Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 11:38 AM EDT

PDB ID	:	7RCJ / pdb_00007rcj
Title	:	Crystal structure of ZnuA from Citrobacter koseri
Authors	:	Yukl, E.T.; Yekwa, E.L.
Deposited on	:	2021-07-07
Resolution	:	3.15 Å(reported)

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

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

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

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

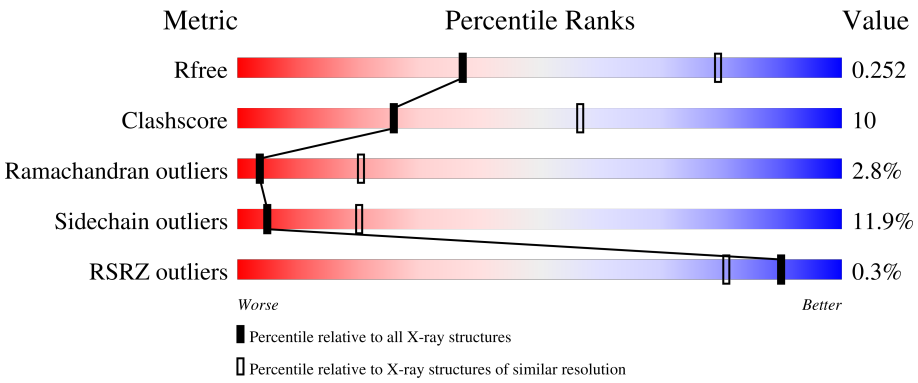
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.15 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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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

Mol	Chain	Length	Quality of chain
1	A	316	60% 18% • • 17%
1	B	316	59% 19% 5% • 16%
1	C	316	58% 21% • • 17%
1	D	316	% 60% 18% 5% • 16%
1	E	316	% 63% 15% 5% • 16%

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Mol	Chain	Length	Quality of chain
1	F	316	59% 19% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12243 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.

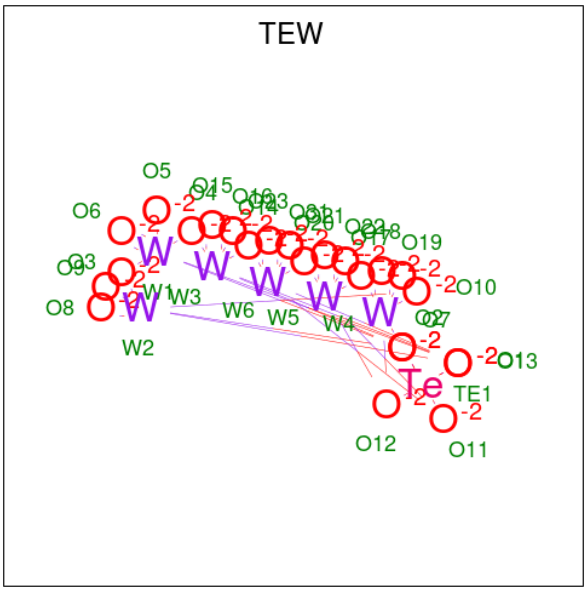
- Molecule 1 is a protein called High-affinity zinc uptake system protein ZnuA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2020	1289	346	377	8	0	0	0
1	B	264	2028	1293	347	380	8	0	0	0
1	C	263	2020	1289	346	377	8	0	0	0
1	D	264	2028	1293	347	380	8	0	0	0
1	E	264	2028	1293	347	380	8	0	0	0
1	F	263	2020	1289	346	377	8	0	0	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0

- Molecule 3 is 6-tungstotellurate(VI) (CCD ID: TEW) (formula: $O_{24}TeW_6$).



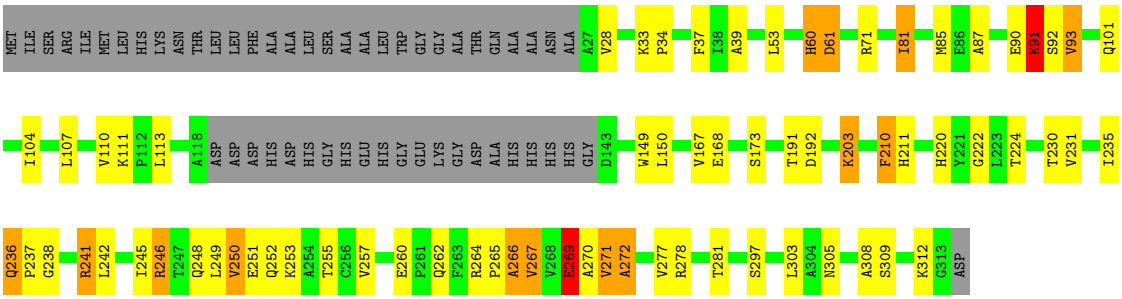
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	Te	W		
3	B	1	31	24	1	6	0	0
			Total	O	Te	W		
3	D	1	31	24	1	6	0	0
			Total	O	Te	W		
3	F	1	31	24	1	6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

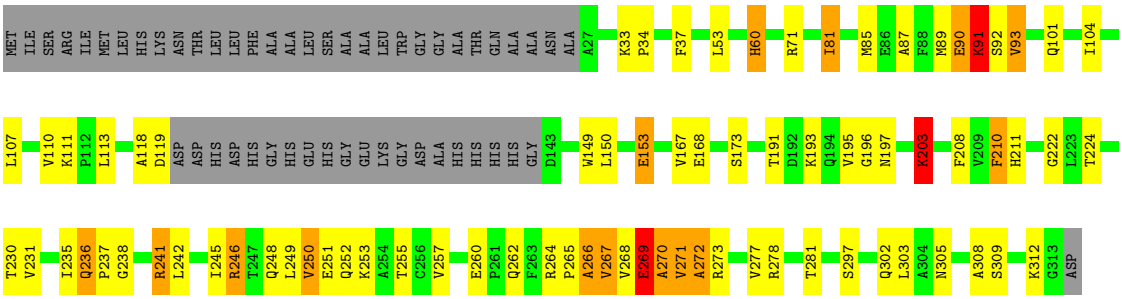
- Molecule 1: High-affinity zinc uptake system protein ZnuA

Chain A:



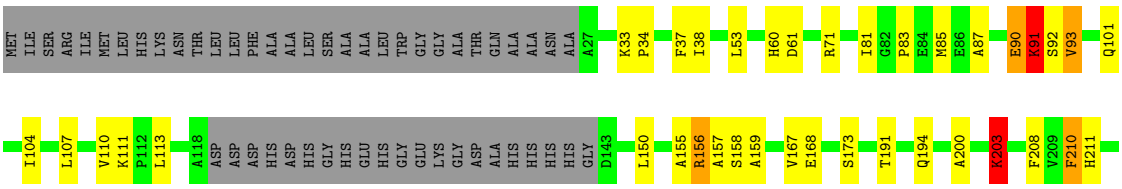
- Molecule 1: High-affinity zinc uptake system protein ZnuA

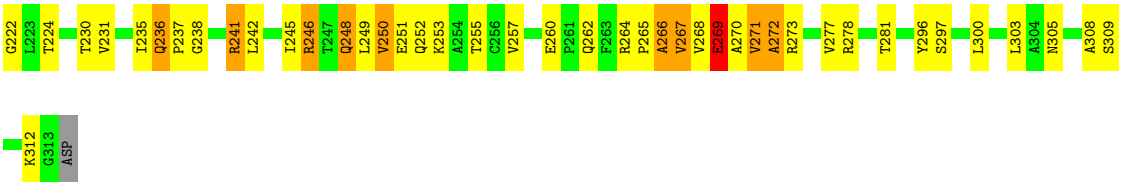
Chain B:



- Molecule 1: High-affinity zinc uptake system protein ZnuA

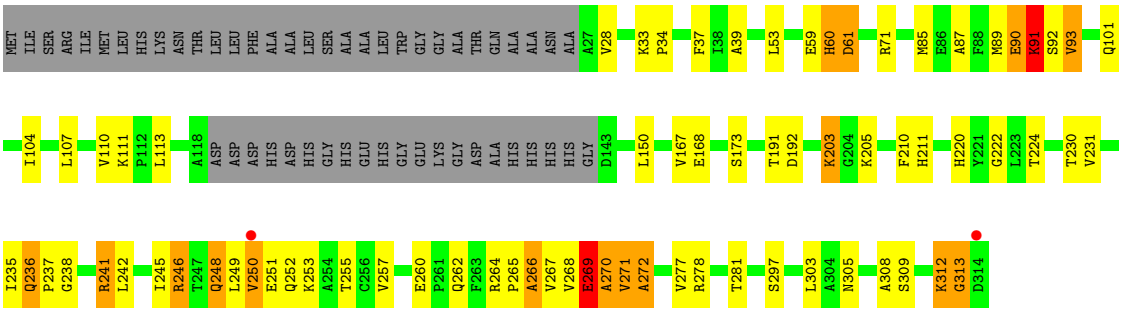
Chain C:





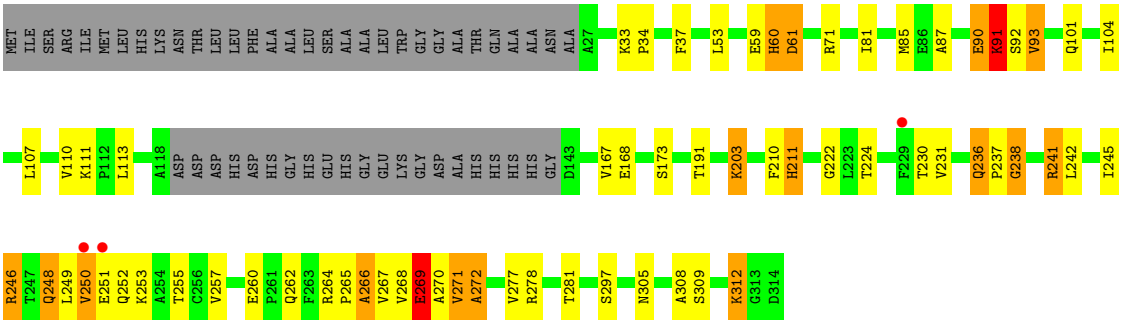
• Molecule 1: High-affinity zinc uptake system protein ZnuA

Chain D:



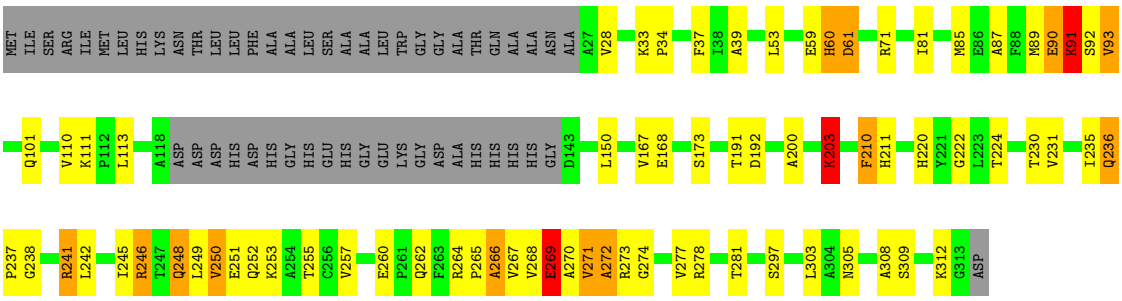
• Molecule 1: High-affinity zinc uptake system protein ZnuA

Chain E:



• Molecule 1: High-affinity zinc uptake system protein ZnuA

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	122.25Å 81.67Å 126.56Å 90.00° 112.99° 90.00°	Depositor
Resolution (Å)	47.47 – 3.15 47.47 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.47-3.15) 99.7 (47.47-3.15)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.217 , 0.254 0.209 , 0.252	Depositor DCC
R_{free} test set	2006 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	89.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 78.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.125 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12243	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.84	0/2062	1.08	7/2796 (0.3%)
1	B	0.82	0/2070	1.11	12/2807 (0.4%)
1	C	0.83	0/2062	1.08	9/2796 (0.3%)
1	D	0.82	0/2070	1.08	8/2807 (0.3%)
1	E	0.82	1/2070 (0.0%)	1.06	5/2807 (0.2%)
1	F	0.80	0/2062	1.06	8/2796 (0.3%)
All	All	0.82	1/12396 (0.0%)	1.08	49/16809 (0.3%)

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	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	211	HIS	CA-C	5.26	1.59	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	90	GLU	N-CA-C	-9.43	99.51	111.02
1	C	269	GLU	N-CA-C	-8.90	98.24	110.35
1	B	269	GLU	N-CA-C	-8.88	98.27	110.35
1	D	313	GLY	N-CA-C	8.82	125.64	112.41
1	D	90	GLU	N-CA-C	-8.70	100.41	111.02
1	C	90	GLU	N-CA-C	-8.58	101.89	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	269	GLU	N-CA-C	-8.14	99.28	110.35
1	F	269	GLU	N-CA-C	-8.10	99.34	110.35
1	E	269	GLU	N-CA-C	-7.98	99.50	110.35
1	D	269	GLU	N-CA-C	-7.91	99.59	110.35
1	B	60	HIS	N-CA-C	7.82	121.25	112.97
1	B	33	LYS	CA-C-N	-7.55	112.02	119.64
1	B	33	LYS	C-N-CA	-7.55	112.02	119.64
1	A	33	LYS	CA-C-N	-7.40	112.17	119.64
1	A	33	LYS	C-N-CA	-7.40	112.17	119.64
1	D	33	LYS	CA-C-N	-7.09	112.48	119.64
1	D	33	LYS	C-N-CA	-7.09	112.48	119.64
1	B	90	GLU	N-CA-C	-6.87	102.64	111.02
1	C	33	LYS	CA-C-N	-6.35	113.23	119.64
1	C	33	LYS	C-N-CA	-6.35	113.23	119.64
1	F	210	PHE	N-CA-C	-6.34	99.68	109.76
1	E	90	GLU	N-CA-C	-6.33	103.30	111.02
1	F	33	LYS	CA-C-N	-6.00	113.58	119.64
1	F	33	LYS	C-N-CA	-6.00	113.58	119.64
1	E	33	LYS	CA-C-N	-5.92	113.66	119.64
1	E	33	LYS	C-N-CA	-5.92	113.66	119.64
1	A	236	GLN	N-CA-C	5.85	122.73	109.81
1	B	302	GLN	N-CA-C	-5.85	104.54	111.03
1	A	90	GLU	N-CA-C	-5.82	104.84	111.07
1	D	236	GLN	N-CA-C	5.70	122.41	109.81
1	C	203	LYS	CG-CD-CE	5.62	124.22	111.30
1	E	236	GLN	N-CA-C	5.51	122.00	109.81
1	F	203	LYS	CG-CD-CE	5.48	123.91	111.30
1	B	236	GLN	N-CA-C	5.47	121.91	109.81
1	D	312	LYS	CA-C-N	5.47	127.69	122.27
1	D	312	LYS	C-N-CA	5.47	127.69	122.27
1	B	267	VAL	CB-CA-C	-5.35	103.59	112.26
1	C	267	VAL	CB-CA-C	-5.31	103.67	112.26
1	A	210	PHE	N-CA-C	-5.30	101.34	109.76
1	A	267	VAL	CB-CA-C	-5.29	103.69	112.26
1	F	236	GLN	N-CA-C	5.24	121.39	109.81
1	B	210	PHE	N-CA-C	-5.22	101.47	109.76
1	C	236	GLN	N-CA-C	5.14	121.17	109.81
1	C	210	PHE	N-CA-C	-5.14	101.59	109.76
1	B	203	LYS	N-CA-C	-5.13	102.46	110.10
1	B	270	ALA	N-CA-C	-5.08	99.98	110.80
1	B	118	ALA	N-CA-C	5.05	117.66	109.79
1	C	203	LYS	N-CA-C	-5.04	102.59	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	203	LYS	N-CA-C	-5.03	102.60	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	312	LYS	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	2020	0	2032	35	0
1	B	2028	0	2036	42	0
1	C	2020	0	2032	49	0
1	D	2028	0	2036	41	0
1	E	2028	0	2036	33	0
1	F	2020	0	2032	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	B	31	0	0	0	0
3	D	31	0	0	0	0
3	F	31	0	0	0	0
All	All	12243	0	12204	233	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 10.

