Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:16 PM GMT

PDB ID	:	1JL4
Title	:	CRYSTAL STRUCTURE OF THE HUMAN CD4 N-TERMINAL TWO DOMAIN FRAGMENT COMPLEXED TO A CLASS II MHC MOLECULE
Authors	:	Wang, J.-H.; Meijers, R.; Reinherz, E.L.
Deposited on	:	2001-07-15
Resolution	:	4.30 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:

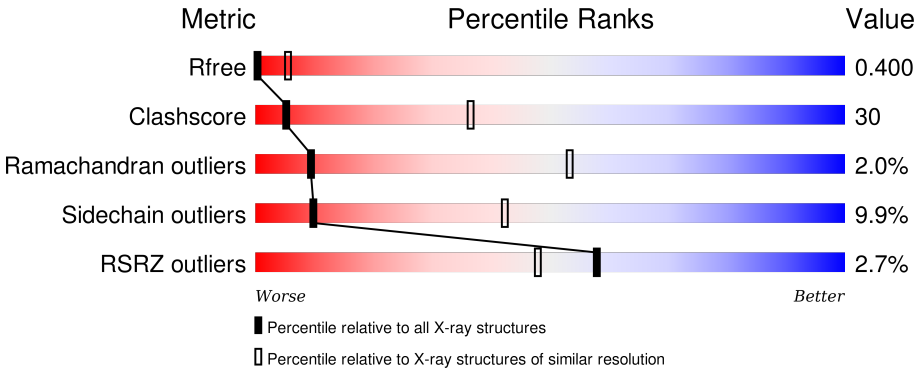
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 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	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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 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	178	3% 64% 34% ·
2	B	185	% 76% 23% ··
3	C	16	6% 38% 25% 38%
4	D	178	3% 39% 39% 20% ·

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4474 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called H-2 CLASS II HISTOCOMPATIBILITY ANTIGEN, A-K ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1447	935	232	277	3			

- Molecule 2 is a protein called H-2 CLASS II HISTOCOMPATIBILITY ANTIGEN, A-K BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	185	Total	C	N	O	S	0	0	0
			1543	972	278	287	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	GLY	-	CLONING ARTIFACT	UNP P06343
B	6	SER	-	CLONING ARTIFACT	UNP P06343
B	181	THR	LYS	CONFLICT	UNP P06343

- Molecule 3 is a protein called OVOTRANSFERRIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	16	Total	C	N	O	0	0	0
			120	71	23	26			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	131	GLY	-	CLONING ARTIFACT	UNP P02789
C	132	ASN	-	CLONING ARTIFACT	UNP P02789
C	133	SER	-	CLONING ARTIFACT	UNP P02789

- Molecule 4 is a protein called T-CELL SURFACE GLYCOPROTEIN CD4.

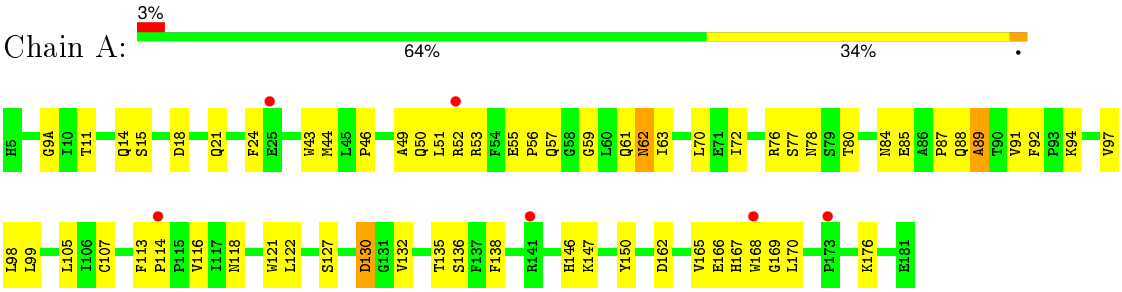
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	178	1364	859	231	270	4	0	0	0

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.

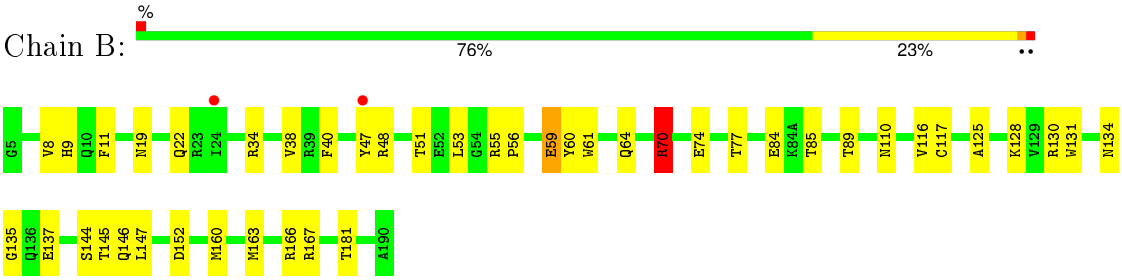
- Molecule 1: H-2 CLASS II HISTOCOMPATIBILITY ANTIGEN, A-K ALPHA CHAIN

Chain A:



