



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:53 PM GMT

PDB ID : 4Q66
Title : Structure of Exomer bound to Arf1.
Authors : Paczkowski, J.E.; Fromme, J.C.
Deposited on : 2014-04-21
Resolution : 3.35 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

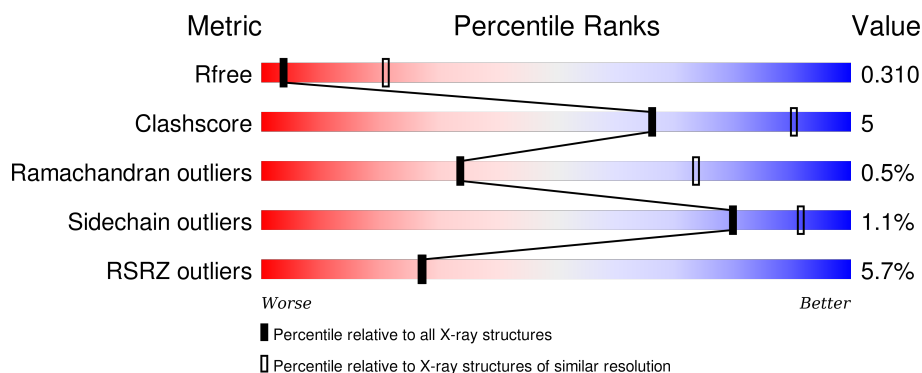
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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 $\leq 5\%$. 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	368	<div> <div>2%</div> <div>53%</div> <div>8%</div> <div>39%</div> </div>
1	D	368	<div> <div>4%</div> <div>41%</div> <div>6%</div> <div>54%</div> </div>
1	G	368	<div> <div>6%</div> <div>49%</div> <div>8%</div> <div>43%</div> </div>
1	J	368	<div> <div>4%</div> <div>36%</div> <div>6%</div> <div>57%</div> </div>
2	B	739	<div> <div>2%</div> <div>60%</div> <div>7%</div> <div>31%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	739	<div><div>%</div><div><div></div><div>66%</div><div>9%</div><div>25%</div></div></div>
2	H	739	<div><div>5%</div><div><div></div><div>42%</div><div></div><div>54%</div></div></div>
2	K	739	<div><div>2%</div><div><div></div><div>68%</div><div>12%</div><div>20%</div></div></div>
3	C	175	<div><div>5%</div><div><div></div><div>68%</div><div>9%</div><div>23%</div></div></div>
3	F	175	<div><div>6%</div><div><div></div><div>74%</div><div>9%</div><div>17%</div></div></div>
3	I	175	<div><div>9%</div><div><div></div><div>44%</div><div>5%</div><div>51%</div></div></div>
3	L	175	<div><div>9%</div><div><div></div><div>65%</div><div>13%</div><div>21%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26303 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 Chs5p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1788	1149	309	323	7			
1	J	158	Total	C	N	O	S	0	0	0
			1240	801	210	226	3			
1	G	211	Total	C	N	O	S	0	0	0
			1655	1064	281	304	6			
1	D	171	Total	C	N	O	S	0	0	0
			1357	878	230	245	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	INITIATING METHIONINE	UNP W7PD87
A	-2	ASP	-	EXPRESSION TAG	UNP W7PD87
A	-1	PRO	-	EXPRESSION TAG	UNP W7PD87
A	0	GLU	-	EXPRESSION TAG	UNP W7PD87
A	1	PHE	-	EXPRESSION TAG	UNP W7PD87
J	-3	MET	-	INITIATING METHIONINE	UNP W7PD87
J	-2	ASP	-	EXPRESSION TAG	UNP W7PD87
J	-1	PRO	-	EXPRESSION TAG	UNP W7PD87
J	0	GLU	-	EXPRESSION TAG	UNP W7PD87
J	1	PHE	-	EXPRESSION TAG	UNP W7PD87
G	-3	MET	-	INITIATING METHIONINE	UNP W7PD87
G	-2	ASP	-	EXPRESSION TAG	UNP W7PD87
G	-1	PRO	-	EXPRESSION TAG	UNP W7PD87
G	0	GLU	-	EXPRESSION TAG	UNP W7PD87
G	1	PHE	-	EXPRESSION TAG	UNP W7PD87
D	-3	MET	-	INITIATING METHIONINE	UNP W7PD87
D	-2	ASP	-	EXPRESSION TAG	UNP W7PD87
D	-1	PRO	-	EXPRESSION TAG	UNP W7PD87
D	0	GLU	-	EXPRESSION TAG	UNP W7PD87
D	1	PHE	-	EXPRESSION TAG	UNP W7PD87

- Molecule 2 is a protein called Protein BCH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	593	Total	C	N	O	S	0	0	0
			4809	3106	792	888	23			
2	E	557	Total	C	N	O	S	0	0	0
			4493	2903	738	830	22			
2	B	507	Total	C	N	O	S	0	0	0
			4108	2656	673	758	21			
2	H	338	Total	C	N	O	S	0	0	0
			2711	1747	447	499	18			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	725	GLY	-	EXPRESSION TAG	UNP Q05029
K	726	THR	-	EXPRESSION TAG	UNP Q05029
K	727	GLU	-	EXPRESSION TAG	UNP Q05029
K	728	ASN	-	EXPRESSION TAG	UNP Q05029
K	729	LEU	-	EXPRESSION TAG	UNP Q05029
K	730	TYR	-	EXPRESSION TAG	UNP Q05029
K	731	PHE	-	EXPRESSION TAG	UNP Q05029
K	732	GLN	-	EXPRESSION TAG	UNP Q05029
K	733	GLY	-	EXPRESSION TAG	UNP Q05029
K	734	HIS	-	EXPRESSION TAG	UNP Q05029
K	735	HIS	-	EXPRESSION TAG	UNP Q05029
K	736	HIS	-	EXPRESSION TAG	UNP Q05029
K	737	HIS	-	EXPRESSION TAG	UNP Q05029
K	738	HIS	-	EXPRESSION TAG	UNP Q05029
K	739	HIS	-	EXPRESSION TAG	UNP Q05029
E	725	GLY	-	EXPRESSION TAG	UNP Q05029
E	726	THR	-	EXPRESSION TAG	UNP Q05029
E	727	GLU	-	EXPRESSION TAG	UNP Q05029
E	728	ASN	-	EXPRESSION TAG	UNP Q05029
E	729	LEU	-	EXPRESSION TAG	UNP Q05029
E	730	TYR	-	EXPRESSION TAG	UNP Q05029
E	731	PHE	-	EXPRESSION TAG	UNP Q05029
E	732	GLN	-	EXPRESSION TAG	UNP Q05029
E	733	GLY	-	EXPRESSION TAG	UNP Q05029
E	734	HIS	-	EXPRESSION TAG	UNP Q05029
E	735	HIS	-	EXPRESSION TAG	UNP Q05029
E	736	HIS	-	EXPRESSION TAG	UNP Q05029
E	737	HIS	-	EXPRESSION TAG	UNP Q05029
E	738	HIS	-	EXPRESSION TAG	UNP Q05029
E	739	HIS	-	EXPRESSION TAG	UNP Q05029

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Chain	Residue	Modelled	Actual	Comment	Reference
B	725	GLY	-	EXPRESSION TAG	UNP Q05029
B	726	THR	-	EXPRESSION TAG	UNP Q05029
B	727	GLU	-	EXPRESSION TAG	UNP Q05029
B	728	ASN	-	EXPRESSION TAG	UNP Q05029
B	729	LEU	-	EXPRESSION TAG	UNP Q05029
B	730	TYR	-	EXPRESSION TAG	UNP Q05029
B	731	PHE	-	EXPRESSION TAG	UNP Q05029
B	732	GLN	-	EXPRESSION TAG	UNP Q05029
B	733	GLY	-	EXPRESSION TAG	UNP Q05029
B	734	HIS	-	EXPRESSION TAG	UNP Q05029
B	735	HIS	-	EXPRESSION TAG	UNP Q05029
B	736	HIS	-	EXPRESSION TAG	UNP Q05029
B	737	HIS	-	EXPRESSION TAG	UNP Q05029
B	738	HIS	-	EXPRESSION TAG	UNP Q05029
B	739	HIS	-	EXPRESSION TAG	UNP Q05029
H	725	GLY	-	EXPRESSION TAG	UNP Q05029
H	726	THR	-	EXPRESSION TAG	UNP Q05029
H	727	GLU	-	EXPRESSION TAG	UNP Q05029
H	728	ASN	-	EXPRESSION TAG	UNP Q05029
H	729	LEU	-	EXPRESSION TAG	UNP Q05029
H	730	TYR	-	EXPRESSION TAG	UNP Q05029
H	731	PHE	-	EXPRESSION TAG	UNP Q05029
H	732	GLN	-	EXPRESSION TAG	UNP Q05029
H	733	GLY	-	EXPRESSION TAG	UNP Q05029
H	734	HIS	-	EXPRESSION TAG	UNP Q05029
H	735	HIS	-	EXPRESSION TAG	UNP Q05029
H	736	HIS	-	EXPRESSION TAG	UNP Q05029
H	737	HIS	-	EXPRESSION TAG	UNP Q05029
H	738	HIS	-	EXPRESSION TAG	UNP Q05029
H	739	HIS	-	EXPRESSION TAG	UNP Q05029

- Molecule 3 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	146	Total 1173	C 745	N 205	O 217	S 6	0	0	0
3	L	139	Total 1115	C 711	N 195	O 203	S 6	0	0	0
3	C	134	Total 1056	C 673	N 177	O 202	S 4	0	0	0
3	I	86	Total 666	C 426	N 113	O 123	S 4	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

