Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2024 – 12:46 PM JST

PDB ID	:	8IF1
Title	:	Complex structure of HLA2402 with recognizing SARS-CoV-2 Y453F epitope NYNYLFRLF
Authors	:	Deng, S.S.; Jin, T.C.; Xu, Z.H.; Wang, M.H.
Deposited on	:	2023-02-16
Resolution	:	2.50 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:

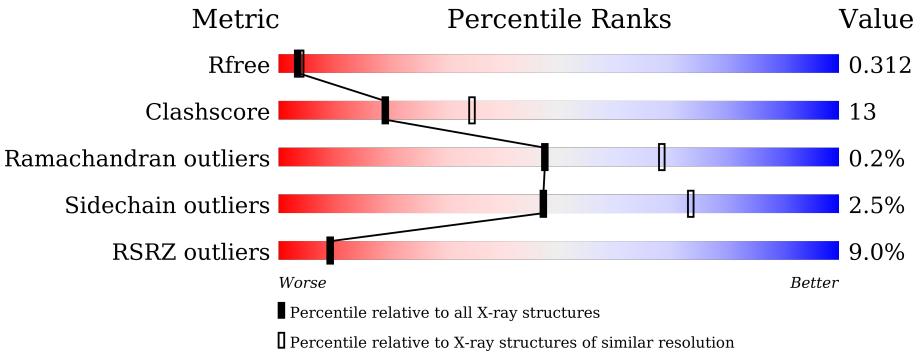
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	308	15% 68% 22% · 10%
1	C	308	6% 67% 23% · 10%
1	G	308	2% 69% 21% · 10%
2	B	101	14% 67% 28% · ·
2	D	101	13% 73% 24% ·
2	H	101	6% 79% 20% ·

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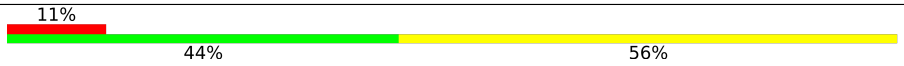
Mol	Chain	Length	Quality of chain
3	E	9	
3	F	9	
3	I	9	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9528 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2251	1399	407	435	10			
1	C	277	Total	C	N	O	S	0	0	0
			2242	1394	406	432	10			
1	G	277	Total	C	N	O	S	0	0	0
			2245	1396	406	433	10			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP D9UAY1
A	-3	ASN	-	expression tag	UNP D9UAY1
A	-2	SER	-	expression tag	UNP D9UAY1
A	-1	VAL	-	expression tag	UNP D9UAY1
A	0	ASP	-	expression tag	UNP D9UAY1
A	277	GLY	-	expression tag	UNP D9UAY1
A	278	SER	-	expression tag	UNP D9UAY1
A	279	GLY	-	expression tag	UNP D9UAY1
A	280	LEU	-	expression tag	UNP D9UAY1
A	281	ASN	-	expression tag	UNP D9UAY1
A	282	ASP	-	expression tag	UNP D9UAY1
A	283	ILE	-	expression tag	UNP D9UAY1
A	284	PHE	-	expression tag	UNP D9UAY1
A	285	GLU	-	expression tag	UNP D9UAY1
A	286	ALA	-	expression tag	UNP D9UAY1
A	287	GLN	-	expression tag	UNP D9UAY1
A	288	LYS	-	expression tag	UNP D9UAY1
A	289	ILE	-	expression tag	UNP D9UAY1
A	290	GLU	-	expression tag	UNP D9UAY1
A	291	TRP	-	expression tag	UNP D9UAY1
A	292	HIS	-	expression tag	UNP D9UAY1
A	293	ALA	-	expression tag	UNP D9UAY1
A	294	ALA	-	expression tag	UNP D9UAY1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	295	ALA	-	expression tag	UNP D9UAY1
A	296	LEU	-	expression tag	UNP D9UAY1
A	297	GLU	-	expression tag	UNP D9UAY1
A	298	HIS	-	expression tag	UNP D9UAY1
A	299	HIS	-	expression tag	UNP D9UAY1
A	300	HIS	-	expression tag	UNP D9UAY1
A	301	HIS	-	expression tag	UNP D9UAY1
A	302	HIS	-	expression tag	UNP D9UAY1
A	303	HIS	-	expression tag	UNP D9UAY1
C	-4	MET	-	initiating methionine	UNP D9UAY1
C	-3	ASN	-	expression tag	UNP D9UAY1
C	-2	SER	-	expression tag	UNP D9UAY1
C	-1	VAL	-	expression tag	UNP D9UAY1
C	0	ASP	-	expression tag	UNP D9UAY1
C	277	GLY	-	expression tag	UNP D9UAY1
C	278	SER	-	expression tag	UNP D9UAY1
C	279	GLY	-	expression tag	UNP D9UAY1
C	280	LEU	-	expression tag	UNP D9UAY1
C	281	ASN	-	expression tag	UNP D9UAY1
C	282	ASP	-	expression tag	UNP D9UAY1
C	283	ILE	-	expression tag	UNP D9UAY1
C	284	PHE	-	expression tag	UNP D9UAY1
C	285	GLU	-	expression tag	UNP D9UAY1
C	286	ALA	-	expression tag	UNP D9UAY1
C	287	GLN	-	expression tag	UNP D9UAY1
C	288	LYS	-	expression tag	UNP D9UAY1
C	289	ILE	-	expression tag	UNP D9UAY1
C	290	GLU	-	expression tag	UNP D9UAY1
C	291	TRP	-	expression tag	UNP D9UAY1
C	292	HIS	-	expression tag	UNP D9UAY1
C	293	ALA	-	expression tag	UNP D9UAY1
C	294	ALA	-	expression tag	UNP D9UAY1
C	295	ALA	-	expression tag	UNP D9UAY1
C	296	LEU	-	expression tag	UNP D9UAY1
C	297	GLU	-	expression tag	UNP D9UAY1
C	298	HIS	-	expression tag	UNP D9UAY1
C	299	HIS	-	expression tag	UNP D9UAY1
C	300	HIS	-	expression tag	UNP D9UAY1
C	301	HIS	-	expression tag	UNP D9UAY1
C	302	HIS	-	expression tag	UNP D9UAY1
C	303	HIS	-	expression tag	UNP D9UAY1
G	-4	MET	-	initiating methionine	UNP D9UAY1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	ASN	-	expression tag	UNP D9UAY1
G	-2	SER	-	expression tag	UNP D9UAY1
G	-1	VAL	-	expression tag	UNP D9UAY1
G	0	ASP	-	expression tag	UNP D9UAY1
G	277	GLY	-	expression tag	UNP D9UAY1
G	278	SER	-	expression tag	UNP D9UAY1
G	279	GLY	-	expression tag	UNP D9UAY1
G	280	LEU	-	expression tag	UNP D9UAY1
G	281	ASN	-	expression tag	UNP D9UAY1
G	282	ASP	-	expression tag	UNP D9UAY1
G	283	ILE	-	expression tag	UNP D9UAY1
G	284	PHE	-	expression tag	UNP D9UAY1
G	285	GLU	-	expression tag	UNP D9UAY1
G	286	ALA	-	expression tag	UNP D9UAY1
G	287	GLN	-	expression tag	UNP D9UAY1
G	288	LYS	-	expression tag	UNP D9UAY1
G	289	ILE	-	expression tag	UNP D9UAY1
G	290	GLU	-	expression tag	UNP D9UAY1
G	291	TRP	-	expression tag	UNP D9UAY1
G	292	HIS	-	expression tag	UNP D9UAY1
G	293	ALA	-	expression tag	UNP D9UAY1
G	294	ALA	-	expression tag	UNP D9UAY1
G	295	ALA	-	expression tag	UNP D9UAY1
G	296	LEU	-	expression tag	UNP D9UAY1
G	297	GLU	-	expression tag	UNP D9UAY1
G	298	HIS	-	expression tag	UNP D9UAY1
G	299	HIS	-	expression tag	UNP D9UAY1
G	300	HIS	-	expression tag	UNP D9UAY1
G	301	HIS	-	expression tag	UNP D9UAY1
G	302	HIS	-	expression tag	UNP D9UAY1
G	303	HIS	-	expression tag	UNP D9UAY1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	D	101	Total	C	N	O	S	0	0	0
			845	537	142	162	4			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ASP	-	expression tag	UNP P61769
B	0	MET	-	expression tag	UNP P61769
D	-1	ASP	-	expression tag	UNP P61769
D	0	MET	-	expression tag	UNP P61769
H	-1	ASP	-	expression tag	UNP P61769
H	0	MET	-	expression tag	UNP P61769