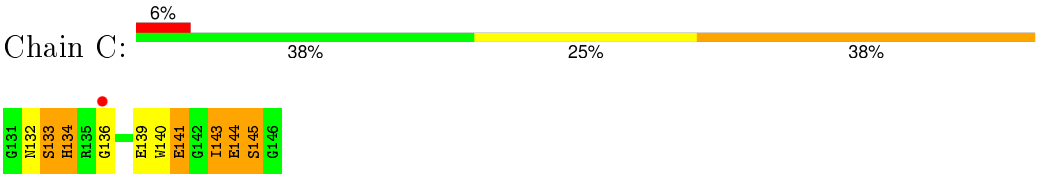
- Molecule 2: H-2 CLASS II HISTOCOMPATIBILITY ANTIGEN, A-K BETA CHAIN

Chain B:



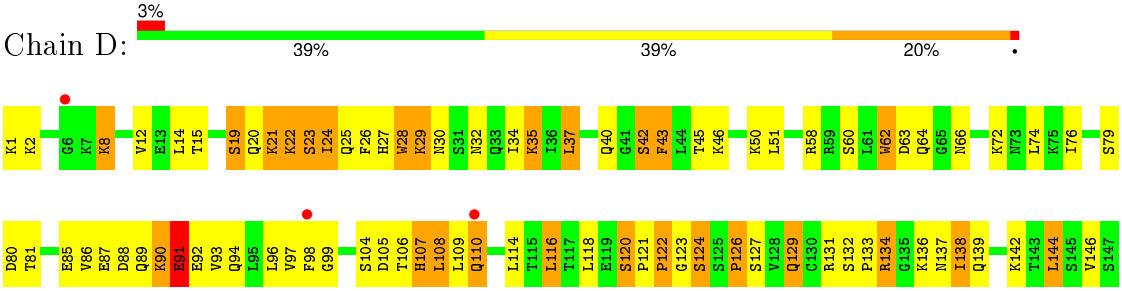
- Molecule 3: OVOTRANSFERRIN

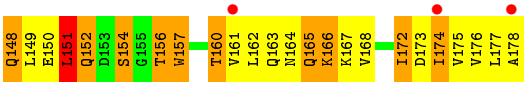
Chain C:



- Molecule 4: T-CELL SURFACE GLYCOPROTEIN CD4

Chain D:




Q148
L149
E150
L151
Q152
D153
S154
G155
T156
W157
T160
V161
L162
Q163
N164
Q165
K166
K167
Y168
I172
D173
I174
V175
V176
L177
A178

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	145.19Å 145.19Å 103.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.30 48.89 – 4.00	Depositor EDS
% Data completeness (in resolution range)	81.0 (20.00-4.30) 75.3 (48.89-4.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 4.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.420 , 0.453 0.376 , 0.400	Depositor DCC
R_{free} test set	645 reflections (11.15%)	DCC
Wilson B-factor (Å^2)	137.3	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 2.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	1 of 7428 reflections (0.013%)	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	4474	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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	0.57	2/1492 (0.1%)	0.75	1/2035 (0.0%)
2	B	0.56	2/1582 (0.1%)	0.83	5/2149 (0.2%)
3	C	0.39	0/122	0.66	0/161
4	D	0.95	2/1379 (0.1%)	1.40	12/1854 (0.6%)
All	All	0.70	6/4575 (0.1%)	1.01	18/6199 (0.3%)

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
4	D	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	99	GLY	C-N	14.16	1.66	1.34
1	A	89	ALA	C-N	10.03	1.57	1.34
2	B	89	THR	C-N	-9.58	1.12	1.34
2	B	84	GLU	C-N	-6.67	1.18	1.34
1	A	80	THR	C-N	6.41	1.46	1.34
4	D	91	GLU	CG-CD	5.37	1.60	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	28	TRP	CD1-CG-CD2	9.87	114.20	106.30
4	D	62	TRP	CD1-CG-CD2	8.80	113.34	106.30
4	D	157	TRP	CD1-CG-CD2	8.76	113.31	106.30
2	B	89	THR	O-C-N	-8.61	108.92	122.70
4	D	28	TRP	CE2-CD2-CG	-8.40	100.58	107.30
2	B	70	ARG	NE-CZ-NH1	-8.27	116.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	62	TRP	CE2-CD2-CG	-7.22	101.52	107.30
4	D	157	TRP	CE2-CD2-CG	-7.04	101.67	107.30
2	B	70	ARG	NE-CZ-NH2	6.95	123.77	120.30
4	D	62	TRP	CG-CD2-CE3	6.89	140.10	133.90
4	D	62	TRP	CB-CG-CD1	-6.35	118.75	127.00
2	B	89	THR	CA-C-N	5.93	130.24	117.20
4	D	28	TRP	CG-CD2-CE3	5.88	139.19	133.90
2	B	89	THR	C-N-CA	5.73	136.03	121.70
4	D	28	TRP	CG-CD1-NE1	-5.72	104.38	110.10
4	D	62	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	A	9(A)	GLY	O-C-N	5.24	131.08	122.70
4	D	28	TRP	CB-CG-CD1	-5.04	120.44	127.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	43	PHE	Sidechain

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	1447	0	1376	71	12
2	B	1543	0	1486	68	23
3	C	120	0	102	47	11
4	D	1364	0	1373	165	23
All	All	4474	0	4337	268	55

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 30.

