



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2014 – 06:01 PM EDT

PDB ID : 3OJ3
Title : Crystal structure of the A20 ZnF4 and ubiquitin complex
Authors : Bosanac, I; Hymowitz, S.G.
Deposited on : 2010-08-20
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

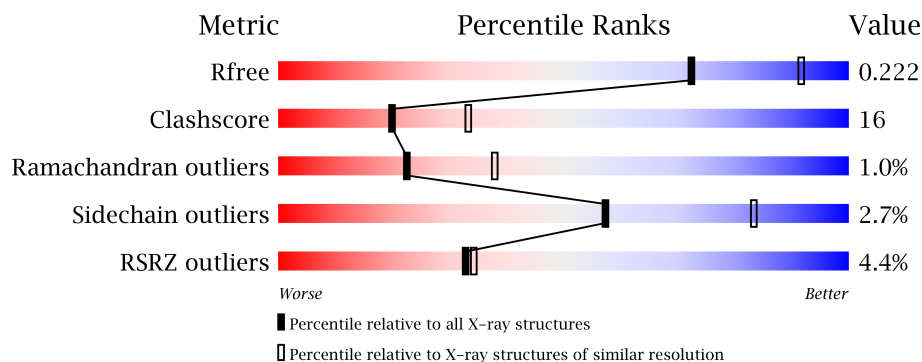
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.50 Å.

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



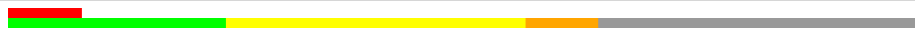
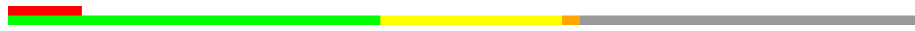
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	79	
1	B	79	
1	C	79	
1	D	79	
1	E	79	
1	F	79	
1	G	79	
1	H	79	
2	I	49	
2	J	49	
2	K	49	
2	L	49	
2	M	49	
2	N	49	

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Mol	Chain	Length	Quality of chain
2	O	49	
2	P	49	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6729 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	73	Total	C	N	O	S	0	0	0
			582	368	99	114	1			
1	B	72	Total	C	N	O	S	0	0	0
			574	362	98	113	1			
1	C	73	Total	C	N	O	S	0	0	0
			582	368	99	114	1			
1	D	73	Total	C	N	O	S	0	0	0
			582	368	99	114	1			
1	E	73	Total	C	N	O	S	0	0	0
			582	368	99	114	1			
1	F	73	Total	C	N	O	S	0	0	0
			582	368	99	114	1			
1	G	71	Total	C	N	O	S	0	0	0
			563	356	94	112	1			
1	H	71	Total	C	N	O	S	0	0	0
			563	356	94	112	1			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P0CG47
A	-1	SER	-	EXPRESSION TAG	UNP P0CG47
A	0	HIS	-	EXPRESSION TAG	UNP P0CG47
B	-2	GLY	-	EXPRESSION TAG	UNP P0CG47
B	-1	SER	-	EXPRESSION TAG	UNP P0CG47
B	0	HIS	-	EXPRESSION TAG	UNP P0CG47
C	-2	GLY	-	EXPRESSION TAG	UNP P0CG47
C	-1	SER	-	EXPRESSION TAG	UNP P0CG47
C	0	HIS	-	EXPRESSION TAG	UNP P0CG47
D	-2	GLY	-	EXPRESSION TAG	UNP P0CG47
D	-1	SER	-	EXPRESSION TAG	UNP P0CG47
D	0	HIS	-	EXPRESSION TAG	UNP P0CG47
E	-2	GLY	-	EXPRESSION TAG	UNP P0CG47

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	EXPRESSION TAG	UNP P0CG47
E	0	HIS	-	EXPRESSION TAG	UNP P0CG47
F	-2	GLY	-	EXPRESSION TAG	UNP P0CG47
F	-1	SER	-	EXPRESSION TAG	UNP P0CG47
F	0	HIS	-	EXPRESSION TAG	UNP P0CG47
G	-2	GLY	-	EXPRESSION TAG	UNP P0CG47
G	-1	SER	-	EXPRESSION TAG	UNP P0CG47
G	0	HIS	-	EXPRESSION TAG	UNP P0CG47
H	-2	GLY	-	EXPRESSION TAG	UNP P0CG47
H	-1	SER	-	EXPRESSION TAG	UNP P0CG47
H	0	HIS	-	EXPRESSION TAG	UNP P0CG47

