Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2025 – 04:15 pm BST

PDB ID	:	9HI7 / pdb_00009hi7
Title	:	Structure of MC.7.G5 T cell receptor in complex with MR1 R9H
Authors	:	Karuppiah, V.
Deposited on	:	2024-11-24
Resolution	:	2.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

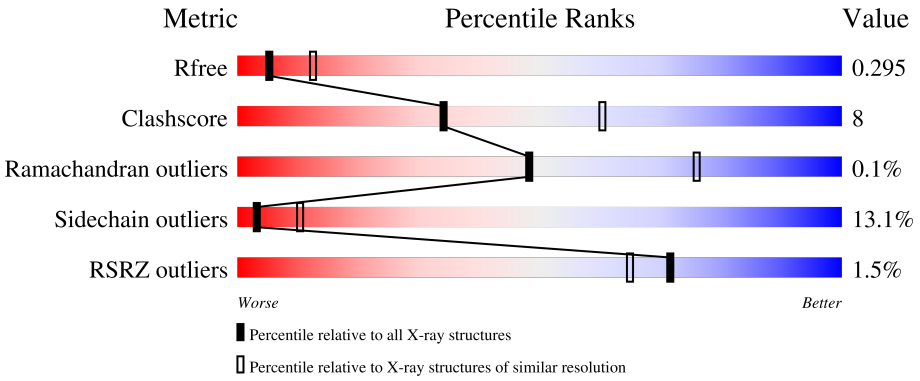
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.81 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}	164625	4293 (2.84-2.80)
Clashscore	180529	4801 (2.84-2.80)
Ramachandran outliers	177936	4739 (2.84-2.80)
Sidechain outliers	177891	4741 (2.84-2.80)
RSRZ outliers	164620	4295 (2.84-2.80)

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	290	2% 69% 19% • 9%
1	F	290	3% 63% 23% 6% 8%
2	B	100	75% 23% •
2	G	100	71% 24% • •
3	D	201	70% 24% • •

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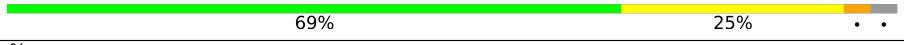
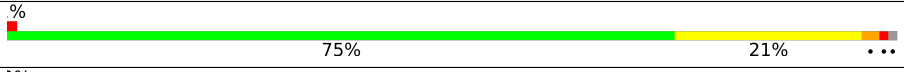
Mol	Chain	Length	Quality of chain
3	H	201	
4	E	248	
4	I	248	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13002 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 Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2175	1390	375	399	11			
1	F	266	Total	C	N	O	S	0	0	0
			2196	1402	378	405	11			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	9	HIS	ARG	engineered mutation	UNP Q95460
A	261	SER	CYS	conflict	UNP Q95460
A	271	GLY	-	expression tag	UNP Q95460
A	272	SER	-	expression tag	UNP Q95460
A	273	GLY	-	expression tag	UNP Q95460
A	274	GLY	-	expression tag	UNP Q95460
A	275	GLY	-	expression tag	UNP Q95460
A	276	LEU	-	expression tag	UNP Q95460
A	277	ASN	-	expression tag	UNP Q95460
A	278	ASP	-	expression tag	UNP Q95460
A	279	ILE	-	expression tag	UNP Q95460
A	280	PHE	-	expression tag	UNP Q95460
A	281	GLU	-	expression tag	UNP Q95460
A	282	ALA	-	expression tag	UNP Q95460
A	283	GLN	-	expression tag	UNP Q95460
A	284	LYS	-	expression tag	UNP Q95460
A	285	ILE	-	expression tag	UNP Q95460
A	286	GLU	-	expression tag	UNP Q95460
A	287	TRP	-	expression tag	UNP Q95460
A	288	HIS	-	expression tag	UNP Q95460
A	289	GLU	-	expression tag	UNP Q95460
F	0	MET	-	initiating methionine	UNP Q95460
F	9	HIS	ARG	engineered mutation	UNP Q95460
F	261	SER	CYS	conflict	UNP Q95460

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Chain	Residue	Modelled	Actual	Comment	Reference
F	271	GLY	-	expression tag	UNP Q95460
F	272	SER	-	expression tag	UNP Q95460
F	273	GLY	-	expression tag	UNP Q95460
F	274	GLY	-	expression tag	UNP Q95460
F	275	GLY	-	expression tag	UNP Q95460
F	276	LEU	-	expression tag	UNP Q95460
F	277	ASN	-	expression tag	UNP Q95460
F	278	ASP	-	expression tag	UNP Q95460
F	279	ILE	-	expression tag	UNP Q95460
F	280	PHE	-	expression tag	UNP Q95460
F	281	GLU	-	expression tag	UNP Q95460
F	282	ALA	-	expression tag	UNP Q95460
F	283	GLN	-	expression tag	UNP Q95460
F	284	LYS	-	expression tag	UNP Q95460
F	285	ILE	-	expression tag	UNP Q95460
F	286	GLU	-	expression tag	UNP Q95460
F	287	TRP	-	expression tag	UNP Q95460
F	288	HIS	-	expression tag	UNP Q95460
F	289	GLU	-	expression tag	UNP Q95460