All (268) 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:88:GLN:HE22	4:D:60:SER:CB	1.26	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLN:NE2	4:D:60:SER:HB3	1.40	1.37
1:A:53:ARG:CG	3:C:132:ASN:O	1.73	1.36
1:A:53:ARG:O	3:C:134:HIS:HB2	1.31	1.26
2:B:85:THR:OG1	3:C:134:HIS:HE1	1.30	1.14
2:B:85:THR:OG1	3:C:134:HIS:CE1	2.00	1.14
1:A:88:GLN:HE22	4:D:60:SER:HB3	0.86	1.02
1:A:53:ARG:HG2	3:C:132:ASN:O	0.84	1.01
4:D:157:TRP:CZ2	4:D:157:TRP:CZ3	2.39	1.00
1:A:88:GLN:NE2	4:D:60:SER:CB	2.03	0.99
4:D:28:TRP:CZ3	4:D:28:TRP:CZ2	2.39	0.99
4:D:126:PRO:HB3	4:D:163:GLN:HG2	1.44	0.98
1:A:53:ARG:HG2	3:C:132:ASN:C	1.83	0.98
2:B:70:ARG:HD2	3:C:140:TRP:CH2	1.99	0.96
4:D:30:ASN:HD21	4:D:34:ILE:HD12	1.26	0.96
4:D:62:TRP:CZ3	4:D:62:TRP:CZ2	2.39	0.95
1:A:53:ARG:O	3:C:134:HIS:CB	2.14	0.95
4:D:98:PHE:CE2	4:D:121:PRO:HD2	2.03	0.94
4:D:21:LYS:HG2	4:D:64:GLN:HA	1.48	0.93
1:A:53:ARG:O	3:C:134:HIS:N	2.01	0.93
2:B:85:THR:CB	3:C:134:HIS:CE1	2.52	0.93
1:A:88:GLN:HE22	4:D:60:SER:HB2	1.35	0.91
1:A:113:PHE:CZ	2:B:34:ARG:HG3	2.06	0.91
1:A:52:ARG:NE	3:C:134:HIS:NE2	2.18	0.90
4:D:85:GLU:HG2	4:D:90:LYS:HG3	1.53	0.90
4:D:30:ASN:HD21	4:D:34:ILE:CD1	1.86	0.88
4:D:98:PHE:HE2	4:D:121:PRO:HD2	1.37	0.87
1:A:52:ARG:NH2	3:C:134:HIS:NE2	2.22	0.87
4:D:20:GLN:HB2	4:D:22:LYS:CE	2.05	0.87
4:D:20:GLN:O	4:D:22:LYS:HD2	1.73	0.86
4:D:129:GLN:O	4:D:129:GLN:HG3	1.74	0.85
1:A:51:LEU:O	3:C:132:ASN:ND2	2.09	0.84
4:D:138:ILE:HD11	4:D:144:LEU:HB3	1.58	0.84
4:D:27:HIS:ND1	4:D:35:LYS:HD3	1.91	0.84
4:D:24:ILE:HG12	4:D:25:GLN:H	1.44	0.83
4:D:21:LYS:CG	4:D:64:GLN:HA	2.08	0.83
4:D:133:PRO:HD3	4:D:157:TRP:NE1	1.94	0.82
2:B:146:GLN:NE2	4:D:46:LYS:HE2	1.97	0.80
2:B:70:ARG:CD	3:C:140:TRP:HH2	1.94	0.79
2:B:70:ARG:CD	3:C:140:TRP:CH2	2.66	0.79
1:A:94:LYS:NZ	2:B:152:ASP:OD2	2.11	0.79
1:A:52:ARG:HE	3:C:134:HIS:CD2	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:SER:O	4:D:45:THR:HB	1.83	0.78
1:A:53:ARG:C	3:C:134:HIS:HB2	2.04	0.77
1:A:113:PHE:CG	2:B:34:ARG:HD2	2.20	0.77
4:D:98:PHE:CE2	4:D:121:PRO:CD	2.69	0.75
4:D:42:SER:HG	4:D:43:PHE:HE1	1.33	0.75
1:A:88:GLN:NE2	4:D:60:SER:HB2	1.95	0.74
1:A:52:ARG:CZ	3:C:134:HIS:NE2	2.51	0.74
4:D:20:GLN:HB2	4:D:22:LYS:HE2	1.69	0.73
4:D:132:SER:HA	4:D:157:TRP:CD2	2.24	0.72
1:A:92:PHE:HB3	4:D:43:PHE:CZ	2.25	0.72
4:D:30:ASN:ND2	4:D:34:ILE:HD12	2.02	0.71
4:D:116:LEU:HD13	4:D:144:LEU:HB2	1.71	0.71
2:B:146:GLN:HE21	4:D:46:LYS:HE2	1.56	0.71
4:D:126:PRO:HB3	4:D:163:GLN:CG	2.21	0.71
4:D:50:LYS:CG	4:D:51:LEU:HD12	2.20	0.70
4:D:108:LEU:HD13	4:D:149:LEU:HD12	1.74	0.70
4:D:131:ARG:HG3	4:D:137:ASN:OD1	1.92	0.69
4:D:134:ARG:CB	4:D:152:GLN:OE1	2.40	0.69
2:B:11:PHE:CD1	3:C:139:GLU:HG3	2.28	0.68
4:D:21:LYS:HG2	4:D:63:ASP:O	1.93	0.68
1:A:53:ARG:HG3	3:C:133:SER:HA	1.75	0.67
2:B:144:SER:O	4:D:45:THR:CB	2.43	0.67
4:D:108:LEU:HD13	4:D:149:LEU:CD1	2.25	0.67
4:D:20:GLN:OE1	4:D:20:GLN:N	2.29	0.66
4:D:22:LYS:O	4:D:24:ILE:HG22	1.95	0.66
1:A:76:ARG:NH1	2:B:53:LEU:O	2.29	0.66
1:A:21:GLN:OE1	1:A:136:SER:HB3	1.95	0.65
2:B:60:TYR:CD2	3:C:143:ILE:HG12	2.32	0.65
4:D:8:LYS:HE3	4:D:76:ILE:CD1	2.27	0.64
2:B:61:TRP:CZ2	3:C:141:GLU:O	2.50	0.64
4:D:21:LYS:HG2	4:D:64:GLN:CA	2.24	0.64
4:D:106:THR:HG22	4:D:107:HIS:H	1.61	0.63
2:B:85:THR:HG21	3:C:134:HIS:CE1	2.34	0.63
4:D:133:PRO:HD3	4:D:157:TRP:CE2	2.33	0.63
4:D:148:GLN:O	4:D:148:GLN:HG2	1.99	0.63
4:D:80:ASP:OD2	4:D:81:THR:N	2.32	0.63
1:A:92:PHE:HB3	4:D:43:PHE:HZ	1.63	0.63
2:B:11:PHE:CG	3:C:139:GLU:HG3	2.34	0.63
4:D:30:ASN:C	4:D:30:ASN:OD1	2.36	0.62
4:D:134:ARG:HB3	4:D:152:GLN:OE1	1.97	0.62
4:D:32:ASN:HB2	4:D:34:ILE:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:HA	3:C:132:ASN:HB3	1.82	0.62
2:B:145:THR:CA	4:D:45:THR:HG22	2.30	0.61
4:D:27:HIS:HB2	4:D:35:LYS:HD2	1.81	0.61
1:A:52:ARG:HH21	3:C:134:HIS:CE1	2.19	0.61
4:D:20:GLN:HB2	4:D:22:LYS:CD	2.29	0.61
