



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:27 PM GMT

PDB ID : 4RRP  
Title : Crystal Structure of the Fab complexed with antigen Asflp, Northeast Structural Genomics Consortium (NESG) Target PdR16  
Authors : Kuzin, A.; Lew, S.; Seetharaman, J.; Mao, L.; Xiao, R.; Oconnell, P.T.; Maglaqui, M.; Bailey, L.; Everett, J.K.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Chaperone-Enabled Studies of Epigenetic Regulation Enzymes (CEBS); Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2014-11-06  
Resolution : 2.79 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](mailto: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.

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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

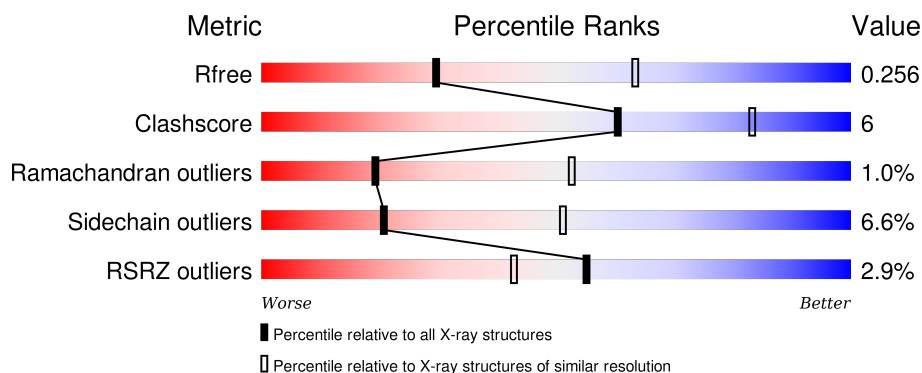
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	216	<div> <div>83%</div> <div>14% ..</div> </div>
1	B	216	<div> <div>85%</div> <div>14%</div> </div>
1	C	216	<div> <div>%</div> <div>73%</div> <div>22% . .</div> </div>
1	D	216	<div> <div>85%</div> <div>14% .</div> </div>
1	E	216	<div> <div>%</div> <div>79%</div> <div>20% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	216	
2	G	238	
2	H	238	
2	I	238	
2	J	238	
2	K	238	
2	L	238	
3	M	160	
3	N	160	
3	O	160	
3	P	160	
3	Q	160	
3	R	160	

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
4	PEG	A	701	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27161 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 Fab antibody, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	2	0
			1655	1035	282	333	5			
1	B	216	Total	C	N	O	S	0	0	0
			1656	1035	278	336	7			
1	C	212	Total	C	N	O	S	0	0	0
			1627	1019	274	329	5			
1	D	214	Total	C	N	O	S	0	1	0
			1650	1032	279	333	6			
1	E	214	Total	C	N	O	S	0	0	0
			1642	1027	276	334	5			
1	F	214	Total	C	N	O	S	0	0	0
			1642	1027	276	333	6			

- Molecule 2 is a protein called Fab antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	219	Total	C	N	O	S	0	1	0
			1633	1031	272	323	7			
2	H	221	Total	C	N	O	S	0	1	0
			1651	1041	276	328	6			
2	I	220	Total	C	N	O	S	0	0	0
			1634	1032	271	325	6			
2	J	222	Total	C	N	O	S	0	0	0
			1646	1038	273	328	7			
2	K	214	Total	C	N	O	S	0	0	0
			1598	1012	264	316	6			
2	L	214	Total	C	N	O	S	0	0	0
			1599	1012	264	316	7			

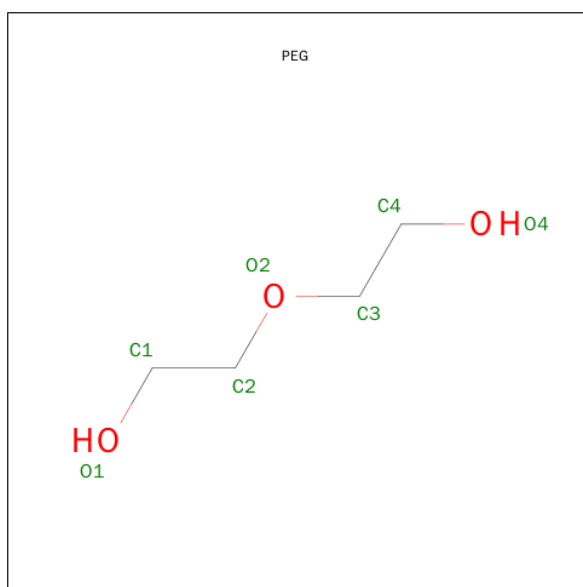
- Molecule 3 is a protein called Antigen Asf1p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	153	Total	C	N	O	S	0	0	0
			1222	784	198	238	2			
3	N	152	Total	C	N	O	S	0	1	0
			1225	788	199	236	2			
3	O	153	Total	C	N	O	S	0	0	0
			1218	781	196	239	2			
3	P	156	Total	C	N	O	S	0	1	0
			1252	802	206	242	2			
3	Q	153	Total	C	N	O	S	0	1	0
			1234	794	201	237	2			
3	R	143	Total	C	N	O	S	0	0	0
			1147	737	187	221	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	GLY	-	EXPRESSION TAG	UNP E7KE71
M	1	SER	-	EXPRESSION TAG	UNP E7KE71
N	0	GLY	-	EXPRESSION TAG	UNP E7KE71
N	1	SER	-	EXPRESSION TAG	UNP E7KE71
O	0	GLY	-	EXPRESSION TAG	UNP E7KE71
O	1	SER	-	EXPRESSION TAG	UNP E7KE71
P	0	GLY	-	EXPRESSION TAG	UNP E7KE71
P	1	SER	-	EXPRESSION TAG	UNP E7KE71
Q	0	GLY	-	EXPRESSION TAG	UNP E7KE71
Q	1	SER	-	EXPRESSION TAG	UNP E7KE71
R	0	GLY	-	EXPRESSION TAG	UNP E7KE71
R	1	SER	-	EXPRESSION TAG	UNP E7KE71

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	G	22	Total	O	0	0
			22	22		
5	B	20	Total	O	0	0
			20	20		
5	H	27	Total	O	0	0
			27	27		
5	C	15	Total	O	0	0
			15	15		
5	I	14	Total	O	0	0
			14	14		
5	D	16	Total	O	0	0
			16	16		
5	J	21	Total	O	0	0
			21	21		
5	K	3	Total	O	0	0
			3	3		
5	F	3	Total	O	0	0
			3	3		
5	L	2	Total	O	0	0
			2	2		

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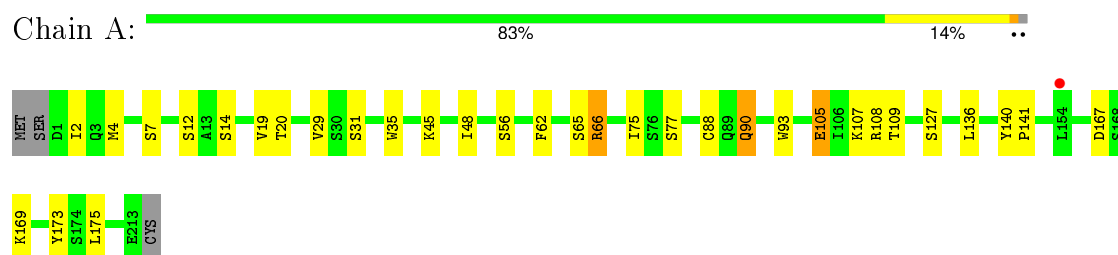
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	10	Total 10	O 10	0	0
5	N	15	Total 15	O 15	0	0
5	O	16	Total 16	O 16	0	0
5	P	13	Total 13	O 13	0	0
5	Q	3	Total 3	O 3	0	0
5	R	2	Total 2	O 2	0	0

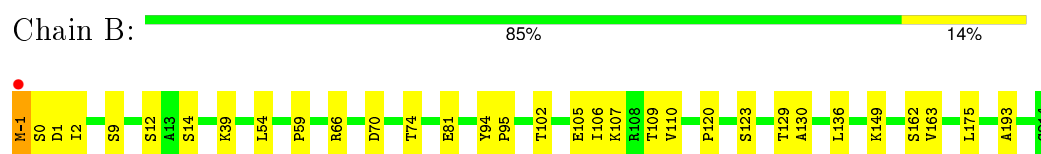
### 3 Residue-property plots

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.