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
2	G	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called T cell receptor alpha chain MC.7.G5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	193	Total	C	N	O	S	0	0	0
			1527	949	256	311	11			
3	H	194	Total	C	N	O	S	0	0	0
			1535	955	257	312	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	167	CYS	THR	conflict	UNP P0DTU3
H	167	CYS	THR	conflict	UNP P0DTU3

- Molecule 4 is a protein called T cell receptor beta chain MC.7.G5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	245	Total	C	N	O	S	0	0	0
			1961	1234	337	382	8			
4	I	246	Total	C	N	O	S	0	0	0
			1966	1237	338	383	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	174	CYS	SER	conflict	UNP P0DTU4
E	192	ALA	CYS	conflict	UNP P0DTU4
E	206	ASP	ASN	conflict	UNP P0DTU4
I	174	CYS	SER	conflict	UNP P0DTU4
I	192	ALA	CYS	conflict	UNP P0DTU4
I	206	ASP	ASN	conflict	UNP P0DTU4

- Molecule 5 is water.

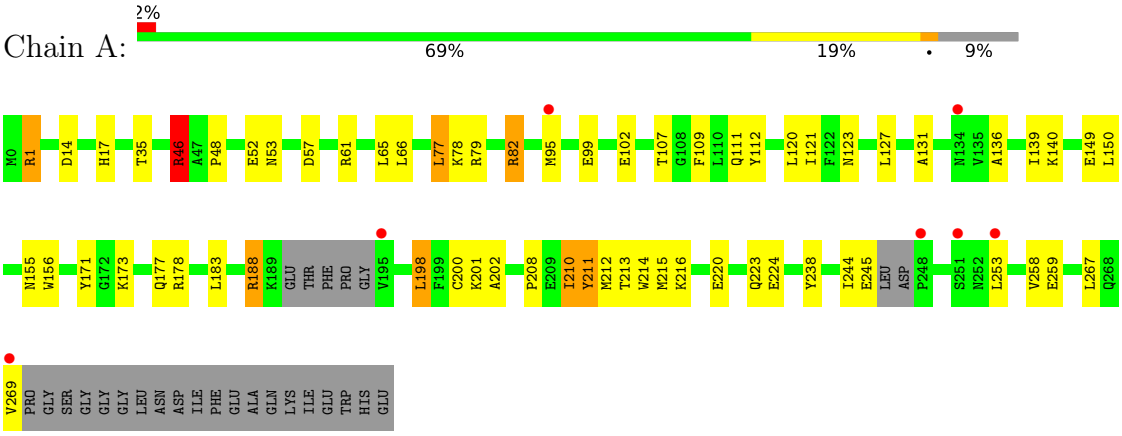
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	H	1	Total	O	0	0
			1	1		

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.

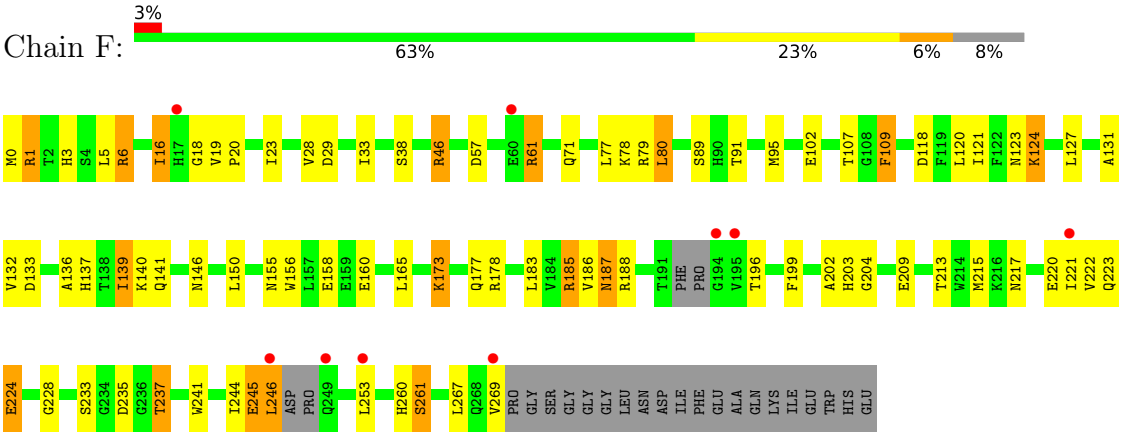
• Molecule 1: Major histocompatibility complex class I-related gene protein

Chain A:



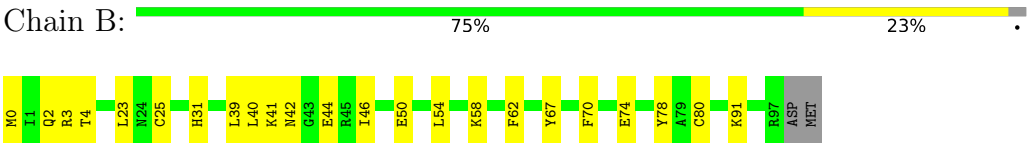
• Molecule 1: Major histocompatibility complex class I-related gene protein

Chain F:



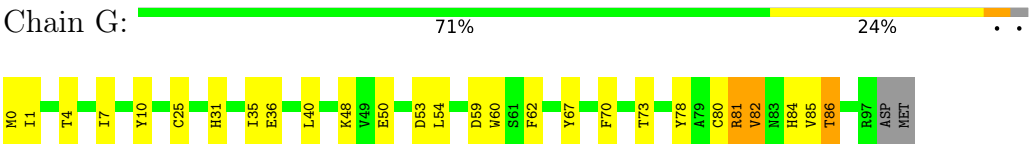
• Molecule 2: Beta-2-microglobulin

Chain B:



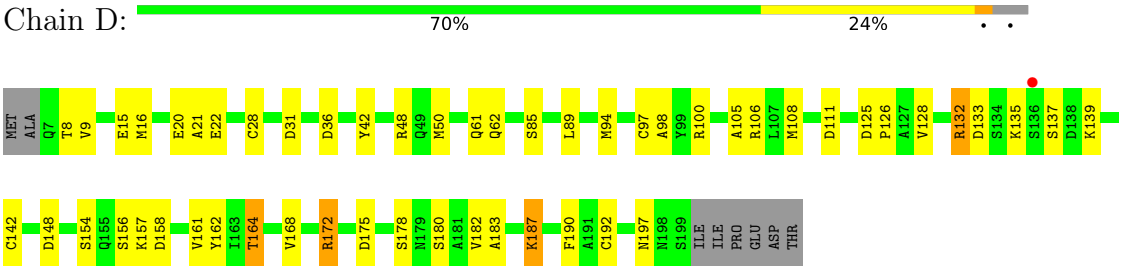
• Molecule 2: Beta-2-microglobulin

Chain G:



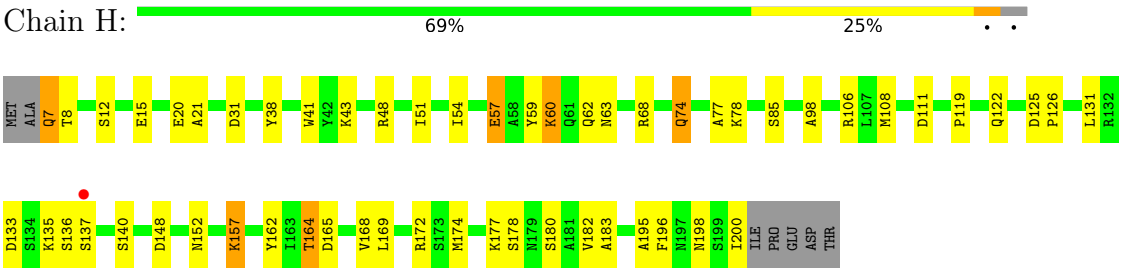
• Molecule 3: T cell receptor alpha chain MC.7.G5

Chain D:



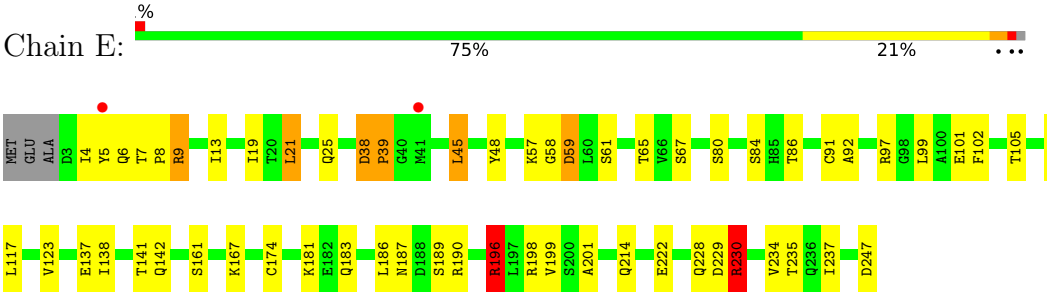
• Molecule 3: T cell receptor alpha chain MC.7.G5

Chain H:



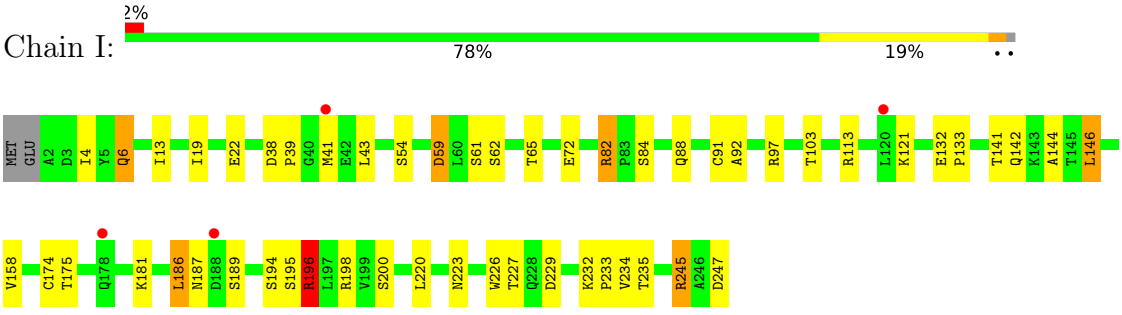
• Molecule 4: T cell receptor beta chain MC.7.G5

Chain E:



• Molecule 4: T cell receptor beta chain MC.7.G5

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.03Å 113.20Å 130.36Å 90.00° 90.73° 90.00°	Depositor
Resolution (Å)	130.35 – 2.81 130.35 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.5 (130.35-2.81) 99.5 (130.35-2.81)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.236 , 0.296 0.252 , 0.295	Depositor DCC
R_{free} test set	2468 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 23.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13002	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.53	0/2240	0.82	0/3041
1	F	0.56	0/2260	0.87	0/3068
2	B	0.54	0/843	0.85	0/1141
2	G	0.62	0/843	0.95	0/1141
3	D	0.59	0/1556	0.94	0/2105
3	H	0.62	0/1564	0.94	0/2116
4	E	0.61	0/2015	0.84	0/2744
4	I	0.58	0/2020	0.85	0/2751
All	All	0.58	0/13341	0.88	0/18107

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	5
1	F	0	3
2	B	0	1
2	G	0	1
3	D	0	3
3	H	0	1
4	E	0	6
4	I	0	6
All	All	0	26

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ARG	Sidechain
1	A	188	ARG	Sidechain
1	A	46	ARG	Sidechain
1	A	61	ARG	Sidechain
1	A	82	ARG	Sidechain
2	B	3	ARG	Sidechain
3	D	106	ARG	Sidechain
3	D	132	ARG	Sidechain
3	D	48	ARG	Sidechain
4	E	190	ARG	Sidechain
4	E	196	ARG	Sidechain
4	E	198	ARG	Sidechain
4	E	230	ARG	Sidechain
4	E	9	ARG	Sidechain
4	E	97	ARG	Sidechain
1	F	185	ARG	Sidechain
1	F	6	ARG	Sidechain
1	F	61	ARG	Sidechain
2	G	81	ARG	Sidechain
3	H	48	ARG	Sidechain
4	I	113	ARG	Sidechain
4	I	196	ARG	Sidechain
4	I	198	ARG	Sidechain
4	I	245	ARG	Sidechain
4	I	82	ARG	Sidechain
4	I	97	ARG	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	2175	0	2067	27	0
1	F	2196	0	2086	43	0
2	B	820	0	792	14	0
2	G	820	0	792	13	0
3	D	1527	0	1453	28	0
3	H	1535	0	1462	31	0
4	E	1961	0	1855	20	0
4	I	1966	0	1860	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	H	1	0	0	0	0
All	All	13002	0	12367	187	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 8.