2:B:145:THR:CG2	4:D:45:THR:HG22	2.31	0.61
4:D:156:THR:HB	4:D:173:ASP:OD1	2.01	0.61
4:D:50:LYS:HG3	4:D:51:LEU:HD12	1.81	0.60
4:D:104:SER:OG	4:D:114:LEU:HD12	2.01	0.60
4:D:164:ASN:HB2	4:D:166:LYS:HG2	1.82	0.60
4:D:22:LYS:O	4:D:24:ILE:N	2.35	0.60
2:B:144:SER:O	4:D:45:THR:CA	2.49	0.60
4:D:50:LYS:HG2	4:D:51:LEU:HD12	1.82	0.60
4:D:43:PHE:CD1	4:D:43:PHE:N	2.70	0.60
4:D:132:SER:HA	4:D:157:TRP:CE2	2.37	0.59
1:A:14:GLN:HE22	1:A:116:VAL:CG2	2.16	0.59
2:B:85:THR:CG2	3:C:134:HIS:CE1	2.86	0.59
1:A:84:ASN:ND2	1:A:168:TRP:HB3	2.17	0.59
2:B:145:THR:HG22	4:D:45:THR:HG22	1.84	0.59
4:D:150:GLU:O	4:D:152:GLN:N	2.36	0.58
4:D:14:LEU:HG	4:D:93:VAL:HG11	1.85	0.58
4:D:12:VAL:HG13	4:D:74:LEU:HD11	1.85	0.58
2:B:85:THR:HG21	3:C:134:HIS:ND1	2.18	0.58
2:B:145:THR:HA	4:D:45:THR:HG22	1.86	0.58
4:D:8:LYS:HG3	4:D:76:ILE:CD1	2.34	0.58
4:D:172:ILE:HG12	4:D:174:ILE:HD12	1.87	0.57
1:A:113:PHE:CD1	2:B:34:ARG:HD2	2.39	0.57
2:B:125:ALA:HB1	2:B:147:LEU:HD21	1.86	0.57
4:D:123:GLY:O	4:D:124:SER:CB	2.53	0.57
2:B:146:GLN:NE2	4:D:46:LYS:CE	2.66	0.56
4:D:156:THR:HB	4:D:173:ASP:CG	2.25	0.56
2:B:70:ARG:NE	3:C:140:TRP:CH2	2.73	0.56
1:A:53:ARG:O	3:C:134:HIS:CA	2.53	0.56
4:D:129:GLN:CG	4:D:129:GLN:O	2.50	0.56
1:A:87:PRO:HD2	1:A:170:LEU:HG	1.87	0.56
4:D:156:THR:HA	4:D:173:ASP:HA	1.87	0.56
4:D:50:LYS:HG2	4:D:51:LEU:CD1	2.35	0.56
1:A:88:GLN:CD	4:D:60:SER:HB3	2.19	0.55
1:A:11:THR:HG23	1:A:63:ILE:HD13	1.88	0.55
2:B:74:GLU:HA	2:B:77:THR:OG1	2.07	0.55
2:B:59:GLU:HG3	2:B:60:TYR:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:THR:HG22	4:D:45:THR:CG2	2.37	0.54
1:A:113:PHE:CE1	2:B:34:ARG:HG3	2.41	0.54
4:D:98:PHE:HD2	4:D:120:SER:HA	1.73	0.54
4:D:161:VAL:HB	4:D:168:VAL:HG12	1.88	0.54
4:D:107:HIS:CE1	4:D:109:LEU:HD11	2.42	0.54
4:D:146:VAL:HG11	4:D:149:LEU:HD23	1.88	0.54
2:B:11:PHE:HB2	3:C:139:GLU:OE1	2.07	0.54
4:D:138:ILE:CD1	4:D:144:LEU:HB3	2.33	0.54
4:D:108:LEU:CD1	4:D:149:LEU:CD1	2.86	0.54
2:B:70:ARG:HD2	3:C:140:TRP:CZ2	2.41	0.54
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.89	0.53
4:D:96:LEU:HD22	4:D:121:PRO:CG	2.39	0.53
4:D:32:ASN:HB2	4:D:34:ILE:HD12	1.90	0.53
4:D:116:LEU:CD1	4:D:144:LEU:HB2	2.36	0.53
2:B:145:THR:HA	4:D:45:THR:HA	1.91	0.53
4:D:2:LYS:NZ	4:D:15:THR:OG1	2.41	0.53
4:D:85:GLU:HA	4:D:89:GLN:O	2.09	0.52
4:D:27:HIS:CG	4:D:35:LYS:HD3	2.43	0.52
4:D:8:LYS:HE3	4:D:76:ILE:HD13	1.91	0.52
4:D:133:PRO:HD3	4:D:157:TRP:CD1	2.44	0.52
2:B:11:PHE:CB	3:C:139:GLU:OE1	2.58	0.52
4:D:42:SER:H	4:D:43:PHE:HD1	1.58	0.51
4:D:42:SER:OG	4:D:43:PHE:CE1	2.57	0.51
4:D:8:LYS:HG3	4:D:76:ILE:HD12	1.92	0.51
4:D:98:PHE:CE2	4:D:120:SER:HB3	2.46	0.51
1:A:72:ILE:O	1:A:76:ARG:HG3	2.10	0.51
4:D:24:ILE:HG12	4:D:25:GLN:N	2.19	0.51
4:D:21:LYS:HE2	4:D:64:GLN:HA	1.92	0.51
4:D:42:SER:OG	4:D:43:PHE:HE1	1.93	0.51
4:D:1:LYS:HE3	4:D:92:GLU:H	1.76	0.51
4:D:150:GLU:O	4:D:151:LEU:C	2.49	0.51
4:D:110:GLN:NE2	4:D:178:ALA:HA	2.26	0.51
4:D:24:ILE:CG1	4:D:25:GLN:H	2.20	0.51
4:D:116:LEU:HD12	4:D:116:LEU:H	1.76	0.50
1:A:76:ARG:HB3	2:B:53:LEU:HD22	1.94	0.50
2:B:60:TYR:HB3	3:C:143:ILE:HD11	1.93	0.50
1:A:43:TRP:HH2	3:C:134:HIS:HD2	1.59	0.50
1:A:14:GLN:HE22	1:A:116:VAL:HG23	1.74	0.50
1:A:62:ASN:ND2	3:C:139:GLU:HB2	2.27	0.50
4:D:19:SER:O	4:D:20:GLN:C	2.50	0.49
2:B:85:THR:HB	3:C:134:HIS:CE1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:98:PHE:CD2	4:D:120:SER:HB3	2.47	0.49
1:A:11:THR:HB	2:B:11:PHE:HB3	1.95	0.49
1:A:91:VAL:HG12	1:A:105:LEU:HD22	1.95	0.49
4:D:40:GLN:HB3	4:D:45:THR:HG23	1.94	0.49
4:D:50:LYS:CG	4:D:51:LEU:CD1	2.89	0.49
4:D:131:ARG:CG	4:D:137:ASN:OD1	2.59	0.48
1:A:97:VAL:O	1:A:98:LEU:HD23	2.13	0.48
1:A:87:PRO:HG2	1:A:167:HIS:CB	2.43	0.48
4:D:21:LYS:O	4:D:22:LYS:HB3	2.13	0.48
4:D:87:GLU:HG2	4:D:88:ASP:N	2.29	0.48
1:A:43:TRP:CD1	1:A:49:ALA:HB2	2.48	0.48
4:D:98:PHE:CD2	4:D:121:PRO:CD	2.96	0.48
2:B:38:VAL:HG23	2:B:48:ARG:O	2.13	0.48