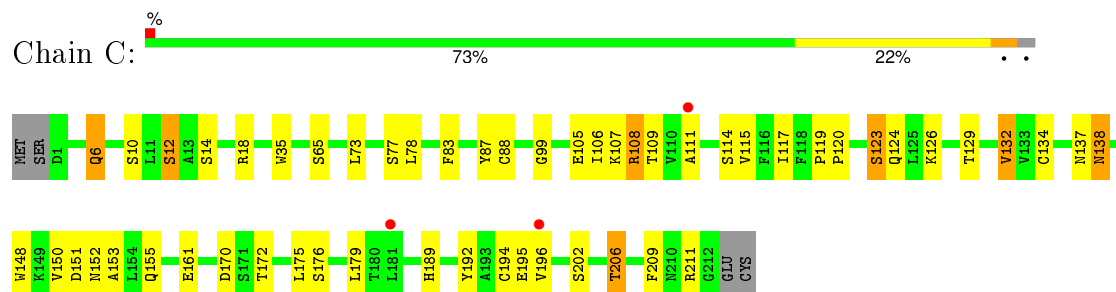
- Molecule 1: Fab antibody, light chain



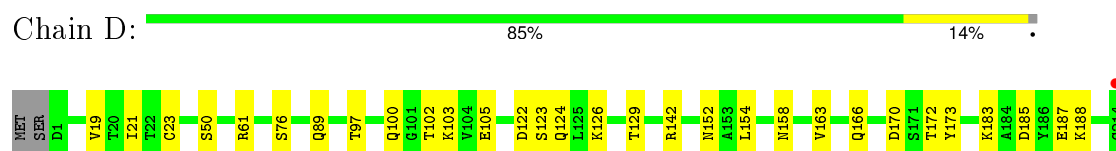
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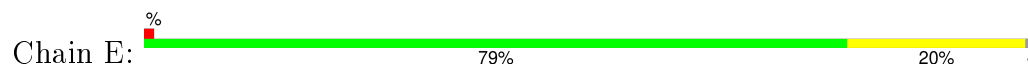
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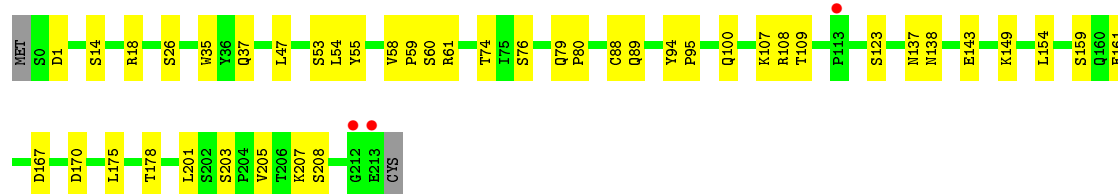
- Molecule 1: Fab antibody, light chain



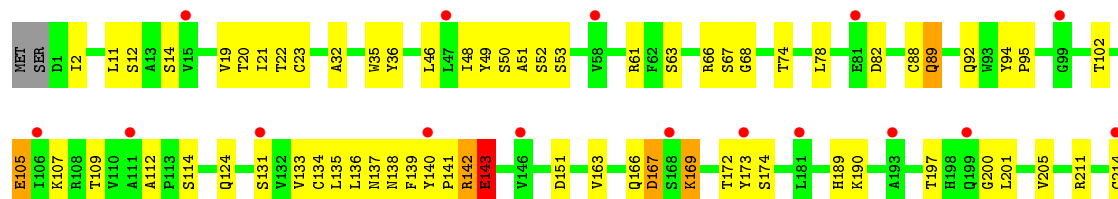
- Molecule 1: Fab antibody, light chain



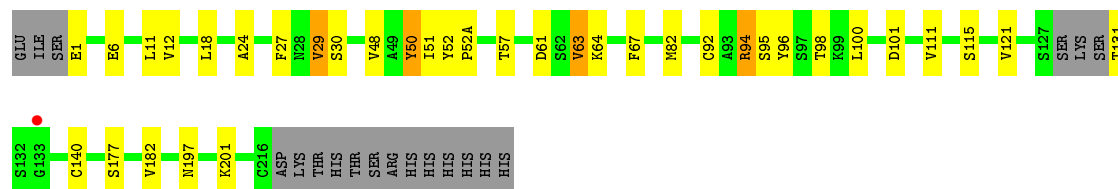
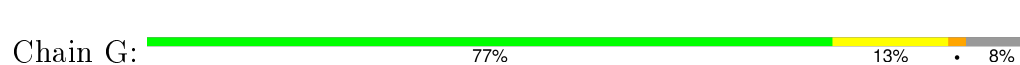




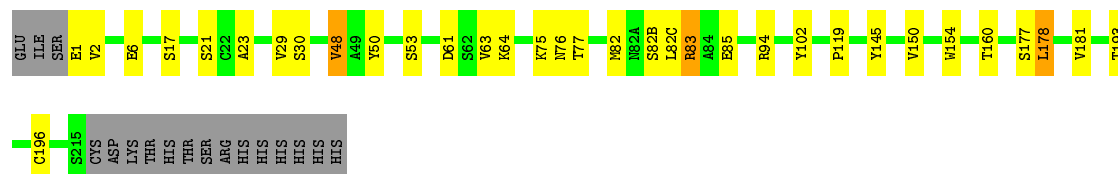
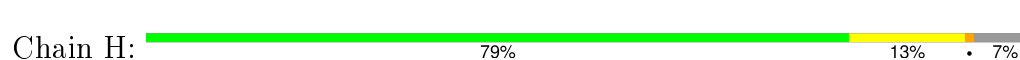
- Molecule 1: Fab antibody, light chain



