125 (100%)	0.24	5 (4%)	38	31	24, 53, 76, 112	0
All	All	248/250 (99%)	0.08	6 (2%)	59	53	24, 54, 76, 112	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	GLY	7.7
1	B	185	PHE	3.2
1	A	262	HIS	2.7
1	B	220	LEU	2.6
1	B	262	HIS	2.5
1	B	141	LYS	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.