4:D:110:GLN:HE21	4:D:178:ALA:HA	1.79	0.48
2:B:125:ALA:HB1	2:B:147:LEU:CD2	2.43	0.48
1:A:52:ARG:NH2	3:C:134:HIS:CE1	2.80	0.48
4:D:96:LEU:HD22	4:D:121:PRO:HG3	1.95	0.48
2:B:144:SER:O	4:D:45:THR:HA	2.14	0.48
1:A:132:VAL:HA	1:A:150:TYR:O	2.14	0.48
1:A:89:ALA:HB2	1:A:165:VAL:HG21	1.97	0.47
4:D:129:GLN:HG2	4:D:160:THR:CG2	2.45	0.47
4:D:87:GLU:HG2	4:D:88:ASP:H	1.80	0.47
4:D:121:PRO:HA	4:D:122:PRO:HD2	1.71	0.47
4:D:134:ARG:HB2	4:D:152:GLN:OE1	2.14	0.46
3:C:143:ILE:HG13	3:C:143:ILE:H	1.39	0.46
4:D:26:PHE:HB2	4:D:86:VAL:HG22	1.98	0.46
4:D:20:GLN:CD	4:D:20:GLN:N	2.69	0.46
1:A:167:HIS:CD2	1:A:169:GLY:H	2.33	0.46
2:B:70:ARG:NE	3:C:140:TRP:HH2	2.11	0.46
4:D:120:SER:CB	4:D:121:PRO:HD2	2.46	0.46
4:D:129:GLN:CG	4:D:160:THR:HG22	2.46	0.46
1:A:77:SER:O	1:A:78:ASN:HB2	2.15	0.46
1:A:113:PHE:CD2	2:B:34:ARG:HD2	2.51	0.46
2:B:146:GLN:HE22	4:D:46:LYS:CE	2.29	0.46
2:B:61:TRP:HZ2	3:C:141:GLU:O	1.97	0.46
4:D:19:SER:C	4:D:20:GLN:CD	2.74	0.46
4:D:98:PHE:CD2	4:D:121:PRO:HD3	2.51	0.45
4:D:37:LEU:HD12	4:D:37:LEU:C	2.36	0.45
4:D:89:GLN:NE2	4:D:91:GLU:HG3	2.31	0.45
4:D:35:LYS:HE2	4:D:35:LYS:HB3	1.71	0.45
4:D:109:LEU:O	4:D:110:GLN:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLN:HG3	2:B:8:VAL:HG22	1.98	0.45
1:A:85:GLU:O	1:A:169:GLY:HA3	2.17	0.45
4:D:79:SER:O	4:D:80:ASP:HB2	2.16	0.45
2:B:110:ASN:OD1	2:B:166:ARG:NH1	2.50	0.45
1:A:44:MET:O	1:A:46:PRO:HD3	2.16	0.45
4:D:20:GLN:HB2	4:D:22:LYS:NZ	2.31	0.45
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.52	0.44
1:A:118:ASN:HB2	1:A:166:GLU:HB3	1.98	0.44
2:B:55:ARG:HB2	2:B:56:PRO:HD3	2.00	0.44
4:D:163:GLN:O	4:D:166:LYS:HG2	2.18	0.44
2:B:60:TYR:CB	3:C:143:ILE:HD11	2.48	0.44
4:D:129:GLN:CG	4:D:160:THR:CG2	2.96	0.44
2:B:61:TRP:CE2	3:C:141:GLU:O	2.70	0.44
4:D:50:LYS:HE2	4:D:51:LEU:HD11	1.99	0.43
4:D:163:GLN:O	4:D:164:ASN:HB2	2.18	0.43
2:B:61:TRP:NE1	3:C:141:GLU:O	2.51	0.43
4:D:79:SER:OG	4:D:97:VAL:N	2.48	0.43
1:A:138:PHE:HB2	1:A:146:HIS:CD2	2.53	0.43
2:B:116:VAL:HG22	2:B:160:MET:HG3	2.00	0.43
4:D:120:SER:O	4:D:122:PRO:HD3	2.18	0.43
4:D:166:LYS:HE3	4:D:166:LYS:HB3	1.51	0.43
2:B:144:SER:C	4:D:45:THR:HB	2.39	0.43
1:A:21:GLN:CD	1:A:136:SER:HB3	2.38	0.42
1:A:107:CYS:HB2	1:A:121:TRP:CZ2	2.54	0.42
1:A:135:THR:O	1:A:147:LYS:HE2	2.19	0.42
4:D:62:TRP:HD1	4:D:66:ASN:O	2.02	0.42
4:D:22:LYS:NZ	4:D:22:LYS:HB3	2.34	0.42
4:D:106:THR:O	4:D:107:HIS:O	2.36	0.42
4:D:85:GLU:HG2	4:D:90:LYS:CG	2.38	0.42
4:D:27:HIS:HB2	4:D:35:LYS:CD	2.50	0.42
2:B:85:THR:HB	3:C:134:HIS:NE2	2.35	0.42
1:A:114:PRO:O	1:A:167:HIS:HE1	2.03	0.42
2:B:167:ARG:HH11	2:B:167:ARG:HG2	1.85	0.42
4:D:107:HIS:HD2	4:D:177:LEU:HD12	1.83	0.42
1:A:176:LYS:HD3	1:A:176:LYS:HA	1.75	0.42
4:D:129:GLN:HG2	4:D:160:THR:HG21	2.02	0.42
4:D:108:LEU:CD1	4:D:149:LEU:HD11	2.49	0.42
4:D:24:ILE:CG1	4:D:25:GLN:N	2.82	0.42
4:D:24:ILE:HD11	4:D:87:GLU:OE2	2.20	0.42
1:A:85:GLU:O	1:A:167:HIS:CD2	2.73	0.42
4:D:164:ASN:C	4:D:166:LYS:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:21:LYS:HE2	4:D:64:GLN:HG2	2.02	0.41
4:D:27:HIS:NE2	4:D:29:LYS:HE3	2.35	0.41
2:B:145:THR:N	4:D:45:THR:HG22	2.35	0.41
4:D:106:THR:HG22	4:D:107:HIS:N	2.33	0.41
2:B:125:ALA:CB	2:B:147:LEU:HD21	2.50	0.41
1:A:56:PRO:O	1:A:59:GLY:N	2.54	0.41
2:B:40:PHE:HB2	2:B:47:TYR:CE1	2.55	0.41
4:D:22:LYS:HZ2	4:D:22:LYS:HB3	1.85	0.41
2:B:60:TYR:HB2	3:C:143:ILE:CD1	2.50	0.41
4:D:1:LYS:CG	4:D:2:LYS:N	2.83	0.41
1:A:55:GLU:HA	1:A:56:PRO:HD2	1.94	0.41
1:A:24:PHE:HZ	3:C:136:GLY:HA2	1.86	0.41
1:A:113:PHE:CE1	2:B:34:ARG:CG	3.03	0.41
2:B:128:LYS:HE3	2:B:130:ARG:HD2	2.01	0.41
4:D:96:LEU:CD2	4:D:121:PRO:HG3	2.51	0.41
1:A:87:PRO:HG2	1:A:167:HIS:HB2	2.02	0.41
1:A:70:LEU:HD13	2:B:9:HIS:HB2	2.03	0.41
4:D:116:LEU:HD12	4:D:116:LEU:N	2.35	0.41
4:D:150:GLU:C	4:D:152:GLN:N	2.74	0.41
1:A:122:LEU:HD23	1:A:127:SER:HA	2.03	0.41
2:B:19:ASN:HB3	2:B:22:GLN:HB3	2.03	0.41