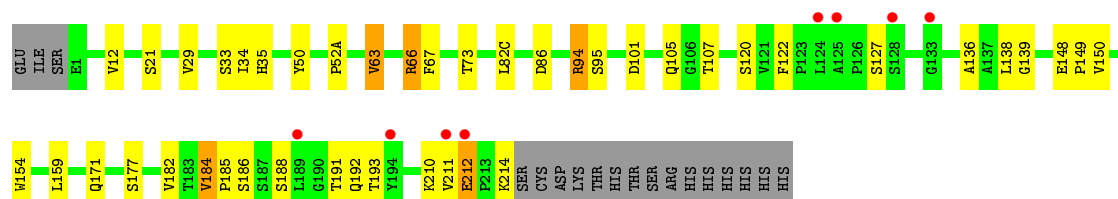
- Molecule 2: Fab antibody, heavy chain



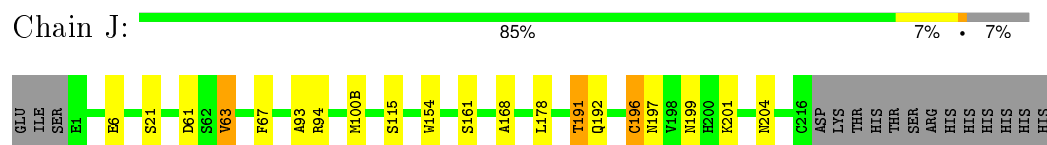
- Molecule 2: Fab antibody, heavy chain



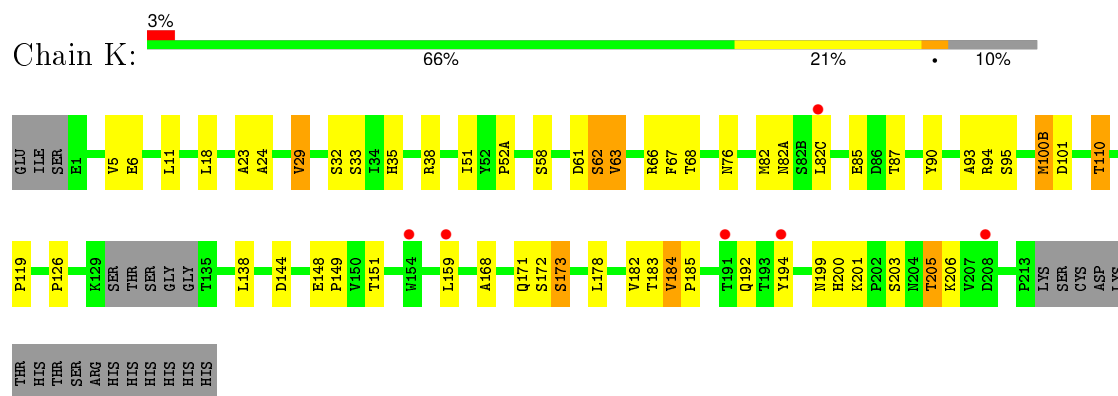
- Molecule 2: Fab antibody, heavy chain



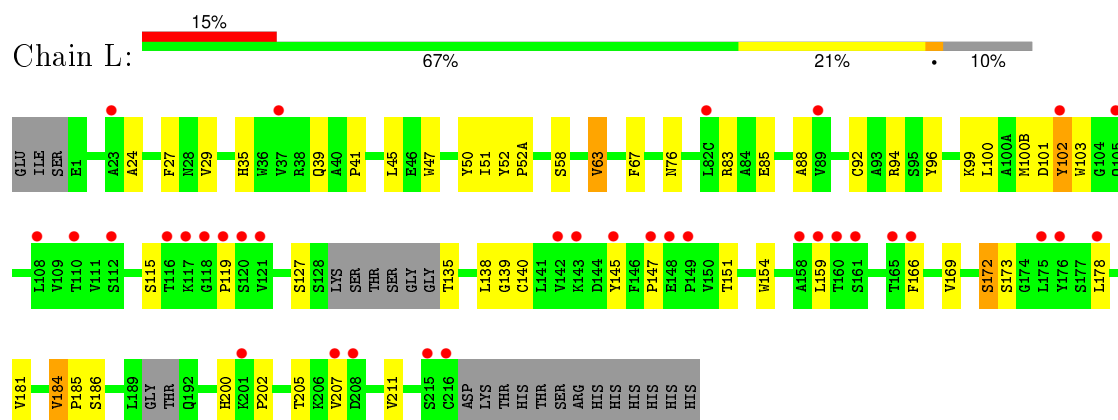
- Molecule 2: Fab antibody, heavy chain



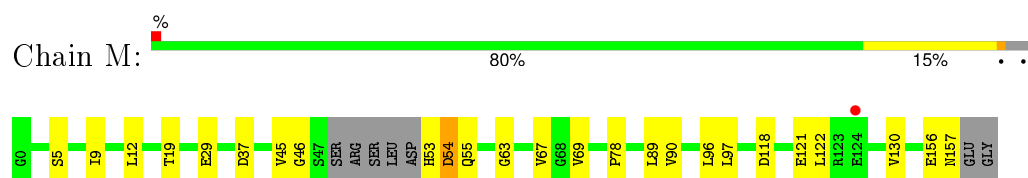
- Molecule 2: Fab antibody, heavy chain



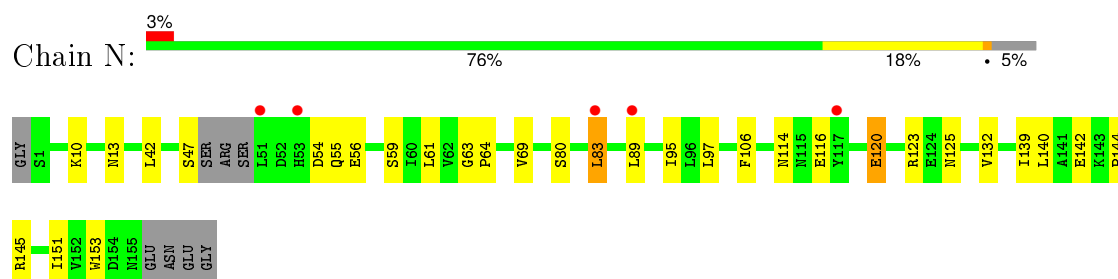
- Molecule 2: Fab antibody, heavy chain



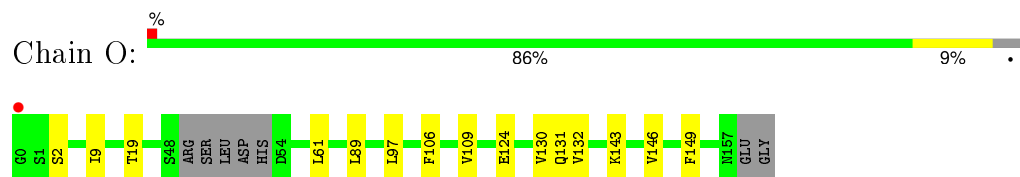
- Molecule 3: Antigen Asf1p



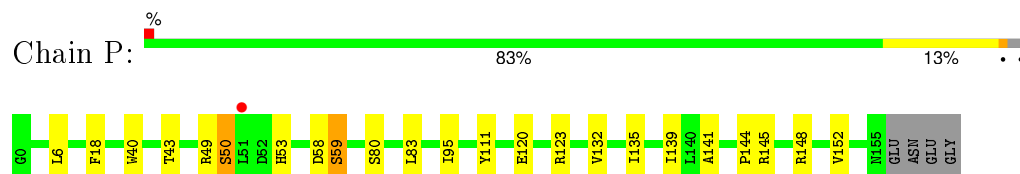
- Molecule 3: Antigen Asf1p



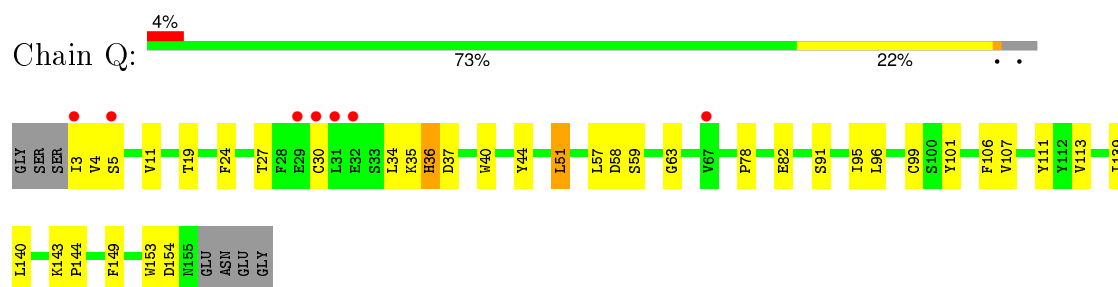
- Molecule 3: Antigen Asf1p



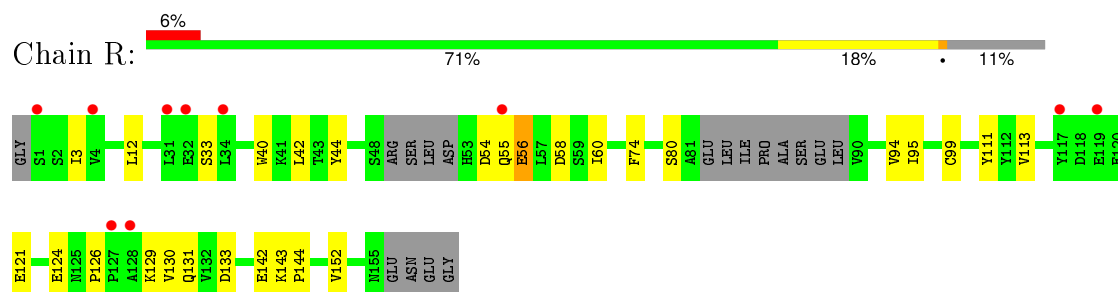
- Molecule 3: Antigen Asf1p



- Molecule 3: Antigen Asf1p



- Molecule 3: Antigen Asf1p



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.72Å 181.31Å 259.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 2.79 49.69 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.69-2.79) 99.4 (49.69-2.79)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.94 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, $R_{free}$	0.183 , 0.253 0.192 , 0.256	Depositor DCC
$R_{free}$ test set	1999 reflections (1.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 108487 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	27161	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

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	0.50	0/1694	0.60	0/2299
1	B	0.52	0/1692	0.60	1/2297 (0.0%)
1	C	0.49	0/1663	0.59	0/2259
1	D	0.52	0/1689	0.61	0/2293
1	E	0.41	0/1678	0.53	0/2279
1	F	0.37	0/1678	0.55	0/2279
2	G	0.53	0/1675	0.63	0/2283
2	H	0.51	0/1691	0.60	1/2305 (0.0%)
2	I	0.51	0/1674	0.67	2/2283 (0.1%)
2	J	0.53	0/1686	0.64	0/2299
2	K	0.38	0/1637	0.51	0/2233
2	L	0.38	0/1637	0.54	0/2231
3	M	0.50	0/1250	0.60	0/1704
3	N	0.47	0/1256	0.61	0/1712
3	O	0.51	0/1245	0.60	0/1697
3	P	0.52	0/1284	0.59	0/1750
3	Q	0.40	0/1266	0.55	0/1727
3	R	0.40	0/1173	0.55	0/1597
All	All	0.47	0/27568	0.59	4/37527 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	138	LEU	CA-CB-CG	5.95	128.97	115.30
2	I	66	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	66	ARG	NE-CZ-NH1	-5.16	117.72	120.30
2	H	178	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	-1	MET	Peptide