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	9	Total C N O 89 62 14 13	0	0	0
3	F	9	Total C N O 89 62 14 13	0	0	0
3	I	9	Total C N O 89 62 14 13	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	6	PHE	TYR	engineered mutation	UNP P0DTC2
F	6	PHE	TYR	engineered mutation	UNP P0DTC2
I	6	PHE	TYR	engineered mutation	UNP P0DTC2

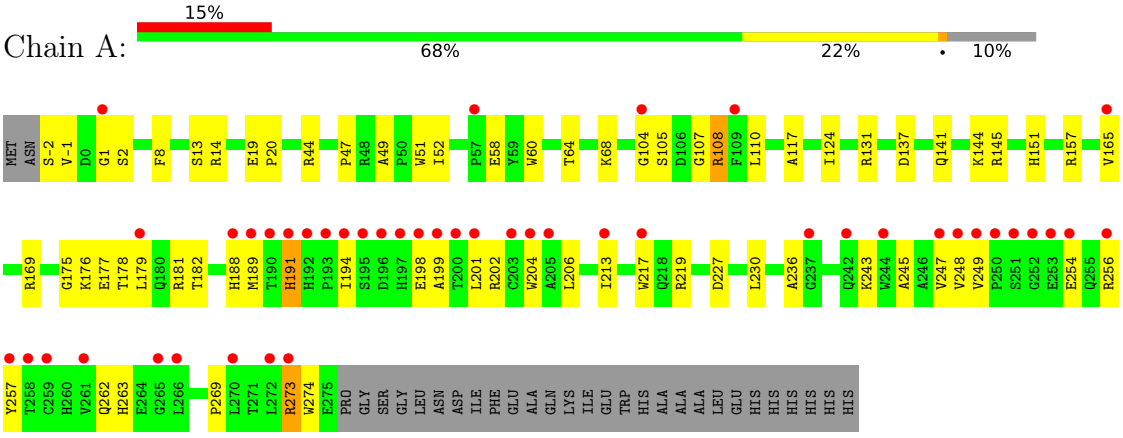
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	2	Total O 2 2	0	0
4	H	1	Total O 1 1	0	0