All (55) 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)
4:D:107:HIS:CD2	4:D:177:LEU:CB[8_665]	0.41	1.79
1:A:57:GLN:CD	1:A:57:GLN:CD[5_555]	0.51	1.69
1:A:57:GLN:CG	1:A:57:GLN:NE2[5_555]	0.91	1.29
2:B:64:GLN:NE2	3:C:144:GLU:CG[5_555]	0.97	1.23
4:D:107:HIS:CG	4:D:177:LEU:CB[8_665]	1.10	1.10
4:D:107:HIS:CG	4:D:177:LEU:CA[8_665]	1.14	1.06
2:B:130:ARG:NH1	2:B:130:ARG:NH2[5_556]	1.18	1.02
4:D:107:HIS:NE2	4:D:177:LEU:CB[8_665]	1.24	0.96
1:A:57:GLN:CG	1:A:57:GLN:CD[5_555]	1.28	0.92
1:A:57:GLN:CD	1:A:57:GLN:NE2[5_555]	1.29	0.91
4:D:107:HIS:C	4:D:177:LEU:CD2[8_665]	1.29	0.91
2:B:64:GLN:CD	3:C:144:GLU:CG[5_555]	1.31	0.89
4:D:107:HIS:O	4:D:177:LEU:CD2[8_665]	1.39	0.81
2:B:135:GLY:N	2:B:181:THR:O[5_556]	1.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:ARG:CZ	2:B:130:ARG:NH1[5_556]	1.54	0.66
4:D:107:HIS:CD2	4:D:177:LEU:CG[8_665]	1.56	0.64
4:D:107:HIS:CD2	4:D:177:LEU:CA[8_665]	1.57	0.63
2:B:64:GLN:OE1	3:C:144:GLU:CG[5_555]	1.63	0.57
1:A:57:GLN:CG	1:A:57:GLN:OE1[5_555]	1.67	0.53
4:D:106:THR:CB	4:D:154:SER:CB[8_665]	1.68	0.52
2:B:51:THR:CG2	4:D:127:SER:OG[8_665]	1.69	0.51
2:B:34:ARG:NH2	4:D:165:GLN:OE1[8_665]	1.71	0.49
1:A:57:GLN:CD	1:A:57:GLN:OE1[5_555]	1.72	0.48
2:B:64:GLN:CA	3:C:144:GLU:OE2[5_555]	1.74	0.46
4:D:107:HIS:CB	4:D:176:VAL:O[8_665]	1.75	0.45
2:B:64:GLN:OE1	3:C:144:GLU:CD[5_555]	1.77	0.43
2:B:64:GLN:CD	3:C:144:GLU:CD[5_555]	1.77	0.43
2:B:128:LYS:NZ	2:B:137:GLU:OE1[5_556]	1.80	0.40
2:B:130:ARG:CZ	2:B:130:ARG:NH2[5_556]	1.80	0.40
4:D:107:HIS:N	4:D:175:VAL:CG1[8_665]	1.82	0.38
4:D:107:HIS:ND1	4:D:177:LEU:CB[8_665]	1.83	0.37
2:B:130:ARG:CZ	2:B:130:ARG:CZ[5_556]	1.83	0.37
2:B:130:ARG:NH1	2:B:130:ARG:NH1[5_556]	1.83	0.37
1:A:57:GLN:OE1	1:A:57:GLN:NE2[5_555]	1.86	0.34
4:D:107:HIS:CE1	4:D:177:LEU:CB[8_665]	1.86	0.34
2:B:64:GLN:CD	3:C:144:GLU:OE2[5_555]	1.86	0.34
1:A:99:LEU:CD2	1:A:130:ASP:OD1[6_565]	1.88	0.32
4:D:107:HIS:CB	4:D:177:LEU:CA[8_665]	1.89	0.31
4:D:107:HIS:CG	4:D:177:LEU:CG[8_665]	1.91	0.29
2:B:134:ASN:C	2:B:181:THR:O[5_556]	1.91	0.29
2:B:64:GLN:NE2	3:C:144:GLU:CB[5_555]	1.91	0.29
4:D:106:THR:OG1	4:D:154:SER:CB[8_665]	1.92	0.28
2:B:64:GLN:NE2	3:C:144:GLU:CD[5_555]	1.93	0.27
2:B:135:GLY:CA	2:B:181:THR:O[5_556]	1.99	0.21
4:D:107:HIS:ND1	4:D:177:LEU:CA[8_665]	2.02	0.18
4:D:108:LEU:N	4:D:177:LEU:CD2[8_665]	2.05	0.15
1:A:61:GLN:OE1	1:A:61:GLN:NE2[5_555]	2.06	0.14
2:B:34:ARG:NH2	4:D:165:GLN:CD[8_665]	2.08	0.12
4:D:107:HIS:C	4:D:177:LEU:CG[8_665]	2.08	0.12
2:B:64:GLN:OE1	3:C:144:GLU:OE2[5_555]	2.12	0.08
4:D:107:HIS:CB	4:D:176:VAL:C[8_665]	2.12	0.08
1:A:57:GLN:CB	1:A:57:GLN:NE2[5_555]	2.14	0.06
2:B:64:GLN:CB	3:C:144:GLU:OE2[5_555]	2.15	0.05
1:A:57:GLN:CB	1:A:57:GLN:OE1[5_555]	2.16	0.04
1:A:57:GLN:CB	1:A:57:GLN:CD[5_555]	2.18	0.02