## 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	1655	0	1619	18	0
1	B	1656	0	1613	17	0
1	C	1627	0	1588	25	0
1	D	1650	0	1612	12	0
1	E	1642	0	1599	17	0
1	F	1642	0	1599	37	0
2	G	1633	0	1601	16	0
2	H	1651	0	1619	15	0
2	I	1634	0	1602	20	0
2	J	1646	0	1612	8	0
2	K	1598	0	1565	36	0
2	L	1599	0	1564	27	0
3	M	1222	0	1197	12	0
3	N	1225	0	1210	13	0
3	O	1218	0	1195	5	0
3	P	1252	0	1237	11	0
3	Q	1234	0	1221	16	0
3	R	1147	0	1124	12	0
4	A	7	0	10	3	0
5	A	21	0	0	0	0
5	B	20	0	0	0	0
5	C	15	0	0	0	0
5	D	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	3	0	0	0	0
5	G	22	0	0	1	0
5	H	27	0	0	0	0
5	I	14	0	0	0	0
5	J	21	0	0	0	0
5	K	3	0	0	0	0
5	L	2	0	0	0	0
5	M	10	0	0	0	0
5	N	15	0	0	0	0
5	O	16	0	0	0	0
5	P	13	0	0	0	0
5	Q	3	0	0	0	0
5	R	2	0	0	0	0
All	All	27161	0	26387	301	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 6.