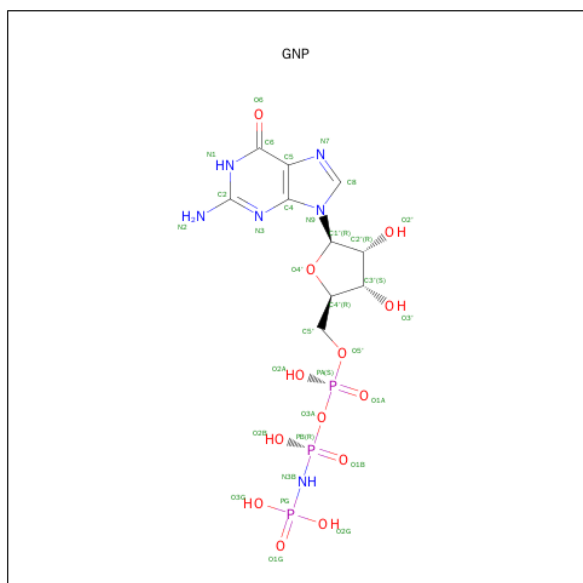
Chain	Residue	Modelled	Actual	Comment	Reference
F	7	MET	-	EXPRESSION TAG	UNP P11076
F	8	THR	-	EXPRESSION TAG	UNP P11076
F	9	GLU	-	EXPRESSION TAG	UNP P11076
F	10	ASN	-	EXPRESSION TAG	UNP P11076
F	11	LEU	-	EXPRESSION TAG	UNP P11076
F	12	TYR	-	EXPRESSION TAG	UNP P11076
F	13	PHE	-	EXPRESSION TAG	UNP P11076
F	14	GLN	-	EXPRESSION TAG	UNP P11076
F	15	GLY	-	EXPRESSION TAG	UNP P11076
F	16	SER	-	EXPRESSION TAG	UNP P11076
F	17	GLY	-	EXPRESSION TAG	UNP P11076
F	71	LEU	GLN	ENGINEERED MUTATION	UNP P11076
L	7	MET	-	EXPRESSION TAG	UNP P11076
L	8	THR	-	EXPRESSION TAG	UNP P11076
L	9	GLU	-	EXPRESSION TAG	UNP P11076
L	10	ASN	-	EXPRESSION TAG	UNP P11076
L	11	LEU	-	EXPRESSION TAG	UNP P11076
L	12	TYR	-	EXPRESSION TAG	UNP P11076
L	13	PHE	-	EXPRESSION TAG	UNP P11076
L	14	GLN	-	EXPRESSION TAG	UNP P11076
L	15	GLY	-	EXPRESSION TAG	UNP P11076
L	16	SER	-	EXPRESSION TAG	UNP P11076
L	17	GLY	-	EXPRESSION TAG	UNP P11076
L	71	LEU	GLN	ENGINEERED MUTATION	UNP P11076
C	7	MET	-	EXPRESSION TAG	UNP P11076
C	8	THR	-	EXPRESSION TAG	UNP P11076
C	9	GLU	-	EXPRESSION TAG	UNP P11076
C	10	ASN	-	EXPRESSION TAG	UNP P11076
C	11	LEU	-	EXPRESSION TAG	UNP P11076
C	12	TYR	-	EXPRESSION TAG	UNP P11076
C	13	PHE	-	EXPRESSION TAG	UNP P11076
C	14	GLN	-	EXPRESSION TAG	UNP P11076
C	15	GLY	-	EXPRESSION TAG	UNP P11076
C	16	SER	-	EXPRESSION TAG	UNP P11076
C	17	GLY	-	EXPRESSION TAG	UNP P11076
C	71	LEU	GLN	ENGINEERED MUTATION	UNP P11076
I	7	MET	-	EXPRESSION TAG	UNP P11076
I	8	THR	-	EXPRESSION TAG	UNP P11076
I	9	GLU	-	EXPRESSION TAG	UNP P11076
I	10	ASN	-	EXPRESSION TAG	UNP P11076
I	11	LEU	-	EXPRESSION TAG	UNP P11076
I	12	TYR	-	EXPRESSION TAG	UNP P11076

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Chain	Residue	Modelled	Actual	Comment	Reference
I	13	PHE	-	EXPRESSION TAG	UNP P11076
I	14	GLN	-	EXPRESSION TAG	UNP P11076
I	15	GLY	-	EXPRESSION TAG	UNP P11076
I	16	SER	-	EXPRESSION TAG	UNP P11076
I	17	GLY	-	EXPRESSION TAG	UNP P11076
I	71	LEU	GLN	ENGINEERED MUTATION	UNP P11076

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



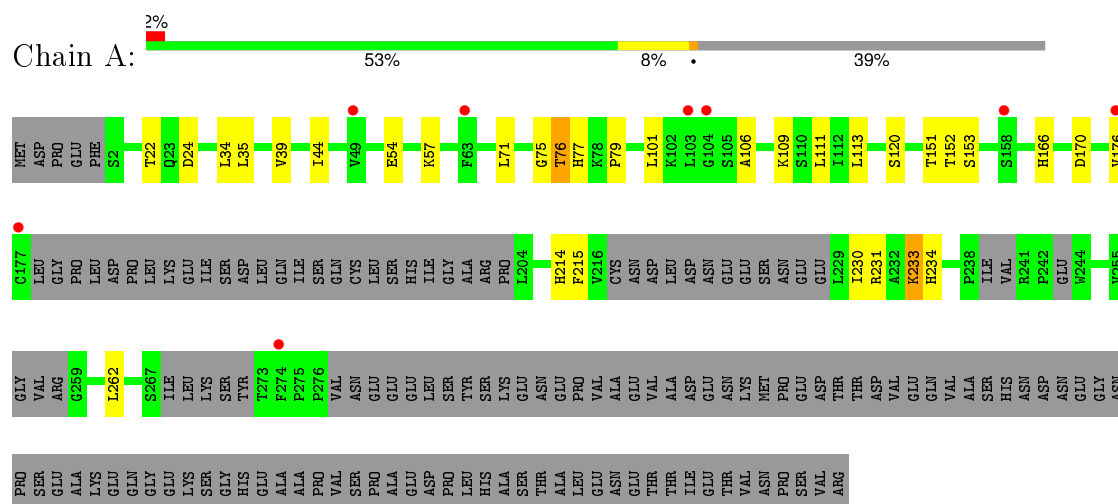
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	1	Total 1	Mg 1	0	0
5	C	1	Total 1	Mg 1	0	0
5	F	1	Total 1	Mg 1	0	0

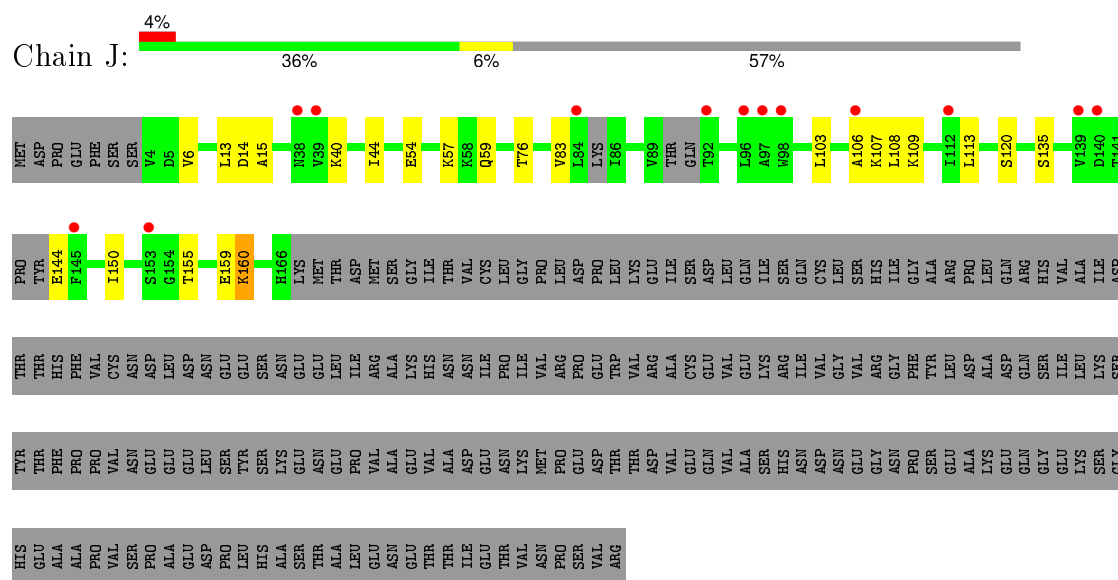
3 Residue-property plots [i](#)