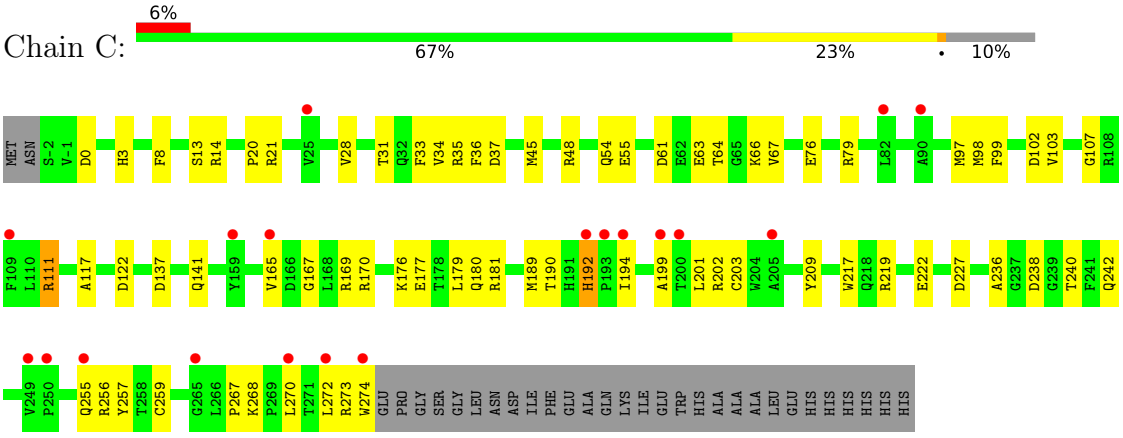
3 Residue-property plots (i)

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.

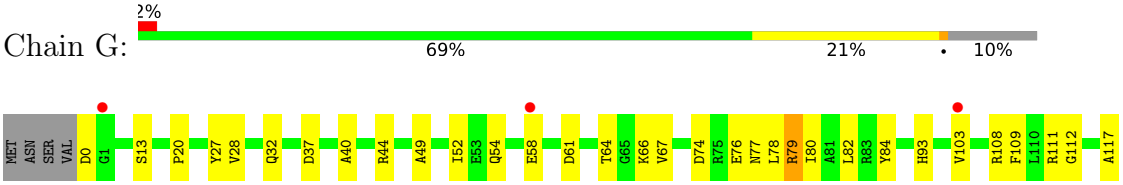
• Molecule 1: MHC class I antigen

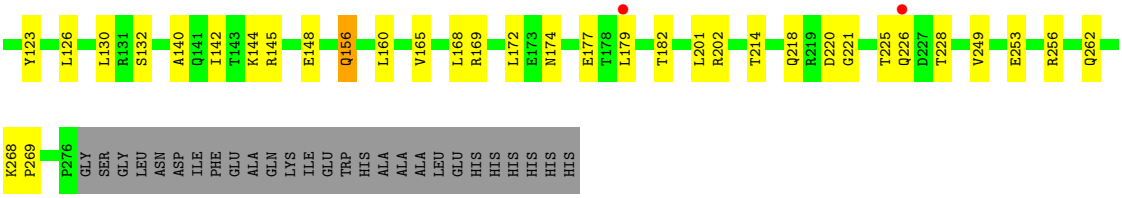


• Molecule 1: MHC class I antigen

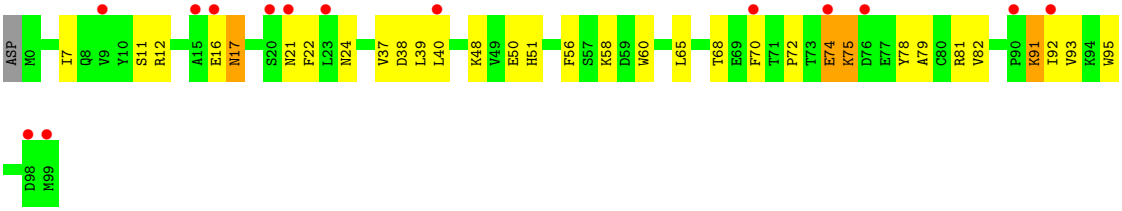


• Molecule 1: MHC class I antigen

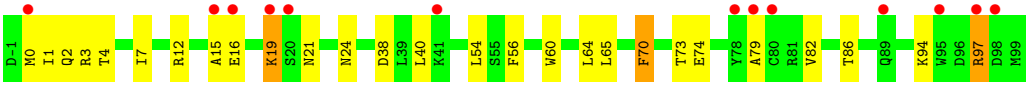




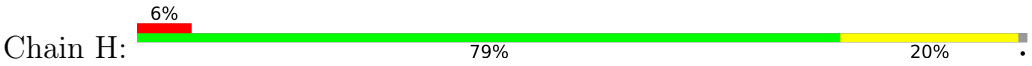
• Molecule 2: Beta-2-microglobulin

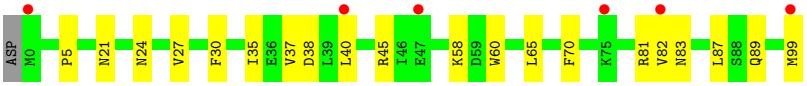


• Molecule 2: Beta-2-microglobulin

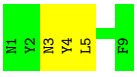


• Molecule 2: Beta-2-microglobulin

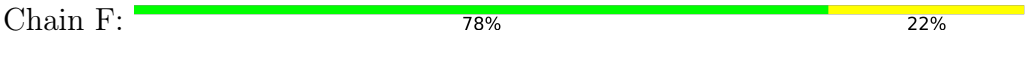


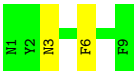


• Molecule 3: Spike protein S1

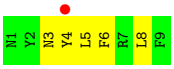


• Molecule 3: Spike protein S1





• Molecule 3: Spike protein S1


N1
Y2
M3
Y4
L5
F6
R7
L8
F9

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	47.05Å 167.49Å 168.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.32 – 2.50 46.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.32-2.50) 91.8 (46.66-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.78 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.251 , 0.309 0.253 , 0.312	Depositor DCC
R_{free} test set	2006 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å^2)	54.2	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9528	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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	0.30	0/2311	0.54	0/3133
1	C	0.28	0/2302	0.48	0/3121
1	G	0.28	0/2306	0.49	0/3127
2	B	0.29	0/860	0.49	0/1162
2	D	0.33	0/868	0.55	0/1173
2	H	0.28	0/860	0.52	0/1162
3	E	0.34	0/92	0.43	0/123
3	F	0.29	0/92	0.37	0/123
3	I	0.27	0/92	0.37	0/123
All	All	0.29	0/9783	0.51	0/13247

There are no bond length outliers.