All (233) 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:A:91:LYS:HE3	1:A:91:LYS:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:LYS:HE3	1:E:91:LYS:HA	1.71	0.72
1:B:91:LYS:HA	1:B:91:LYS:HE3	1.72	0.71
1:C:83:PRO:HB3	1:C:90:GLU:HG3	1.72	0.71
1:D:203:LYS:HG3	1:D:222:GLY:O	1.91	0.71
1:F:91:LYS:HE3	1:F:91:LYS:HA	1.72	0.71
1:D:205:LYS:NZ	1:D:313:GLY:HA2	2.06	0.71
1:C:269:GLU:O	1:C:270:ALA:HB3	1.91	0.71
1:B:273:ARG:NH1	1:D:192:ASP:OD2	2.25	0.70
1:E:269:GLU:O	1:E:270:ALA:HB3	1.91	0.70
1:D:269:GLU:O	1:D:270:ALA:HB3	1.91	0.70
1:C:91:LYS:HE3	1:C:91:LYS:HA	1.72	0.70
1:D:91:LYS:HE3	1:D:91:LYS:HA	1.72	0.69
1:A:203:LYS:HG3	1:A:222:GLY:O	1.91	0.69
1:B:203:LYS:HG3	1:B:222:GLY:O	1.93	0.69
1:E:203:LYS:HG3	1:E:222:GLY:O	1.92	0.69
1:C:203:LYS:HG3	1:C:222:GLY:O	1.93	0.68
1:A:269:GLU:O	1:A:270:ALA:HB3	1.92	0.68
1:F:269:GLU:O	1:F:270:ALA:HB3	1.94	0.68
1:F:203:LYS:HG3	1:F:222:GLY:O	1.93	0.67
1:A:192:ASP:OD2	1:C:273:ARG:NH1	2.28	0.67
1:B:269:GLU:O	1:B:270:ALA:HB3	1.93	0.67
1:A:91:LYS:HA	1:A:91:LYS:CE	2.25	0.66
1:C:257:VAL:HG23	1:C:277:VAL:HG11	1.78	0.65
1:E:91:LYS:HA	1:E:91:LYS:CE	2.26	0.65
1:F:257:VAL:HG23	1:F:277:VAL:HG11	1.79	0.65
1:B:91:LYS:HA	1:B:91:LYS:CE	2.27	0.64
1:B:257:VAL:HG23	1:B:277:VAL:HG11	1.78	0.64
1:E:257:VAL:HG23	1:E:277:VAL:HG11	1.79	0.64
1:C:91:LYS:HA	1:C:91:LYS:CE	2.27	0.64
1:F:91:LYS:HA	1:F:91:LYS:CE	2.27	0.64
1:D:91:LYS:HA	1:D:91:LYS:CE	2.27	0.63
1:C:270:ALA:O	1:C:272:ALA:N	2.31	0.63
1:E:270:ALA:O	1:E:272:ALA:N	2.32	0.63
1:D:257:VAL:HG23	1:D:277:VAL:HG11	1.81	0.62
1:C:269:GLU:O	1:C:270:ALA:CB	2.48	0.62
1:B:269:GLU:O	1:B:270:ALA:CB	2.49	0.61
1:B:270:ALA:O	1:B:272:ALA:N	2.34	0.61
1:B:153:GLU:OE1	1:B:153:GLU:HA	2.00	0.61
1:A:249:LEU:HD12	1:A:271:VAL:O	2.01	0.61
1:D:269:GLU:O	1:D:270:ALA:CB	2.49	0.61
1:E:269:GLU:O	1:E:270:ALA:CB	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:GLU:O	1:D:91:LYS:C	2.43	0.60
1:D:249:LEU:HD12	1:D:271:VAL:O	2.02	0.60
1:E:34:PRO:HA	1:E:37:PHE:CD2	2.37	0.60
1:C:249:LEU:HD12	1:C:271:VAL:O	2.02	0.59
1:D:270:ALA:O	1:D:272:ALA:N	2.34	0.59
1:F:249:LEU:HD12	1:F:271:VAL:O	2.03	0.59
1:B:249:LEU:HD12	1:B:271:VAL:O	2.02	0.59
1:C:156:ARG:O	1:C:159:ALA:N	2.36	0.59
1:E:249:LEU:HD12	1:E:271:VAL:O	2.02	0.59
1:F:269:GLU:O	1:F:270:ALA:CB	2.51	0.58
1:A:269:GLU:O	1:A:270:ALA:CB	2.49	0.57
1:B:90:GLU:O	1:B:91:LYS:C	2.48	0.57
1:A:251:GLU:O	1:A:253:LYS:HB2	2.05	0.56
1:D:34:PRO:HA	1:D:37:PHE:CD2	2.40	0.56
1:E:251:GLU:O	1:E:253:LYS:HB2	2.05	0.56
1:A:270:ALA:O	1:A:272:ALA:N	2.39	0.56
1:D:251:GLU:O	1:D:253:LYS:HB2	2.06	0.56
1:C:251:GLU:O	1:C:253:LYS:HB2	2.06	0.56
1:F:270:ALA:O	1:F:272:ALA:N	2.38	0.56
1:F:251:GLU:O	1:F:253:LYS:HB2	2.06	0.56
1:F:257:VAL:HG11	1:F:268:VAL:HG13	1.89	0.55
1:B:251:GLU:O	1:B:253:LYS:HB2	2.07	0.54
1:A:34:PRO:HA	1:A:37:PHE:CD2	2.41	0.54
1:B:257:VAL:HG11	1:B:268:VAL:HG13	1.89	0.54
1:E:257:VAL:HG11	1:E:268:VAL:HG13	1.91	0.53
1:F:192:ASP:OD1	1:F:220:HIS:HE1	1.92	0.53
1:F:34:PRO:HA	1:F:37:PHE:CD2	2.44	0.53
1:C:90:GLU:O	1:C:91:LYS:C	2.52	0.52
1:C:34:PRO:HA	1:C:37:PHE:CD2	2.45	0.52
1:C:257:VAL:HG11	1:C:268:VAL:HG13	1.90	0.52
1:B:34:PRO:HA	1:B:37:PHE:CD2	2.44	0.51
1:C:270:ALA:O	1:C:271:VAL:C	2.53	0.51
1:F:90:GLU:O	1:F:91:LYS:C	2.55	0.50
1:B:246:ARG:NH1	1:D:220:HIS:O	2.45	0.50
1:D:257:VAL:HG11	1:D:268:VAL:HG13	1.94	0.49
1:E:270:ALA:O	1:E:271:VAL:C	2.55	0.49
1:C:155:ALA:O	1:C:156:ARG:C	2.51	0.49
1:D:265:PRO:O	1:D:266:ALA:C	2.55	0.48
1:B:270:ALA:O	1:B:271:VAL:C	2.55	0.48
1:A:238:GLY:HA2	1:A:242:LEU:HD12	1.96	0.48
1:E:238:GLY:HA2	1:E:242:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ARG:O	1:C:158:SER:N	2.47	0.48
1:A:257:VAL:HG13	1:A:277:VAL:HG11	1.95	0.47
1:B:238:GLY:HA2	1:B:242:LEU:HD12	1.96	0.47
1:C:296:TYR:CD1	1:C:296:TYR:C	2.92	0.47
1:E:265:PRO:O	1:E:266:ALA:C	2.56	0.47
1:F:238:GLY:HA2	1:F:242:LEU:HD12	1.97	0.47
1:C:210:PHE:O	1:C:260:GLU:OE1	2.32	0.47
1:D:89:MET:O	1:D:90:GLU:C	2.56	0.47
1:D:238:GLY:HA2	1:D:242:LEU:HD12	1.95	0.47
1:F:265:PRO:O	1:F:266:ALA:C	2.57	0.47
1:E:210:PHE:O	1:E:260:GLU:OE1	2.33	0.47
1:D:270:ALA:O	1:D:271:VAL:C	2.57	0.47
1:E:93:VAL:HG13	1:E:101:GLN:HE22	1.80	0.46
1:E:91:LYS:CE	1:E:91:LYS:CA	2.93	0.46
1:B:210:PHE:O	1:B:260:GLU:OE1	2.33	0.46
1:F:93:VAL:HG13	1:F:101:GLN:HE22	1.80	0.46
1:C:93:VAL:HG13	1:C:101:GLN:HE22	1.80	0.46
1:B:265:PRO:O	1:B:266:ALA:C	2.57	0.46
1:D:93:VAL:HG13	1:D:101:GLN:HE22	1.79	0.46
1:A:220:HIS:O	1:C:246:ARG:NH1	2.47	0.46
1:A:248:GLN:O	1:A:253:LYS:HB3	2.16	0.46
1:C:156:ARG:O	1:C:157:ALA:C	2.57	0.46
1:C:248:GLN:O	1:C:253:LYS:HB3	2.16	0.46
1:B:91:LYS:CE	1:B:91:LYS:CA	2.93	0.46
1:B:235:ILE:HD12	1:B:235:ILE:N	2.31	0.46
1:F:270:ALA:O	1:F:271:VAL:C	2.58	0.45
1:A:246:ARG:O	1:A:250:VAL:HG22	2.17	0.45
1:B:195:VAL:O	1:B:196:GLY:C	2.60	0.45
1:C:91:LYS:CE	1:C:91:LYS:CA	2.93	0.45
1:C:238:GLY:HA2	1:C:242:LEU:HD12	1.97	0.45
1:F:91:LYS:CE	1:F:91:LYS:CA	2.94	0.45
1:A:270:ALA:O	1:A:271:VAL:C	2.58	0.45
1:C:257:VAL:CG1	1:C:268:VAL:HG13	2.46	0.45
1:D:210:PHE:O	1:D:260:GLU:OE1	2.34	0.45
1:A:192:ASP:HB3	1:C:273:ARG:NH1	2.31	0.45
1:F:60:HIS:O	1:F:61:ASP:CB	2.65	0.45
1:F:248:GLN:O	1:F:253:LYS:HB3	2.16	0.45
1:F:257:VAL:CG1	1:F:268:VAL:HG13	2.46	0.45