- Molecule 2 is a protein called Tumor necrosis factor alpha-induced protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	33	Total	C	N	O	S	0	0	0
			260	164	45	47	4			
2	J	30	Total	C	N	O	S	0	0	0
			240	152	41	43	4			
2	K	31	Total	C	N	O	S	0	0	0
			249	158	43	44	4			
2	L	31	Total	C	N	O	S	0	0	0
			249	158	43	44	4			
2	M	31	Total	C	N	O	S	0	0	0
			249	158	43	44	4			
2	N	30	Total	C	N	O	S	0	0	0
			240	152	41	43	4			
2	O	32	Total	C	N	O	S	0	0	0
			256	162	44	46	4			
2	P	31	Total	C	N	O	S	0	0	0
			249	158	43	44	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	587	GLY	-	EXPRESSION TAG	UNP P21580
I	588	SER	-	EXPRESSION TAG	UNP P21580
I	589	PRO	-	EXPRESSION TAG	UNP P21580
I	590	GLU	-	EXPRESSION TAG	UNP P21580
I	591	PHE	-	EXPRESSION TAG	UNP P21580
J	587	GLY	-	EXPRESSION TAG	UNP P21580
J	588	SER	-	EXPRESSION TAG	UNP P21580

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Chain	Residue	Modelled	Actual	Comment	Reference
J	589	PRO	-	EXPRESSION TAG	UNP P21580
J	590	GLU	-	EXPRESSION TAG	UNP P21580
J	591	PHE	-	EXPRESSION TAG	UNP P21580
K	587	GLY	-	EXPRESSION TAG	UNP P21580
K	588	SER	-	EXPRESSION TAG	UNP P21580
K	589	PRO	-	EXPRESSION TAG	UNP P21580
K	590	GLU	-	EXPRESSION TAG	UNP P21580
K	591	PHE	-	EXPRESSION TAG	UNP P21580
L	587	GLY	-	EXPRESSION TAG	UNP P21580
L	588	SER	-	EXPRESSION TAG	UNP P21580
L	589	PRO	-	EXPRESSION TAG	UNP P21580
L	590	GLU	-	EXPRESSION TAG	UNP P21580
L	591	PHE	-	EXPRESSION TAG	UNP P21580
M	587	GLY	-	EXPRESSION TAG	UNP P21580
M	588	SER	-	EXPRESSION TAG	UNP P21580
M	589	PRO	-	EXPRESSION TAG	UNP P21580
M	590	GLU	-	EXPRESSION TAG	UNP P21580
M	591	PHE	-	EXPRESSION TAG	UNP P21580
N	587	GLY	-	EXPRESSION TAG	UNP P21580
N	588	SER	-	EXPRESSION TAG	UNP P21580
N	589	PRO	-	EXPRESSION TAG	UNP P21580
N	590	GLU	-	EXPRESSION TAG	UNP P21580
N	591	PHE	-	EXPRESSION TAG	UNP P21580
O	587	GLY	-	EXPRESSION TAG	UNP P21580
O	588	SER	-	EXPRESSION TAG	UNP P21580
O	589	PRO	-	EXPRESSION TAG	UNP P21580
O	590	GLU	-	EXPRESSION TAG	UNP P21580
O	591	PHE	-	EXPRESSION TAG	UNP P21580
P	587	GLY	-	EXPRESSION TAG	UNP P21580
P	588	SER	-	EXPRESSION TAG	UNP P21580
P	589	PRO	-	EXPRESSION TAG	UNP P21580
P	590	GLU	-	EXPRESSION TAG	UNP P21580
P	591	PHE	-	EXPRESSION TAG	UNP P21580

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0
3	K	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total 1	Zn 1	0	0
3	N	1	Total 1	Zn 1	0	0
3	O	1	Total 1	Zn 1	0	0
3	L	1	Total 1	Zn 1	0	0
3	M	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total 12	O 12	0	0
4	B	11	Total 11	O 11	0	0
4	C	18	Total 18	O 18	0	0
4	D	7	Total 7	O 7	0	0
4	E	9	Total 9	O 9	0	0
4	F	15	Total 15	O 15	0	0
4	G	12	Total 12	O 12	0	0
4	H	7	Total 7	O 7	0	0
4	I	4	Total 4	O 4	0	0
4	J	3	Total 3	O 3	0	0
4	K	3	Total 3	O 3	0	0
4	L	2	Total 2	O 2	0	0
4	M	4	Total 4	O 4	0	0
4	N	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	6	Total	O	0	0
			6	6		
4	P	2	Total	O	0	0
			2	2		

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: Ubiquitin

Chain A:



• Molecule 1: Ubiquitin

Chain B:



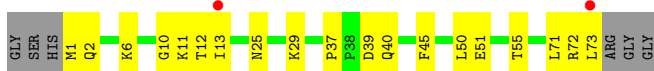
• Molecule 1: Ubiquitin

Chain C:



• Molecule 1: Ubiquitin

Chain D:



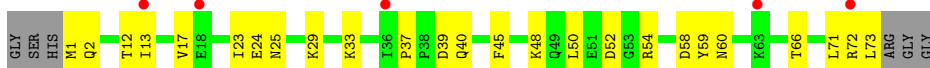
• Molecule 1: Ubiquitin

Chain E:



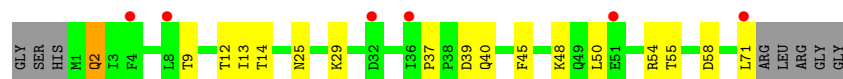
• Molecule 1: Ubiquitin

Chain F:



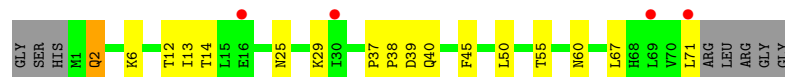
- Molecule 1: Ubiquitin

Chain G: 



- Molecule 1: Ubiquitin

Chain H: 



- Molecule 2: Tumor necrosis factor alpha-induced protein 3

Chain I: 



- Molecule 2: Tumor necrosis factor alpha-induced protein 3

Chain J: 



- Molecule 2: Tumor necrosis factor alpha-induced protein 3

Chain K: 



- Molecule 2: Tumor necrosis factor alpha-induced protein 3

Chain L: 



- Molecule 2: Tumor necrosis factor alpha-induced protein 3

Chain M: 



- Molecule 2: Tumor necrosis factor alpha-induced protein 3

Chain N: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.83Å 170.03Å 66.24Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	43.06 – 2.50 43.06 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (43.06-2.50) 95.7 (43.06-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.203 , 0.226 0.200 , 0.222	Depositor DCC
R_{free} test set	1631 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.5	EDS
Estimated twinning fraction	0.351 for "H,-K,-L' 0.317 for h,-k,-l	Xtriage
Reported twinning fraction	0.351 for "H,-K,-L'	Depositor
L-test for twinning	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 31426 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6729	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.43	0/588	0.56	0/792
1	B	0.43	0/580	0.57	0/781
1	C	0.44	0/588	0.55	0/792
1	D	0.44	0/588	0.56	0/792
1	E	0.44	0/588	0.57	0/792
1	F	0.44	0/588	0.54	0/792
1	G	0.42	0/569	0.56	0/767
1	H	0.42	0/569	0.54	0/767
2	I	0.52	0/265	0.56	0/352
2	J	0.46	0/245	0.57	0/326
2	K	0.51	0/254	0.58	0/337
2	L	0.50	0/254	0.61	0/337
2	M	0.50	0/254	0.58	0/337
2	N	0.60	1/245 (0.4%)	0.57	0/326
2	O	0.53	0/261	0.62	0/347
2	P	0.47	0/254	0.57	0/337
All	All	0.46	1/6690 (0.0%)	0.56	0/8974