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	176/178 (99%)	168 (96%)	8 (4%)	0	100 100
2	B	183/185 (99%)	175 (96%)	8 (4%)	0	100 100
3	C	14/16 (88%)	12 (86%)	1 (7%)	1 (7%)	1 23
4	D	176/178 (99%)	145 (82%)	21 (12%)	10 (6%)	2 28
All	All	549/557 (99%)	500 (91%)	38 (7%)	11 (2%)	9 53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	124	SER
4	D	21	LYS
4	D	126	PRO
4	D	151	LEU
3	C	145	SER
4	D	23	SER
4	D	24	ILE
4	D	136	LYS
4	D	105	ASP
4	D	107	HIS
4	D	122	PRO

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	162/162 (100%)	157 (97%)	5 (3%)	47 78
2	B	171/171 (100%)	168 (98%)	3 (2%)	66 87
3	C	11/11 (100%)	5 (46%)	6 (54%)	0 0
4	D	159/161 (99%)	123 (77%)	36 (23%)	1 9
All	All	503/505 (100%)	453 (90%)	50 (10%)	10 42

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	18	ASP
1	A	50	GLN
1	A	62	ASN
1	A	130	ASP
2	B	59	GLU
2	B	70	ARG
2	B	163	MET
3	C	133	SER
3	C	134	HIS
3	C	141	GLU
3	C	143	ILE
3	C	144	GLU
3	C	145	SER
4	D	8	LYS
4	D	19	SER
4	D	22	LYS
4	D	23	SER
4	D	29	LYS
4	D	35	LYS
4	D	37	LEU
4	D	42	SER
4	D	58	ARG
4	D	72	LYS
4	D	90	LYS
4	D	91	GLU
4	D	94	GLN
4	D	108	LEU
4	D	110	GLN
4	D	116	LEU
4	D	118	LEU
4	D	120	SER
4	D	129	GLN

