Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2023 – 06:15 AM EDT

PDB ID	:	5DCX
Title	:	Structural studies of AAV2 Rep68 reveal a partially structured linker and compact domain conformation
Authors	:	Musayev, F.N.; Zarate-Perez, F.
Deposited on	:	2015-08-24
Resolution	:	2.60 Å(reported)

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

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

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

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

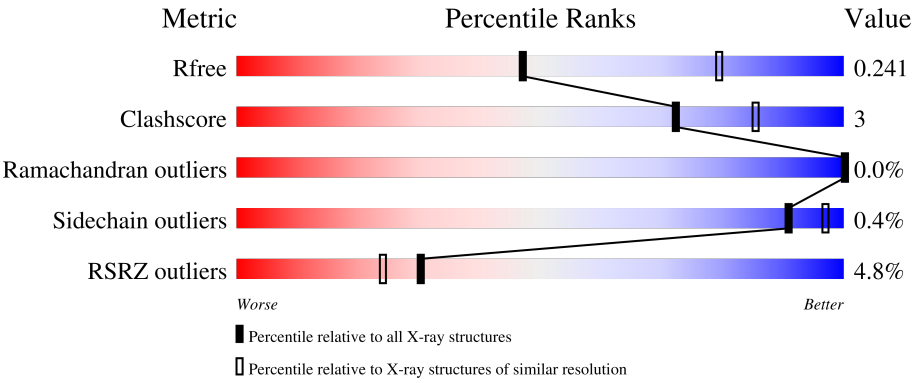
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	227	4% 83% 9% 8%
1	B	227	2% 80% 10% 10%
1	C	227	81% 8% 11%
1	D	227	% 82% 7% 11%
1	E	227	4% 80% 6% 14%

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Mol	Chain	Length	Quality of chain
1	F	227	% 77% 6% 17%
1	G	227	3% 81% 8% 11%
1	H	227	14% 82% 7% 11%
1	I	227	4% 74% 9% 17%
1	J	227	5% 70% 11% 19%
1	K	227	10% 72% 11% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	B	301	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17626 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 Protein Rep68.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1698	1091	288	314	5			
1	B	205	Total	C	N	O	S	0	0	0
			1675	1076	284	310	5			
1	C	202	Total	C	N	O	S	0	0	0
			1622	1046	272	298	6			
1	D	202	Total	C	N	O	S	0	0	0
			1643	1057	276	305	5			
1	E	195	Total	C	N	O	S	0	0	0
			1594	1030	267	291	6			
1	F	188	Total	C	N	O	S	0	0	0
			1524	988	252	278	6			
1	G	203	Total	C	N	O	S	0	0	0
			1620	1044	276	295	5			
1	H	202	Total	C	N	O	S	0	0	0
			1609	1036	268	300	5			
1	I	189	Total	C	N	O	S	0	0	0
			1541	998	255	282	6			
1	J	185	Total	C	N	O	S	0	0	0
			1478	957	249	268	4			
1	K	189	Total	C	N	O	S	0	0	0
			1438	939	237	256	6			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P03132
A	-1	SER	-	expression tag	UNP P03132
A	0	HIS	-	expression tag	UNP P03132
A	151	SER	CYS	engineered mutation	UNP P03132
B	-2	GLY	-	expression tag	UNP P03132
B	-1	SER	-	expression tag	UNP P03132
B	0	HIS	-	expression tag	UNP P03132

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Chain	Residue	Modelled	Actual	Comment	Reference
B	151	SER	CYS	engineered mutation	UNP P03132
C	-2	GLY	-	expression tag	UNP P03132
C	-1	SER	-	expression tag	UNP P03132
C	0	HIS	-	expression tag	UNP P03132
C	151	SER	CYS	engineered mutation	UNP P03132
D	-2	GLY	-	expression tag	UNP P03132
D	-1	SER	-	expression tag	UNP P03132
D	0	HIS	-	expression tag	UNP P03132
D	151	SER	CYS	engineered mutation	UNP P03132
E	-2	GLY	-	expression tag	UNP P03132
E	-1	SER	-	expression tag	UNP P03132
E	0	HIS	-	expression tag	UNP P03132
E	151	SER	CYS	engineered mutation	UNP P03132
F	-2	GLY	-	expression tag	UNP P03132
F	-1	SER	-	expression tag	UNP P03132
F	0	HIS	-	expression tag	UNP P03132
F	151	SER	CYS	engineered mutation	UNP P03132
G	-2	GLY	-	expression tag	UNP P03132
G	-1	SER	-	expression tag	UNP P03132
G	0	HIS	-	expression tag	UNP P03132
G	151	SER	CYS	engineered mutation	UNP P03132
H	-2	GLY	-	expression tag	UNP P03132
H	-1	SER	-	expression tag	UNP P03132
H	0	HIS	-	expression tag	UNP P03132
H	151	SER	CYS	engineered mutation	UNP P03132
I	-2	GLY	-	expression tag	UNP P03132
I	-1	SER	-	expression tag	UNP P03132
I	0	HIS	-	expression tag	UNP P03132
I	151	SER	CYS	engineered mutation	UNP P03132
J	-2	GLY	-	expression tag	UNP P03132
J	-1	SER	-	expression tag	UNP P03132
J	0	HIS	-	expression tag	UNP P03132
J	151	SER	CYS	engineered mutation	UNP P03132
K	-2	GLY	-	expression tag	UNP P03132
K	-1	SER	-	expression tag	UNP P03132
K	0	HIS	-	expression tag	UNP P03132
K	151	SER	CYS	engineered mutation	UNP P03132