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	624	CYS	CB-SG	-5.48	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	582	0	610	14	0
1	B	574	0	599	22	0
1	C	582	0	610	16	0
1	D	582	0	610	16	0
1	E	582	0	610	21	0
1	F	582	0	610	29	0
1	G	563	0	586	13	0
1	H	563	0	586	13	0
2	I	260	0	249	20	0
2	J	240	0	226	7	0
2	K	249	0	239	16	0
2	L	249	0	239	8	0
2	M	249	0	240	12	0
2	N	240	0	226	18	0
2	O	256	0	246	28	0
2	P	249	0	239	12	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	A	12	0	0	2	0
4	B	11	0	0	7	0
4	C	18	0	0	0	0
4	D	7	0	0	3	0
4	E	9	0	0	1	0
4	F	15	0	0	6	0
4	G	12	0	0	3	0
4	H	7	0	0	1	0
4	I	4	0	0	3	0
4	J	3	0	0	0	0
4	K	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	2	0	0	0	0
4	M	4	0	0	0	0
4	N	4	0	0	0	0
4	O	6	0	0	1	0
4	P	2	0	0	0	0
All	All	6729	0	6725	213	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (213) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:618:PRO:HD2	4:O:28:HOH:O	1.52	1.08
2:O:629:ILE:O	2:O:633:GLU:HG2	1.76	0.84
2:M:631:TYR:HE2	2:M:635:LYS:HZ1	1.22	0.83
2:O:607:CYS:SG	2:O:624:CYS:N	2.55	0.79
1:G:9:THR:HG23	4:G:109:HOH:O	1.84	0.77
1:F:60:ASN:HB2	2:N:615:PHE:CG	2.22	0.75
2:I:634:ASN:O	2:I:635:LYS:HB2	1.87	0.74
1:F:48:LYS:NZ	2:N:613:VAL:HG11	2.04	0.72
1:E:44:ILE:HD11	2:P:629:ILE:HG21	1.71	0.71
2:O:620:ASN:O	2:O:623:PHE:HB2	1.91	0.71
1:D:11:LYS:HE3	2:I:606:LYS:HB2	1.75	0.68
1:F:54:ARG:CZ	2:N:626:LEU:HD12	2.24	0.68
2:N:609:LYS:HD3	2:N:627:CYS:SG	2.33	0.68
1:F:52:ASP:HA	4:F:81:HOH:O	1.92	0.68
1:H:55:THR:HG21	2:P:625:THR:HG21	1.77	0.68
1:F:72:ARG:O	1:F:73:LEU:HD23	1.94	0.67
1:D:55:THR:CG2	2:L:625:THR:HG21	2.25	0.67
1:B:32:ASP:HB3	4:B:106:HOH:O	1.95	0.66
1:B:54:ARG:NH1	4:B:77:HOH:O	2.25	0.66
2:P:609:LYS:HD3	2:P:627:CYS:SG	2.36	0.65
1:H:55:THR:CG2	2:P:625:THR:HG21	2.28	0.64
1:F:25:ASN:O	1:F:29:LYS:HG3	1.97	0.64
1:H:6:LYS:HG2	4:H:116:HOH:O	1.97	0.64
1:E:54:ARG:NH1	4:E:77:HOH:O	2.31	0.64
2:O:609:LYS:HB3	2:O:612:CYS:HB2	1.78	0.63
2:M:609:LYS:HD3	2:M:627:CYS:SG	2.38	0.63
2:L:609:LYS:HD3	2:L:627:CYS:SG	2.37	0.63
1:C:25:ASN:O	1:C:29:LYS:HG3	1.99	0.63
2:I:609:LYS:HD3	2:I:627:CYS:SG	2.41	0.61
2:I:604:THR:HG23	2:I:605:SER:H	1.63	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:55:THR:HG21	2:L:625:THR:HG21	1.83	0.61
1:F:48:LYS:HZ2	2:N:613:VAL:HG11	1.64	0.61
2:O:609:LYS:NZ	2:O:630:GLU:OE2	2.34	0.60
1:B:25:ASN:O	1:B:29:LYS:HG3	2.01	0.60
1:D:72:ARG:O	1:D:73:LEU:HD23	2.01	0.60
1:E:72:ARG:NH1	1:E:73:LEU:HD22	2.16	0.60
1:E:60:ASN:HB2	2:M:615:PHE:CG	2.37	0.60
1:E:72:ARG:HH12	1:E:73:LEU:HD22	1.67	0.59
1:B:70:VAL:HG11	2:K:630:GLU:HA	1.84	0.59
1:F:48:LYS:NZ	2:N:613:VAL:CG1	2.65	0.59
2:M:613:VAL:HG12	2:M:613:VAL:O	2.02	0.59
1:E:72:ARG:HG3	2:P:633:GLU:O	2.02	0.59
1:C:73:LEU:HG	2:I:634:ASN:HD21	1.68	0.58
1:F:54:ARG:HD3	4:F:78:HOH:O	2.03	0.58
1:H:25:ASN:O	1:H:29:LYS:HG3	2.03	0.58
1:B:49:GLN:HE22	2:K:633:GLU:CD	2.06	0.58
1:D:25:ASN:O	1:D:29:LYS:HG3	2.03	0.58
1:G:25:ASN:O	1:G:29:LYS:HG3	2.04	0.58
1:C:73:LEU:HG	2:I:634:ASN:ND2	2.19	0.57
2:P:613:VAL:O	2:P:613:VAL:HG12	2.05	0.57
1:A:25:ASN:O	1:A:29:LYS:HG3	2.05	0.57
1:B:32:ASP:CB	4:B:106:HOH:O	2.52	0.56
1:E:37:PRO:HD2	1:E:40:GLN:OE1	2.06	0.56
2:M:621:LYS:NZ	2:M:635:LYS:NZ	2.53	0.56
1:E:25:ASN:O	1:E:29:LYS:HG3	2.06	0.56
2:K:609:LYS:HD3	2:K:627:CYS:SG	2.45	0.56
1:H:37:PRO:HB2	1:H:39:ASP:OD1	2.04	0.56
1:E:44:ILE:CD1	2:P:629:ILE:HG21	2.35	0.56
2:O:623:PHE:HE2	2:O:631:TYR:CD1	2.23	0.56
2:J:609:LYS:HD3	2:J:627:CYS:SG	2.46	0.56
1:C:55:THR:HG21	2:K:625:THR:HG21	1.88	0.56
1:F:48:LYS:HZ2	2:N:613:VAL:CG1	2.18	0.55
1:G:37:PRO:HB2	1:G:39:ASP:OD1	2.06	0.55
2:N:613:VAL:HG12	2:N:613:VAL:O	2.05	0.55
1:D:11:LYS:HB2	2:I:608:ARG:HA	1.87	0.55