There are no bond angle outliers.

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	2251	0	2106	66	0
1	C	2242	0	2100	60	0
1	G	2245	0	2099	48	0
2	B	837	0	803	31	0
2	D	845	0	807	29	0
2	H	837	0	803	14	0
3	E	89	0	85	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	89	0	85	2	0
3	I	89	0	85	6	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	H	1	0	0	0	0
All	All	9528	0	8973	240	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 13.

All (240) 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:16:GLU:CG	2:D:19:LYS:HE2	1.36	1.53
2:D:16:GLU:HG3	2:D:19:LYS:CE	1.59	1.30
2:D:16:GLU:HB2	2:D:19:LYS:CE	1.67	1.22
2:D:16:GLU:CB	2:D:19:LYS:CE	2.27	1.13
2:D:16:GLU:CG	2:D:19:LYS:CE	2.20	1.12
2:D:16:GLU:CB	2:D:19:LYS:HE3	1.80	1.11
2:B:16:GLU:O	2:B:17:ASN:HB2	1.51	1.09
1:G:142:ILE:HG22	1:G:145:ARG:HH12	1.24	0.98
2:D:16:GLU:HB2	2:D:19:LYS:HE3	0.98	0.96
1:A:191:HIS:HE1	1:A:199:ALA:HB1	1.31	0.93
2:D:16:GLU:CB	2:D:19:LYS:HE2	1.93	0.93
2:B:48:LYS:NZ	2:B:50:GLU:HG3	1.92	0.85
1:C:45:MET:H	1:C:64:THR:HG22	1.44	0.83
1:A:191:HIS:CE1	1:A:199:ALA:HB1	2.13	0.83
2:D:15:ALA:HB3	2:D:97:ARG:HG3	1.62	0.81
2:B:16:GLU:O	2:B:17:ASN:CB	2.30	0.79
1:G:74:ASP:HA	1:G:77:ASN:HB2	1.67	0.77
1:G:84:TYR:CE1	1:G:142:ILE:HD11	2.20	0.77
2:B:79:ALA:HB1	2:B:92:ILE:HD11	1.68	0.76
2:B:48:LYS:HZ1	2:B:50:GLU:HG3	1.50	0.75
2:B:12:ARG:HD3	2:B:22:PHE:HB2	1.69	0.75
2:B:91:LYS:HE3	2:B:93:VAL:HG23	1.70	0.73
1:A:175:GLY:O	1:A:179:LEU:N	2.20	0.72
2:H:37:VAL:HG22	2:H:82:VAL:HG22	1.71	0.72
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.71	0.70
1:G:54:GLN:OE1	1:G:174:ASN:ND2	2.22	0.68
1:C:33:PHE:CD2	1:C:34:VAL:HG23	2.32	0.65
2:H:83:ASN:HA	2:H:87:LEU:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:ILE:HG22	1:G:145:ARG:NH1	2.05	0.65
1:C:177:GLU:OE2	1:C:177:GLU:N	2.24	0.65
1:A:217:TRP:HE1	1:A:245:ALA:HB3	1.63	0.64
1:C:76:GLU:OE2	1:C:79:ARG:NH2	2.32	0.63
1:C:102:ASP:OD2	1:C:111:ARG:NH1	2.31	0.63
2:B:12:ARG:HB2	2:B:22:PHE:HB2	1.80	0.62
2:D:4:THR:HG22	2:D:86:THR:HB	1.80	0.62
1:A:247:VAL:HG13	1:A:249:VAL:HG13	1.81	0.62
1:A:64:THR:HG22	1:A:68:LYS:HE2	1.82	0.62
1:C:13:SER:HA	1:C:20:PRO:HB3	1.81	0.62
1:G:144:LYS:NZ	1:G:148:GLU:OE2	2.34	0.61
2:H:38:ASP:OD2	2:H:45:ARG:CZ	2.49	0.61
1:A:189:MET:SD	1:A:201:LEU:HD21	2.41	0.61
2:D:16:GLU:HG3	2:D:19:LYS:HE2	0.64	0.60
1:A:202:ARG:HD2	1:A:204:TRP:NE1	2.16	0.60
2:D:16:GLU:HB2	2:D:19:LYS:HG3	1.82	0.59
2:D:21:ASN:HB3	2:D:70:PHE:CE1	2.38	0.59
1:A:213:ILE:HD12	1:A:263:HIS:HB2	1.85	0.58
2:B:48:LYS:HZ3	2:B:50:GLU:HG3	1.67	0.58
1:A:-2:SER:OG	1:A:-1:VAL:N	2.25	0.57
1:A:107:GLY:O	1:A:169:ARG:NH2	2.30	0.57
1:A:227:ASP:HB3	1:A:247:VAL:HG23	1.86	0.57
1:G:66:LYS:HE3	3:I:4:TYR:HA	1.84	0.57
1:G:13:SER:HA	1:G:20:PRO:HB3	1.85	0.57
1:G:58:GLU:HA	1:G:61:ASP:HB2	1.85	0.57
1:A:227:ASP:HB3	1:A:247:VAL:CG2	2.35	0.57
2:B:7:ILE:HD13	2:B:91:LYS:HE2	1.87	0.57