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: Chs5p

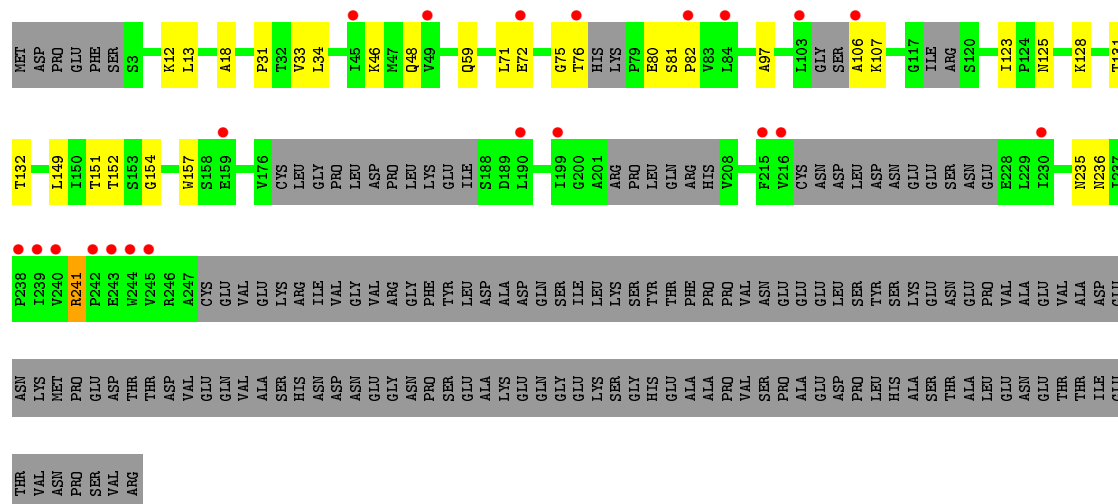


• Molecule 1: Chs5p

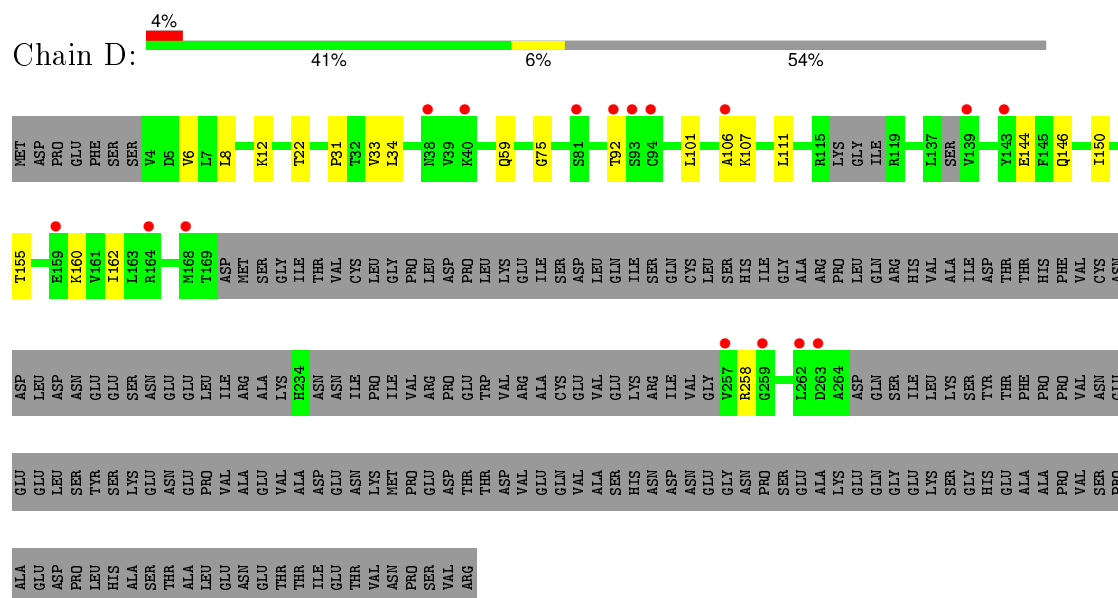


• Molecule 1: Chs5p

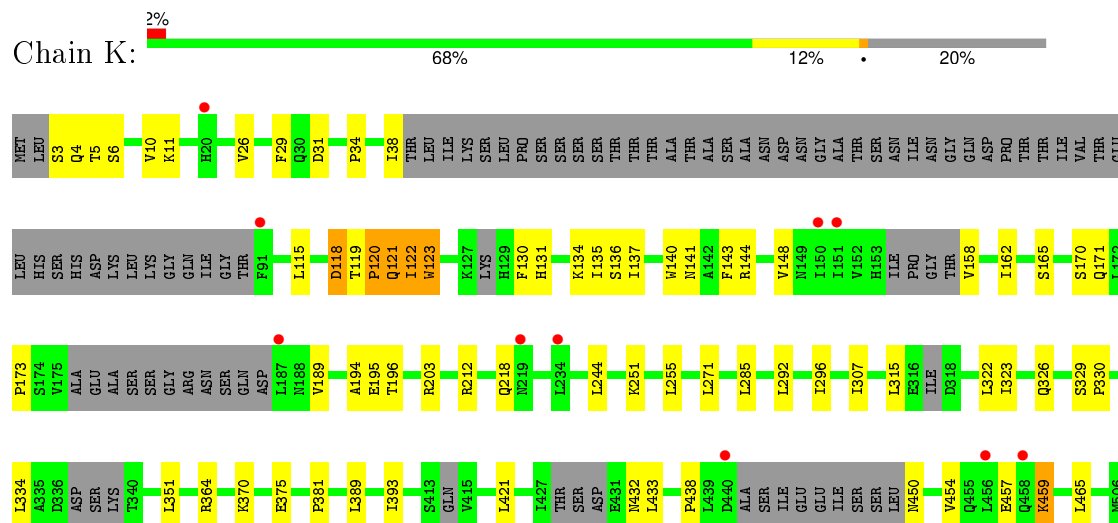


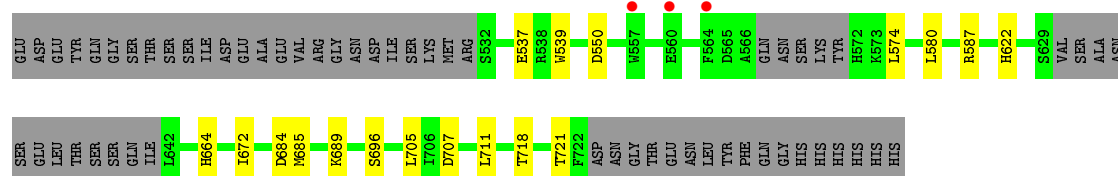


- Molecule 1: Chs5p

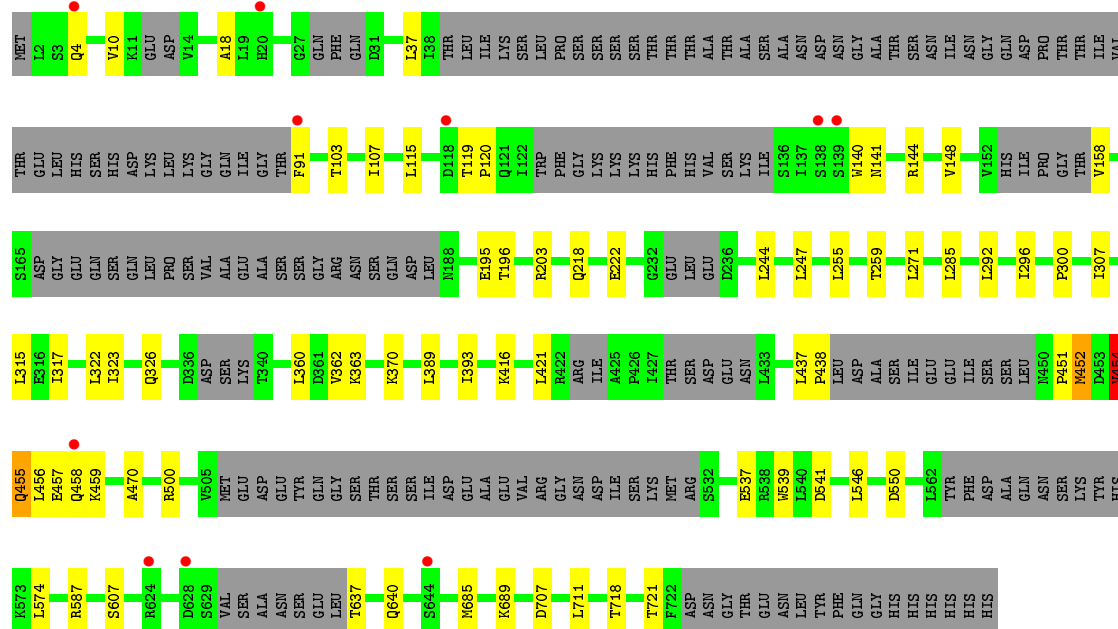


- Molecule 2: Protein BCH1

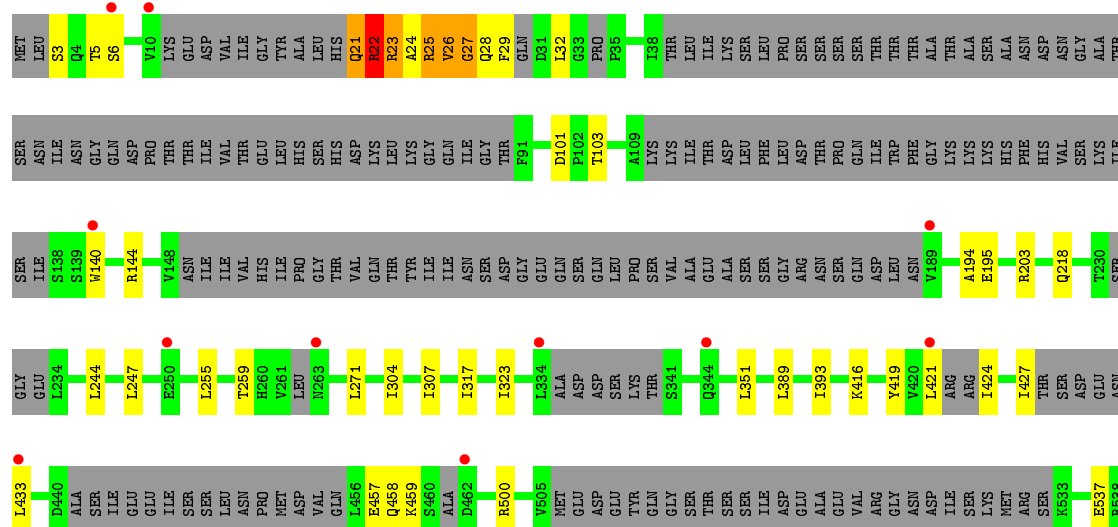


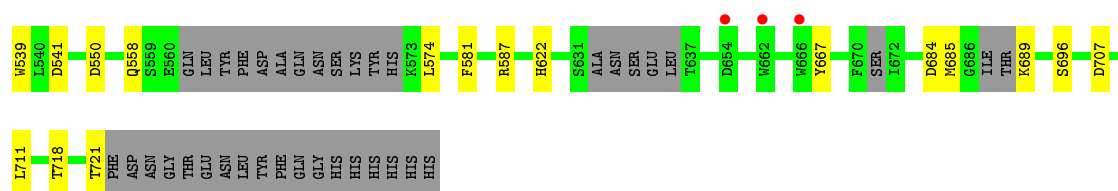


• Molecule 2: Protein BCH1

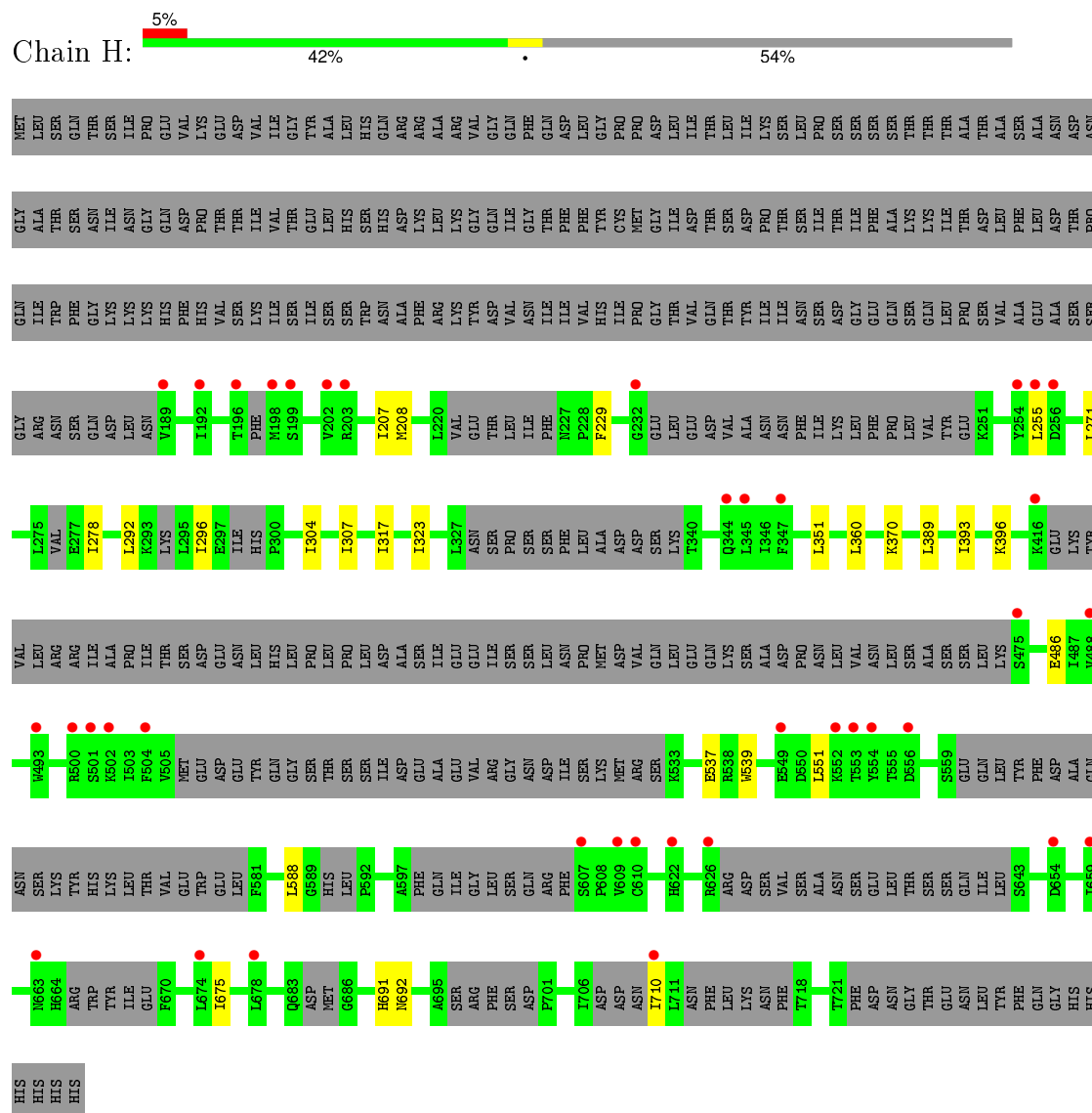


• Molecule 2: Protein BCH1

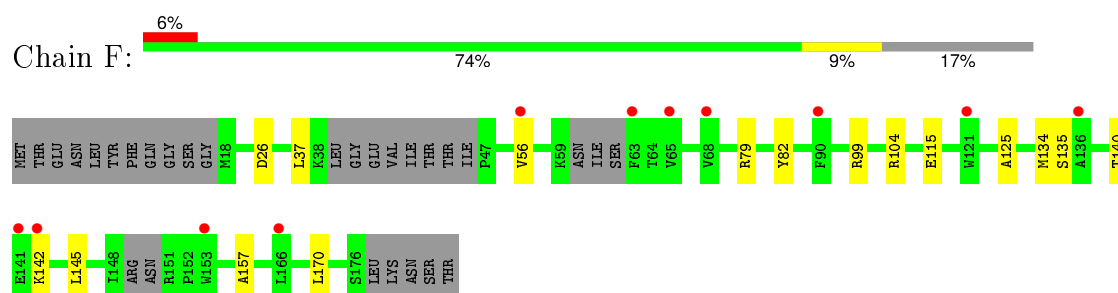




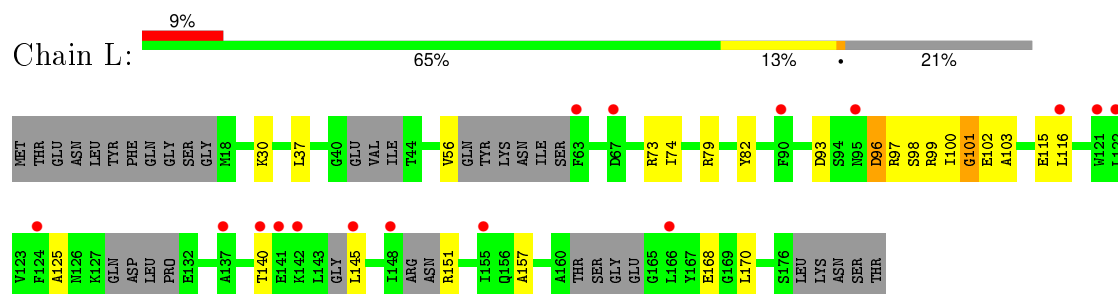
• Molecule 2: Protein BCH1



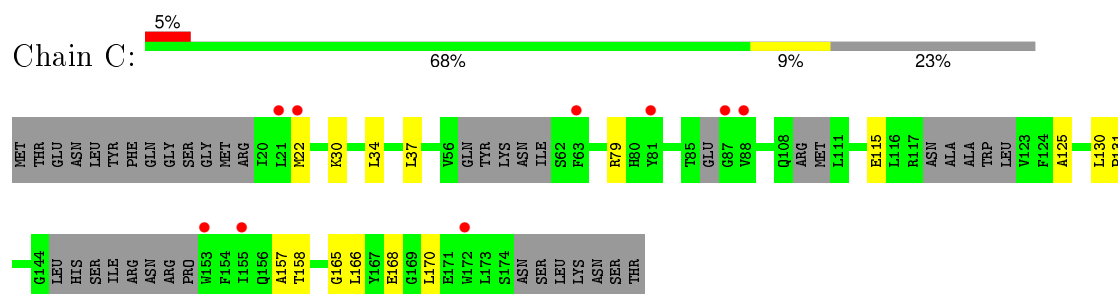
• Molecule 3: ADP-ribosylation factor 1



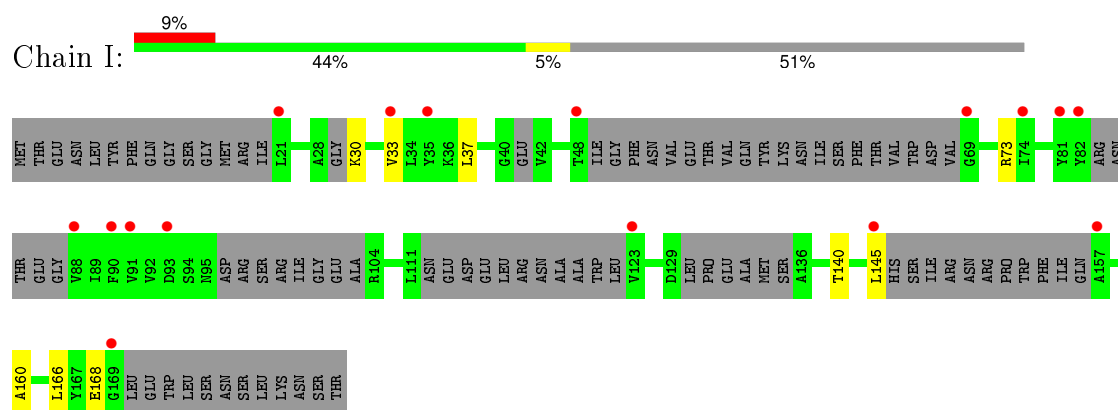
- Molecule 3: ADP-ribosylation factor 1



- Molecule 3: ADP-ribosylation factor 1



- Molecule 3: ADP-ribosylation factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.66Å 208.17Å 155.08Å 90.00° 105.48° 90.00°	Depositor
Resolution (Å)	43.17 – 3.35 50.00 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (43.17-3.35) 91.2 (50.00-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.279 , 0.310 0.281 , 0.310	Depositor DCC
R_{free} test set	2418 reflections (2.65%)	DCC