1:C:38:ILE:HG13	1:C:296:TYR:CD2	2.52	0.45
1:C:270:ALA:C	1:C:272:ALA:N	2.75	0.45
1:A:210:PHE:O	1:A:260:GLU:OE1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ILE:N	1:C:235:ILE:HD12	2.32	0.44
1:E:257:VAL:CG1	1:E:268:VAL:HG13	2.47	0.44
1:F:89:MET:O	1:F:90:GLU:C	2.57	0.44
1:F:210:PHE:O	1:F:260:GLU:OE1	2.35	0.44
1:C:104:ILE:HA	1:C:107:LEU:HG	2.00	0.44
1:D:277:VAL:HG12	1:D:278:ARG:O	2.17	0.44
1:E:270:ALA:C	1:E:272:ALA:N	2.75	0.44
1:B:248:GLN:O	1:B:253:LYS:HB3	2.17	0.44
1:B:257:VAL:CG1	1:B:268:VAL:HG13	2.47	0.44
1:B:270:ALA:C	1:B:272:ALA:N	2.76	0.44
1:E:85:MET:O	1:E:87:ALA:N	2.50	0.44
1:E:90:GLU:O	1:E:91:LYS:C	2.60	0.44
1:E:248:GLN:O	1:E:253:LYS:HB3	2.17	0.44
1:A:93:VAL:HG13	1:A:101:GLN:HE22	1.82	0.44
1:C:241:ARG:O	1:C:245:ILE:HG12	2.18	0.44
1:D:270:ALA:C	1:D:272:ALA:N	2.76	0.44
1:D:110:VAL:O	1:D:111:LYS:C	2.61	0.44
1:D:236:GLN:N	1:D:237:PRO:HA	2.33	0.44
1:D:246:ARG:O	1:D:250:VAL:HG22	2.18	0.44
1:A:265:PRO:O	1:A:266:ALA:C	2.61	0.43
1:D:85:MET:O	1:D:87:ALA:N	2.51	0.43
1:D:248:GLN:O	1:D:253:LYS:HB3	2.18	0.43
1:D:205:LYS:NZ	1:D:313:GLY:CA	2.77	0.43
1:E:277:VAL:HG12	1:E:278:ARG:O	2.18	0.43
1:A:277:VAL:HG12	1:A:278:ARG:O	2.19	0.43
1:C:150:LEU:HD23	1:C:303:LEU:HD21	1.99	0.43
1:E:246:ARG:O	1:E:250:VAL:HG22	2.18	0.43
1:B:93:VAL:HG13	1:B:101:GLN:HE22	1.82	0.43
1:C:246:ARG:O	1:C:250:VAL:HG22	2.19	0.43
1:E:308:ALA:O	1:E:312:LYS:HG3	2.19	0.43
1:F:277:VAL:HG12	1:F:278:ARG:O	2.18	0.43
1:A:150:LEU:HD23	1:A:303:LEU:HD21	1.99	0.43
1:F:150:LEU:HD23	1:F:303:LEU:HD21	2.00	0.43
1:B:89:MET:O	1:B:90:GLU:C	2.59	0.43
1:A:91:LYS:CE	1:A:91:LYS:CA	2.92	0.43
1:A:236:GLN:N	1:A:237:PRO:HA	2.34	0.43
1:F:308:ALA:O	1:F:312:LYS:HG3	2.19	0.43
1:C:208:PHE:CE1	1:C:245:ILE:HD13	2.54	0.43
1:B:208:PHE:CE1	1:B:245:ILE:HD13	2.54	0.42
1:B:236:GLN:N	1:B:237:PRO:HA	2.34	0.42
1:D:257:VAL:CG1	1:D:268:VAL:HG13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:VAL:O	1:F:111:LYS:C	2.62	0.42
1:B:85:MET:O	1:B:87:ALA:N	2.52	0.42
1:D:241:ARG:O	1:D:245:ILE:HG12	2.19	0.42
1:A:81:ILE:CD1	1:A:149:TRP:HE3	2.33	0.42
1:A:85:MET:O	1:A:87:ALA:N	2.51	0.42
1:A:305:ASN:O	1:A:309:SER:HB2	2.20	0.42
1:B:241:ARG:O	1:B:245:ILE:HG12	2.20	0.42
1:C:265:PRO:O	1:C:266:ALA:C	2.62	0.42
1:A:110:VAL:O	1:A:111:LYS:C	2.62	0.42
1:B:150:LEU:HD23	1:B:303:LEU:HD21	2.01	0.42
1:C:236:GLN:N	1:C:237:PRO:HA	2.33	0.42
1:C:245:ILE:O	1:C:246:ARG:C	2.62	0.42
1:F:235:ILE:N	1:F:235:ILE:HD12	2.34	0.42
1:F:241:ARG:O	1:F:245:ILE:HG12	2.20	0.42
1:F:246:ARG:O	1:F:250:VAL:HG22	2.19	0.42
1:D:150:LEU:HD23	1:D:303:LEU:HD21	2.02	0.42
1:D:235:ILE:HD12	1:D:235:ILE:N	2.35	0.42
1:E:241:ARG:O	1:E:245:ILE:HG12	2.19	0.42
1:E:110:VAL:O	1:E:111:LYS:C	2.63	0.42
1:F:236:GLN:N	1:F:237:PRO:HA	2.34	0.42
1:B:277:VAL:HG12	1:B:278:ARG:O	2.19	0.42
1:C:85:MET:O	1:C:87:ALA:N	2.52	0.42
1:C:308:ALA:O	1:C:312:LYS:HG3	2.20	0.42
1:D:308:ALA:O	1:D:312:LYS:HG3	2.19	0.42
1:B:104:ILE:HA	1:B:107:LEU:HG	2.01	0.42
1:B:308:ALA:O	1:B:312:LYS:HG3	2.20	0.42
1:B:246:ARG:O	1:B:250:VAL:HG22	2.19	0.41
1:E:60:HIS:O	1:E:61:ASP:CB	2.69	0.41
1:F:191:THR:OG1	1:F:297:SER:HB3	2.20	0.41
1:A:104:ILE:HA	1:A:107:LEU:HG	2.02	0.41
1:B:81:ILE:CD1	1:B:149:TRP:HE3	2.34	0.41
1:D:191:THR:OG1	1:D:297:SER:HB3	2.21	0.41
1:F:200:ALA:O	1:F:203:LYS:HD3	2.21	0.41
1:A:241:ARG:O	1:A:245:ILE:HG12	2.20	0.41
1:B:191:THR:OG1	1:B:297:SER:HB3	2.20	0.41
1:C:277:VAL:HG12	1:C:278:ARG:O	2.19	0.41
1:D:91:LYS:CE	1:D:91:LYS:CA	2.94	0.41
1:E:236:GLN:N	1:E:237:PRO:HA	2.34	0.41
1:B:193:LYS:HB2	1:F:273:ARG:HD2	2.01	0.41
1:D:60:HIS:O	1:D:61:ASP:CB	2.67	0.41
1:F:85:MET:O	1:F:87:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ASN:O	1:C:309:SER:HB2	2.20	0.41
1:D:104:ILE:HA	1:D:107:LEU:HG	2.03	0.41
1:A:28:VAL:HG11	1:A:39:ALA:HB1	2.03	0.41
1:A:191:THR:OG1	1:A:297:SER:HB3	2.21	0.41
1:A:308:ALA:O	1:A:312:LYS:HG3	2.20	0.41
1:C:155:ALA:O	1:C:156:ARG:O	2.38	0.41
1:C:296:TYR:HE1	1:C:300:LEU:HD11	1.85	0.41
1:E:104:ILE:HA	1:E:107:LEU:HG	2.02	0.41
1:F:238:GLY:O	1:F:241:ARG:HB2	2.21	0.41
1:A:60:HIS:O	1:A:61:ASP:CB	2.68	0.41
1:C:303:LEU:HD12	1:C:303:LEU:HA	1.91	0.41
1:B:110:VAL:O	1:B:111:LYS:C	2.63	0.40
1:B:197:ASN:OD1	1:F:274:GLY:HA2	2.21	0.40
1:B:305:ASN:O	1:B:309:SER:HB2	2.22	0.40
1:C:110:VAL:O	1:C:111:LYS:C	2.64	0.40
1:F:305:ASN:O	1:F:309:SER:HB2	2.21	0.40
1:A:235:ILE:N	1:A:235:ILE:HD12	2.36	0.40
1:D:305:ASN:O	1:D:309:SER:HB2	2.21	0.40
1:E:191:THR:OG1	1:E:297:SER:HB3	2.21	0.40
1:F:270:ALA:C	1:F:272:ALA:N	2.79	0.40
1:C:200:ALA:O	1:C:203:LYS:HD3	2.22	0.40
1:D:303:LEU:HD12	1:D:303:LEU:HA	1.92	0.40
1:E:305:ASN:O	1:E:309:SER:HB2	2.21	0.40
1:C:191:THR:OG1	1:C:297:SER:HB3	2.22	0.40
1:E:238:GLY:O	1:E:241:ARG:HB2	2.22	0.40
1:D:28:VAL:HG11	1:D:39:ALA:HB1	2.04	0.40
1:F:28:VAL:HG11	1:F:39:ALA:HB1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/316 (82%)	228 (88%)	24 (9%)	7 (3%)	4	21
1	B	260/316 (82%)	230 (88%)	24 (9%)	6 (2%)	5	24
1	C	259/316 (82%)	226 (87%)	25 (10%)	8 (3%)	3	18
1	D	260/316 (82%)	230 (88%)	22 (8%)	8 (3%)	3	18
1	E	260/316 (82%)	231 (89%)	21 (8%)	8 (3%)	3	18
1	F	259/316 (82%)	228 (88%)	24 (9%)	7 (3%)	4	21
All	All	1557/1896 (82%)	1373 (88%)	140 (9%)	44 (3%)	4	20