1:F:60:ASN:HB2	2:N:615:PHE:CD1	2.40	0.55
1:B:37:PRO:HB2	1:B:39:ASP:OD1	2.07	0.54
1:C:37:PRO:HB2	1:C:39:ASP:OD1	2.08	0.54
1:C:55:THR:CG2	2:K:625:THR:HG21	2.38	0.54
1:E:37:PRO:HB2	1:E:39:ASP:OD1	2.06	0.54
2:I:613:VAL:HG12	2:I:613:VAL:O	2.08	0.54
1:A:37:PRO:HB2	1:A:39:ASP:OD1	2.06	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:37:PRO:HD2	1:G:40:GLN:OE1	2.07	0.54
1:F:37:PRO:HB2	1:F:39:ASP:OD1	2.08	0.54
1:F:58:ASP:OD1	2:N:625:THR:HG23	2.07	0.54
1:F:54:ARG:NH1	2:N:626:LEU:HD12	2.22	0.54
1:H:37:PRO:HD2	1:H:40:GLN:OE1	2.08	0.54
2:I:607:CYS:HB3	2:I:612:CYS:HB3	1.88	0.54
2:K:613:VAL:HG12	2:K:613:VAL:O	2.08	0.54
1:D:51:GLU:HA	4:D:79:HOH:O	2.08	0.54
1:C:37:PRO:HD2	1:C:40:GLN:OE1	2.09	0.53
2:K:607:CYS:HB3	2:K:612:CYS:HB3	1.91	0.53
2:M:621:LYS:HZ1	2:M:635:LYS:NZ	2.07	0.53
2:O:628:PHE:C	2:O:628:PHE:CD2	2.82	0.53
1:A:37:PRO:HD2	1:A:40:GLN:OE1	2.09	0.53
1:G:58:ASP:OD1	2:O:625:THR:HB	2.08	0.53
1:A:63:LYS:HE3	4:A:107:HOH:O	2.09	0.53
1:D:37:PRO:HD2	1:D:40:GLN:OE1	2.09	0.53
1:E:40:GLN:O	1:E:71:LEU:HA	2.09	0.53
1:G:48:LYS:NZ	4:G:79:HOH:O	2.28	0.52
2:L:613:VAL:O	2:L:613:VAL:HG12	2.09	0.52
2:J:607:CYS:HB3	2:J:612:CYS:HB3	1.91	0.52
1:D:37:PRO:HB2	1:D:39:ASP:OD1	2.11	0.51
2:M:617:THR:HG23	2:M:620:ASN:HB2	1.92	0.51
2:J:613:VAL:O	2:J:613:VAL:HG12	2.09	0.51
1:D:72:ARG:NH1	4:D:82:HOH:O	2.43	0.51
1:B:55:THR:HG21	2:J:625:THR:HG21	1.93	0.51
2:O:632:ARG:O	2:O:632:ARG:HG2	2.11	0.51
2:M:607:CYS:HB3	2:M:612:CYS:HB3	1.92	0.51
1:E:72:ARG:O	1:E:73:LEU:C	2.49	0.51
1:D:10:GLY:HA3	2:I:608:ARG:HD2	1.93	0.51
2:O:620:ASN:HB3	2:O:628:PHE:HD1	1.75	0.51
1:D:1:MET:N	4:D:77:HOH:O	2.43	0.50
1:A:63:LYS:CE	4:A:107:HOH:O	2.58	0.50
1:E:70:VAL:HG11	2:P:630:GLU:HA	1.93	0.50
1:F:48:LYS:HZ1	2:N:613:VAL:HG11	1.75	0.50
1:F:24:GLU:CD	4:F:81:HOH:O	2.50	0.50
1:B:44:ILE:HD11	2:K:629:ILE:HG21	1.92	0.50
2:J:617:THR:HG23	2:J:620:ASN:HB2	1.94	0.50
1:C:60:ASN:HB2	2:K:615:PHE:CG	2.46	0.49
1:A:55:THR:CG2	2:I:625:THR:HG21	2.42	0.49
1:F:72:ARG:HG2	1:F:73:LEU:N	2.26	0.49
1:F:37:PRO:HD2	1:F:40:GLN:OE1	2.12	0.49
1:F:66:THR:O	4:F:118:HOH:O	2.20	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:40:GLN:O	1:G:71:LEU:HA	2.12	0.49
2:O:607:CYS:HB2	2:O:614:TYR:O	2.13	0.49
2:O:623:PHE:CE2	2:O:631:TYR:CD1	3.00	0.49
1:F:40:GLN:O	1:F:71:LEU:HA	2.13	0.49
1:A:40:GLN:O	1:A:71:LEU:HA	2.13	0.49
2:P:629:ILE:O	2:P:633:GLU:HG2	2.12	0.49
1:H:40:GLN:O	1:H:71:LEU:HA	2.12	0.48
2:O:618:PRO:O	2:O:621:LYS:N	2.38	0.48
2:N:617:THR:HG23	2:N:620:ASN:HB2	1.95	0.48
2:I:629:ILE:O	2:I:633:GLU:HG2	2.13	0.48
2:M:621:LYS:NZ	2:M:635:LYS:HZ3	2.12	0.48
2:L:607:CYS:HB3	2:L:612:CYS:HB3	1.96	0.48
1:B:37:PRO:HD2	1:B:40:GLN:OE1	2.14	0.48
1:G:54:ARG:NH1	4:G:78:HOH:O	2.46	0.47
1:C:72:ARG:HG3	2:I:633:GLU:O	2.14	0.47
2:N:607:CYS:HB3	2:N:612:CYS:HB3	1.96	0.47
2:O:606:LYS:HD3	2:O:606:LYS:HA	1.66	0.47
2:I:617:THR:HG23	2:I:620:ASN:HB2	1.96	0.47
1:E:72:ARG:HG2	1:E:73:LEU:N	2.29	0.47
2:M:629:ILE:O	2:M:633:GLU:HG2	2.14	0.47
1:F:45:PHE:HB3	1:F:50:LEU:HD21	1.97	0.47
1:B:40:GLN:O	1:B:71:LEU:HA	2.15	0.47
1:F:33:LYS:NZ	2:O:619:GLU:OE2	2.35	0.47
1:C:44:ILE:HD11	2:I:629:ILE:HG21	1.98	0.46
1:H:45:PHE:HB3	1:H:50:LEU:HD21	1.96	0.46
2:I:618:PRO:HB2	4:I:98:HOH:O	2.14	0.46
2:O:620:ASN:HA	2:O:628:PHE:CD1	2.50	0.46
1:D:40:GLN:O	1:D:71:LEU:HA	2.15	0.46
2:P:617:THR:HG23	2:P:620:ASN:HB2	1.97	0.46
1:C:12:THR:HG22	1:C:13:ILE:N	2.31	0.46
1:G:45:PHE:HB3	1:G:50:LEU:HD21	1.97	0.46
2:O:620:ASN:CB	2:O:628:PHE:HD1	2.29	0.46
1:A:55:THR:HG21	2:I:625:THR:HG21	1.96	0.46
1:C:40:GLN:O	1:C:71:LEU:HA	2.15	0.46
1:E:55:THR:HG21	2:M:625:THR:HG21	1.97	0.46
2:K:605:SER:N	4:K:14:HOH:O	2.49	0.46
1:E:12:THR:HG22	1:E:13:ILE:N	2.30	0.46