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	0	0
3	B	35	Total O 35 35	0	0
3	C	16	Total O 16 16	0	0
3	D	18	Total O 18 18	0	0
3	E	19	Total O 19 19	0	0
3	F	18	Total O 18 18	0	0
3	G	15	Total O 15 15	0	0

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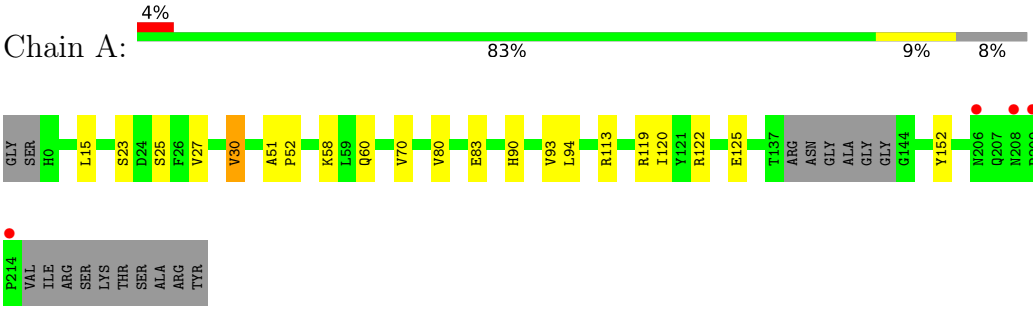
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	10	Total O 10 10	0	0
3	I	6	Total O 6 6	0	0
3	J	11	Total O 11 11	0	0
3	K	3	Total O 3 3	0	0

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.

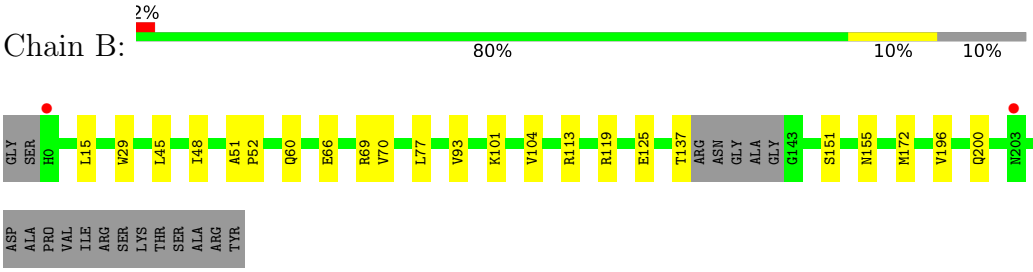
• Molecule 1: Protein Rep68

Chain A:



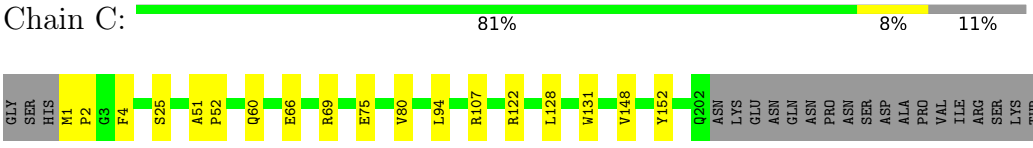
• Molecule 1: Protein Rep68

Chain B:



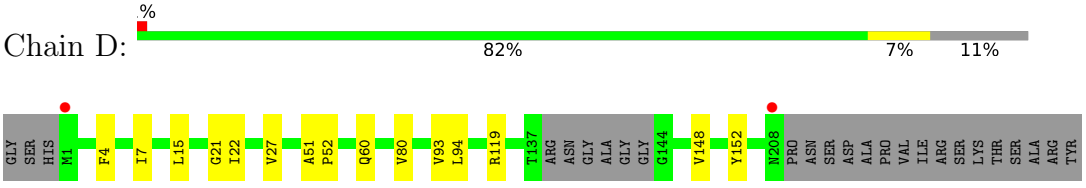
• Molecule 1: Protein Rep68

Chain C:



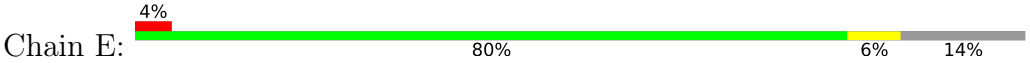
• Molecule 1: Protein Rep68

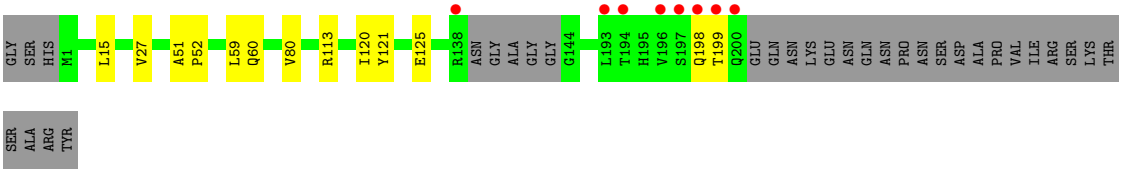
Chain D:



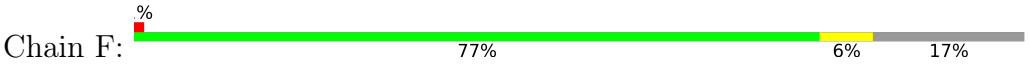
• Molecule 1: Protein Rep68

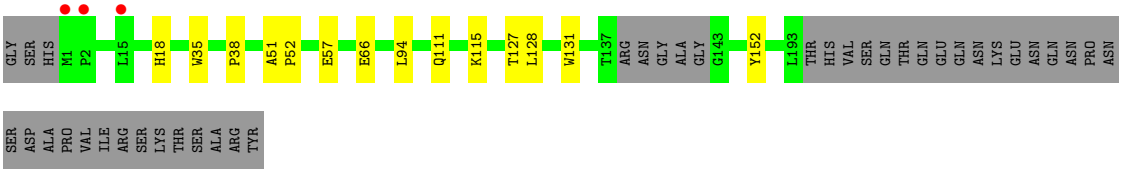
Chain E:



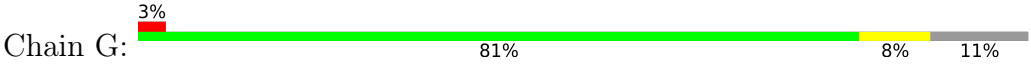


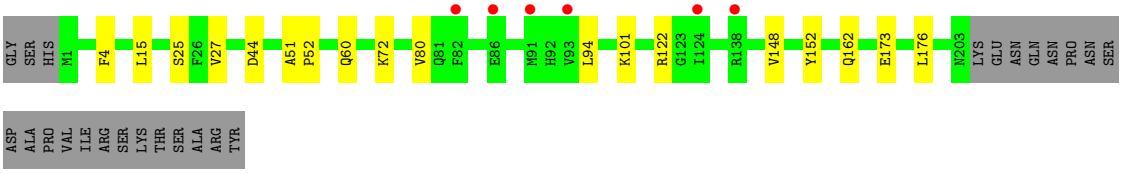
• Molecule 1: Protein Rep68



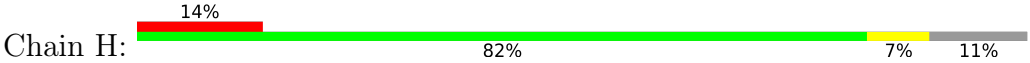


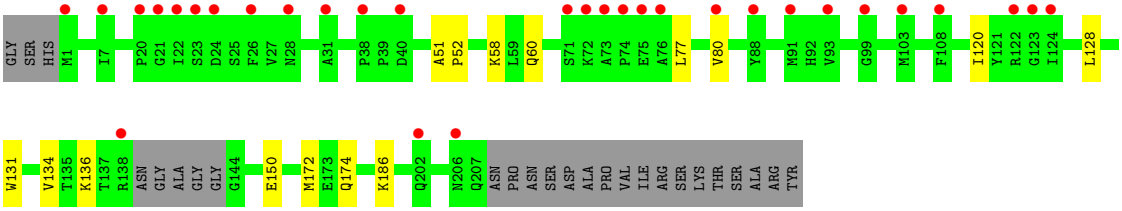
• Molecule 1: Protein Rep68



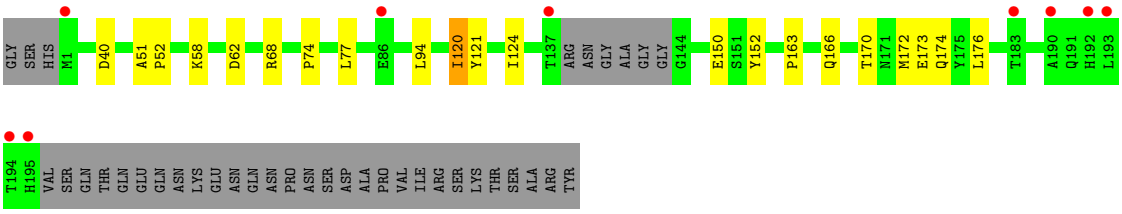


• Molecule 1: Protein Rep68

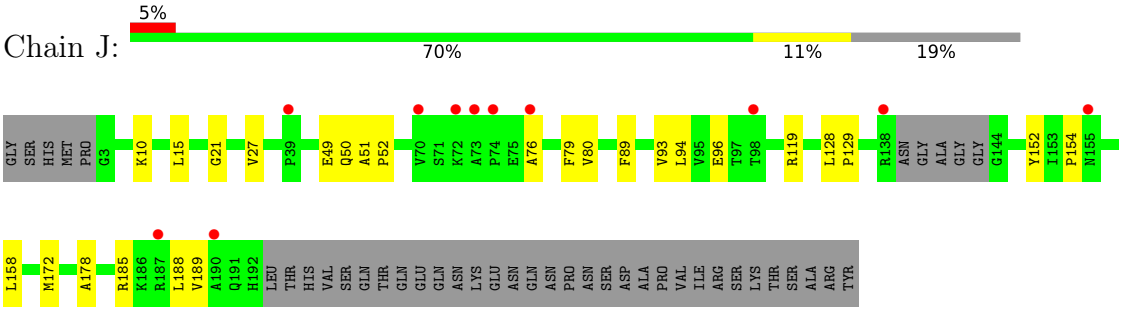




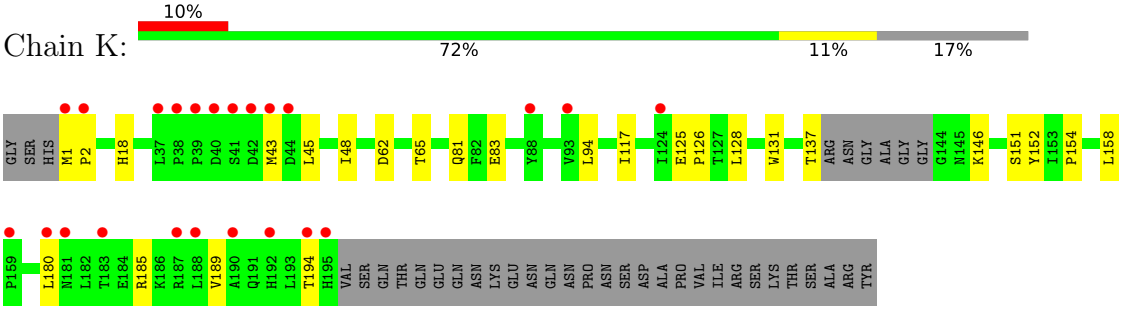
• Molecule 1: Protein Rep68



• Molecule 1: Protein Rep68



• Molecule 1: Protein Rep68



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.64Å 178.71Å 130.36Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	29.81 – 2.60 29.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.81-2.60) 98.7 (29.81-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.40 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.237 0.199 , 0.241	Depositor DCC
R_{free} test set	5239 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17626	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.22	0/1743	0.40	0/2372