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASP
1	A	266	ALA
1	B	266	ALA
1	C	61	ASP
1	C	266	ALA
1	D	61	ASP
1	D	266	ALA
1	E	61	ASP
1	E	266	ALA
1	F	61	ASP
1	F	266	ALA
1	A	272	ALA
1	B	91	LYS
1	B	272	ALA
1	C	272	ALA
1	D	91	LYS
1	D	271	VAL
1	D	272	ALA
1	E	271	VAL
1	E	272	ALA
1	F	91	LYS
1	F	272	ALA
1	A	91	LYS
1	A	271	VAL
1	B	271	VAL
1	C	91	LYS
1	C	156	ARG
1	C	271	VAL
1	E	91	LYS
1	A	211	HIS

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Mol	Chain	Res	Type
1	A	252	GLN
1	B	211	HIS
1	C	211	HIS
1	D	211	HIS
1	E	211	HIS
1	F	211	HIS
1	F	271	VAL
1	B	252	GLN
1	C	252	GLN
1	D	252	GLN
1	E	252	GLN
1	F	252	GLN
1	D	270	ALA
1	E	238	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	213/251 (85%)	189 (89%)	24 (11%)	5 21
1	B	214/251 (85%)	188 (88%)	26 (12%)	5 20
1	C	213/251 (85%)	187 (88%)	26 (12%)	5 19
1	D	214/251 (85%)	189 (88%)	25 (12%)	5 20
1	E	214/251 (85%)	188 (88%)	26 (12%)	5 20
1	F	213/251 (85%)	187 (88%)	26 (12%)	5 19
All	All	1281/1506 (85%)	1128 (88%)	153 (12%)	5 20

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	60	HIS
1	A	71	ARG
1	A	81	ILE

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Mol	Chain	Res	Type
1	A	91	LYS
1	A	92	SER
1	A	93	VAL
1	A	113	LEU
1	A	167	VAL
1	A	168	GLU
1	A	173	SER
1	A	203	LYS
1	A	224	THR
1	A	230	THR
1	A	231	VAL
1	A	241	ARG
1	A	246	ARG
1	A	250	VAL
1	A	255	THR
1	A	262	GLN
1	A	264	ARG
1	A	267	VAL
1	A	269	GLU
1	A	281	THR
1	B	53	LEU
1	B	60	HIS
1	B	71	ARG
1	B	81	ILE
1	B	91	LYS
1	B	92	SER
1	B	93	VAL
1	B	113	LEU
1	B	119	ASP
1	B	153	GLU
1	B	167	VAL
1	B	168	GLU
1	B	173	SER
1	B	203	LYS
1	B	224	THR
1	B	230	THR
1	B	231	VAL
1	B	241	ARG
1	B	246	ARG
1	B	250	VAL
1	B	255	THR
1	B	262	GLN

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Mol	Chain	Res	Type
1	B	264	ARG
1	B	267	VAL
1	B	269	GLU
1	B	281	THR
1	C	53	LEU
1	C	60	HIS
1	C	71	ARG
1	C	81	ILE
1	C	91	LYS
1	C	92	SER
1	C	93	VAL
1	C	113	LEU
1	C	167	VAL
1	C	168	GLU
1	C	173	SER
1	C	194	GLN
1	C	203	LYS
1	C	224	THR
1	C	230	THR
1	C	231	VAL
1	C	241	ARG
1	C	246	ARG
1	C	248	GLN
1	C	250	VAL
1	C	255	THR
1	C	262	GLN
1	C	264	ARG
1	C	267	VAL
1	C	269	GLU
1	C	281	THR
1	D	53	LEU
1	D	59	GLU
1	D	60	HIS
1	D	71	ARG
1	D	91	LYS
1	D	92	SER
1	D	93	VAL
1	D	113	LEU
1	D	167	VAL
1	D	168	GLU
1	D	173	SER
1	D	203	LYS