All (301) 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:C:189:HIS:O	1:C:211:ARG:NH1	2.12	0.81
3:Q:35:LYS:O	3:Q:36:HIS:ND1	2.17	0.76
1:F:214:CYS:HG	2:L:127:SER:HG	1.34	0.75
1:F:12:SER:HB2	1:F:107:LYS:HD3	1.70	0.73
1:C:120:PRO:HD3	1:C:132:VAL:HG13	1.70	0.73
1:E:167:ASP:HB3	1:E:170:ASP:HB3	1.70	0.72
3:P:132:VAL:HA	3:P:135:ILE:HD12	1.72	0.70
1:C:12:SER:HB2	1:C:107:LYS:HE3	1.72	0.69
2:G:61:ASP:HA	2:G:64:LYS:HD3	1.74	0.69
1:C:195:GLU:HB2	1:C:206:THR:HG23	1.72	0.69
2:K:62:SER:O	2:K:66:ARG:NH2	2.26	0.68
2:K:148:GLU:HG2	2:K:149:PRO:HA	1.75	0.68
2:G:63:VAL:HG13	2:G:67:PHE:HB2	1.76	0.68
2:I:29:VAL:HG13	2:I:52(A):PRO:HG2	1.76	0.67
2:G:29:VAL:HG13	2:G:52(A):PRO:HG2	1.77	0.67
2:J:63:VAL:HG13	2:J:67:PHE:HB2	1.78	0.66
3:P:95:ILE:HG22	3:P:111:TYR:HB2	1.78	0.66
2:I:66:ARG:NH2	2:I:86:ASP:OD2	2.28	0.65
2:H:82:MET:HE2	2:H:82(C):LEU:HD21	1.76	0.65
2:L:119:PRO:HB3	2:L:145:TYR:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:ILE:HG23	1:F:53:SER:H	1.62	0.64
1:F:36:TYR:OH	1:F:89:GLN:NE2	2.31	0.64
1:C:137:ASN:OD1	1:C:138:ASN:ND2	2.31	0.64
3:O:109:VAL:HG22	3:O:146:VAL:HG22	1.80	0.63
2:I:154:TRP:HZ3	2:I:211:VAL:HG21	1.63	0.63
2:I:184:VAL:HG22	2:I:185:PRO:HD2	1.80	0.62
2:K:144:ASP:OD1	2:K:171:GLN:NE2	2.30	0.62
1:E:37:GLN:HB2	1:E:47:LEU:HD11	1.81	0.62
2:L:63:VAL:HG13	2:L:67:PHE:HB2	1.82	0.61
2:H:23:ALA:HA	2:H:77:THR:HG22	1.82	0.61
1:F:23:CYS:HB2	1:F:35:TRP:CH2	2.36	0.61
1:B:-1:MET:HB2	1:B:95:PRO:HD3	1.82	0.61
2:L:184:VAL:HG22	2:L:185:PRO:HD2	1.83	0.61
1:B:136:LEU:HD22	1:B:175:LEU:HD22	1.83	0.61
3:Q:37:ASP:HB3	3:Q:63:GLY:HA3	1.83	0.60
3:O:124:GLU:HA	3:Q:51:LEU:HD11	1.81	0.60
1:A:90:GLN:OE1	1:A:93:TRP:N	2.28	0.60
2:K:168:ALA:HA	2:K:178:LEU:HB3	1.84	0.59
1:C:115:VAL:HG21	1:C:196:VAL:HG21	1.84	0.59
2:K:119:PRO:HD2	2:K:205:THR:HG21	1.84	0.59
1:B:-1:MET:H2	1:B:1:ASP:H	1.50	0.59
3:N:120:GLU:HA	3:N:123[A]:ARG:HE	1.66	0.59
2:K:151:THR:HB	2:K:199:ASN:HB3	1.86	0.58
2:K:171:GLN:O	2:K:173:SER:N	2.36	0.58
2:I:136:ALA:HB2	2:I:186:SER:HB3	1.85	0.58
2:L:135:THR:N	2:L:186:SER:HG	2.03	0.57
1:E:18:ARG:HG3	1:E:76:SER:HA	1.86	0.56
3:Q:111:TYR:CE2	3:Q:144:PRO:HB3	2.41	0.56
1:F:66:ARG:NH2	1:F:68:GLY:O	2.36	0.56
3:P:80:SER:HB3	3:P:83:LEU:HD12	1.86	0.56
1:F:135:LEU:HD21	1:F:137:ASN:HB2	1.88	0.56
2:K:168:ALA:HB2	2:K:178:LEU:HD23	1.88	0.55
1:A:62:PHE:HE2	4:A:701:PEG:H42	1.71	0.55
3:N:139:ILE:H	3:N:139:ILE:HD12	1.73	0.54
2:L:138:LEU:HB2	2:L:211:VAL:HG11	1.88	0.54
3:P:6:LEU:H	3:P:148[B]:ARG:HH12	1.56	0.54
1:C:83:PHE:CZ	1:C:106:ILE:HG13	2.43	0.54
1:A:35:TRP:HD1	1:A:48:ILE:HD11	1.73	0.54
3:M:45:VAL:HG22	3:M:53:HIS:HA	1.89	0.53
1:D:21:ILE:HG12	1:D:102:THR:HG21	1.91	0.53
3:N:106:PHE:HB3	3:N:151:ILE:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:154:TRP:HB2	2:L:159:LEU:HB3	1.91	0.53
1:D:166:GLN:HG3	1:D:173:TYR:CZ	2.44	0.53
3:R:129:LYS:O	3:R:131:GLN:N	2.42	0.53
2:G:96:TYR:O	2:G:98:THR:HG23	2.09	0.53
1:C:170:ASP:OD1	1:C:172:THR:OG1	2.19	0.52
1:F:124:GLN:OE1	1:F:131:SER:N	2.43	0.52
1:A:105:GLU:HG3	1:A:173:TYR:OH	2.10	0.52
2:L:94:ARG:HH21	2:L:96:TYR:HD2	1.58	0.52
3:N:80:SER:HB2	3:N:83:LEU:HD22	1.92	0.52
2:L:27:PHE:CZ	2:L:94:ARG:HD2	2.45	0.52
3:M:9:ILE:HD13	3:M:97:LEU:HD23	1.91	0.52
1:E:138:ASN:ND2	1:E:170:ASP:OD2	2.43	0.52
3:P:120:GLU:OE1	3:P:123:ARG:NH2	2.43	0.52
1:F:142:ARG:NH2	1:F:163:VAL:HG21	2.25	0.52
3:O:9:ILE:HD13	3:O:97:LEU:HD13	1.92	0.52
3:Q:3:ILE:HG13	3:Q:153:TRP:CG	2.45	0.52
1:B:-1:MET:N	1:B:1:ASP:H	2.07	0.52
1:A:62:PHE:CE2	4:A:701:PEG:H42	2.45	0.51
1:A:108:ARG:HG3	1:A:109:THR:O	2.09	0.51
1:D:100:GLN:HB2	5:D:310:HOH:O	2.10	0.51
2:H:48:VAL:HG23	2:H:63:VAL:HG21	1.92	0.51
1:A:29:VAL:O	1:A:66:ARG:NH2	2.43	0.51
2:J:93:ALA:HB1	2:J:100(B):MET:HB3	1.92	0.51
2:H:75:LYS:O	2:H:77:THR:HG23	2.10	0.51
2:L:103:TRP:CD1	2:L:103:TRP:N	2.79	0.51
2:J:191:THR:OG1	2:J:192:GLN:N	2.43	0.51
2:K:200:HIS:HB3	2:K:205:THR:HG23	1.91	0.51
3:R:55:GLN:HG2	3:R:56:GLU:H	1.76	0.51
2:L:63:VAL:HG22	2:L:67:PHE:CD1	2.46	0.51
1:C:153:ALA:O	1:C:155:GLN:NE2	2.40	0.51
1:C:123:SER:O	1:C:126:LYS:HG2	2.11	0.51
1:D:126:LYS:HD2	3:N:61:LEU:HD11	1.93	0.51
3:M:19:THR:O	3:M:78:PRO:HG3	2.11	0.51
1:C:161:GLU:OE2	1:C:175:LEU:HD11	2.10	0.50
2:L:27:PHE:CE2	2:L:94:ARG:HD2	2.45	0.50
2:H:1:GLU:HG3	2:H:2:VAL:H	1.76	0.50
2:K:33:SER:HG	2:K:35:HIS:HE2	1.55	0.50
1:B:12:SER:HB2	1:B:107:LYS:HG3	1.94	0.50
1:C:6:GLN:HG3	1:C:99:GLY:HA3	1.93	0.50
1:E:79:GLN:HB3	1:E:80:PRO:HD2	1.94	0.50
2:I:171:GLN:OE1	2:I:177:SER:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:39:GLN:H	2:L:88:ALA:HB1	1.76	0.50
2:G:48:VAL:HG13	2:G:63:VAL:HG11	1.94	0.49
1:C:6:GLN:OE1	1:C:87:TYR:HA	2.12	0.49
2:K:82:MET:HB3	2:K:82(C):LEU:HD21	1.95	0.49
3:Q:106:PHE:HA	3:Q:149:PHE:HB2	1.95	0.49
3:P:139:ILE:O	3:P:141:ALA:N	2.46	0.49
1:F:63:SER:O	1:F:74:THR:N	2.44	0.49
1:C:124:GLN:HG3	2:I:122:PHE:CE2	2.48	0.49
1:D:122:ASP:O	1:D:126:LYS:HG2	2.13	0.49
2:K:93:ALA:HB1	2:K:100(B):MET:HB2	1.93	0.49
1:A:19:VAL:HG22	1:A:75:ILE:HB	1.94	0.49
3:Q:44:TYR:HB2	3:Q:57:LEU:HD11	1.93	0.49
1:F:23:CYS:HB2	1:F:35:TRP:HH2	1.74	0.49
1:F:35:TRP:CZ3	1:F:88:CYS:HB3	2.48	0.49
1:D:142[A]:ARG:NH2	1:D:163:VAL:HG21	2.28	0.49
1:F:201:LEU:HD13	1:F:205:VAL:HG23	1.94	0.49
1:F:133:VAL:HG12	1:F:134:CYS:H	1.78	0.48
3:R:42:LEU:HD11	3:R:95:ILE:HG23	1.95	0.48
1:E:201:LEU:HD13	1:E:205:VAL:HG23	1.95	0.48
1:A:108:ARG:NH1	1:A:109:THR:O	2.44	0.48
1:F:135:LEU:O	1:F:136:LEU:HD12	2.13	0.48
3:R:94:VAL:O	3:R:95:ILE:HD12	2.13	0.48
2:L:24:ALA:HB3	2:L:76:ASN:ND2	2.28	0.48
2:G:94:ARG:NH2	5:G:821:HOH:O	2.45	0.48
1:F:32:ALA:HB3	1:F:92:GLN:HB2	1.95	0.48
2:I:29:VAL:HG22	2:I:34:ILE:HD11	1.96	0.48
3:M:54:ASP:HB3	3:M:55:GLN:HG3	1.95	0.48
3:Q:4:VAL:HG12	3:Q:30:CYS:HA	1.96	0.48
2:L:200:HIS:CD2	2:L:202:PRO:HD2	2.49	0.48
2:K:87:THR:HG23	2:K:110:THR:HA	1.95	0.48
3:Q:99:CYS:HB3	3:Q:107:VAL:HG12	1.96	0.48
1:D:170:ASP:OD1	1:D:172:THR:OG1	2.30	0.48
1:F:107:LYS:HD2	1:F:140:TYR:OH	2.14	0.47
2:I:94:ARG:HG2	2:I:95:SER:N	2.27	0.47
1:F:167:ASP:C	1:F:169:LYS:H	2.17	0.47
3:M:69:VAL:HG11	3:N:69:VAL:HG11	1.95	0.47
2:K:63:VAL:HG13	2:K:67:PHE:HB2	1.95	0.47
3:M:89:LEU:HD12	3:M:130:VAL:HG11	1.96	0.47
1:F:36:TYR:CE2	1:F:46:LEU:HD13	2.50	0.47
2:L:83:ARG:HB2	2:L:85:GLU:HG2	1.97	0.47
3:R:111:TYR:CE1	3:R:144:PRO:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:113:VAL:HG22	3:Q:139:ILE:HG12	1.97	0.47
3:Q:3:ILE:HB	3:Q:153:TRP:CE2	2.49	0.47
1:F:61:ARG:NE	1:F:82:ASP:OD2	2.42	0.47
1:B:-1:MET:SD	1:B:95:PRO:HG3	2.55	0.46
3:M:29:GLU:OE2	3:N:10:LYS:NZ	2.39	0.46
2:G:24:ALA:HB1	2:G:27:PHE:CE1	2.49	0.46
2:I:212:GLU:C	2:I:214:LYS:H	2.19	0.46
3:N:42:LEU:HD11	3:N:95:ILE:HB	1.97	0.46
3:N:142:GLU:O	3:N:144:PRO:HD3	2.14	0.46
3:Q:40:TRP:O	3:Q:59:SER:HA	2.15	0.46
1:F:21:ILE:HD13	1:F:102:THR:HG21	1.97	0.46
1:B:149:LYS:HB2	1:B:193:ALA:HB3	1.97	0.46
1:E:149:LYS:HG2	1:E:154:LEU:HA	1.97	0.46
1:F:140:TYR:CG	1:F:141:PRO:HA	2.50	0.46
1:A:45:LYS:HD2	4:A:701:PEG:O1	2.14	0.46
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.51	0.46
2:I:148:GLU:HG3	2:I:149:PRO:HA	1.96	0.46