1	B	0.22	0/1719	0.40	0/2337
1	C	0.22	0/1665	0.39	0/2266
1	D	0.22	0/1685	0.40	0/2291
1	E	0.22	0/1635	0.41	0/2222
1	F	0.24	0/1565	0.41	0/2129
1	G	0.23	0/1663	0.42	0/2264
1	H	0.22	0/1651	0.39	0/2253
1	I	0.22	0/1583	0.40	0/2154
1	J	0.21	0/1518	0.40	0/2069
1	K	0.24	0/1478	0.46	0/2025
All	All	0.22	0/17905	0.41	0/24382

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	1698	0	1660	13	0
1	B	1675	0	1645	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1622	0	1594	11	0
1	D	1643	0	1608	10	0
1	E	1594	0	1584	9	0
1	F	1524	0	1499	9	0
1	G	1620	0	1585	10	0
1	H	1609	0	1539	8	0
1	I	1541	0	1514	12	0
1	J	1478	0	1420	16	0
1	K	1438	0	1345	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
3	A	22	0	0	1	0
3	B	35	0	0	1	0
3	C	16	0	0	1	0
3	D	18	0	0	0	0
3	E	19	0	0	0	0
3	F	18	0	0	0	0
3	G	15	0	0	1	0
3	H	10	0	0	0	0
3	I	6	0	0	0	0
3	J	11	0	0	0	0
3	K	3	0	0	0	0
All	All	17626	0	16993	118	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 3.