Wilson B-factor (Å ²)	93.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 57.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 97164 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	26303	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, 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	0.21	0/1818	0.42	0/2456
1	D	0.21	0/1379	0.39	0/1862
1	G	0.20	0/1679	0.40	0/2269
1	J	0.20	0/1258	0.39	0/1699
2	B	0.21	0/4175	0.36	0/5634
2	E	0.21	0/4571	0.37	0/6183
2	H	0.20	0/2740	0.33	0/3682
2	K	0.21	0/4901	0.36	0/6630
3	C	0.20	0/1070	0.35	0/1442
3	F	0.20	0/1194	0.34	0/1609
3	I	0.20	0/667	0.34	0/887
3	L	0.20	0/1131	0.36	0/1521
All	All	0.21	0/26583	0.37	0/35874

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 [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	1788	0	1872	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1357	0	1435	15	0
1	G	1655	0	1743	21	0
1	J	1240	0	1325	16	0
2	B	4108	0	4150	52	0
2	E	4493	0	4560	40	0
2	H	2711	0	2781	15	0
2	K	4809	0	4841	46	0
3	C	1056	0	1042	10	0
3	F	1173	0	1158	10	0
3	I	666	0	681	6	0
3	L	1115	0	1109	23	0
4	C	32	0	13	1	0
4	F	32	0	13	0	0
4	I	32	0	13	1	0
4	L	32	0	13	1	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
5	L	1	0	0	0	0
All	All	26303	0	26749	259	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 5.