1:D:183:LYS:O	1:D:187:GLU:HG3	2.16	0.46
2:K:206:LYS:HE2	2:K:206:LYS:HB2	1.75	0.46
3:P:111:TYR:CE1	3:P:144:PRO:HB3	2.51	0.46
3:Q:11:VAL:HG22	3:Q:24:PHE:CE2	2.51	0.46
1:C:108:ARG:HH21	1:C:111:ALA:HB2	1.81	0.46
2:L:139:GLY:HA3	2:L:181:VAL:HG12	1.98	0.46
2:L:45:LEU:HA	2:L:45:LEU:HD23	1.70	0.46
1:F:166:GLN:HB2	1:F:173:TYR:CZ	2.51	0.46
1:F:112:ALA:HB2	1:F:200:GLY:O	2.15	0.46
3:R:44:TYR:HB3	3:R:55:GLN:HB3	1.98	0.45
2:K:126:PRO:HG3	2:K:138:LEU:HB3	1.97	0.45
3:P:18:PHE:HB2	3:P:135:ILE:HG22	1.97	0.45
2:H:154:TRP:CZ3	2:H:196:CYS:HB3	2.51	0.45
2:K:32:SER:HB2	2:K:95:SER:O	2.16	0.45
2:K:63:VAL:HG22	2:K:67:PHE:CG	2.52	0.45
1:C:148:TRP:CG	1:C:179:LEU:HD13	2.51	0.45
3:N:114:ASN:OD1	3:N:116:GLU:HG3	2.17	0.45
2:I:193:THR:HG23	2:I:210:LYS:HE3	1.98	0.45
2:J:199:ASN:HD21	2:J:201:LYS:HG3	1.80	0.45
2:I:139:GLY:HA2	2:I:154:TRP:CH2	2.51	0.45
2:L:51:ILE:O	2:L:52(A):PRO:HD3	2.15	0.45
1:E:108:ARG:NH1	1:E:170:ASP:O	2.47	0.45
2:K:33:SER:HG	2:K:35:HIS:CD2	2.34	0.45
2:G:95:SER:OG	2:G:100:LEU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:HIS:O	1:F:211:ARG:HD3	2.17	0.45
3:R:40:TRP:HB2	3:R:60:ILE:HG22	1.97	0.45
2:K:6:GLU:N	2:K:6:GLU:OE1	2.49	0.45
2:K:29:VAL:HG13	2:K:52(A):PRO:HG2	1.99	0.45
1:E:55:TYR:OH	2:K:101:ASP:HB2	2.17	0.45
1:E:35:TRP:CZ3	1:E:88:CYS:HB3	2.51	0.45
2:K:66:ARG:HB3	2:K:82(A):ASN:O	2.17	0.45
1:F:151:ASP:OD1	1:F:189:HIS:HB3	2.17	0.45
2:K:51:ILE:O	2:K:52(A):PRO:HD3	2.17	0.45
2:I:63:VAL:HG13	2:I:67:PHE:HB2	1.98	0.45
1:F:46:LEU:HD21	1:F:49:TYR:HB3	1.99	0.44
1:F:105:GLU:HB2	1:F:166:GLN:HE22	1.82	0.44
1:E:55:TYR:CZ	2:K:101:ASP:HB2	2.53	0.44
2:G:94:ARG:HG2	2:G:95:SER:N	2.33	0.44
3:R:40:TRP:CE3	3:R:99:CYS:HB2	2.53	0.44
2:H:6:GLU:HA	2:H:21:SER:O	2.17	0.44
2:K:184:VAL:HG22	2:K:185:PRO:HD2	1.99	0.44
1:A:12:SER:HB3	1:A:107:LYS:HG3	2.00	0.44
2:H:83[B]:ARG:HB3	2:H:85:GLU:OE2	2.18	0.44
1:F:142:ARG:HD2	1:F:143:GLU:N	2.33	0.43
1:C:117:ILE:HD12	1:C:194:CYS:HB2	1.99	0.43
3:P:95:ILE:HD12	3:P:95:ILE:HA	1.88	0.43
1:B:39:LYS:NZ	1:B:81:GLU:O	2.48	0.43
1:B:9:SER:O	1:B:102:THR:HA	2.17	0.43
1:C:134:CYS:HB2	1:C:148:TRP:CZ2	2.53	0.43
1:A:140:TYR:CG	1:A:141:PRO:HA	2.53	0.43
1:B:120:PRO:HG3	1:B:130:ALA:HB1	1.99	0.43
2:I:188:SER:HB2	2:I:192:GLN:HB3	2.00	0.43
2:L:172:SER:OG	2:L:172:SER:O	2.31	0.43
1:F:105:GLU:HB2	1:F:166:GLN:NE2	2.33	0.43
2:G:51:ILE:HG13	2:G:57:THR:HG22	2.01	0.43
2:G:50:TYR:C	2:G:50:TYR:CD1	2.92	0.43
2:H:2:VAL:HB	2:H:102:TYR:CE2	2.53	0.43
2:I:12:VAL:HG21	2:I:82(C):LEU:HD13	1.99	0.43
2:J:154:TRP:CZ3	2:J:196:CYS:HB3	2.53	0.43
2:J:154:TRP:CH2	2:J:196:CYS:HB3	2.54	0.43
3:M:90:VAL:O	3:M:90:VAL:HG12	2.19	0.43
2:K:203:SER:OG	2:K:205:THR:HG22	2.18	0.43
2:K:200:HIS:HB3	2:K:205:THR:CG2	2.48	0.43
3:R:124:GLU:O	3:R:126:PRO:HD3	2.19	0.43
2:K:24:ALA:O	2:K:76:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASP:OD2	1:A:169:LYS:HG2	2.19	0.43
1:C:83:PHE:CE2	1:C:106:ILE:HA	2.54	0.43
2:L:35:HIS:ND1	2:L:50:TYR:HB3	2.34	0.43
2:G:6:GLU:OE2	2:G:92:CYS:N	2.38	0.43
3:O:106:PHE:HA	3:O:149:PHE:HB2	2.01	0.43
1:C:119:PRO:HB3	1:C:209:PHE:CZ	2.53	0.43
1:B:0:SER:HB2	1:B:94:TYR:O	2.19	0.43
3:N:63:GLY:HA2	3:N:64:PRO:C	2.39	0.42
1:E:59:PRO:HB3	1:E:61:ARG:NH1	2.34	0.42
2:L:99:LYS:O	2:L:100:LEU:HB2	2.19	0.42
3:Q:34:LEU:HD12	3:Q:36:HIS:H	1.84	0.42
1:E:143:GLU:N	1:E:143:GLU:OE2	2.46	0.42
1:D:185:ASP:HA	1:D:188:LYS:HE3	2.00	0.42
1:F:174:SER:HB3	2:L:166:PHE:CZ	2.54	0.42
1:F:94:TYR:HA	1:F:95:PRO:HA	1.77	0.42
1:B:109:THR:HG22	1:B:110:VAL:O	2.19	0.42
2:H:64:LYS:HD3	3:M:67:VAL:O	2.19	0.42
2:H:119:PRO:HB3	2:H:145:TYR:HB3	2.00	0.42
1:A:4:MET:SD	1:A:90:GLN:HB2	2.59	0.42
1:C:124:GLN:HB2	2:I:122:PHE:CG	2.54	0.42
2:H:64:LYS:CG	3:M:67:VAL:HB	2.50	0.42
3:N:13:ASN:N	3:N:13:ASN:OD1	2.48	0.42
2:K:5:VAL:HG22	2:K:23:ALA:HB3	2.01	0.42
1:B:163:VAL:HG22	1:B:175:LEU:HD12	2.01	0.42
2:K:5:VAL:CG2	2:K:23:ALA:HB3	2.49	0.42
2:I:35:HIS:ND1	2:I:50:TYR:HB3	2.35	0.42
1:A:108:ARG:HH11	1:A:108:ARG:HG3	1.84	0.42
2:K:159:LEU:HD21	2:K:182:VAL:HG21	2.01	0.42
2:K:63:VAL:HG22	2:K:67:PHE:CD1	2.55	0.42
1:E:159:SER:HA	1:E:178:THR:O	2.19	0.42
2:K:38:ARG:HD3	2:K:90:TYR:CE2	2.55	0.42
2:G:52:TYR:CE1	3:M:12:LEU:HD13	2.53	0.42
3:P:6:LEU:O	3:P:148[B]:ARG:NH2	2.53	0.42
1:F:19:VAL:HG21	1:F:78:LEU:HD22	2.02	0.42
1:D:61:ARG:HB2	1:D:76:SER:O	2.20	0.42
1:E:161:GLU:OE2	1:E:175:LEU:HD11	2.20	0.42
1:E:54:LEU:HD11	1:E:58:VAL:HG12	2.01	0.42
1:F:50:SER:O	1:F:52:SER:N	2.45	0.42
2:H:29:VAL:HG22	2:H:76:ASN:OD1	2.19	0.42
2:J:168:ALA:HA	2:J:178:LEU:HB3	2.02	0.42
1:F:142:ARG:C	1:F:142:ARG:HD2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:40:TRP:CZ3	3:R:99:CYS:HB2	2.54	0.41
3:P:40:TRP:O	3:P:59:SER:HA	2.20	0.41
2:G:12:VAL:O	2:G:111:VAL:HA	2.20	0.41
1:F:135:LEU:HD13	2:L:181:VAL:HG21	2.01	0.41
2:I:33:SER:OG	2:I:35:HIS:NE2	2.51	0.41
2:G:11:LEU:HD12	2:G:12:VAL:N	2.34	0.41
1:A:136:LEU:HD22	1:A:175:LEU:HD22	2.03	0.41
3:O:89:LEU:HD23	3:O:89:LEU:HA	1.95	0.41
1:C:151:ASP:CG	1:C:189:HIS:HB3	2.41	0.41
3:M:37:ASP:OD1	3:M:63:GLY:HA3	2.20	0.41
3:N:89:LEU:CD2	3:N:132:VAL:HG22	2.51	0.41
2:K:192:GLN:HG3	2:K:194:TYR:CZ	2.55	0.41
1:C:150:VAL:HG13	1:C:192:TYR:CE1	2.55	0.41
2:K:149:PRO:O	2:K:200:HIS:HD2	2.03	0.41
1:B:106:ILE:HD12	1:B:107:LYS:H	1.86	0.41
3:R:95:ILE:HD13	3:R:113:VAL:HG21	2.01	0.41
1:B:81:GLU:OE1	1:B:81:GLU:N	2.38	0.41
2:L:35:HIS:HD1	2:L:47:TRP:HE1	1.69	0.41
3:Q:19:THR:O	3:Q:78:PRO:HG3	2.20	0.41
1:C:35:TRP:CD2	1:C:73:LEU:HB2	2.55	0.41
2:L:52:TYR:CE1	3:R:12:LEU:HB3	2.56	0.41
1:F:36:TYR:HE1	1:F:89:GLN:HB3	1.86	0.40
1:B:-1:MET:HB3	2:H:61:ASP:OD2	2.21	0.40
3:Q:36:HIS:HB2	3:Q:101:TYR:CE1	2.56	0.40
1:A:169:LYS:HG2	1:A:169:LYS:H	1.71	0.40
1:E:94:TYR:HA	1:E:95:PRO:HA	1.77	0.40
1:B:54:LEU:HD12	1:B:54:LEU:HA	1.86	0.40
2:J:6:GLU:HA	2:J:21:SER:O	2.22	0.40
1:D:124:GLN:HG2	1:D:129:THR:O	2.21	0.40
1:D:89:GLN:HA	1:D:97:THR:O	2.21	0.40
2:L:94:ARG:NH1	2:L:101:ASP:OD1	2.54	0.40
1:C:35:TRP:CZ3	1:C:88:CYS:HB3	2.57	0.40
2:I:159:LEU:HD21	2:I:182:VAL:HG21	2.04	0.40
2:H:30:SER:O	2:H:53:SER:HB3	2.21	0.40
2:G:82:MET:HB2	2:G:82:MET:HE2	1.86	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	213/216 (99%)	201 (94%)	10 (5%)	2 (1%)	21	55
1	B	214/216 (99%)	201 (94%)	12 (6%)	1 (0%)	34	69
1	C	210/216 (97%)	197 (94%)	12 (6%)	1 (0%)	34	69
1	D	213/216 (99%)	198 (93%)	15 (7%)	0	100	100
1	E	212/216 (98%)	189 (89%)	22 (10%)	1 (0%)	34	69
1	F	212/216 (98%)	182 (86%)	27 (13%)	3 (1%)	14	42
2	G	216/238 (91%)	212 (98%)	3 (1%)	1 (0%)	34	69
2	H	220/238 (92%)	213 (97%)	7 (3%)	0	100	100
2	I	218/238 (92%)	203 (93%)	14 (6%)	1 (0%)	34	69
2	J	220/238 (92%)	212 (96%)	8 (4%)	0	100	100
2	K	210/238 (88%)	189 (90%)	18 (9%)	3 (1%)	14	42
2	L	208/238 (87%)	184 (88%)	18 (9%)	6 (3%)	6	19
3	M	149/160 (93%)	142 (95%)	3 (2%)	4 (3%)	6	21
3	N	149/160 (93%)	139 (93%)	8 (5%)	2 (1%)	15	44
3	O	149/160 (93%)	142 (95%)	5 (3%)	2 (1%)	15	44
3	P	155/160 (97%)	146 (94%)	8 (5%)	1 (1%)	30	65
3	Q	152/160 (95%)	137 (90%)	14 (9%)	1 (1%)	26	62
3	R	137/160 (86%)	121 (88%)	12 (9%)	4 (3%)	6	19
All	All	3457/3684 (94%)	3208 (93%)	216 (6%)	33 (1%)	19	52