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Mol	Chain	Res	Type
1	D	224	THR
1	D	230	THR
1	D	231	VAL
1	D	241	ARG
1	D	246	ARG
1	D	248	GLN
1	D	250	VAL
1	D	255	THR
1	D	262	GLN
1	D	264	ARG
1	D	267	VAL
1	D	269	GLU
1	D	281	THR
1	E	53	LEU
1	E	59	GLU
1	E	60	HIS
1	E	71	ARG
1	E	81	ILE
1	E	91	LYS
1	E	92	SER
1	E	93	VAL
1	E	113	LEU
1	E	167	VAL
1	E	168	GLU
1	E	173	SER
1	E	203	LYS
1	E	224	THR
1	E	230	THR
1	E	231	VAL
1	E	241	ARG
1	E	246	ARG
1	E	248	GLN
1	E	250	VAL
1	E	255	THR
1	E	262	GLN
1	E	264	ARG
1	E	267	VAL
1	E	269	GLU
1	E	281	THR
1	F	53	LEU
1	F	59	GLU
1	F	60	HIS

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Mol	Chain	Res	Type
1	F	71	ARG
1	F	81	ILE
1	F	91	LYS
1	F	92	SER
1	F	93	VAL
1	F	113	LEU
1	F	167	VAL
1	F	168	GLU
1	F	173	SER
1	F	203	LYS
1	F	224	THR
1	F	230	THR
1	F	231	VAL
1	F	241	ARG
1	F	246	ARG
1	F	248	GLN
1	F	250	VAL
1	F	255	THR
1	F	262	GLN
1	F	264	ARG
1	F	267	VAL
1	F	269	GLU
1	F	281	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	211	HIS
1	B	101	GLN
1	B	187	GLN
1	C	187	GLN
1	D	187	GLN
1	E	187	GLN
1	E	211	HIS
1	E	243	HIS
1	F	101	GLN
1	F	187	GLN
1	F	220	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	TEW	B	402	-	24,42,42	1.06	0	12,129,129	1.92	4 (33%)
3	TEW	F	402	-	24,42,42	1.06	0	12,129,129	2.19	5 (41%)
3	TEW	D	402	-	24,42,42	1.06	0	12,129,129	1.97	4 (33%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	TEW	O12-TE1-O7	-3.72	80.81	85.21
3	F	402	TEW	O12-TE1-O11	-3.61	80.94	85.21
3	F	402	TEW	O13-TE1-O1	3.46	97.77	94.65
3	D	402	TEW	O7-TE1-O1	-3.30	81.31	85.21
3	B	402	TEW	O13-TE1-O1	3.28	97.61	94.65
3	D	402	TEW	O13-TE1-O12	3.14	97.48	94.65
3	F	402	TEW	O12-TE1-O7	-3.14	81.51	85.21
3	F	402	TEW	O11-TE1-O2	3.02	97.37	94.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	402	TEW	O1-TE1-O2	-2.73	81.98	85.21
3	B	402	TEW	O7-TE1-O1	-2.54	82.20	85.21
3	D	402	TEW	O11-TE1-O2	2.42	96.83	94.65
3	F	402	TEW	O13-TE1-O12	2.34	96.76	94.65
3	B	402	TEW	O13-TE1-O12	2.04	96.49	94.65

There are no chirality outliers.

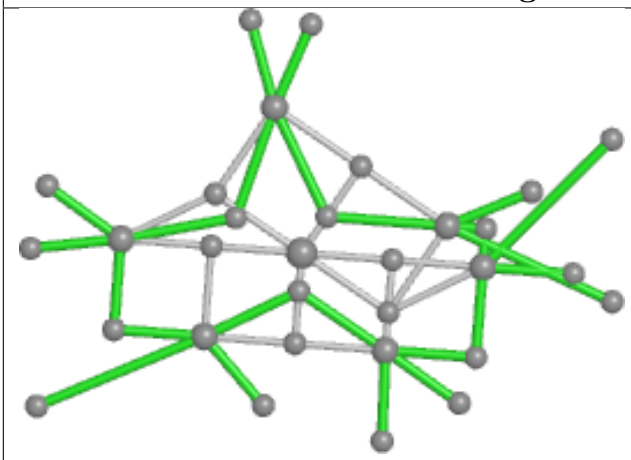
There are no torsion outliers.

There are no ring outliers.

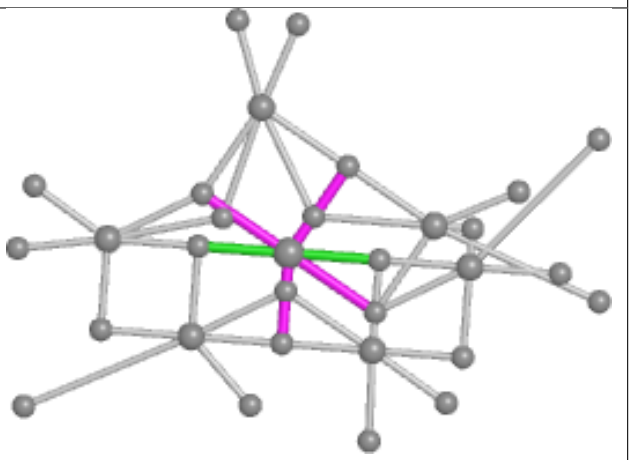
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