All (259) 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:B:26:VAL:O	2:B:28:GLN:N	1.72	1.19
3:L:100:ILE:O	3:L:103:ALA:N	1.85	1.09
2:B:22:ARG:O	2:B:23:ARG:NE	1.88	1.06
3:L:100:ILE:HG23	3:L:101:GLY:H	1.31	0.96
3:L:100:ILE:HG23	3:L:101:GLY:N	1.81	0.93
3:L:100:ILE:CG2	3:L:101:GLY:H	1.83	0.90
1:A:151:THR:HG22	1:A:153:SER:H	1.42	0.85
2:B:21:GLN:HE22	2:B:22:ARG:HD3	1.42	0.81
3:L:100:ILE:O	3:L:102:GLU:N	2.15	0.79
2:B:24:ALA:O	2:B:26:VAL:HG23	1.88	0.74
2:K:218:GLN:HE22	2:K:421:LEU:HD12	1.53	0.73
1:D:75:GLY:HA2	2:E:317:ILE:HG23	1.69	0.73
1:G:72:GLU:O	1:G:76:THR:OG1	2.06	0.73
2:B:24:ALA:O	2:B:26:VAL:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:362:VAL:HG13	2:E:363:LYS:HG2	1.73	0.70
2:B:26:VAL:HG12	2:B:27:GLY:N	2.06	0.70
3:L:96:ASP:N	3:L:96:ASP:OD2	2.25	0.69
2:K:162:ILE:HB	2:K:170:SER:HB3	1.74	0.69
1:G:241:ARG:HD3	1:G:241:ARG:H	1.60	0.67
2:B:21:GLN:OE1	2:B:22:ARG:HB3	1.96	0.66
2:B:21:GLN:HE22	2:B:22:ARG:CD	2.08	0.65
1:G:71:LEU:O	1:G:76:THR:HG23	1.97	0.64
2:E:685:MET:HB2	2:E:689:LYS:HD3	1.80	0.64
3:L:99:ARG:O	3:L:99:ARG:HG3	1.97	0.64
2:K:459:LYS:HE3	2:K:574:LEU:HD13	1.79	0.64
1:G:33:VAL:HG13	1:G:34:LEU:HD12	1.81	0.63
3:L:100:ILE:CG2	3:L:101:GLY:N	2.44	0.63
3:L:100:ILE:O	3:L:101:GLY:C	2.37	0.63
2:B:21:GLN:NE2	2:B:22:ARG:HG2	2.13	0.62
3:L:73:ARG:HG3	3:L:74:ILE:HG12	1.80	0.62
1:A:71:LEU:O	1:A:76:THR:OG1	2.17	0.62
2:E:452:MET:N	2:E:452:MET:SD	2.72	0.61
2:E:637:THR:OG1	2:E:640:GLN:OE1	2.18	0.61
1:A:166:HIS:ND1	1:A:170:ASP:OD2	2.34	0.60
1:A:34:LEU:HD22	1:D:6:VAL:HG11	1.82	0.60
3:C:125:ALA:HB3	3:C:157:ALA:HA	1.82	0.60
1:A:35:LEU:HB3	1:A:39:VAL:HG21	1.84	0.60
2:E:218:GLN:HE22	2:E:421:LEU:HD12	1.67	0.60
2:E:144:ARG:NH1	2:E:195:GLU:OE2	2.34	0.60
2:E:550:ASP:OD2	2:E:587:ARG:NH1	2.35	0.59
2:B:459:LYS:HD3	2:B:574:LEU:HD13	1.85	0.59
2:E:4:GLN:H	2:E:115:LEU:HD11	1.68	0.59
2:K:144:ARG:NH1	2:K:195:GLU:OE2	2.36	0.59
3:F:37:LEU:HB3	3:F:56:VAL:HG11	1.85	0.59
1:J:59:GLN:NE2	2:K:375:GLU:OE2	2.35	0.58
1:D:33:VAL:HG13	1:D:34:LEU:HD12	1.84	0.58
3:L:140:THR:HG22	3:L:145:LEU:HD12	1.86	0.58
2:K:118:ASP:N	2:K:118:ASP:OD1	2.37	0.58
2:E:500:ARG:NH2	2:E:541:ASP:OD1	2.36	0.58
2:B:25:ARG:O	2:B:25:ARG:HG3	2.04	0.57
2:K:3:SER:O	2:K:5:THR:N	2.35	0.57
2:K:685:MET:HB2	2:K:689:LYS:HD3	1.86	0.57
1:A:22:THR:OG1	1:A:24:ASP:OD1	2.19	0.57
1:A:75:GLY:HA2	2:B:317:ILE:HG23	1.87	0.57
2:K:140:TRP:O	2:K:203:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:307:ILE:HD13	2:H:323:ILE:HG12	1.87	0.57
1:G:75:GLY:HA2	2:H:317:ILE:HG23	1.87	0.57
2:B:500:ARG:NH2	2:B:541:ASP:OD1	2.38	0.57
3:L:100:ILE:C	3:L:102:GLU:N	2.59	0.56
1:A:109:LYS:HE3	1:A:152:THR:HB	1.88	0.56
3:L:93:ASP:CG	3:L:96:ASP:OD2	2.43	0.56
1:A:176:VAL:HG12	1:A:214:HIS:HB2	1.88	0.56
3:F:104:ARG:NH1	3:F:142:LYS:O	2.39	0.56
1:J:144:GLU:OE1	1:J:160:LYS:NZ	2.39	0.55
2:H:255:LEU:HD12	2:H:271:LEU:HB2	1.88	0.55
1:J:103:LEU:HD21	1:J:108:LEU:HB3	1.87	0.55
2:B:685:MET:HB2	2:B:689:LYS:HD3	1.89	0.55
2:B:550:ASP:OD2	2:B:587:ARG:NH1	2.40	0.54
2:B:457:GLU:OE2	2:B:458:GLN:N	2.41	0.54
2:K:148:VAL:HG21	2:K:196:THR:HG21	1.89	0.53
3:C:37:LEU:HD21	3:C:166:LEU:HB3	1.89	0.53
1:G:151:THR:OG1	1:G:154:GLY:O	2.24	0.53
2:E:459:LYS:HD2	2:E:574:LEU:HD13	1.90	0.53
2:B:144:ARG:NH1	2:B:195:GLU:OE2	2.42	0.53
1:G:71:LEU:O	1:G:76:THR:CG2	2.57	0.53
2:K:696:SER:HB3	3:L:79:ARG:HD2	1.90	0.53
3:I:37:LEU:HD21	3:I:166:LEU:HB3	1.91	0.53
3:F:125:ALA:HB3	3:F:157:ALA:HA	1.91	0.53
1:D:8:LEU:HD22	1:D:22:THR:HG22	1.90	0.53
3:L:125:ALA:HB3	3:L:157:ALA:HA	1.90	0.52
2:E:18:ALA:HB1	2:E:37:LEU:HD21	1.91	0.52
2:K:120:PRO:O	2:K:122:ILE:HG13	2.09	0.52
2:B:307:ILE:HD13	2:B:323:ILE:HG12	1.91	0.52
2:B:218:GLN:HE22	2:B:421:LEU:HD12	1.75	0.52
2:B:21:GLN:CG	2:B:22:ARG:N	2.73	0.52
3:F:26:ASP:O	3:F:99:ARG:NH2	2.42	0.52
2:B:21:GLN:NE2	2:B:22:ARG:CG	2.73	0.51
2:E:259:THR:HA	2:E:416:LYS:HD2	1.92	0.51
2:B:696:SER:O	3:C:79:ARG:NE	2.44	0.51
2:B:537:GLU:O	2:B:539:TRP:N	2.43	0.51
2:B:244:LEU:HD12	2:B:247:LEU:HD12	1.91	0.51
1:J:83:VAL:HG12	1:J:159:GLU:HG3	1.91	0.51
1:G:12:LYS:HG3	2:K:381:PRO:HD2	1.93	0.51
2:B:255:LEU:HD12	2:B:271:LEU:HB2	1.92	0.50
1:A:54:GLU:HA	1:A:57:LYS:HE2	1.91	0.50
2:K:195:GLU:OE2	2:K:251:LYS:NZ	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:GLN:HG3	2:B:22:ARG:H	1.77	0.50
2:K:550:ASP:OD2	2:K:587:ARG:NH1	2.44	0.50
2:H:692:ASN:HD22	3:I:73:ARG:HB3	1.76	0.50
3:F:37:LEU:HD13	3:F:170:LEU:HD11	1.94	0.49
2:H:396:LYS:NZ	2:H:486:GLU:OE2	2.43	0.49
1:D:144:GLU:HB3	1:D:162:ILE:HG22	1.94	0.49
2:H:370:LYS:HB2	2:H:393:ILE:HG21	1.94	0.49
1:J:54:GLU:HA	1:J:57:LYS:HZ3	1.77	0.49
2:E:454:VAL:HG22	2:E:455:GLN:H	1.77	0.49
3:C:30:LYS:NZ	4:C:201:GNP:O1B	2.36	0.49
1:D:101:LEU:HD11	1:D:111:LEU:HD22	1.94	0.49
3:C:37:LEU:HD13	3:C:170:LEU:HD11	1.95	0.49
2:E:244:LEU:HD12	2:E:247:LEU:HD12	1.95	0.49
2:E:707:ASP:HA	2:E:711:LEU:HB3	1.94	0.49
2:K:38:ILE:HG12	2:K:137:ILE:HG23	1.95	0.48
2:B:21:GLN:HE22	2:B:22:ARG:HG2	1.78	0.48
2:K:322:LEU:O	2:K:326:GLN:HG2	2.14	0.48
2:K:307:ILE:HD13	2:K:323:ILE:HG12	1.96	0.48
2:K:194:ALA:HA	2:K:244:LEU:HD21	1.95	0.48
2:K:664:HIS:CG	2:K:705:LEU:HD11	2.49	0.48
2:E:4:GLN:HA	2:E:115:LEU:HD21	1.95	0.47
2:E:457:GLU:HA	2:E:459:LYS:HE2	1.96	0.47
2:B:427:ILE:HG21	2:B:433:LEU:HD11	1.96	0.47
2:B:3:SER:O	2:B:5:THR:N	2.45	0.47
2:K:255:LEU:HD12	2:K:271:LEU:HB2	1.95	0.47
2:B:21:GLN:HE22	2:B:22:ARG:CG	2.26	0.47
2:B:707:ASP:HA	2:B:711:LEU:HB3	1.97	0.47
2:E:307:ILE:HD13	2:E:323:ILE:HG12	1.96	0.47
2:K:26:VAL:HG12	2:K:165:SER:HA	1.97	0.47
2:E:370:LYS:HB2	2:E:393:ILE:HG21	1.95	0.47
1:G:13:LEU:HD23	1:G:18:ALA:HB2	1.96	0.47
2:B:622:HIS:NE2	2:B:684:ASP:OD2	2.46	0.47
2:K:389:LEU:O	2:K:393:ILE:HG12	2.14	0.47