All (118) 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:I:173:GLU:HA	1:I:176:LEU:HG	1.63	0.80
1:A:119:ARG:NH1	1:D:21:GLY:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLU:OE2	1:B:69:ARG:NH2	2.29	0.66
1:C:66:GLU:OE2	1:C:69:ARG:NH1	2.30	0.64
1:A:25:SER:OG	1:A:122:ARG:NH2	2.31	0.63
1:D:119:ARG:NH2	1:F:38:PRO:O	2.31	0.63
1:A:15:LEU:HD21	1:A:27:VAL:HG22	1.83	0.61
1:H:150:GLU:OE2	1:H:174:GLN:NE2	2.34	0.60
1:G:94:LEU:HD11	1:G:152:TYR:HD2	1.66	0.59
1:G:25:SER:OG	1:G:122:ARG:NH1	2.35	0.58
1:I:58:LYS:HG2	1:I:120:ILE:HD12	1.85	0.58
1:E:198:GLN:OE1	1:E:199:THR:OG1	2.21	0.57
1:G:15:LEU:HD13	1:G:27:VAL:HG22	1.86	0.56
1:I:150:GLU:OE1	1:I:174:GLN:NE2	2.39	0.56
1:A:113:ARG:NH2	1:A:125:GLU:OE1	2.40	0.55
1:F:35:TRP:HH2	1:F:57:GLU:HG3	1.70	0.55
1:I:77:LEU:HD22	1:I:172:MET:HG2	1.89	0.55
1:B:29:TRP:HA	1:J:129:PRO:HG3	1.90	0.54
1:H:58:LYS:HD3	1:H:120:ILE:HG13	1.90	0.54
1:K:154:PRO:HA	1:K:158:LEU:HB2	1.90	0.54
1:J:76:ALA:HB1	1:J:96:GLU:HG2	1.91	0.53
1:I:94:LEU:HD11	1:I:152:TYR:HD2	1.74	0.53
1:C:94:LEU:HD11	1:C:152:TYR:HD2	1.74	0.52
1:H:134:VAL:HG13	1:H:136:LYS:HE2	1.92	0.52
1:K:18:HIS:CG	1:K:128:LEU:HD21	2.44	0.51
1:I:68:ARG:HD3	1:I:74:PRO:HA	1.92	0.51
1:C:4:PHE:HB2	1:C:148:VAL:HG22	1.93	0.51
1:E:59:LEU:HD23	1:E:120:ILE:HD12	1.93	0.51
1:J:79:PHE:HB2	1:J:172:MET:HE3	1.93	0.51
1:J:178:ALA:HB2	1:J:188:LEU:HD12	1.94	0.50
1:D:80:VAL:HG22	1:D:93:VAL:HB	1.94	0.50
1:C:25:SER:OG	1:C:122:ARG:NH1	2.45	0.50
1:I:94:LEU:HD11	1:I:152:TYR:CD2	2.47	0.50
1:B:113:ARG:NH2	1:B:125:GLU:OE1	2.45	0.49
1:D:7:ILE:O	1:D:93:VAL:HG13	2.12	0.49
1:J:154:PRO:HA	1:J:158:LEU:HD12	1.94	0.49
1:J:185:ARG:O	1:J:189:VAL:HG23	2.12	0.49
1:K:94:LEU:HD11	1:K:152:TYR:CD2	2.48	0.49
1:B:104:VAL:HG12	1:E:15:LEU:HD22	1.94	0.49
1:D:94:LEU:HD11	1:D:152:TYR:HD2	1.77	0.48
1:A:30:VAL:HG13	1:A:51:ALA:HB1	1.95	0.48
1:D:4:PHE:HB2	1:D:148:VAL:HG22	1.95	0.48
1:E:15:LEU:HD21	1:E:27:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:PHE:HB2	1:G:148:VAL:HG22	1.95	0.48
1:I:51:ALA:HB3	1:I:52:PRO:HD3	1.95	0.48
1:B:77:LEU:HG	1:B:172:MET:HG2	1.94	0.48
1:C:75:GLU:CD	1:J:119:ARG:HH12	2.17	0.48
1:J:51:ALA:HB3	1:J:52:PRO:HD3	1.94	0.48
1:D:15:LEU:HD13	1:D:27:VAL:HG22	1.96	0.48
1:I:163:PRO:O	1:I:166:GLN:NE2	2.44	0.48
1:A:60:GLN:NE2	3:A:403:HOH:O	2.46	0.47
1:B:60:GLN:NE2	3:B:401:HOH:O	2.33	0.46
1:H:51:ALA:HB3	1:H:52:PRO:HD3	1.97	0.46
1:D:51:ALA:HB3	1:D:52:PRO:HD3	1.98	0.46
1:F:66:GLU:OE2	1:F:115:LYS:HD2	2.15	0.46
1:I:121:TYR:HB3	1:I:124:ILE:O	2.15	0.46
1:B:101:LYS:HD3	1:E:51:ALA:HB2	1.98	0.46
1:K:94:LEU:HD11	1:K:152:TYR:HD2	1.81	0.46
1:G:44:ASP:H	1:G:162:GLN:HE22	1.63	0.46
1:H:128:LEU:HB2	1:H:131:TRP:HB3	1.98	0.46
1:B:151:SER:O	1:B:155:ASN:HB2	2.16	0.46
1:G:72:LYS:NZ	3:G:401:HOH:O	2.48	0.46
1:K:125:GLU:HA	1:K:126:PRO:HD3	1.72	0.46
1:F:128:LEU:HB2	1:F:131:TRP:HB3	1.97	0.45
1:G:51:ALA:HB3	1:G:52:PRO:HD3	1.98	0.45
1:C:51:ALA:HB3	1:C:52:PRO:HD3	1.97	0.45