1:C:60:ASN:HB2	2:K:615:PHE:CD1	2.51	0.46
1:B:19:PRO:HB3	4:B:122:HOH:O	2.15	0.45
1:A:12:THR:HG22	1:A:13:ILE:N	2.32	0.45
1:F:12:THR:HG22	1:F:13:ILE:N	2.30	0.45
2:I:618:PRO:CD	4:I:98:HOH:O	2.65	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:617:THR:HG23	2:K:620:ASN:HB2	1.98	0.45
2:K:629:ILE:O	2:K:633:GLU:HG2	2.17	0.45
1:A:8:LEU:HD22	1:F:54:ARG:HH22	1.80	0.45
1:C:45:PHE:HB3	1:C:50:LEU:HD21	1.99	0.45
1:H:60:ASN:HB2	2:P:615:PHE:CG	2.52	0.45
1:B:12:THR:HG22	1:B:13:ILE:N	2.32	0.44
2:L:617:THR:HG23	2:L:620:ASN:HB2	1.98	0.44
1:E:70:VAL:CG1	2:P:630:GLU:HA	2.47	0.44
2:L:629:ILE:O	2:L:633:GLU:HG2	2.17	0.44
1:E:37:PRO:HA	1:E:38:PRO:HD3	1.85	0.44
2:O:620:ASN:HB3	2:O:628:PHE:CD1	2.53	0.44
1:G:12:THR:HG22	1:G:13:ILE:N	2.32	0.43
1:D:45:PHE:HB3	1:D:50:LEU:HD21	2.00	0.43
2:O:617:THR:HB	2:O:619:GLU:OE1	2.18	0.43
1:D:12:THR:HG22	1:D:13:ILE:N	2.33	0.43
1:B:49:GLN:NE2	2:K:633:GLU:OE2	2.51	0.43
1:A:40:GLN:NE2	1:A:73:LEU:HD23	2.34	0.43
1:G:54:ARG:CZ	2:O:614:TYR:CE2	3.02	0.43
2:N:629:ILE:O	2:N:633:GLU:HG2	2.18	0.43
1:B:37:PRO:HA	1:B:38:PRO:HD3	1.85	0.43
2:O:625:THR:O	2:O:628:PHE:HB3	2.18	0.43
2:O:628:PHE:O	2:O:631:TYR:HB3	2.19	0.43
2:K:631:TYR:CE2	2:K:635:LYS:HD2	2.54	0.43
1:C:71:LEU:N	1:C:71:LEU:HD12	2.35	0.42
2:I:621:LYS:HD3	4:I:20:HOH:O	2.18	0.42
1:A:45:PHE:HB3	1:A:50:LEU:HD21	2.01	0.42
1:F:58:ASP:O	2:N:614:TYR:HB3	2.20	0.42
1:E:63:LYS:O	1:E:64:GLU:HB2	2.20	0.42
1:G:2:GLN:HG3	1:G:14:THR:HG23	2.02	0.42
1:B:55:THR:CG2	2:J:625:THR:HG21	2.50	0.42
1:B:18:GLU:OE1	4:B:125:HOH:O	2.22	0.42
1:G:55:THR:HG23	2:O:625:THR:HG21	2.02	0.42
1:B:70:VAL:HG12	1:B:71:LEU:N	2.35	0.42
1:E:45:PHE:HB3	1:E:50:LEU:HD21	2.02	0.42
1:F:23:ILE:HB	4:F:81:HOH:O	2.18	0.41
2:L:623:PHE:HB2	2:L:628:PHE:HB2	2.02	0.41
1:E:55:THR:CG2	2:M:625:THR:HG21	2.50	0.41
1:F:1:MET:HG2	1:F:17:VAL:O	2.21	0.41
2:J:629:ILE:O	2:J:633:GLU:HG2	2.21	0.41
1:B:44:ILE:CD1	2:K:629:ILE:HG21	2.49	0.41
1:C:37:PRO:HA	1:C:38:PRO:HD3	1.86	0.41
1:H:12:THR:HG22	1:H:13:ILE:N	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:11:LYS:HA	2:I:608:ARG:HG3	2.02	0.41
2:O:609:LYS:O	2:O:610:ALA:O	2.39	0.41
1:B:33:LYS:N	4:B:106:HOH:O	2.53	0.41
2:O:620:ASN:CB	2:O:628:PHE:CD1	3.04	0.41
1:H:2:GLN:HG3	1:H:14:THR:HG23	2.02	0.41
2:O:618:PRO:C	2:O:620:ASN:N	2.74	0.41
2:O:619:GLU:H	2:O:619:GLU:CD	2.24	0.41
1:F:59:TYR:CE1	2:N:614:TYR:HE1	2.38	0.40
1:A:70:VAL:HG11	2:N:630:GLU:HA	2.04	0.40
1:F:72:ARG:NH1	4:F:77:HOH:O	2.55	0.40
1:B:1:MET:HG2	1:B:17:VAL:O	2.20	0.40
1:A:72:ARG:O	1:A:73:LEU:C	2.59	0.40
1:H:45:PHE:HB2	1:H:67:LEU:HD22	2.03	0.40
1:B:25:ASN:ND2	4:B:105:HOH:O	2.54	0.40
1:H:37:PRO:HA	1:H:38:PRO:HD3	1.85	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	71/79 (90%)	70 (99%)	1 (1%)	0	100	100
1	B	70/79 (89%)	68 (97%)	2 (3%)	0	100	100
1	C	71/79 (90%)	69 (97%)	2 (3%)	0	100	100
1	D	71/79 (90%)	70 (99%)	1 (1%)	0	100	100
1	E	71/79 (90%)	69 (97%)	2 (3%)	0	100	100
1	F	71/79 (90%)	69 (97%)	2 (3%)	0	100	100
1	G	69/79 (87%)	68 (99%)	1 (1%)	0	100	100
1	H	69/79 (87%)	67 (97%)	2 (3%)	0	100	100
2	I	31/49 (63%)	27 (87%)	3 (10%)	1 (3%)	6	8
2	J	28/49 (57%)	25 (89%)	2 (7%)	1 (4%)	5	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	29/49 (59%)	26 (90%)	2 (7%)	1 (3%)	6	7
2	L	29/49 (59%)	26 (90%)	2 (7%)	1 (3%)	6	7
2	M	29/49 (59%)	25 (86%)	3 (10%)	1 (3%)	6	7
2	N	28/49 (57%)	25 (89%)	2 (7%)	1 (4%)	5	6
2	O	30/49 (61%)	25 (83%)	4 (13%)	1 (3%)	6	7
2	P	29/49 (59%)	26 (90%)	2 (7%)	1 (3%)	6	7
All	All	796/1024 (78%)	755 (95%)	33 (4%)	8 (1%)	22	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	610	ALA
2	I	610	ALA
2	J	610	ALA
2	K	610	ALA
2	L	610	ALA
2	M	610	ALA
2	P	610	ALA
2	N	610	ALA