2:B:304:ILE:HG12	2:B:351:LEU:HD21	1.95	0.47
3:I:140:THR:HG23	3:I:145:LEU:HB2	1.96	0.47
3:L:115:GLU:N	3:L:115:GLU:OE1	2.46	0.47
2:E:437:LEU:HD12	2:E:438:PRO:HD2	1.95	0.47
2:E:255:LEU:HD12	2:E:271:LEU:HB2	1.97	0.47
1:G:235:ASN:O	1:G:236:ASN:HB2	2.15	0.47
2:K:173:PRO:HG2	2:K:189:VAL:HG22	1.97	0.47
2:B:389:LEU:O	2:B:393:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:HD11	1:D:59:GLN:HG3	1.97	0.46
1:D:106:ALA:HB3	2:E:363:LYS:HZ3	1.81	0.46
2:K:718:THR:O	2:K:721:THR:OG1	2.28	0.46
2:K:292:LEU:O	2:K:296:ILE:HG13	2.15	0.46
2:H:229:PHE:HE1	2:H:278:ILE:HG23	1.80	0.46
1:J:106:ALA:HB1	1:J:107:LYS:HB2	1.96	0.46
1:G:106:ALA:N	1:G:107:LYS:HA	2.31	0.46
1:J:14:ASP:OD1	1:J:15:ALA:N	2.40	0.46
1:J:44:ILE:HD11	1:G:59:GLN:HG3	1.98	0.46
2:B:21:GLN:HG3	2:B:22:ARG:N	2.31	0.46
1:D:106:ALA:HA	1:D:107:LYS:HA	1.77	0.46
2:K:622:HIS:NE2	2:K:684:ASP:OD2	2.46	0.46
1:A:77:HIS:O	1:A:79:PRO:HD3	2.16	0.46
2:B:21:GLN:OE1	2:B:22:ARG:HD2	2.16	0.45
2:K:131:HIS:HA	2:K:134:LYS:HD2	1.97	0.45
2:H:389:LEU:O	2:H:393:ILE:HG12	2.17	0.45
3:F:134:MET:HE1	3:F:142:LYS:HG3	1.99	0.45
2:K:537:GLU:O	2:K:539:TRP:N	2.44	0.45
1:A:106:ALA:HB1	1:A:151:THR:CG2	2.47	0.45
1:D:106:ALA:HB1	1:D:107:LYS:HB2	1.99	0.45
1:A:233:LYS:HB3	1:A:234:HIS:H	1.56	0.45
2:K:707:ASP:HA	2:K:711:LEU:HB3	1.99	0.45
2:H:207:ILE:HG23	2:H:208:MET:HG2	1.98	0.45
2:K:170:SER:OG	2:K:171:GLN:N	2.44	0.45
3:L:30:LYS:NZ	4:L:201:GNP:O1B	2.46	0.45
3:F:140:THR:HG23	3:F:145:LEU:HD12	1.99	0.45
2:E:718:THR:O	2:E:721:THR:OG1	2.31	0.45
2:B:23:ARG:HA	2:B:23:ARG:HD3	1.72	0.44
1:D:31:PRO:HG2	1:D:34:LEU:HD13	1.99	0.44
3:L:116:LEU:O	3:L:151:ARG:NH1	2.49	0.44
1:J:113:LEU:O	1:J:120:SER:HB2	2.17	0.44
2:E:537:GLU:O	2:E:539:TRP:N	2.45	0.44
2:E:389:LEU:O	2:E:393:ILE:HG12	2.16	0.44
3:L:37:LEU:HB3	3:L:56:VAL:HG11	1.99	0.44
1:G:82:PRO:HG3	1:G:149:LEU:HB2	1.98	0.44
2:K:465:LEU:HG	2:K:580:LEU:HD23	2.00	0.44
2:E:148:VAL:HG21	2:E:196:THR:HG21	1.98	0.44
2:E:296:ILE:HG23	2:E:300:PRO:HA	2.00	0.44
2:K:334:LEU:HD11	2:K:351:LEU:HD12	1.99	0.44
2:B:558:GLN:HE21	2:B:581:PHE:HZ	1.65	0.44
2:B:21:GLN:NE2	2:B:22:ARG:CD	2.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:PRO:HG2	1:G:34:LEU:HD13	2.00	0.44
3:C:115:GLU:OE1	3:C:115:GLU:N	2.46	0.44
2:B:194:ALA:HA	2:B:244:LEU:HD21	2.00	0.43
1:J:6:VAL:HG21	1:G:34:LEU:HG	1.99	0.43
1:G:97:ALA:HB2	1:G:131:THR:HG22	2.00	0.43
2:H:537:GLU:O	2:H:539:TRP:N	2.47	0.43
3:I:30:LYS:NZ	4:I:201:GNP:O3G	2.39	0.43
1:A:231:ARG:HB2	1:A:233:LYS:HG2	2.00	0.43
3:F:79:ARG:HA	3:F:82:TYR:CD2	2.53	0.43
1:A:106:ALA:HB1	1:A:151:THR:HG21	2.00	0.43
2:K:134:LYS:HB3	2:K:135:ILE:HA	1.99	0.43
2:E:292:LEU:O	2:E:296:ILE:HG13	2.18	0.43
2:E:119:THR:HA	2:E:120:PRO:HD2	1.94	0.43
2:H:675:ILE:HG12	2:H:710:ILE:HG23	2.01	0.43
2:K:11:LYS:HB2	2:K:432:ASN:HD21	1.83	0.43
2:K:212:ARG:HH22	2:K:672:ILE:HG21	1.83	0.43
2:B:21:GLN:NE2	2:B:22:ARG:HD3	2.21	0.43
1:D:146:GLN:HB3	1:D:160:LYS:HA	2.01	0.43
2:K:11:LYS:HE2	2:K:123:TRP:HE1	1.84	0.42
3:C:168:GLU:OE1	3:C:168:GLU:N	2.49	0.42
2:B:23:ARG:HG3	2:B:424:ILE:HG22	2.00	0.42
1:D:150:ILE:HG23	1:D:155:THR:HG22	2.00	0.42
2:B:21:GLN:CD	2:B:22:ARG:N	2.73	0.42
2:B:6:SER:HA	2:B:667:TYR:HD1	1.83	0.42
2:K:329:SER:HA	2:K:330:PRO:HD3	1.84	0.42
2:E:470:ALA:HA	2:E:546:LEU:HD23	2.00	0.42
2:E:360:LEU:HD13	2:E:393:ILE:HD13	2.02	0.42
1:J:106:ALA:HA	1:J:107:LYS:HA	1.77	0.42
2:E:140:TRP:O	2:E:203:ARG:NH1	2.50	0.42
1:J:135:SER:CB	3:L:99:ARG:HD2	2.49	0.42
2:H:360:LEU:HD13	2:H:393:ILE:HD13	2.00	0.42
2:K:143:PHE:CZ	2:K:255:LEU:HD11	2.54	0.42
1:D:258:ARG:HD3	3:F:135:SER:HB3	2.02	0.42
3:F:115:GLU:N	3:F:115:GLU:OE1	2.46	0.42
1:G:123:ILE:HD12	1:G:132:THR:HG21	2.01	0.42
2:K:6:SER:HB3	2:K:438:PRO:HB3	2.01	0.42
2:E:285:LEU:HD21	2:E:315:LEU:HD11	2.01	0.42
2:K:141:ASN:HB3	2:K:196:THR:HA	2.01	0.41
2:E:141:ASN:HB3	2:E:196:THR:HA	2.00	0.41
1:A:113:LEU:O	1:A:120:SER:OG	2.36	0.41
2:B:29:PHE:HA	2:B:29:PHE:HD1	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:29:PHE:CZ	2:K:34:PRO:HG3	2.54	0.41
2:E:103:THR:O	2:E:107:ILE:HG13	2.20	0.41
3:L:37:LEU:HD13	3:L:170:LEU:HD11	2.01	0.41
1:G:46:LYS:HE2	1:G:48:GLN:HE21	1.84	0.41
3:L:100:ILE:HG22	3:L:101:GLY:H	1.80	0.41
1:A:101:LEU:HD11	1:A:111:LEU:HD22	2.02	0.41
1:J:109:LYS:HB2	1:J:150:ILE:HG22	2.01	0.41
2:B:259:THR:HA	2:B:416:LYS:HD2	2.01	0.41
2:H:304:ILE:HG12	2:H:351:LEU:HD21	2.01	0.41
1:D:12:LYS:HE2	1:D:12:LYS:HB3	1.91	0.41
2:B:32:LEU:HB2	2:B:419:TYR:CE1	2.56	0.41
2:B:140:TRP:O	2:B:203:ARG:NH1	2.42	0.41
2:B:26:VAL:C	2:B:28:GLN:H	2.03	0.41
1:A:215:PHE:CZ	1:A:233:LYS:HE2	2.56	0.41
2:K:285:LEU:HD21	2:K:315:LEU:HD11	2.03	0.41
2:H:551:LEU:HD23	2:H:588:LEU:HD13	2.03	0.41
3:C:130:LEU:HA	3:C:131:PRO:HD3	1.92	0.41
3:L:79:ARG:HA	3:L:82:TYR:CD2	2.54	0.41
2:B:21:GLN:O	2:B:22:ARG:HB3	2.21	0.41
2:E:222:GLU:OE1	2:E:222:GLU:N	2.50	0.41
2:B:101:ASP:OD1	2:B:103:THR:OG1	2.30	0.41
2:E:457:GLU:HB3	2:E:458:GLN:H	1.62	0.41
2:E:322:LEU:O	2:E:326:GLN:HG2	2.21	0.41
2:B:718:THR:O	2:B:721:THR:OG1	2.28	0.41
3:I:168:GLU:N	3:I:168:GLU:OE1	2.49	0.41
1:A:106:ALA:O	1:A:153:SER:OG	2.27	0.40
2:K:370:LYS:HB2	2:K:393:ILE:HG21	2.01	0.40
2:K:10:VAL:HG22	2:K:433:LEU:HB3	2.02	0.40
1:J:13:LEU:HD22	1:J:40:LYS:O	2.22	0.40
1:G:125:ASN:HB3	1:G:128:LYS:HB2	2.04	0.40
3:C:158:THR:HG22	3:C:165:GLY:O	2.22	0.40
3:C:22:MET:HE1	3:C:34:LEU:HB2	2.04	0.40
3:I:33:VAL:HG22	3:I:160:ALA:HB2	2.03	0.40
2:H:292:LEU:O	2:H:296:ILE:HG13	2.20	0.40
1:G:107:LYS:HE3	1:G:107:LYS:HB2	1.90	0.40
1:J:109:LYS:N	1:J:150:ILE:O	2.46	0.40
2:K:4:GLN:H	2:K:115:LEU:HD13	1.86	0.40
1:G:81:SER:HA	1:G:82:PRO:HD3	1.91	0.40
1:J:150:ILE:HG23	1:J:155:THR:HG22	2.02	0.40
2:E:10:VAL:HB	2:E:91:PHE:CD1	2.56	0.40