All (187) 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)
3:D:8:THR:CG2	3:D:31:ASP:HB3	2.15	0.76
1:A:208:PRO:HG3	1:A:238:TYR:CE2	2.23	0.74
1:F:124:LYS:HE2	1:F:158:GLU:HG2	1.72	0.71
2:B:25:CYS:CB	2:B:80:CYS:HG	2.04	0.70
3:D:28:CYS:SG	3:D:97:CYS:CB	2.80	0.69
2:G:84:HIS:ND1	2:G:86:THR:CG2	2.55	0.69
1:F:188:ARG:HH11	1:F:188:ARG:HG3	1.58	0.68
1:A:212:MET:HG2	1:A:258:VAL:HG22	1.75	0.67
1:F:3:HIS:ND1	1:F:29:ASP:OD2	2.25	0.67
3:D:89:LEU:HD12	3:D:168:VAL:HG11	1.76	0.67
1:F:131:ALA:HB1	1:F:136:ALA:HB3	1.77	0.67
3:D:28:CYS:HG	3:D:97:CYS:CB	2.07	0.66
4:I:13:ILE:HG21	4:I:19:ILE:HD11	1.76	0.66
3:D:8:THR:HG22	3:D:31:ASP:HB3	1.76	0.66
2:B:25:CYS:SG	2:B:80:CYS:CB	2.84	0.66
4:I:186:LEU:HD23	4:I:187:ASN:H	1.60	0.66
1:F:118:ASP:O	1:F:132:VAL:HG11	1.97	0.65
2:B:41:LYS:HB2	2:B:46:ILE:HD11	1.78	0.64
2:G:25:CYS:SG	2:G:80:CYS:CB	2.86	0.64
3:H:41:TRP:HB2	3:H:54:ILE:HG22	1.78	0.64
3:H:131:LEU:HB3	4:I:132:GLU:O	1.98	0.64
4:I:133:PRO:HG2	4:I:144:ALA:HB1	1.80	0.64
2:G:54:LEU:HD11	2:G:62:PHE:HB3	1.79	0.64
1:F:120:LEU:C	1:F:121:ILE:HD12	2.19	0.63
2:G:25:CYS:HG	2:G:80:CYS:CB	2.11	0.63
1:A:210:ILE:HD11	1:A:258:VAL:HG13	1.83	0.61
4:E:38:ASP:O	4:E:39:PRO:C	2.39	0.61
4:I:38:ASP:O	4:I:39:PRO:C	2.38	0.61
1:F:71:GLN:NE2	1:F:71:GLN:HA	2.15	0.61
2:B:54:LEU:HD11	2:B:62:PHE:HB3	1.84	0.60
2:G:84:HIS:ND1	2:G:86:THR:HG22	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:195:ALA:O	3:H:196:PHE:HB2	2.01	0.59
3:H:60:LYS:HE3	3:H:60:LYS:HA	1.84	0.59
3:D:128:VAL:CG1	3:D:192:CYS:HB3	2.33	0.59
4:I:38:ASP:HB2	4:I:41:MET:HB3	1.85	0.58
3:H:98:ALA:HA	3:H:108:MET:O	2.03	0.58
3:D:164:THR:HG22	3:D:182:VAL:H	1.68	0.58
3:H:164:THR:HG22	3:H:182:VAL:H	1.67	0.58
2:G:50:GLU:HB2	2:G:67:TYR:CZ	2.39	0.58
1:A:173:LYS:HA	1:A:177:GLN:HG3	1.87	0.57
1:F:233:SER:HB2	1:F:237:THR:HG22	1.87	0.57
3:H:38:TYR:CE2	4:I:103:THR:HA	2.39	0.56
3:H:106:ARG:NH1	4:I:59:ASP:HB2	2.21	0.56
1:A:48:PRO:O	1:A:52:GLU:HG3	2.07	0.55
3:D:172:ARG:HH12	3:D:175:ASP:HA	1.72	0.54
3:H:133:ASP:C	3:H:135:LYS:H	2.10	0.54
3:D:42:TYR:HB3	3:D:50:MET:HE3	1.88	0.54
1:F:20:PRO:HD2	1:F:23:ILE:HD11	1.89	0.53
3:D:156:SER:HB2	3:D:161:VAL:HG13	1.90	0.53
3:D:125:ASP:N	3:D:126:PRO:HD3	2.23	0.53
1:F:260:HIS:O	1:F:261:SER:C	2.47	0.53
3:D:125:ASP:N	3:D:126:PRO:CD	2.71	0.53
4:E:174:CYS:HB3	4:E:196:ARG:HD2	1.90	0.52
3:D:133:ASP:HB3	3:D:137:SER:H	1.75	0.52
3:D:162:TYR:O	3:D:183:ALA:HA	2.10	0.51
1:A:131:ALA:HB1	1:A:136:ALA:HB3	1.92	0.51
4:E:13:ILE:HG21	4:E:19:ILE:HD11	1.93	0.51
4:I:6:GLN:HA	4:I:22:GLU:O	2.11	0.51
3:H:162:TYR:O	3:H:183:ALA:HA	2.10	0.51
1:F:16:ILE:HG22	1:F:19:VAL:HG23	1.93	0.51
4:E:6:GLN:HB2	4:E:110:PRO:HD2	1.92	0.50
3:H:125:ASP:N	3:H:126:PRO:HD3	2.25	0.50
3:D:8:THR:HG23	3:D:31:ASP:HB3	1.93	0.50
3:H:119:PRO:HG3	3:H:168:VAL:CG1	2.42	0.50
1:F:28:VAL:HG23	1:F:33:ILE:HD13	1.94	0.49
1:F:71:GLN:HA	1:F:71:GLN:HE21	1.76	0.49
1:F:91:THR:HG21	2:G:31:HIS:CE1	2.47	0.49
1:F:204:GLY:HA2	1:F:237:THR:HG21	1.95	0.49
1:F:204:GLY:HA2	1:F:237:THR:CG2	2.42	0.49
4:I:133:PRO:CG	4:I:144:ALA:HB1	2.42	0.49
3:H:62:GLN:O	3:H:63:ASN:HB2	2.12	0.49
2:B:41:LYS:HG3	2:B:78:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:ARG:HH11	1:F:188:ARG:CG	2.24	0.49
3:H:20:GLU:O	3:H:21:ALA:HB3	2.13	0.49
1:A:65:LEU:HD11	4:E:101:GLU:HG3	1.94	0.49
1:A:112:TYR:HB2	1:A:120:LEU:HB2	1.94	0.49
3:H:106:ARG:HG2	3:H:108:MET:HE2	1.94	0.49
3:H:43:LYS:HG2	3:H:51:ILE:HB	1.95	0.49
1:F:156:TRP:HA	1:F:160:GLU:HB2	1.94	0.49
1:F:245:GLU:HG2	1:F:246:LEU:N	2.28	0.48
1:F:246:LEU:C	1:F:246:LEU:HD12	2.33	0.48
3:H:106:ARG:HH11	4:I:59:ASP:HB2	1.77	0.48
3:H:57:GLU:HG3	3:H:59:TYR:CE1	2.49	0.48
1:F:120:LEU:O	1:F:121:ILE:HD12	2.13	0.48
2:B:50:GLU:HB2	2:B:67:TYR:CZ	2.48	0.48
1:F:133:ASP:C	1:F:133:ASP:OD1	2.51	0.48
3:D:187:LYS:HD2	3:D:190:PHE:HB2	1.94	0.48
1:A:53:ASN:ND2	1:A:171:TYR:CD1	2.82	0.48
3:D:89:LEU:HD22	3:D:89:LEU:N	2.29	0.48
1:F:1:ARG:HA	1:F:102:GLU:HG2	1.96	0.47
1:F:136:ALA:O	1:F:139:ILE:HG12	2.14	0.47
1:A:200:CYS:HB2	1:A:214:TRP:CZ2	2.49	0.47
1:F:223:GLN:HG2	1:F:224:GLU:N	2.29	0.47
3:H:57:GLU:H	3:H:57:GLU:CD	2.18	0.47
1:A:223:GLN:HG2	1:A:224:GLU:HG2	1.96	0.47
4:I:91:CYS:SG	4:I:92:ALA:N	2.87	0.47
3:H:125:ASP:N	3:H:126:PRO:CD	2.77	0.47
3:D:98:ALA:HA	3:D:108:MET:O	2.14	0.47
1:F:187:ASN:ND2	1:F:199:PHE:HB2	2.29	0.47