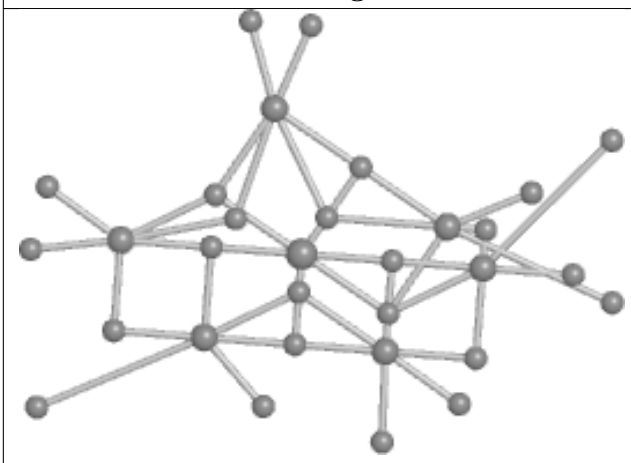
Ligand TEW B 402



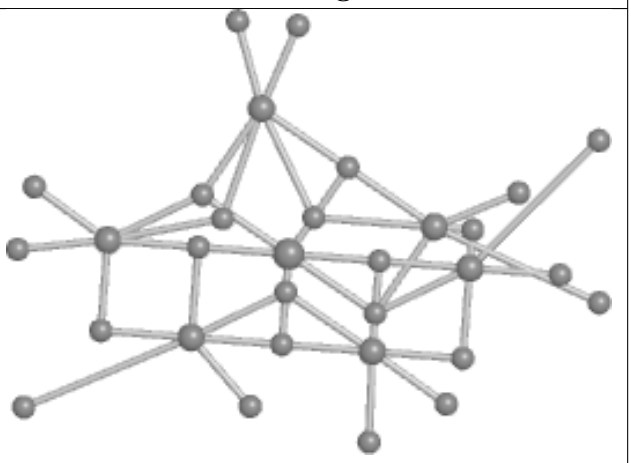
Bond lengths



Bond angles

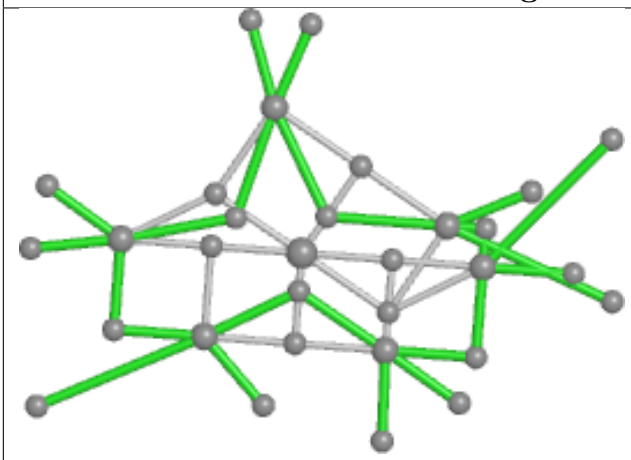


Torsions

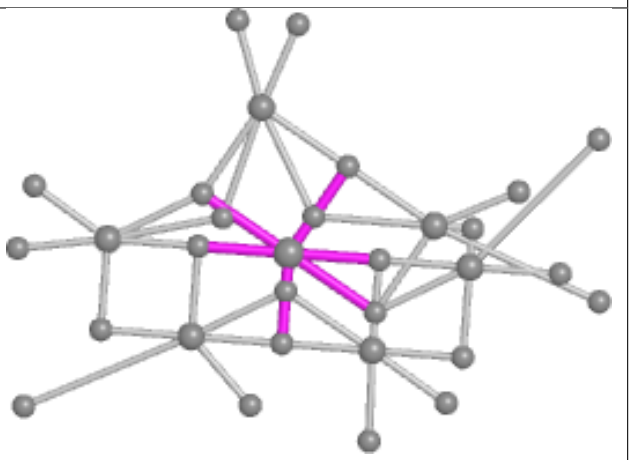


Rings

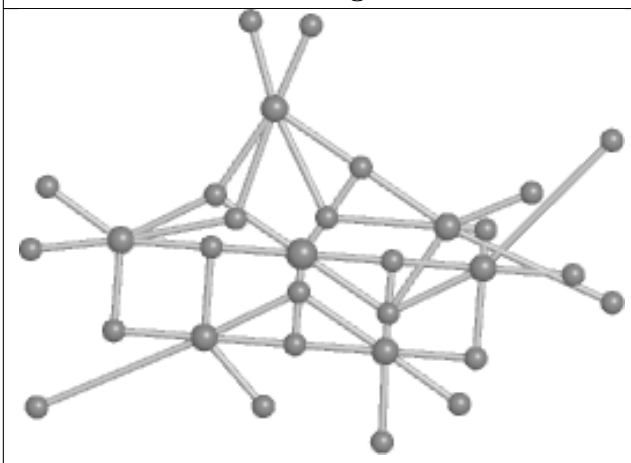
Ligand TEW F 402



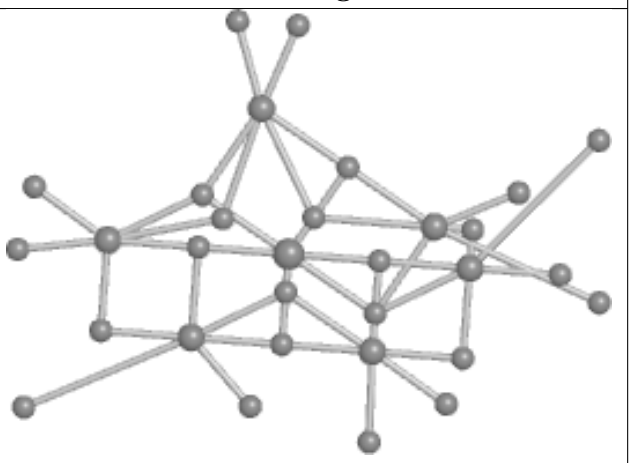
Bond lengths



Bond angles

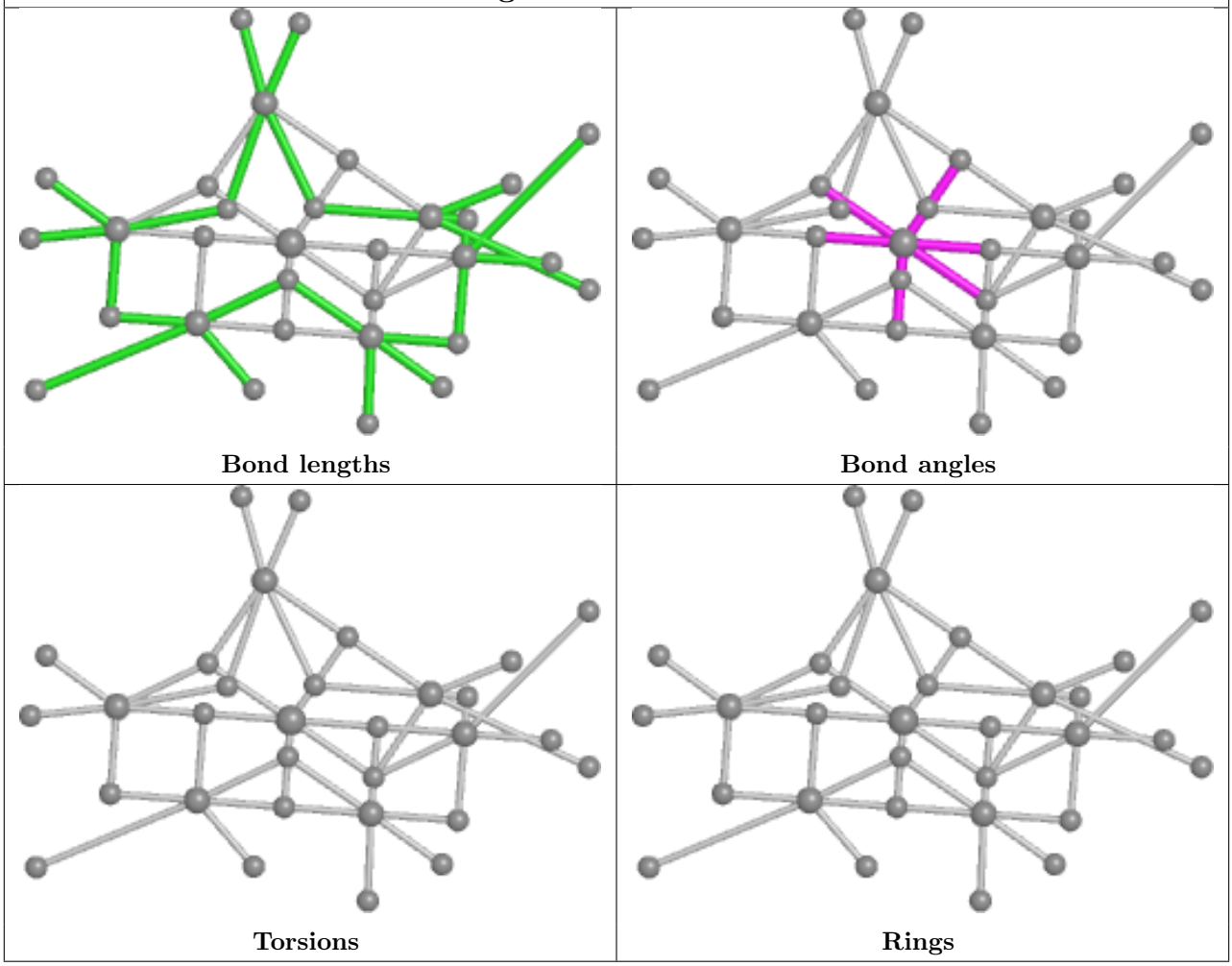


Torsions



Rings

Ligand TEW D 402



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	263/316 (83%)	-0.55	0	100	100	66, 92, 120, 152	0
1	B	264/316 (83%)	-0.44	0	100	100	69, 95, 127, 150	0
1	C	263/316 (83%)	-0.44	0	100	100	72, 98, 130, 155	0
1	D	264/316 (83%)	-0.33	2 (0%)	82	66	69, 102, 162, 236	0
1	E	264/316 (83%)	-0.26	3 (1%)	78	60	72, 102, 170, 222	0
1	F	263/316 (83%)	-0.37	0	100	100	72, 106, 143, 167	0
All	All	1581/1896 (83%)	-0.40	5 (0%)	90	81	66, 99, 144, 236	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	250	VAL	5.0
1	D	250	VAL	3.6
1	E	251	GLU	3.0
1	D	314	ASP	2.2
1	E	229	PHE	2.1

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 oligosaccharides in this entry.