There are no symmetry-related clashes.

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	212/368 (58%)	190 (90%)	22 (10%)	0	100	100
1	D	162/368 (44%)	152 (94%)	10 (6%)	0	100	100
1	G	197/368 (54%)	183 (93%)	13 (7%)	1 (0%)	34	74
1	J	150/368 (41%)	139 (93%)	11 (7%)	0	100	100
2	B	469/739 (64%)	446 (95%)	19 (4%)	4 (1%)	21	63
2	E	527/739 (71%)	503 (95%)	21 (4%)	3 (1%)	30	70
2	H	300/739 (41%)	290 (97%)	10 (3%)	0	100	100
2	K	567/739 (77%)	536 (94%)	25 (4%)	6 (1%)	17	58
3	C	122/175 (70%)	120 (98%)	2 (2%)	0	100	100
3	F	138/175 (79%)	136 (99%)	2 (1%)	0	100	100
3	I	68/175 (39%)	66 (97%)	2 (3%)	0	100	100
3	L	125/175 (71%)	119 (95%)	5 (4%)	1 (1%)	24	65
All	All	3037/5128 (59%)	2880 (95%)	142 (5%)	15 (0%)	34	74

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	454	VAL
2	B	22	ARG
2	B	25	ARG
2	B	27	GLY
2	E	451	PRO
3	L	101	GLY
1	G	80	GLU
2	K	31	ASP
2	E	607	SER
2	K	119	THR
2	K	120	PRO
2	K	121	GLN

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Mol	Chain	Res	Type
2	K	136	SER
2	K	364	ARG
2	B	26	VAL

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	207/333 (62%)	203 (98%)	4 (2%)	65	86
1	D	157/333 (47%)	156 (99%)	1 (1%)	90	96
1	G	193/333 (58%)	190 (98%)	3 (2%)	70	88
1	J	145/333 (44%)	143 (99%)	2 (1%)	74	89
2	B	467/672 (70%)	464 (99%)	3 (1%)	90	96
2	E	512/672 (76%)	507 (99%)	5 (1%)	82	92
2	H	307/672 (46%)	306 (100%)	1 (0%)	94	98
2	K	545/672 (81%)	535 (98%)	10 (2%)	66	87
3	C	113/150 (75%)	113 (100%)	0	100	100
3	F	124/150 (83%)	124 (100%)	0	100	100
3	I	71/150 (47%)	71 (100%)	0	100	100
3	L	118/150 (79%)	114 (97%)	4 (3%)	44	78
All	All	2959/4620 (64%)	2926 (99%)	33 (1%)	80	91

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	THR
1	A	230	ILE
1	A	233	LYS
1	A	262	LEU
1	J	76	THR
1	J	160	LYS
1	G	152	THR

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Mol	Chain	Res	Type
1	G	157	TRP
1	G	241	ARG
1	D	92	THR
2	K	118	ASP
2	K	121	GLN
2	K	122	ILE
2	K	123	TRP
2	K	130	PHE
2	K	158	VAL
2	K	450	ASN
2	K	454	VAL
2	K	457	GLU
2	K	459	LYS
2	E	158	VAL
2	E	452	MET
2	E	454	VAL
2	E	455	GLN
2	E	456	LEU
2	B	21	GLN
2	B	22	ARG
2	B	23	ARG
2	H	691	HIS
3	L	96	ASP
3	L	97	ARG
3	L	98	SER
3	L	168	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	J	146	GLN
1	G	48	GLN
1	D	166	HIS
2	K	21	GLN
2	K	28	GLN
2	K	218	GLN
2	K	342	HIS
2	K	432	ASN
2	K	495	GLN
2	K	664	HIS
2	E	218	GLN

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Mol	Chain	Res	Type
2	E	342	HIS
2	E	495	GLN
2	B	218	GLN
2	B	342	HIS
2	B	640	GLN
2	B	664	HIS
2	H	478	GLN
2	H	495	GLN
2	H	616	GLN
2	H	692	ASN
2	H	704	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GNP	C	201	5	28,34,34	1.88	5 (17%)	33,54,54	2.39	8 (24%)
4	GNP	F	201	5	28,34,34	1.89	5 (17%)	33,54,54	2.39	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GNP	I	201	5	28,34,34	1.88	5 (17%)	33,54,54	2.38	8 (24%)
4	GNP	L	201	5	28,34,34	1.88	5 (17%)	33,54,54	2.37	8 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GNP	C	201	5	-	1/12/38/38	0/3/3/3
4	GNP	F	201	5	-	0/12/38/38	0/3/3/3
4	GNP	I	201	5	-	0/12/38/38	0/3/3/3
4	GNP	L	201	5	-	1/12/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	GNP	PB-O3A	-5.28	1.52	1.59
4	F	201	GNP	PB-O3A	-5.27	1.52	1.59
4	L	201	GNP	PB-O3A	-5.23	1.52	1.59
4	I	201	GNP	PB-O3A	-5.15	1.52	1.59
4	I	201	GNP	PB-O2B	-2.95	1.48	1.56
4	C	201	GNP	PB-O2B	-2.94	1.48	1.56
4	F	201	GNP	PB-O2B	-2.94	1.48	1.56
4	L	201	GNP	PB-O2B	-2.91	1.48	1.56
4	C	201	GNP	PB-O1B	2.03	1.48	1.46
4	L	201	GNP	PB-O1B	2.08	1.48	1.46
4	F	201	GNP	PB-O1B	2.09	1.48	1.46
4	I	201	GNP	PB-O1B	2.09	1.48	1.46
4	C	201	GNP	C6-N1	3.55	1.39	1.33
4	L	201	GNP	C6-N1	3.56	1.39	1.33
4	F	201	GNP	C6-N1	3.57	1.39	1.33
4	I	201	GNP	C6-N1	3.61	1.39	1.33
4	C	201	GNP	PG-O1G	4.57	1.51	1.46
4	L	201	GNP	PG-O1G	4.60	1.51	1.46
4	I	201	GNP	PG-O1G	4.62	1.51	1.46
4	F	201	GNP	PG-O1G	4.66	1.51	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	201	GNP	C5-C6-N1	-8.71	111.68	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	201	GNP	C5-C6-N1	-8.70	111.70	123.59
4	C	201	GNP	C5-C6-N1	-8.67	111.74	123.59
4	I	201	GNP	C5-C6-N1	-8.66	111.75	123.59
4	C	201	GNP	PA-O3A-PB	-3.72	120.18	132.67
4	F	201	GNP	PA-O3A-PB	-3.62	120.54	132.67
4	L	201	GNP	PA-O3A-PB	-3.52	120.86	132.67
4	I	201	GNP	PA-O3A-PB	-3.51	120.90	132.67
4	I	201	GNP	O3G-PG-O1G	-3.17	105.08	113.49
4	C	201	GNP	O3G-PG-O1G	-3.16	105.08	113.49
4	F	201	GNP	O3G-PG-O1G	-3.14	105.14	113.49
4	L	201	GNP	O3G-PG-O1G	-3.12	105.21	113.49
4	F	201	GNP	N3-C2-N1	-2.28	123.97	127.44
4	F	201	GNP	O1G-PG-N3B	-2.27	108.42	111.90
4	I	201	GNP	N3-C2-N1	-2.26	124.00	127.44
4	C	201	GNP	N3-C2-N1	-2.26	124.01	127.44
4	L	201	GNP	N3-C2-N1	-2.25	124.02	127.44
4	I	201	GNP	O1G-PG-N3B	-2.21	108.50	111.90
4	L	201	GNP	O1G-PG-N3B	-2.14	108.62	111.90
4	C	201	GNP	O1G-PG-N3B	-2.07	108.73	111.90
4	I	201	GNP	O3G-PG-O2G	2.77	115.79	107.58
4	F	201	GNP	O3G-PG-O2G	2.77	115.80	107.58
4	L	201	GNP	O3G-PG-O2G	2.78	115.81	107.58
4	C	201	GNP	O3G-PG-O2G	2.79	115.84	107.58
4	I	201	GNP	O2B-PB-O1B	3.79	117.92	110.00
4	L	201	GNP	O2B-PB-O1B	3.83	118.00	110.00
4	C	201	GNP	O2B-PB-O1B	3.84	118.01	110.00
4	F	201	GNP	O2B-PB-O1B	3.90	118.14	110.00
4	I	201	GNP	C6-N1-C2	6.42	124.85	115.94
4	L	201	GNP	C6-N1-C2	6.45	124.90	115.94
4	F	201	GNP	C6-N1-C2	6.45	124.90	115.94
4	C	201	GNP	C6-N1-C2	6.46	124.90	115.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	201	GNP	O1B-PB-N3B-PG
4	L	201	GNP	O1B-PB-N3B-PG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	201	GNP	1	0
4	I	201	GNP	1	0
4	L	201	GNP	1	0