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	67/70 (96%)	66 (98%)	1 (2%)	76	93
1	B	66/70 (94%)	65 (98%)	1 (2%)	76	93
1	C	67/70 (96%)	66 (98%)	1 (2%)	76	93
1	D	67/70 (96%)	65 (97%)	2 (3%)	53	80
1	E	67/70 (96%)	66 (98%)	1 (2%)	76	93
1	F	67/70 (96%)	66 (98%)	1 (2%)	76	93
1	G	65/70 (93%)	64 (98%)	1 (2%)	76	93
1	H	65/70 (93%)	64 (98%)	1 (2%)	76	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	28/40 (70%)	27 (96%)	1 (4%)	47	73
2	J	26/40 (65%)	25 (96%)	1 (4%)	44	71
2	K	27/40 (68%)	26 (96%)	1 (4%)	45	72
2	L	27/40 (68%)	26 (96%)	1 (4%)	45	72
2	M	27/40 (68%)	25 (93%)	2 (7%)	20	35
2	N	26/40 (65%)	25 (96%)	1 (4%)	44	71
2	O	28/40 (70%)	25 (89%)	3 (11%)	10	17
2	P	27/40 (68%)	26 (96%)	1 (4%)	45	72
All	All	747/880 (85%)	727 (97%)	20 (3%)	57	83