1:G:165:VAL:O	1:G:169:ARG:HG3	2.05	0.57
1:A:262:GLN:NE2	1:A:269:PRO:HG3	2.20	0.57
1:G:156:GLN:HA	1:G:156:GLN:NE2	2.19	0.57
1:G:202:ARG:HH12	2:H:99:MET:HG2	1.70	0.56
1:A:108:ARG:H	1:A:108:ARG:HD2	1.70	0.56
2:H:27:VAL:HG11	2:H:35:ILE:HD13	1.87	0.56
1:A:189:MET:CE	1:A:273:ARG:HA	2.34	0.56
1:A:201:LEU:HD12	1:A:254:GLU:HG2	1.88	0.56
1:C:165:VAL:O	1:C:169:ARG:HG3	2.06	0.56
1:C:35:ARG:HB3	1:C:48:ARG:HD2	1.87	0.56
1:G:79:ARG:HA	1:G:82:LEU:HD13	1.88	0.56
1:A:182:THR:O	1:A:182:THR:OG1	2.17	0.56
1:A:256:ARG:HE	1:A:257:TYR:HE1	1.53	0.56
2:H:58:LYS:H	2:H:58:LYS:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ALA:HB3	1:A:249:VAL:HG23	1.88	0.55
1:A:13:SER:HA	1:A:20:PRO:HB3	1.89	0.55
1:C:217:TRP:CH2	1:C:259:CYS:HB2	2.42	0.55
2:B:17:ASN:O	2:B:72:PRO:O	2.25	0.55
1:C:270:LEU:HD12	1:C:272:LEU:HD11	1.88	0.55
1:C:270:LEU:CD1	1:C:272:LEU:HD11	2.38	0.54
2:H:24:ASN:HB3	2:H:65:LEU:HD11	1.88	0.54
1:A:178:THR:HA	1:A:181:ARG:HG3	1.88	0.54
1:C:189:MET:HE3	1:C:201:LEU:HD21	1.88	0.54
1:A:274:TRP:HA	1:A:274:TRP:CE3	2.42	0.53
1:A:230:LEU:HG	1:A:243:LYS:HE3	1.91	0.53
1:C:176:LYS:HD2	1:C:180:GLN:HB2	1.90	0.53
2:B:11:SER:HB3	2:B:21:ASN:ND2	2.24	0.53
1:C:35:ARG:HG2	1:C:36:PHE:N	2.24	0.53
1:G:78:LEU:HD21	1:G:93:HIS:HB2	1.91	0.53
3:I:5:LEU:C	3:I:5:LEU:HD13	2.28	0.53
1:A:194:ILE:HG21	1:A:198:GLU:HB2	1.90	0.53
1:C:45:MET:H	1:C:64:THR:CG2	2.17	0.53
1:A:2:SER:HA	1:A:104:GLY:HA2	1.91	0.52
2:B:79:ALA:CB	2:B:92:ILE:HD11	2.39	0.52
1:G:28:VAL:HG11	1:G:179:LEU:HD13	1.90	0.52
1:A:191:HIS:NE2	1:A:254:GLU:OE2	2.41	0.52
1:A:165:VAL:O	1:A:169:ARG:HG2	2.10	0.52
1:C:219:ARG:HD2	1:C:257:TYR:OH	2.10	0.52
1:A:58:GLU:N	1:A:58:GLU:OE2	2.41	0.51
1:C:21:ARG:HH21	1:C:37:ASP:CG	2.12	0.51
1:A:201:LEU:HD22	1:A:217:TRP:HH2	1.75	0.51
1:C:255:GLN:OE1	1:C:255:GLN:N	2.41	0.51
1:C:28:VAL:HG11	1:C:179:LEU:HD13	1.92	0.51
1:C:194:ILE:H	1:C:199:ALA:HA	1.75	0.51
1:C:203:CYS:HB2	1:C:217:TRP:CZ2	2.45	0.51
2:B:70:PHE:CD2	2:B:78:TYR:HE2	2.29	0.51
2:D:15:ALA:CB	2:D:97:ARG:HG3	2.34	0.51
2:D:54:LEU:HA	2:D:64:LEU:HD21	1.93	0.51
1:G:64:THR:HA	1:G:67:VAL:HG12	1.93	0.51
1:A:1:GLY:HA3	1:A:105:SER:HB3	1.92	0.51
1:G:103:VAL:HG13	1:G:168:LEU:HD23	1.93	0.51
1:A:124:ILE:HD11	1:A:144:LYS:HB2	1.92	0.51
3:F:3:ASN:HB3	3:F:6:PHE:CZ	2.46	0.51
1:A:-2:SER:HG	1:A:-1:VAL:H	1.56	0.50
1:C:21:ARG:NH2	1:C:37:ASP:OD2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:HD22	1:A:217:TRP:CH2	2.47	0.50
1:G:168:LEU:O	1:G:172:LEU:HG	2.12	0.50
1:C:35:ARG:HH21	1:C:48:ARG:CZ	2.23	0.50
2:D:21:ASN:N	2:D:70:PHE:O	2.32	0.50
2:H:27:VAL:HG12	2:H:30:PHE:CE1	2.47	0.50
1:C:63:GLU:O	1:C:67:VAL:HG12	2.12	0.50
1:G:177:GLU:OE1	1:G:177:GLU:N	2.33	0.50
1:G:0:ASP:OD1	1:G:0:ASP:N	2.45	0.49
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.47	0.49
1:C:270:LEU:HD12	1:C:272:LEU:CD1	2.42	0.49
2:D:16:GLU:CB	2:D:19:LYS:HG3	2.42	0.49