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Mol	Chain	Res	Type
4	D	134	ARG
4	D	138	ILE
4	D	139	GLN
4	D	142	LYS
4	D	144	LEU
4	D	148	GLN
4	D	151	LEU
4	D	152	GLN
4	D	154	SER
4	D	156	THR
4	D	160	THR
4	D	162	LEU
4	D	165	GLN
4	D	166	LYS
4	D	167	LYS
4	D	172	ILE
4	D	174	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	57	GLN
1	A	88	GLN
1	A	167	HIS
2	B	96	GLN
2	B	146	GLN
4	D	32	ASN
4	D	66	ASN
4	D	73	ASN
4	D	89	GLN
4	D	103	ASN
4	D	107	HIS
4	D	110	GLN
4	D	148	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	178/178 (100%)	0.02	6 (3%)	49	39	52, 52, 57, 57	0
2	B	185/185 (100%)	0.08	2 (1%)	82	76	47, 47, 63, 63	0
3	C	16/16 (100%)	0.31	1 (6%)	23	16	82, 82, 82, 82	0
4	D	178/178 (100%)	0.17	6 (3%)	49	39	73, 73, 100, 100	0
All	All	557/557 (100%)	0.10	15 (2%)	58	48	47, 57, 100, 100	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	110	GLN	3.1
4	D	161	VAL	3.1
2	B	47	TYR	2.9
2	B	24	ILE	2.9
1	A	52	ARG	2.9
4	D	174	ILE	2.8
4	D	178	ALA	2.4
1	A	141	ARG	2.3
1	A	168	TRP	2.3
1	A	25	GLU	2.3
4	D	98	PHE	2.3
4	D	6	GLY	2.2
1	A	173	PRO	2.2
1	A	114	PRO	2.1
3	C	136	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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.