4:I:141:THR:O	4:I:142:GLN:HB2	2.14	0.47
4:E:141:THR:O	4:E:142:GLN:HB2	2.15	0.47
4:I:175:THR:HG23	4:I:195:SER:HB2	1.97	0.47
4:I:234:VAL:HG23	4:I:235:THR:O	2.14	0.47
4:I:226:TRP:HB2	4:I:232:LYS:HD2	1.97	0.46
2:G:84:HIS:CE1	2:G:86:THR:HG22	2.49	0.46
3:D:168:VAL:O	4:E:174:CYS:SG	2.74	0.46
3:H:119:PRO:HG3	3:H:168:VAL:HG11	1.98	0.46
1:A:35:THR:HB	1:A:46:ARG:HD2	1.98	0.46
4:E:8:PRO:HD2	4:E:21:LEU:HD12	1.98	0.46
4:E:234:VAL:HG23	4:E:235:THR:O	2.16	0.45
1:A:111:GLN:HE21	1:A:121:ILE:HG12	1.80	0.45
1:A:127:LEU:HB3	1:A:150:LEU:HD23	1.97	0.45
3:D:89:LEU:CD1	3:D:168:VAL:HG11	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:181:LYS:HE3	4:I:189:SER:HB3	1.97	0.45
4:I:220:LEU:HD22	4:I:233:PRO:HG2	1.99	0.45
2:B:91:LYS:HE3	2:B:91:LYS:HB2	1.84	0.45
2:B:2:GLN:HB3	2:B:31:HIS:O	2.17	0.45
1:F:5:LEU:HB2	1:F:165:LEU:HD13	1.98	0.45
1:F:71:GLN:NE2	1:F:71:GLN:CA	2.79	0.45
2:G:10:TYR:CD1	2:G:10:TYR:N	2.85	0.44
4:E:91:CYS:SG	4:E:92:ALA:N	2.89	0.44
4:E:137:GLU:O	4:E:141:THR:OG1	2.31	0.44
2:B:25:CYS:CB	2:B:80:CYS:SG	3.00	0.44
3:H:106:ARG:NH1	4:I:59:ASP:CB	2.81	0.44
3:H:133:ASP:C	3:H:135:LYS:N	2.71	0.44
4:I:186:LEU:CD2	4:I:187:ASN:H	2.29	0.44
1:A:183:LEU:O	1:A:202:ALA:HA	2.18	0.44
1:A:223:GLN:H	1:A:223:GLN:CD	2.21	0.44
4:E:229:ASP:O	4:E:230:ARG:C	2.56	0.44
3:H:74:GLN:HB2	3:H:77:ALA:HB3	2.00	0.44
4:I:194:SER:OG	4:I:196:ARG:NH2	2.51	0.44
1:F:123:ASN:C	1:F:123:ASN:OD1	2.56	0.44
1:F:18:GLY:O	1:F:19:VAL:C	2.55	0.44
1:A:53:ASN:HD22	1:A:171:TYR:HB3	1.82	0.43
1:F:80:LEU:HD12	1:F:80:LEU:HA	1.82	0.43
2:B:39:LEU:O	2:B:46:ILE:HG12	2.18	0.43
3:H:131:LEU:HD22	4:I:133:PRO:HA	1.99	0.43
2:B:23:LEU:O	2:B:67:TYR:HA	2.18	0.43
1:A:77:LEU:HD13	1:A:77:LEU:HA	1.72	0.43
1:F:183:LEU:O	1:F:202:ALA:HA	2.18	0.43
3:D:158:ASP:HB3	3:D:161:VAL:HG12	2.01	0.43
4:E:86:THR:HG23	4:E:115:THR:HA	2.00	0.43
4:E:138:ILE:HG23	4:E:201:ALA:HB1	2.00	0.43
2:B:40:LEU:O	2:B:78:TYR:HA	2.19	0.43
1:F:6:ARG:HG2	1:F:109:PHE:HE2	1.84	0.43
3:D:142:CYS:CB	3:D:192:CYS:HG	2.29	0.43
1:F:71:GLN:HE21	1:F:71:GLN:CA	2.31	0.43
2:G:59:ASP:O	2:G:60:TRP:HB2	2.18	0.43
3:H:7:GLN:O	3:H:8:THR:HB	2.19	0.43
1:F:71:GLN:HG2	4:I:54:SER:HB2	2.00	0.43
1:F:137:HIS:O	1:F:141:GLN:HG2	2.19	0.43
3:H:168:VAL:O	4:I:174:CYS:SG	2.77	0.43
1:A:149:GLU:HG2	4:E:99:LEU:HD12	2.01	0.42
4:E:181:LYS:HE2	4:E:189:SER:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:LYS:HE3	1:F:173:LYS:HB2	1.45	0.42
3:H:152:ASN:O	3:H:200:ILE:HB	2.19	0.42
1:A:123:ASN:OD1	1:A:123:ASN:C	2.58	0.42
3:D:172:ARG:NH1	3:D:175:ASP:HA	2.33	0.42
2:G:7:ILE:HG12	2:G:82:VAL:HG11	2.02	0.42
2:B:41:LYS:HD3	2:B:78:TYR:OH	2.20	0.42
1:A:155:ASN:O	1:A:156:TRP:C	2.56	0.42
1:A:99:GLU:HB2	1:A:107:THR:OG1	2.19	0.41
1:A:173:LYS:HB2	1:A:173:LYS:HE3	1.87	0.41
1:A:198:LEU:HD12	1:A:214:TRP:CH2	2.55	0.41
1:A:198:LEU:HG	1:A:244:ILE:HG13	2.01	0.41
1:F:228:GLY:HA3	1:F:241:TRP:CE2	2.55	0.41
3:H:195:ALA:O	3:H:196:PHE:CB	2.68	0.41
4:I:146:LEU:H	4:I:146:LEU:HG	1.69	0.41
3:D:20:GLU:O	3:D:21:ALA:HB3	2.20	0.41
1:F:127:LEU:HD12	1:F:150:LEU:HB3	2.03	0.41
3:D:158:ASP:HB3	3:D:161:VAL:CG1	2.50	0.41
4:E:45:LEU:HD11	4:E:48:TYR:HB3	2.02	0.41
1:F:146:ASN:OD1	1:F:146:ASN:C	2.59	0.41
1:F:155:ASN:O	1:F:156:TRP:C	2.57	0.41
1:F:235:ASP:OD1	1:F:237:THR:HG22	2.20	0.41
3:H:157:LYS:N	3:H:157:LYS:HD3	2.36	0.41
1:F:46:ARG:NH2	2:G:53:ASP:OD2	2.31	0.41
3:D:22:GLU:HA	3:D:22:GLU:OE1	2.21	0.41
4:E:214:GLN:HG3	4:E:237:ILE:HG23	2.02	0.41
4:E:58:GLY:O	4:E:59:ASP:C	2.60	0.40
1:A:210:ILE:HD13	1:A:211:TYR:N	2.37	0.40
3:D:105:ALA:HB2	4:E:102:PHE:CZ	2.56	0.40
3:H:8:THR:CG2	3:H:31:ASP:HB3	2.52	0.40
3:D:128:VAL:HG12	3:D:192:CYS:HB3	2.02	0.40
2:G:40:LEU:O	2:G:78:TYR:HA	2.20	0.40
1:A:208:PRO:HG3	1:A:238:TYR:CD2	2.56	0.40
2:B:41:LYS:HG2	2:B:42:ASN:ND2	2.37	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	257/290 (89%)	243 (95%)	14 (5%)	0	100 100
1	F	260/290 (90%)	240 (92%)	20 (8%)	0	100 100
2	B	96/100 (96%)	93 (97%)	3 (3%)	0	100 100
2	G	96/100 (96%)	92 (96%)	4 (4%)	0	100 100
3	D	191/201 (95%)	176 (92%)	15 (8%)	0	100 100
3	H	192/201 (96%)	172 (90%)	20 (10%)	0	100 100
4	E	243/248 (98%)	224 (92%)	18 (7%)	1 (0%)	30 59
4	I	244/248 (98%)	231 (95%)	13 (5%)	0	100 100
All	All	1579/1678 (94%)	1471 (93%)	107 (7%)	1 (0%)	48 76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	39	PRO