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	B	2	GLN
1	C	2	GLN
1	D	2	GLN
1	D	6	LYS
1	E	2	GLN
1	F	2	GLN
1	G	2	GLN
1	H	2	GLN
2	I	617	THR
2	J	617	THR
2	K	617	THR
2	L	617	THR
2	M	617	THR
2	M	635	LYS
2	N	617	THR
2	O	617	THR
2	O	624	CYS
2	O	625	THR
2	P	617	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN

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Mol	Chain	Res	Type
1	A	62	GLN
1	B	25	ASN
1	B	49	GLN
1	B	60	ASN
1	B	62	GLN
1	C	60	ASN
1	C	62	GLN
1	D	60	ASN
1	D	62	GLN
1	E	60	ASN
1	E	62	GLN
1	F	60	ASN
1	F	62	GLN
1	G	49	GLN
1	G	60	ASN
1	G	62	GLN
1	H	60	ASN
1	H	62	GLN
2	K	620	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	73/79 (92%)	0.51	1 (1%) 72 74	36, 54, 71, 78	0
1	B	72/79 (91%)	0.47	0 100 100	36, 53, 72, 80	0
1	C	73/79 (92%)	0.64	4 (5%) 24 24	35, 52, 71, 81	0
1	D	73/79 (92%)	0.48	2 (2%) 52 54	36, 52, 74, 79	0
1	E	73/79 (92%)	0.43	1 (1%) 72 74	37, 53, 73, 80	0
1	F	73/79 (92%)	0.66	5 (6%) 17 17	36, 53, 74, 79	0
1	G	71/79 (89%)	0.83	6 (8%) 11 10	36, 54, 74, 79	0
1	H	71/79 (89%)	0.76	4 (5%) 24 24	36, 53, 73, 80	0
2	I	33/49 (67%)	0.55	1 (3%) 48 50	44, 57, 71, 79	0
2	J	30/49 (61%)	0.47	1 (3%) 44 45	43, 57, 71, 74	0
2	K	31/49 (63%)	0.54	0 100 100	43, 58, 70, 72	0
2	L	31/49 (63%)	0.77	3 (9%) 8 7	44, 56, 72, 82	0
2	M	31/49 (63%)	0.81	1 (3%) 45 47	45, 58, 72, 75	0
2	N	30/49 (61%)	0.45	0 100 100	44, 57, 71, 72	0
2	O	32/49 (65%)	0.72	4 (12%) 5 4	43, 67, 79, 84	0
2	P	31/49 (63%)	0.76	4 (12%) 4 4	44, 58, 72, 78	0
All	All	828/1024 (80%)	0.61	37 (4%) 33 33	35, 56, 74, 84	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	8	LEU	6.3
1	G	71	LEU	4.1
1	H	71	LEU	3.7
1	F	13	ILE	3.4
1	H	69	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	30	ILE	3.3
2	P	635	LYS	3.3
1	G	36	ILE	3.2
1	A	73	LEU	3.2
2	O	631	TYR	3.2
1	D	73	LEU	3.1
1	C	71	LEU	3.1
1	F	63	LYS	3.1
2	L	633	GLU	3.0
2	L	635	LYS	2.9
1	C	36	ILE	2.8
1	F	18	GLU	2.6
2	M	635	LYS	2.6
1	H	16	GLU	2.6
1	G	32	ASP	2.6
2	I	635	LYS	2.5
2	L	631	TYR	2.5
2	P	633	GLU	2.5
1	G	4	PHE	2.5
2	P	631	TYR	2.4
1	F	72	ARG	2.4
1	D	13	ILE	2.4
1	G	51	GLU	2.3
1	C	39	ASP	2.2
2	J	631	TYR	2.2
1	F	36	ILE	2.2
1	C	13	ILE	2.1
1	E	39	ASP	2.1
2	O	616	GLY	2.0
2	P	634	ASN	2.0
2	O	621	LYS	2.0
2	O	611	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	P	908	1/1	0.18	0.12	60,60,60,60	0
3	ZN	I	901	1/1	0.17	0.07	46,46,46,46	0
3	ZN	L	904	1/1	0.15	-0.41	48,48,48,48	0
3	ZN	N	906	1/1	0.14	-0.46	55,55,55,55	0
3	ZN	J	902	1/1	0.13	-0.75	53,53,53,53	0
3	ZN	K	903	1/1	0.12	-1.17	53,53,53,53	0
3	ZN	O	907	1/1	0.08	-1.19	73,73,73,73	0
3	ZN	M	905	1/1	0.11	-1.21	50,50,50,50	0

6.5 Other polymers

There are no such residues in this entry.