1:C:267:PRO:HB2	1:C:268:LYS:HD2	1.94	0.49
1:C:8:PHE:HB3	2:D:56:PHE:CE2	2.48	0.49
2:B:12:ARG:HD3	2:B:22:PHE:CB	2.42	0.49
1:A:236:ALA:O	2:B:24:ASN:ND2	2.42	0.48
2:H:38:ASP:OD2	2:H:45:ARG:NH1	2.47	0.48
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.49	0.48
1:A:194:ILE:CG2	1:A:198:GLU:HB2	2.44	0.48
2:B:40:LEU:HD21	2:B:92:ILE:HD13	1.95	0.48
2:D:24:ASN:HB3	2:D:65:LEU:HD21	1.95	0.48
1:C:267:PRO:C	1:C:268:LYS:HD2	2.35	0.47
1:A:137:ASP:O	1:A:141:GLN:HG2	2.13	0.47
1:A:104:GLY:N	1:A:110:LEU:CD2	2.78	0.47
1:C:219:ARG:HH21	1:C:256:ARG:HH22	1.62	0.47
1:C:219:ARG:HB2	1:C:257:TYR:CE2	2.48	0.47
1:C:219:ARG:HD2	1:C:257:TYR:CZ	2.50	0.47
1:A:217:TRP:HE1	1:A:245:ALA:CB	2.27	0.47
2:B:70:PHE:HE2	2:B:72:PRO:HB3	1.79	0.47
1:A:108:ARG:O	1:A:110:LEU:HD22	2.15	0.47
1:C:61:ASP:O	1:C:64:THR:OG1	2.31	0.47
1:A:151:HIS:CE1	1:C:222:GLU:HB3	2.50	0.47
1:C:189:MET:CE	1:C:201:LEU:HD21	2.44	0.47
1:A:14:ARG:NH1	1:A:19:GLU:O	2.49	0.46
1:C:242:GLN:NE2	2:D:12:ARG:O	2.48	0.46
1:G:80:ILE:HG22	1:G:84:TYR:CE2	2.51	0.46
1:G:202:ARG:NH1	2:H:99:MET:HG2	2.29	0.46
1:G:214:THR:OG1	1:G:262:GLN:HB2	2.15	0.46
1:G:220:ASP:OD2	1:G:256:ARG:NH2	2.47	0.46
1:G:225:THR:HA	1:G:228:THR:HG22	1.97	0.46
1:G:268:LYS:HE3	1:G:269:PRO:HD2	1.98	0.46
1:G:126:LEU:HD12	1:G:132:SER:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ARG:NE	1:C:48:ARG:HD2	2.31	0.46
1:C:238:ASP:OD1	1:C:240:THR:HG22	2.15	0.46
2:B:39:LEU:HD12	2:B:68:THR:HG22	1.98	0.45
1:G:253:GLU:OE2	1:G:256:ARG:NH1	2.49	0.45
2:B:11:SER:HB3	2:B:21:ASN:HD21	1.81	0.45
1:C:236:ALA:HB1	2:D:12:ARG:HG3	1.97	0.45
1:G:44:ARG:HA	1:G:64:THR:HG21	1.99	0.45
1:A:49:ALA:O	1:A:52:ILE:HG22	2.16	0.45
2:D:1:ILE:O	2:D:3:ARG:HG2	2.16	0.45
1:G:66:LYS:HZ2	3:I:6:PHE:HE1	1.63	0.45
1:G:156:GLN:OE1	3:I:3:ASN:ND2	2.33	0.45
2:B:51:HIS:HA	2:B:65:LEU:O	2.17	0.45
2:D:73:THR:HG22	2:D:74:GLU:H	1.81	0.45
1:A:44:ARG:HA	1:A:64:THR:HG23	1.99	0.45
3:E:5:LEU:HD23	3:E:5:LEU:HA	1.82	0.45
1:C:0:ASP:OD1	1:C:0:ASP:N	2.49	0.45
2:H:87:LEU:HD13	2:H:89:GLN:O	2.17	0.45
1:C:45:MET:SD	1:C:67:VAL:HG11	2.56	0.45
1:C:122:ASP:OD1	2:D:60:TRP:NE1	2.41	0.45
3:E:3:ASN:OD1	3:E:4:TYR:N	2.49	0.45
1:G:123:TYR:CZ	1:G:140:ALA:HA	2.52	0.44
1:G:156:GLN:NE2	1:G:156:GLN:CA	2.80	0.44
1:A:249:VAL:HG12	1:A:257:TYR:CE1	2.53	0.44
1:C:35:ARG:NH2	1:C:48:ARG:NE	2.64	0.44
1:A:131:ARG:HG2	1:A:157:ARG:NH1	2.33	0.44
1:A:51:TRP:CD1	1:A:178:THR:HG21	2.52	0.44
2:B:38:ASP:HB2	2:B:81:ARG:HG3	2.00	0.44
1:A:51:TRP:HD1	1:A:178:THR:HG21	1.83	0.44
1:C:31:THR:HG23	1:C:209:TYR:CE2	2.52	0.44
1:G:27:TYR:CE2	1:G:32:GLN:HB2	2.53	0.44
1:G:37:ASP:HB3	1:G:40:ALA:HB2	2.00	0.44
1:A:189:MET:HE3	1:A:273:ARG:HA	1.99	0.44
2:B:37:VAL:HG22	2:B:82:VAL:HG12	2.00	0.44
2:B:40:LEU:HD11	2:B:79:ALA:HB3	1.99	0.44
1:A:227:ASP:OD1	1:A:248:VAL:HG22	2.18	0.43
1:C:66:LYS:HE2	1:C:66:LYS:HB2	1.81	0.43
2:D:64:LEU:HD23	2:D:64:LEU:HA	1.76	0.43