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	234/255 (92%)	204 (87%)	30 (13%)	3 11
1	F	236/255 (92%)	194 (82%)	42 (18%)	1 4
2	B	93/95 (98%)	87 (94%)	6 (6%)	14 38
2	G	93/95 (98%)	81 (87%)	12 (13%)	3 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	174/181 (96%)	152 (87%)	22 (13%)	3 11
3	H	175/181 (97%)	150 (86%)	25 (14%)	2 8
4	E	216/218 (99%)	187 (87%)	29 (13%)	3 10
4	I	216/218 (99%)	194 (90%)	22 (10%)	6 18
All	All	1437/1498 (96%)	1249 (87%)	188 (13%)	3 10

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	14	ASP
1	A	17	HIS
1	A	46	ARG
1	A	57	ASP
1	A	66	LEU
1	A	77	LEU
1	A	78	LYS
1	A	79	ARG
1	A	82	ARG
1	A	95	MET
1	A	102	GLU
1	A	109	PHE
1	A	139	ILE
1	A	140	LYS
1	A	178	ARG
1	A	188	ARG
1	A	198	LEU
1	A	201	LYS
1	A	210	ILE
1	A	211	TYR
1	A	213	THR
1	A	215	MET
1	A	216	LYS
1	A	220	GLU
1	A	245	GLU
1	A	253	LEU
1	A	259	GLU
1	A	267	LEU
1	A	269	VAL
2	B	0	MET
2	B	4	THR