1:K:45:LEU:HA	1:K:48:ILE:HD12	1.99	0.45
1:D:60:GLN:HG3	1:D:80:VAL:HG11	1.97	0.45
1:C:107:ARG:NH2	1:D:22:ILE:O	2.40	0.45
1:E:51:ALA:HB3	1:E:52:PRO:HD3	1.99	0.45
1:K:137:THR:HG23	1:K:146:LYS:HB2	1.99	0.45
1:B:51:ALA:HB3	1:B:52:PRO:HD3	1.99	0.45
1:F:51:ALA:HB3	1:F:52:PRO:HD3	1.97	0.45
1:B:119:ARG:HG2	1:J:21:GLY:HA3	1.99	0.44
1:E:60:GLN:HG3	1:E:80:VAL:HG11	1.98	0.44
1:K:117:ILE:HD13	1:K:125:GLU:HB2	1.99	0.44
1:H:60:GLN:HG3	1:H:80:VAL:HG11	1.99	0.44
1:K:81:GLN:NE2	1:K:83:GLU:OE1	2.48	0.44
1:B:196:VAL:O	1:B:200:GLN:HG3	2.18	0.44
1:F:18:HIS:HA	1:F:127:THR:HB	1.99	0.44
1:K:43:MET:HG3	1:K:180:LEU:O	2.18	0.44
1:B:137:THR:O	1:B:137:THR:OG1	2.33	0.44
1:C:1:MET:HA	1:C:2:PRO:HD3	1.86	0.44
1:A:25:SER:HG	1:A:122:ARG:NH2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:94:LEU:HD11	1:J:152:TYR:CD1	2.53	0.43
1:I:170:THR:HG23	1:I:176:LEU:HD23	2.00	0.43
1:F:94:LEU:HD11	1:F:152:TYR:HD2	1.83	0.43
1:J:10:LYS:NZ	1:J:129:PRO:O	2.39	0.43
1:J:15:LEU:HD13	1:J:27:VAL:HG22	2.01	0.43
1:K:1:MET:HG3	1:K:2:PRO:HD2	2.01	0.43
1:K:185:ARG:O	1:K:189:VAL:HG23	2.18	0.43
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.89	0.42
1:G:60:GLN:HG3	1:G:80:VAL:HG11	2.01	0.42
1:A:23:SER:O	1:A:27:VAL:HG23	2.18	0.42
1:C:60:GLN:NE2	3:C:401:HOH:O	2.52	0.42
1:J:49:GLU:HG3	1:J:89:PHE:HZ	1.83	0.42
1:A:51:ALA:HB3	1:A:52:PRO:HD3	2.00	0.42
1:A:83:GLU:OE2	1:A:90:HIS:NE2	2.53	0.42
1:C:128:LEU:HB2	1:C:131:TRP:HB3	2.02	0.42
1:K:154:PRO:HA	1:K:158:LEU:HD22	2.02	0.42
1:G:173:GLU:HA	1:G:176:LEU:HG	2.01	0.42
1:H:77:LEU:HD22	1:H:172:MET:HG2	2.02	0.42
1:E:59:LEU:HD11	1:E:121:TYR:OH	2.20	0.42
1:K:128:LEU:HB2	1:K:131:TRP:HB3	2.02	0.42
1:F:111:GLN:O	1:F:115:LYS:HG3	2.20	0.41
1:A:58:LYS:HD3	1:A:120:ILE:HG12	2.02	0.41
1:A:94:LEU:HD11	1:A:152:TYR:HD2	1.85	0.41
1:K:62:ASP:HA	1:K:65:THR:HG22	2.02	0.41
1:B:45:LEU:HA	1:B:48:ILE:HD12	2.01	0.41
1:F:94:LEU:HD11	1:F:152:TYR:CD2	2.55	0.41
1:E:113:ARG:NH2	1:E:125:GLU:OE2	2.54	0.41
1:J:128:LEU:HA	1:J:129:PRO:HD3	1.90	0.41
1:G:101:LYS:HE2	1:J:50:GLN:HB2	2.01	0.40
1:I:58:LYS:NZ	1:I:62:ASP:OD2	2.54	0.40
1:A:80:VAL:HG13	1:A:93:VAL:HG22	2.04	0.40
1:C:60:GLN:HG3	1:C:80:VAL:HG11	2.03	0.40
1:H:186:LYS:HB2	1:H:186:LYS:HE3	1.78	0.40
1:J:80:VAL:HG22	1:J:93:VAL:HG13	2.04	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	205/227 (90%)	203 (99%)	2 (1%)	0	100	100
1	B	201/227 (88%)	200 (100%)	1 (0%)	0	100	100
1	C	200/227 (88%)	197 (98%)	3 (2%)	0	100	100
1	D	198/227 (87%)	196 (99%)	2 (1%)	0	100	100
1	E	191/227 (84%)	189 (99%)	2 (1%)	0	100	100
1	F	184/227 (81%)	184 (100%)	0	0	100	100
1	G	201/227 (88%)	198 (98%)	3 (2%)	0	100	100
1	H	198/227 (87%)	196 (99%)	2 (1%)	0	100	100
1	I	185/227 (82%)	182 (98%)	3 (2%)	0	100	100
1	J	181/227 (80%)	175 (97%)	6 (3%)	0	100	100
1	K	185/227 (82%)	179 (97%)	5 (3%)	1 (0%)	29	52
All	All	2129/2497 (85%)	2099 (99%)	29 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	194	THR