1:C:45:MET:N	1:C:64:THR:HG22	2.24	0.43
1:C:55:GLU:CD	1:C:170:ARG:HH12	2.21	0.43
1:G:77:ASN:OD1	3:I:8:LEU:HA	2.18	0.43
1:A:256:ARG:NE	1:A:257:TYR:HE1	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:THR:HB	1:C:202:ARG:HB3	1.99	0.43
1:A:141:GLN:O	1:A:145:ARG:HG3	2.18	0.43
1:A:204:TRP:CE3	1:A:206:LEU:HD11	2.53	0.43
1:A:202:ARG:HD2	1:A:204:TRP:HE1	1.80	0.43
1:A:274:TRP:HA	1:A:274:TRP:HE3	1.81	0.43
1:C:3:HIS:HB2	1:C:103:VAL:HG12	2.01	0.43
1:G:76:GLU:O	1:G:80:ILE:HG13	2.19	0.43
1:C:273:ARG:HG2	1:C:274:TRP:H	1.84	0.43
1:G:49:ALA:O	1:G:52:ILE:HG22	2.19	0.42
1:C:35:ARG:NH2	1:C:48:ARG:CZ	2.82	0.42
1:G:109:PHE:CZ	1:G:130:LEU:HD11	2.54	0.42
1:A:199:ALA:O	1:A:248:VAL:HA	2.19	0.42
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.54	0.42
1:G:109:PHE:HZ	1:G:130:LEU:HD11	1.83	0.42
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.54	0.42
1:A:201:LEU:HD12	1:A:254:GLU:CG	2.50	0.42
1:A:8:PHE:HB3	2:B:56:PHE:CE2	2.55	0.42
1:G:66:LYS:HA	1:G:66:LYS:HD2	1.67	0.42
2:H:40:LEU:HD11	2:H:81:ARG:HB2	2.01	0.42
1:C:34:VAL:CG1	1:C:45:MET:HG3	2.50	0.41
1:C:167:GLY:HA2	1:C:170:ARG:HG2	2.02	0.41
1:G:182:THR:O	1:G:182:THR:OG1	2.33	0.41
1:A:104:GLY:N	1:A:110:LEU:HD23	2.35	0.41
1:C:99:PHE:CE2	3:F:3:ASN:HB2	2.55	0.41
2:B:78:TYR:HB2	2:B:95:TRP:CE3	2.56	0.41
1:C:137:ASP:O	1:C:141:GLN:HG3	2.21	0.41
1:G:112:GLY:HA3	1:G:160:LEU:HD13	2.03	0.41
1:G:218:GLN:HE21	1:G:221:GLY:C	2.23	0.41
1:A:52:ILE:HG13	1:A:52:ILE:O	2.21	0.41
2:B:38:ASP:HB2	2:B:81:ARG:CG	2.51	0.41
1:C:107:GLY:O	1:C:169:ARG:HD2	2.20	0.41
1:C:192:HIS:ND1	1:C:192:HIS:C	2.74	0.41
1:G:44:ARG:HA	1:G:64:THR:CG2	2.51	0.41
1:G:201:LEU:HD12	1:G:249:VAL:HG11	2.03	0.41
2:D:38:ASP:HB3	2:D:40:LEU:HD21	2.03	0.41
1:G:66:LYS:HE3	3:I:4:TYR:CA	2.50	0.40
1:A:227:ASP:O	1:A:247:VAL:HA	2.20	0.40
2:B:74:GLU:C	2:B:75:LYS:HD2	2.42	0.40
1:C:97:MET:HG2	1:C:98:MET:N	2.37	0.40
1:A:176:LYS:HG3	1:A:177:GLU:N	2.37	0.40
2:D:7:ILE:HD11	2:D:82:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:PRO:HB3	2:H:30:PHE:HB3	2.03	0.40
1:A:47:PRO:HB3	1:A:60:TRP:CH2	2.56	0.40
1:A:108:ARG:HD2	1:A:108:ARG:N	2.36	0.40
1:A:201:LEU:HD23	1:A:202:ARG:N	2.37	0.40
1:C:14:ARG:CZ	1:C:21:ARG:HB2	2.51	0.40
1:C:255:GLN:O	1:C:273:ARG:NH1	2.51	0.40
2:D:79:ALA:HA	2:D:94:LYS:HA	2.03	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	276/308 (90%)	261 (95%)	15 (5%)	0	100	100
1	C	275/308 (89%)	265 (96%)	10 (4%)	0	100	100
1	G	275/308 (89%)	270 (98%)	5 (2%)	0	100	100
2	B	98/101 (97%)	97 (99%)	0	1 (1%)	15	28
2	D	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	28
2	H	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
3	E	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
3	I	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1142/1254 (91%)	1103 (97%)	37 (3%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	ASN
2	D	2	GLN