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	172	SER
1	F	138	ASN
2	L	207	VAL
3	O	130	VAL

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Mol	Chain	Res	Type
3	R	3	ILE
3	R	130	VAL
2	K	173	SER
1	F	143	GLU
3	M	118	ASP
1	C	138	ASN
3	M	156	GLU
3	N	55	GLN
3	Q	140	LEU
1	A	31	SER
2	I	191	THR
1	F	51	ALA
2	L	102	TYR
2	L	173	SER
3	O	143	LYS
3	P	50	SER
3	R	121	GLU
1	B	59	PRO
2	L	41	PRO
2	L	172	SER
3	N	153	TRP
3	R	33	SER
1	A	77	SER
2	G	63	VAL
1	E	26	SER
2	K	62	SER
3	M	54	ASP
3	M	46	GLY
2	L	147	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	190/191 (100%)	180 (95%)	10 (5%)	28 61
1	B	191/191 (100%)	183 (96%)	8 (4%)	36 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	187/191 (98%)	168 (90%)	19 (10%)	9	26
1	D	190/191 (100%)	181 (95%)	9 (5%)	32	67
1	E	189/191 (99%)	175 (93%)	14 (7%)	17	43
1	F	189/191 (99%)	171 (90%)	18 (10%)	11	30
2	G	183/201 (91%)	168 (92%)	15 (8%)	14	38
2	H	185/201 (92%)	172 (93%)	13 (7%)	19	47
2	I	183/201 (91%)	171 (93%)	12 (7%)	21	51
2	J	185/201 (92%)	176 (95%)	9 (5%)	31	65
2	K	179/201 (89%)	164 (92%)	15 (8%)	14	37
2	L	180/201 (90%)	167 (93%)	13 (7%)	18	45
3	M	140/146 (96%)	135 (96%)	5 (4%)	42	76
3	N	141/146 (97%)	131 (93%)	10 (7%)	18	46
3	O	140/146 (96%)	135 (96%)	5 (4%)	42	76
3	P	144/146 (99%)	136 (94%)	8 (6%)	26	59
3	Q	142/146 (97%)	130 (92%)	12 (8%)	13	36
3	R	132/146 (90%)	123 (93%)	9 (7%)	20	49
All	All	3070/3228 (95%)	2866 (93%)	204 (7%)	21	51

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	7	SER
1	A	14	SER
1	A	20	THR
1	A	56	SER
1	A	65	SER
1	A	66	ARG
1	A	90	GLN
1	A	105	GLU
1	A	127	SER
2	G	1	GLU
2	G	18	LEU
2	G	29	VAL
2	G	30	SER
2	G	50	TYR

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Mol	Chain	Res	Type
2	G	94	ARG
2	G	101	ASP
2	G	115	SER
2	G	121	VAL
2	G	131	THR
2	G	140	CYS
2	G	177	SER
2	G	182	VAL
2	G	197	ASN
2	G	201	LYS
1	B	2	ILE
1	B	14	SER
1	B	70	ASP
1	B	74	THR
1	B	105	GLU
1	B	123	SER
1	B	129	THR
1	B	162	SER
2	H	17	SER
2	H	48	VAL
2	H	50	TYR
2	H	82(B)	SER
2	H	83[A]	ARG
2	H	83[B]	ARG
2	H	94	ARG
2	H	150	VAL
2	H	160	THR
2	H	177	SER
2	H	178	LEU
2	H	181	VAL
2	H	193	THR
1	C	6	GLN
1	C	10	SER
1	C	12	SER
1	C	14	SER
1	C	18	ARG
1	C	65	SER
1	C	77	SER
1	C	78	LEU
1	C	105	GLU
1	C	108	ARG
1	C	109	THR

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Mol	Chain	Res	Type
1	C	114	SER
1	C	123	SER
1	C	129	THR
1	C	132	VAL
1	C	152	ASN
1	C	176	SER
1	C	202	SER
1	C	206	THR
2	I	21	SER
2	I	63	VAL
2	I	73	THR
2	I	94	ARG
2	I	101	ASP
2	I	105	GLN
2	I	107	THR
2	I	120	SER
2	I	127	SER
2	I	150	VAL
2	I	184	VAL
2	I	212	GLU
1	D	19	VAL
1	D	23	CYS
1	D	50	SER
1	D	103	LYS
1	D	105	GLU
1	D	123	SER
1	D	152	ASN
1	D	154	LEU
1	D	158	ASN
2	J	61	ASP
2	J	63	VAL
2	J	94	ARG
2	J	115	SER
2	J	161	SER
2	J	191	THR
2	J	196	CYS
2	J	197	ASN
2	J	204	ASN
1	E	1	ASP
1	E	14	SER
1	E	53	SER
1	E	60	SER