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	186/203 (92%)	184 (99%)	2 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	185/203 (91%)	183 (99%)	2 (1%)	73 88
1	C	176/203 (87%)	176 (100%)	0	100 100
1	D	180/203 (89%)	180 (100%)	0	100 100
1	E	176/203 (87%)	176 (100%)	0	100 100
1	F	166/203 (82%)	166 (100%)	0	100 100
1	G	173/203 (85%)	173 (100%)	0	100 100
1	H	172/203 (85%)	172 (100%)	0	100 100
1	I	169/203 (83%)	167 (99%)	2 (1%)	71 87
1	J	155/203 (76%)	155 (100%)	0	100 100
1	K	142/203 (70%)	141 (99%)	1 (1%)	84 94
All	All	1880/2233 (84%)	1873 (100%)	7 (0%)	91 97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	70	VAL
1	B	70	VAL
1	B	93	VAL
1	I	40	ASP
1	I	120	ILE
1	K	151	SER

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

Mol	Chain	Res	Type
1	G	118	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	209/227 (92%)	-0.10	8 (3%) 40 33	28, 46, 82, 166	0
1	B	205/227 (90%)	-0.20	4 (1%) 65 60	27, 43, 70, 112	0
1	C	202/227 (88%)	-0.25	0 100 100	28, 45, 76, 118	0
1	D	202/227 (88%)	-0.23	2 (0%) 82 80	29, 43, 78, 114	0
1	E	195/227 (85%)	-0.20	8 (4%) 37 30	32, 48, 93, 176	0
1	F	188/227 (82%)	-0.21	3 (1%) 72 68	28, 49, 82, 96	0
1	G	203/227 (89%)	0.01	6 (2%) 50 43	36, 57, 90, 125	0
1	H	202/227 (88%)	0.54	31 (15%) 2 1	49, 73, 102, 123	0
1	I	189/227 (83%)	-0.02	9 (4%) 30 24	42, 67, 97, 133	0
1	J	185/227 (81%)	0.18	11 (5%) 22 17	33, 69, 111, 138	0
1	K	189/227 (83%)	0.58	23 (12%) 4 2	41, 82, 138, 188	0
All	All	2169/2497 (86%)	0.00	105 (4%) 30 24	27, 55, 104, 188	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	ALA	9.7
1	A	212	ASP	8.2
1	A	211	SER	7.9
1	K	43	MET	6.2
1	A	214	PRO	6.2
1	A	210	ASN	5.4
1	K	39	PRO	4.9
1	I	194	THR	4.9
1	A	209	PRO	4.9
1	K	192	HIS	4.4
1	E	198	GLN	4.4
1	K	42	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	208	ASN	4.0
1	E	196	VAL	3.9
1	J	187	ARG	3.9
1	K	188	LEU	3.9
1	H	1	MET	3.9
1	B	209	PRO	3.8
1	K	180	LEU	3.8
1	K	194	THR	3.7
1	H	138	ARG	3.7
1	H	99	GLY	3.6
1	I	195	HIS	3.6
1	H	73	ALA	3.6
1	G	124	ILE	3.5
1	H	74	PRO	3.5
1	K	1	MET	3.5
1	K	38	PRO	3.5
1	J	138	ARG	3.4
1	K	181	ASN	3.4
1	H	71	SER	3.3
1	K	187	ARG	3.3
1	J	190	ALA	3.3
1	H	93	VAL	3.3
1	K	37	LEU	3.3
1	A	208	ASN	3.3
1	E	138	ARG	3.3
1	E	199	THR	3.3
1	H	28	ASN	3.2
1	J	74	PRO	3.2
1	H	24	ASP	3.2
1	H	80	VAL	3.1
1	D	1	MET	3.1
1	K	41	SER	3.1
1	I	190	ALA	3.1
1	K	183	THR	3.1
1	B	0	HIS	3.0
1	H	76	ALA	3.0
1	K	93	VAL	2.9
1	H	26	PHE	2.9
1	I	137	THR	2.9
1	I	1	MET	2.9
1	G	91	MET	2.9
1	H	23	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	192	HIS	2.8
1	F	2	PRO	2.8
1	H	20	PRO	2.7
1	B	208	ASN	2.7
1	J	98	THR	2.7
1	E	200	GLN	2.7
1	K	40	ASP	2.7
1	K	190	ALA	2.7
1	H	91	MET	2.7
1	K	2	PRO	2.6
1	K	195	HIS	2.6
1	I	86	GLU	2.6
1	H	40	ASP	2.6
1	H	124	ILE	2.6
1	K	124	ILE	2.6
1	G	138	ARG	2.6
1	H	75	GLU	2.5
1	J	73	ALA	2.5
1	K	159	PRO	2.5
1	H	31	ALA	2.5
1	E	194	THR	2.5
1	J	39	PRO	2.4
1	H	122	ARG	2.4
1	F	15	LEU	2.4
1	G	86	GLU	2.4
1	G	82	PHE	2.4
1	H	202	GLN	2.4
1	H	206	ASN	2.3
1	H	7	ILE	2.3
1	H	103	MET	2.3
1	E	193	LEU	2.3
1	F	1	MET	2.3
1	H	108	PHE	2.3
1	H	88	TYR	2.3
1	K	88	TYR	2.2
1	J	70	VAL	2.2
1	I	183	THR	2.2
1	A	206	ASN	2.2
1	E	197	SER	2.2
1	J	155	ASN	2.1
1	H	21	GLY	2.1
1	H	38	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	203	ASN	2.1
1	I	193	LEU	2.1
1	G	93	VAL	2.1
1	H	123	GLY	2.1
1	J	72	LYS	2.0
1	J	76	ALA	2.0
1	K	44	ASP	2.0
1	H	22	ILE	2.0
1	H	72	LYS	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	301	1/1	0.59	0.83	443,443,443,443	0
2	MG	F	301	1/1	0.92	0.19	39,39,39,39	0
2	MG	H	301	1/1	0.93	0.22	46,46,46,46	0
2	MG	C	301	1/1	0.95	0.20	34,34,34,34	0
2	MG	I	301	1/1	0.95	0.21	57,57,57,57	0
2	MG	J	301	1/1	0.95	0.16	48,48,48,48	0
2	MG	K	301	1/1	0.95	0.14	63,63,63,63	0
2	MG	A	301	1/1	0.96	0.68	95,95,95,95	0
2	MG	G	301	1/1	0.96	0.28	36,36,36,36	0
2	MG	E	301	1/1	0.96	0.12	36,36,36,36	0
2	MG	D	301	1/1	0.97	0.34	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.