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	234/258 (91%)	229 (98%)	5 (2%)	53 78
1	C	233/258 (90%)	228 (98%)	5 (2%)	53 78
1	G	233/258 (90%)	228 (98%)	5 (2%)	53 78
2	B	95/96 (99%)	91 (96%)	4 (4%)	30 54
2	D	96/96 (100%)	92 (96%)	4 (4%)	30 54
2	H	95/96 (99%)	93 (98%)	2 (2%)	53 78
3	E	9/9 (100%)	9 (100%)	0	100 100
3	F	9/9 (100%)	9 (100%)	0	100 100
3	I	9/9 (100%)	9 (100%)	0	100 100
All	All	1013/1089 (93%)	988 (98%)	25 (2%)	47 73

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	188	HIS
1	A	191	HIS
1	A	219	ARG
1	A	273	ARG
2	B	58	LYS
2	B	74	GLU
2	B	75	LYS
2	B	91	LYS
1	C	54	GLN
1	C	111	ARG
1	C	181	ARG
1	C	192	HIS
1	C	227	ASP
2	D	0	MET
2	D	19	LYS
2	D	70	PHE
2	D	97	ARG

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Mol	Chain	Res	Type
1	G	79	ARG
1	G	108	ARG
1	G	111	ARG
1	G	156	GLN
1	G	226	GLN
2	H	21	ASN
2	H	70	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	278/308 (90%)	0.96	46 (16%) 1 1	36, 70, 152, 238	0
1	C	277/308 (89%)	0.76	19 (6%) 16 17	57, 83, 120, 145	0
1	G	277/308 (89%)	0.36	5 (1%) 68 71	52, 78, 105, 131	0
2	B	100/101 (99%)	0.84	14 (14%) 2 2	41, 80, 137, 161	0
2	D	101/101 (100%)	0.92	13 (12%) 3 3	64, 99, 138, 157	0
2	H	100/101 (99%)	0.62	6 (6%) 21 22	57, 83, 116, 125	0
3	E	9/9 (100%)	0.24	0 100 100	43, 53, 64, 72	0
3	F	9/9 (100%)	0.84	0 100 100	64, 81, 87, 104	0
3	I	9/9 (100%)	0.79	1 (11%) 5 5	73, 87, 101, 102	0
All	All	1160/1254 (92%)	0.72	104 (8%) 9 9	36, 81, 129, 238	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	GLU	12.6
1	A	249	VAL	9.4
1	A	199	ALA	8.3
1	A	266	LEU	6.6
1	A	265	GLY	6.4
1	A	196	ASP	5.8
1	A	200	THR	5.7
1	C	194	ILE	5.6
1	A	192	HIS	5.1
1	A	256	ARG	4.7
1	A	195	SER	4.7
1	A	248	VAL	4.7
1	A	201	LEU	4.7
2	B	99	MET	4.6
1	C	199	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	191	HIS	4.4
1	A	252	GLY	4.3
1	A	204	TRP	4.3
1	A	194	ILE	4.2
1	A	193	PRO	3.9
1	A	250	PRO	3.9
1	C	249	VAL	3.8
2	D	20	SER	3.8
1	C	200	THR	3.7
1	C	250	PRO	3.7
1	A	217	TRP	3.7
1	A	270	LEU	3.7
1	C	270	LEU	3.6
2	D	15	ALA	3.6
1	C	272	LEU	3.5
1	C	274	TRP	3.5
2	D	16	GLU	3.5
1	A	203	CYS	3.4
1	A	188	HIS	3.4
2	D	95	TRP	3.4
1	G	1	GLY	3.2
1	A	257	TYR	3.1
1	A	179	LEU	3.1
1	A	205	ALA	3.1
1	A	57	PRO	3.1
1	A	247	VAL	3.0
1	A	104	GLY	3.0
2	D	89	GLN	2.9
1	C	109	PHE	2.9
2	B	74	GLU	2.9
1	G	179	LEU	2.8
2	B	15	ALA	2.8
1	A	261	VAL	2.8
2	B	98	ASP	2.8
1	A	272	LEU	2.7
2	H	99	MET	2.7
2	B	9	VAL	2.7
2	H	40	LEU	2.6
1	A	197	HIS	2.5
1	C	265	GLY	2.5
1	A	251	SER	2.5
1	A	244	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	165	VAL	2.5
1	A	273	ARG	2.4
2	B	40	LEU	2.4
1	A	253	GLU	2.4
2	B	16	GLU	2.4
2	B	21	ASN	2.4
2	B	23	LEU	2.4
3	I	4	TYR	2.3
1	G	103	VAL	2.3
2	D	19	LYS	2.3
1	A	189	MET	2.3
2	D	0	MET	2.3
1	C	193	PRO	2.3
2	D	78	TYR	2.3
2	H	75	LYS	2.2
1	C	255	GLN	2.2
1	A	258	THR	2.2
1	C	25	VAL	2.2
1	C	90	ALA	2.2
2	D	97	ARG	2.2
1	A	1	GLY	2.2
2	B	90	PRO	2.2
1	C	192	HIS	2.1
2	H	0	MET	2.1
1	G	226	GLN	2.1
1	A	198	GLU	2.1
1	G	58	GLU	2.1
1	A	259	CYS	2.1
2	D	80	CYS	2.1
2	H	82	VAL	2.1
2	B	20	SER	2.1
2	D	79	ALA	2.1
1	A	165	VAL	2.1
2	D	41	LYS	2.1
1	C	159	TYR	2.1
2	B	92	ILE	2.1
2	B	76	ASP	2.0
2	D	98	ASP	2.0
1	A	213	ILE	2.0
2	H	47	GLU	2.0
1	A	190	THR	2.0
1	A	237	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	109	PHE	2.0
1	C	205	ALA	2.0
1	C	82	LEU	2.0
2	B	70	PHE	2.0
1	A	242	GLN	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 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.