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Mol	Chain	Res	Type
2	B	44	GLU
2	B	58	LYS
2	B	70	PHE
2	B	74	GLU
3	D	9	VAL
3	D	15	GLU
3	D	16	MET
3	D	36	ASP
3	D	61	GLN
3	D	62	GLN
3	D	85	SER
3	D	94	MET
3	D	100	ARG
3	D	111	ASP
3	D	132	ARG
3	D	135	LYS
3	D	139	LYS
3	D	148	ASP
3	D	154	SER
3	D	157	LYS
3	D	164	THR
3	D	172	ARG
3	D	178	SER
3	D	180	SER
3	D	187	LYS
3	D	197	ASN
4	E	4	ILE
4	E	5	TYR
4	E	7	THR
4	E	9	ARG
4	E	21	LEU
4	E	25	GLN
4	E	38	ASP
4	E	45	LEU
4	E	57	LYS
4	E	59	ASP
4	E	61	SER
4	E	65	THR
4	E	67	SER
4	E	80	SER
4	E	84	SER
4	E	105	THR

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Mol	Chain	Res	Type
4	E	117	LEU
4	E	123	VAL
4	E	161	SER
4	E	167	LYS
4	E	183	GLN
4	E	186	LEU
4	E	187	ASN
4	E	196	ARG
4	E	199	VAL
4	E	222	GLU
4	E	228	GLN
4	E	230	ARG
4	E	247	ASP
1	F	0	MET
1	F	1	ARG
1	F	16	ILE
1	F	38	SER
1	F	46	ARG
1	F	57	ASP
1	F	61	ARG
1	F	77	LEU
1	F	78	LYS
1	F	79	ARG
1	F	80	LEU
1	F	89	SER
1	F	95	MET
1	F	107	THR
1	F	109	PHE
1	F	124	LYS
1	F	139	ILE
1	F	140	LYS
1	F	173	LYS
1	F	177	GLN
1	F	178	ARG
1	F	185	ARG
1	F	186	VAL
1	F	187	ASN
1	F	196	THR
1	F	203	HIS
1	F	209	GLU
1	F	213	THR
1	F	215	MET

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Mol	Chain	Res	Type
1	F	217	ASN
1	F	220	GLU
1	F	221	ILE
1	F	222	VAL
1	F	224	GLU
1	F	237	THR
1	F	244	ILE
1	F	245	GLU
1	F	246	LEU
1	F	253	LEU
1	F	261	SER
1	F	267	LEU
1	F	269	VAL
2	G	0	MET
2	G	1	ILE
2	G	4	THR
2	G	35	ILE
2	G	36	GLU
2	G	48	LYS
2	G	70	PHE
2	G	73	THR
2	G	81	ARG
2	G	82	VAL
2	G	85	VAL
2	G	86	THR
3	H	7	GLN
3	H	12	SER
3	H	15	GLU
3	H	57	GLU
3	H	60	LYS
3	H	68	ARG
3	H	74	GLN
3	H	78	LYS
3	H	85	SER
3	H	111	ASP
3	H	122	GLN
3	H	136	SER
3	H	137	SER
3	H	140	SER
3	H	148	ASP
3	H	157	LYS
3	H	164	THR

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Mol	Chain	Res	Type
3	H	165	ASP
3	H	169	LEU
3	H	172	ARG
3	H	174	MET
3	H	177	LYS
3	H	178	SER
3	H	180	SER
3	H	198	ASN
4	I	4	ILE
4	I	6	GLN
4	I	43	LEU
4	I	59	ASP
4	I	61	SER
4	I	62	SER
4	I	65	THR
4	I	72	GLU
4	I	82	ARG
4	I	84	SER
4	I	88	GLN
4	I	121	LYS
4	I	146	LEU
4	I	158	VAL
4	I	186	LEU
4	I	196	ARG
4	I	200	SER
4	I	223	ASN
4	I	227	THR
4	I	229	ASP
4	I	245	ARG
4	I	247	ASP

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

Mol	Chain	Res	Type
1	F	71	GLN

5.3.3 RNA

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, 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	263/290 (90%)	0.00	7 (2%) 56 48	46, 60, 103, 128	0
1	F	266/290 (91%)	-0.06	9 (3%) 48 40	46, 61, 105, 129	0
2	B	98/100 (98%)	-0.06	0 100 100	57, 73, 91, 95	0
2	G	98/100 (98%)	-0.33	0 100 100	49, 60, 76, 79	0
3	D	193/201 (96%)	-0.08	1 (0%) 87 83	44, 54, 85, 99	0
3	H	194/201 (96%)	-0.12	1 (0%) 87 83	46, 56, 70, 76	0
4	E	245/248 (98%)	-0.15	2 (0%) 82 77	41, 53, 76, 93	0
4	I	246/248 (99%)	-0.10	4 (1%) 70 63	49, 57, 78, 91	0
All	All	1603/1678 (95%)	-0.10	24 (1%) 71 65	41, 58, 90, 129	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	VAL	5.5
1	A	248	PRO	4.2
1	F	194	GLY	3.4
1	A	253	LEU	3.3
3	H	137	SER	3.0
4	E	41	MET	2.9
1	F	249	GLN	2.9
4	I	41	MET	2.9
1	F	253	LEU	2.8
1	F	17	HIS	2.7
1	F	195	VAL	2.7
1	A	251	SER	2.6
1	F	269	VAL	2.6
3	D	136	SER	2.6
4	I	178	GLN	2.4
4	E	5	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	246	LEU	2.3
1	F	60	GLU	2.2
1	A	195	VAL	2.2
1	A	95	MET	2.2
4	I	120	LEU	2.2
4	I	188	ASP	2.2
1	A	134	ASN	2.1
1	F	221	ILE	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.