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Mol	Chain	Res	Type
1	E	74	THR
1	E	89	GLN
1	E	100	GLN
1	E	107	LYS
1	E	109	THR
1	E	123	SER
1	E	137	ASN
1	E	203	SER
1	E	207	LYS
1	E	208	SER
2	K	11	LEU
2	K	18	LEU
2	K	29	VAL
2	K	58	SER
2	K	61	ASP
2	K	63	VAL
2	K	68	THR
2	K	85	GLU
2	K	94	ARG
2	K	100(B)	MET
2	K	110	THR
2	K	183	THR
2	K	184	VAL
2	K	201	LYS
2	K	205	THR
1	F	2	ILE
1	F	11	LEU
1	F	14	SER
1	F	20	THR
1	F	22	THR
1	F	67	SER
1	F	89	GLN
1	F	105	GLU
1	F	109	THR
1	F	114	SER
1	F	139	PHE
1	F	142	ARG
1	F	143	GLU
1	F	167	ASP
1	F	169	LYS
1	F	172	THR
1	F	190	LYS

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Mol	Chain	Res	Type
1	F	197	THR
2	L	29	VAL
2	L	58	SER
2	L	63	VAL
2	L	92	CYS
2	L	100(B)	MET
2	L	102	TYR
2	L	115	SER
2	L	140	CYS
2	L	151	THR
2	L	169	VAL
2	L	178	LEU
2	L	184	VAL
2	L	205	THR
3	M	5	SER
3	M	96	LEU
3	M	121	GLU
3	M	122	LEU
3	M	157	ASN
3	N	47	SER
3	N	54	ASP
3	N	56	GLU
3	N	59	SER
3	N	83	LEU
3	N	97	LEU
3	N	120	GLU
3	N	125	ASN
3	N	140	LEU
3	N	145	ARG
3	O	2	SER
3	O	19	THR
3	O	61	LEU
3	O	131	GLN
3	O	132	VAL
3	P	43	THR
3	P	49	ARG
3	P	50	SER
3	P	53	HIS
3	P	58	ASP
3	P	59	SER
3	P	145	ARG
3	P	152	VAL

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Mol	Chain	Res	Type
3	Q	5	SER
3	Q	27	THR
3	Q	36	HIS
3	Q	51	LEU
3	Q	58	ASP
3	Q	82	GLU
3	Q	91	SER
3	Q	95	ILE
3	Q	96	LEU
3	Q	143[A]	LYS
3	Q	143[B]	LYS
3	Q	154	ASP
3	R	54	ASP
3	R	56	GLU
3	R	58	ASP
3	R	74	PHE
3	R	80	SER
3	R	133	ASP
3	R	142	GLU
3	R	143	LYS
3	R	152	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	137	ASN
2	H	28	ASN
1	C	6	GLN
2	I	164	HIS
2	I	199	ASN
1	F	89	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](#)

1 ligand is modelled in this entry.

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	PEG	A	701	-	6,6,6	0.49	0	5,5,5	0.87	0

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	PEG	A	701	-	-	0/4/4/4	0/0/0/0

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	PEG	3	0

## 5.7 Other polymers [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	213/216 (98%)	-0.20	1 (0%) 91 88	13, 26, 42, 61	0
1	B	216/216 (100%)	-0.28	1 (0%) 91 88	15, 33, 53, 76	0
1	C	212/216 (98%)	0.06	3 (1%) 78 69	12, 41, 71, 80	0
1	D	214/216 (99%)	-0.21	1 (0%) 91 88	14, 25, 43, 74	0
1	E	214/216 (99%)	0.04	3 (1%) 78 69	32, 52, 68, 83	0
1	F	214/216 (99%)	0.71	16 (7%) 17 9	50, 71, 86, 104	0
2	G	219/238 (92%)	-0.32	1 (0%) 91 88	14, 23, 47, 74	0
2	H	221/238 (92%)	-0.19	0 100 100	15, 26, 59, 86	0
2	I	220/238 (92%)	0.04	8 (3%) 46 34	12, 28, 75, 89	0
2	J	222/238 (93%)	-0.42	0 100 100	11, 25, 45, 70	0
2	K	214/238 (89%)	0.25	6 (2%) 56 44	26, 63, 87, 106	0
2	L	214/238 (89%)	0.82	35 (16%) 2 1	31, 68, 96, 104	0
3	M	153/160 (95%)	-0.06	1 (0%) 89 84	16, 29, 64, 81	0
3	N	152/160 (95%)	0.08	5 (3%) 50 38	17, 34, 79, 88	1 (0%)
3	O	153/160 (95%)	-0.12	1 (0%) 89 84	15, 27, 68, 79	0
3	P	156/160 (97%)	-0.23	1 (0%) 90 86	16, 25, 54, 76	0
3	Q	153/160 (95%)	0.30	7 (4%) 36 25	28, 54, 86, 95	0
3	R	143/160 (89%)	0.56	10 (6%) 19 11	32, 64, 96, 106	0
All	All	3503/3684 (95%)	0.04	100 (2%) 55 43	11, 36, 82, 106	1 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	112	SER	5.8
2	L	119	PRO	4.7
2	L	149	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
2	L	161	SER	4.2
1	F	106	ILE	4.2
1	B	-1	MET	4.1
3	Q	29	GLU	3.9
2	K	154	TRP	3.9
2	K	208	ASP	3.9
2	L	178	LEU	3.8
2	L	118	GLY	3.7
3	N	53	HIS	3.6
1	F	140	TYR	3.6
2	L	160	THR	3.5
3	R	1	SER	3.4
2	L	159	LEU	3.3
2	L	117	LYS	3.3
2	L	176	TYR	3.3
2	I	128	SER	3.2
2	L	142	VAL	3.2
3	O	0	GLY	3.1
2	L	148	GLU	3.1
2	L	147	PRO	3.0
3	N	89	LEU	3.0
3	Q	3	ILE	3.0
1	E	212	GLY	3.0
2	K	191	THR	3.0
1	F	199	GLN	3.0
2	L	105	GLN	2.9
3	N	51	LEU	2.9
1	D	214	CYS	2.9
2	L	158	ALA	2.9
1	F	15	VAL	2.9
3	N	83	LEU	2.9
2	L	166	PHE	2.9
2	L	143	LYS	2.8
1	F	81	GLU	2.8
3	R	127	PRO	2.8
1	C	196	VAL	2.7
3	R	34	LEU	2.7
2	L	145	TYR	2.7
2	L	165	THR	2.7
3	Q	31	LEU	2.7
2	G	133	GLY	2.6
2	L	116	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	47	LEU	2.6
3	R	117	TYR	2.6
3	R	31	LEU	2.6
2	L	121	VAL	2.6
2	I	211	VAL	2.5
2	L	216	CYS	2.5
1	F	99	GLY	2.5
3	R	119	GLU	2.5
2	I	125	ALA	2.5
2	L	23	ALA	2.4
3	R	32	GLU	2.4
2	L	89	VAL	2.4
2	L	215	SER	2.4
3	Q	5	SER	2.4
3	M	124	GLU	2.4
3	Q	67	VAL	2.4
2	L	102	TYR	2.3
1	F	193	ALA	2.3
2	K	159	LEU	2.3
2	L	120	SER	2.3
1	C	181	LEU	2.3
2	I	124	LEU	2.3
1	F	111	ALA	2.3
2	L	175	LEU	2.3
1	F	173	TYR	2.2
2	K	82(C)	LEU	2.2
1	F	146	VAL	2.2
2	K	194	TYR	2.2
2	I	194	TYR	2.2
2	I	189	LEU	2.2
2	L	208	ASP	2.1
1	F	214	CYS	2.1
2	I	133	GLY	2.1
3	N	117	TYR	2.1
1	C	111	ALA	2.1
1	F	131	SER	2.1
1	F	181	LEU	2.1
2	I	212	GLU	2.1
1	F	168	SER	2.1
2	L	201	LYS	2.1
3	R	55	GLN	2.1
3	R	128	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	P	51	LEU	2.1
1	E	113	PRO	2.1
3	Q	30	CYS	2.1
1	A	154	LEU	2.0
2	L	207	VAL	2.0
1	F	58	VAL	2.0
2	L	37	VAL	2.0
3	Q	32	GLU	2.0
2	L	108	LEU	2.0
2	L	82(C)	LEU	2.0
1	E	213	GLU	2.0
2	L	110	THR	2.0
3	R	4	VAL	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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
4	PEG	A	701	7/7	0.95	0.31	7.28	31,37,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.