6.4 Ligands (i)

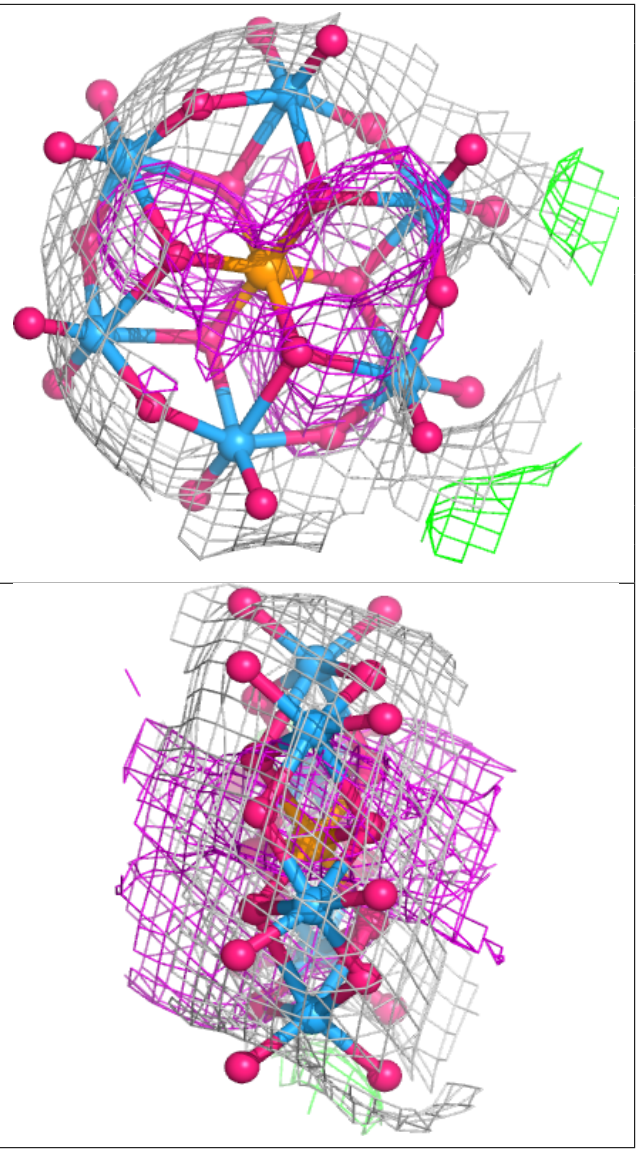
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TEW	F	402	31/31	0.56	0.12	355,376,414,434	31
3	TEW	B	402	31/31	0.60	0.13	324,343,356,382	31
3	TEW	D	402	31/31	0.66	0.12	312,334,349,370	31
2	ZN	D	401	1/1	1.00	0.02	96,96,96,96	0
2	ZN	E	401	1/1	1.00	0.02	93,93,93,93	0
2	ZN	F	401	1/1	1.00	0.03	91,91,91,91	0
2	ZN	A	401	1/1	1.00	0.02	84,84,84,84	0
2	ZN	B	401	1/1	1.00	0.03	89,89,89,89	0
2	ZN	C	401	1/1	1.00	0.02	80,80,80,80	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

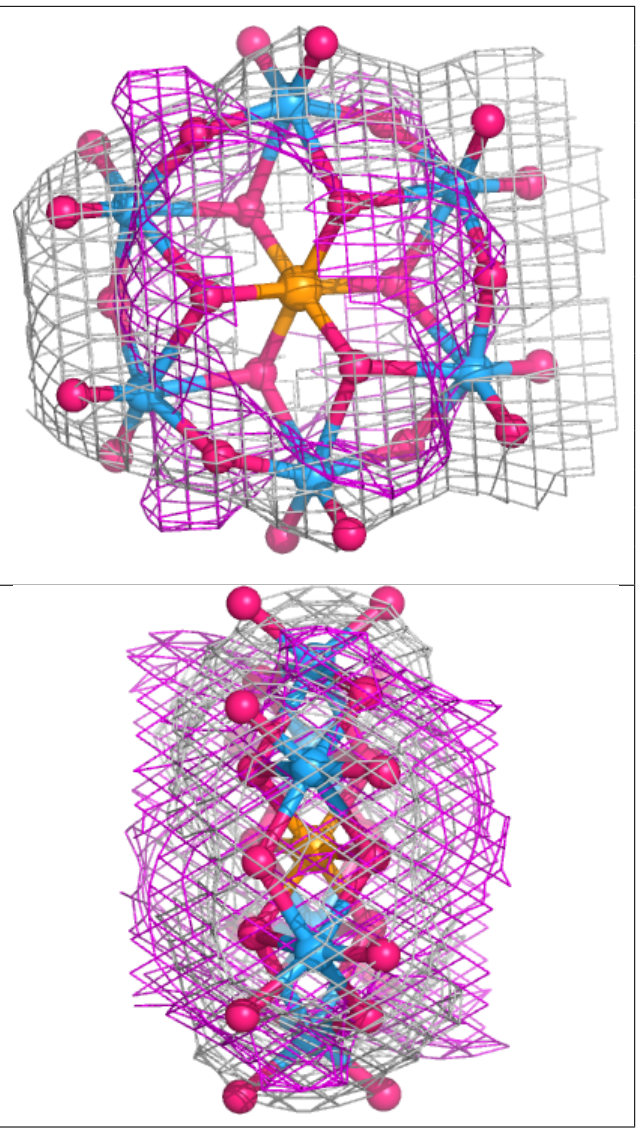
Electron density around TEW F 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TEW B 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TEW D 402:

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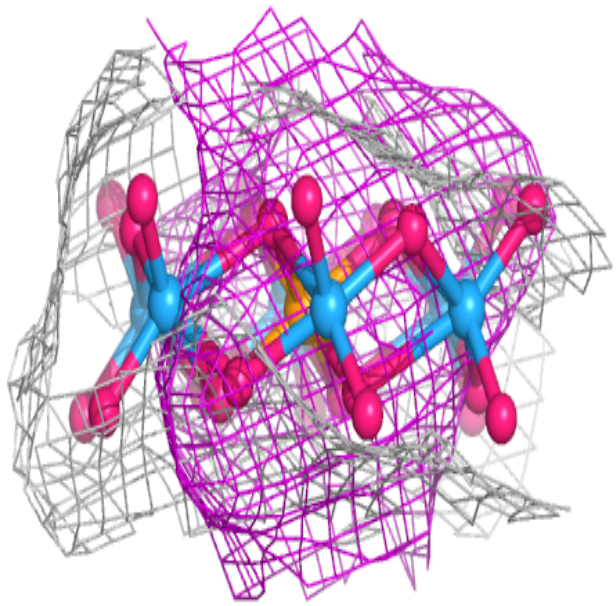
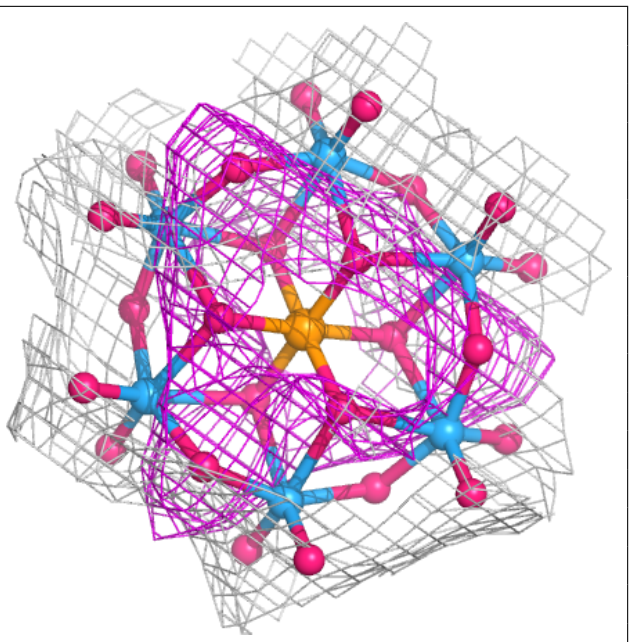
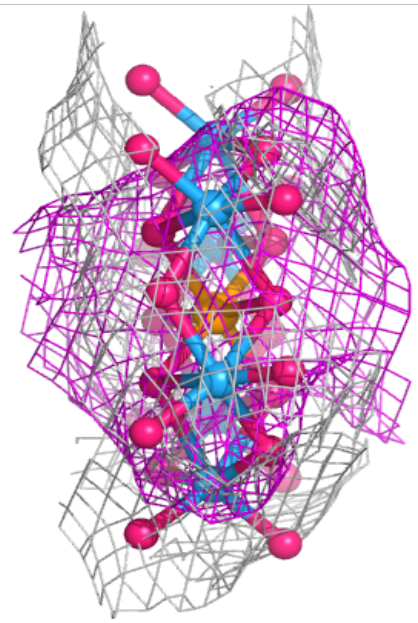
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.