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, 95th 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	226/368 (61%)	0.30	8 (3%) 48 47	63, 102, 153, 199	0
1	D	171/368 (46%)	0.65	16 (9%) 11 11	58, 103, 174, 290	0
1	G	211/368 (57%)	0.61	21 (9%) 9 10	61, 108, 176, 203	0
1	J	158/368 (42%)	0.44	13 (8%) 14 14	62, 93, 159, 233	0
2	B	507/739 (68%)	0.26	14 (2%) 56 57	24, 102, 149, 204	0
2	E	557/739 (75%)	0.17	10 (1%) 71 71	53, 90, 147, 273	0
2	H	338/739 (45%)	0.55	38 (11%) 7 6	86, 133, 179, 213	0
2	K	593/739 (80%)	0.20	13 (2%) 65 65	53, 79, 143, 231	0
3	C	134/175 (76%)	0.37	9 (6%) 21 21	79, 123, 176, 197	0
3	F	146/175 (83%)	0.53	11 (7%) 17 18	76, 118, 157, 185	0
3	I	86/175 (49%)	0.79	16 (18%) 2 2	92, 127, 179, 204	0
3	L	139/175 (79%)	0.69	16 (11%) 6 6	24, 115, 147, 174	0
All	All	3266/5128 (63%)	0.36	185 (5%) 27 27	24, 103, 163, 290	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	187	LEU	7.4
3	F	121	TRP	6.5
1	D	106	ALA	6.0
1	G	243	GLU	6.0
2	E	628	ASP	5.5
3	I	88	VAL	5.4
3	C	87	GLY	5.3
1	J	38	ASN	4.9
1	D	92	THR	4.8
3	F	63	PHE	4.6
2	B	250	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
3	L	124	PHE	4.6
2	H	196	THR	4.6
2	E	118	ASP	4.6
2	B	433	LEU	4.5
1	J	145	PHE	4.4
1	J	96	LEU	4.3
3	L	122	LEU	4.3
1	G	215	PHE	4.2
1	D	263	ASP	4.2
1	J	92	THR	4.1
2	H	202	VAL	4.1
1	G	199	ILE	4.0
2	K	458	GLN	4.0
1	G	242	PRO	3.9
3	C	153	TRP	3.8
1	G	72	GLU	3.8
3	I	69	GLY	3.8
3	L	121	TRP	3.8
2	H	610	CYS	3.8
3	L	140	THR	3.7
1	G	103	LEU	3.7
1	A	104	GLY	3.6
2	H	189	VAL	3.6
3	I	21	LEU	3.5
3	C	63	PHE	3.5
3	F	65	VAL	3.4
2	K	219	ASN	3.4
3	C	21	LEU	3.4
3	F	141	GLU	3.4
1	G	49	VAL	3.4
1	J	106	ALA	3.4
1	D	143	TYR	3.3
2	H	192	ILE	3.3
2	H	659	ILE	3.3
2	H	256	ASP	3.3
1	G	238	PRO	3.3
2	H	502	LYS	3.2
3	F	166	LEU	3.2
2	H	556	ASP	3.2
1	D	139	VAL	3.1
2	K	564	PHE	3.1
1	D	164	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	155	ILE	3.0
1	D	40	LYS	3.0
3	L	166	LEU	3.0
1	G	84	LEU	3.0
1	J	39	VAL	3.0
1	J	97	ALA	3.0
2	H	493	TRP	3.0
3	C	88	VAL	3.0
3	I	91	VAL	3.0
1	J	98	TRP	3.0
2	E	139	SER	3.0
2	B	10	VAL	3.0
2	E	458	GLN	2.9
3	I	93	ASP	2.9
2	K	456	LEU	2.9
2	B	666	TRP	2.9
3	L	142	LYS	2.9
2	K	440	ASP	2.8
1	J	140	ASP	2.8
3	I	90	PHE	2.8
1	G	239	ILE	2.8
2	H	710	ILE	2.8
2	H	553	THR	2.8
3	I	145	LEU	2.8
2	K	557	TRP	2.8
2	H	552	LYS	2.8
3	L	145	LEU	2.8
1	J	112	ILE	2.8
2	H	607	SER	2.8
3	C	22	MET	2.7
1	D	262	LEU	2.7
2	H	232	GLY	2.7
2	B	344	GLN	2.7
2	B	654	ASP	2.7
2	H	549	GLU	2.7
2	K	91	PHE	2.6
3	L	148	ILE	2.6
3	L	63	PHE	2.6
1	A	176	VAL	2.6
1	D	81	SER	2.6
2	B	421	LEU	2.6
1	A	49	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	347	PHE	2.6
3	I	123	VAL	2.6
2	H	678	LEU	2.6
1	G	106	ALA	2.6
2	H	500	ARG	2.6
2	K	20	HIS	2.6
2	H	501	SER	2.6
2	K	151	ILE	2.6
1	D	93	SER	2.6
2	H	199	SER	2.6
1	G	159	GLU	2.6
3	F	153	TRP	2.5
2	H	344	GLN	2.5
2	E	624	ARG	2.5
2	H	488	VAL	2.5
2	H	254	TYR	2.5
1	G	190	LEU	2.5
3	F	142	LYS	2.5
2	E	20	HIS	2.5
2	K	150	ILE	2.5
1	D	159	GLU	2.5
2	E	4	GLN	2.5
2	E	91	PHE	2.4
3	L	90	PHE	2.4
1	A	63	PHE	2.4
1	J	139	VAL	2.4
2	H	345	LEU	2.4
2	H	255	LEU	2.4
1	G	82	PRO	2.4
3	L	67	ASP	2.4
3	I	35	TYR	2.4
1	G	216	VAL	2.4
2	H	198	MET	2.4
1	G	240	VAL	2.4
3	L	137	ALA	2.3
1	G	230	ILE	2.3
1	A	103	LEU	2.3
3	C	81	TYR	2.3
1	A	158	SER	2.3
2	B	140	TRP	2.3
2	H	654	ASP	2.3
2	B	189	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	K	234	LEU	2.3
2	H	416	LYS	2.3
2	K	560	GLU	2.3
2	B	462	ASP	2.3
2	E	138	SER	2.3
1	G	245	VAL	2.3
3	C	172	TRP	2.3
2	B	263	ASN	2.2
1	J	84	LEU	2.2
3	I	157	ALA	2.2
3	L	155	ILE	2.2
2	B	6	SER	2.2
2	H	554	TYR	2.2
3	I	33	VAL	2.2
1	D	94	CYS	2.2
3	L	141	GLU	2.2
1	J	153	SER	2.2
3	F	56	VAL	2.2
3	I	74	ILE	2.2
3	F	90	PHE	2.2
1	G	45	ILE	2.2
1	D	257	VAL	2.2
2	B	662	TRP	2.1
3	F	68	VAL	2.1
3	L	95	ASN	2.1
2	E	644	SER	2.1
2	H	475	SER	2.1
3	I	81	TYR	2.1
3	L	116	LEU	2.1
1	D	259	GLY	2.1
2	B	334	LEU	2.1
1	D	168	MET	2.1
3	F	136	ALA	2.1
1	A	177	CYS	2.1
2	H	609	VAL	2.1
3	I	82	TYR	2.1
2	H	663	ASN	2.1
1	D	38	ASN	2.1
3	I	48	THR	2.1
1	G	76	THR	2.1
1	G	244	TRP	2.1
2	H	203	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	626	ARG	2.0
3	I	169	GLY	2.0
2	H	622	HIS	2.0
2	H	504	PHE	2.0
2	H	674	LEU	2.0
1	A	274	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
5	MG	L	202	1/1	0.97	0.18	-0.39	51,51,51,51	0
4	GNP	C	201	32/32	0.95	0.15	-0.87	53,82,103,108	0
4	GNP	L	201	32/32	0.93	0.18	-0.90	86,112,138,201	0
4	GNP	F	201	32/32	0.94	0.15	-1.07	98,129,153,381	0
4	GNP	I	201	32/32	0.96	0.15	-1.15	50,94,122,244	0
5	MG	C	202	1/1	0.91	0.16	-1.56	60,60,60,60	0
5	MG	I	202	1/1	0.98	0.11	-	83,83,83,83	0
5	MG	F	202	1/1	0.97	0.19	-	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.