



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 10:17 PM EDT

PDB ID : 6Z8O
Title : Structure of [NiFeSe] hydrogenase G491A variant from *Desulfovibrio vulgaris* Hildenborough pressurized with Krypton gas - structure G491A-Kr
Authors : Zacarias, S.; Temporao, A.; Carpentier, P.; van der Linden, P.; Pereira, I.A.C.; Matias, P.M.
Deposited on : 2020-06-02
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

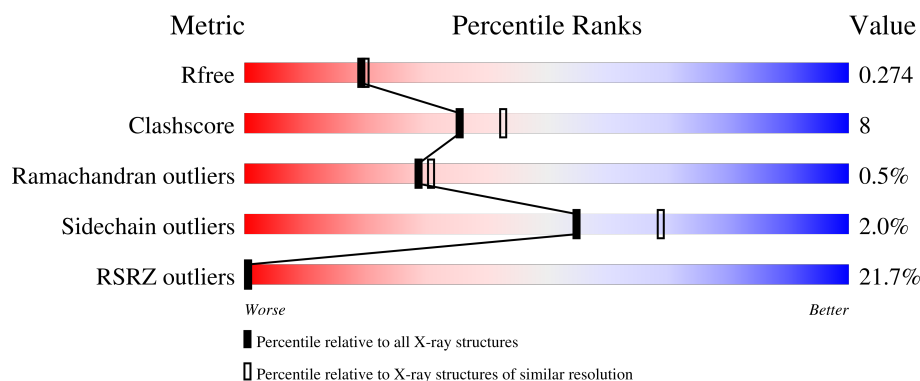
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. 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	283	<div> <div>15%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
1	C	283	<div> <div>10%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
2	B	484	<div> <div>25%</div> <div>80%</div> <div>20%</div> <div>.</div> </div>
2	D	484	<div> <div>28%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>

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
5	KR	A	306	-	-	X	-
5	KR	C	310	-	-	X	-
6	FCO	D	501	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 23485 atoms, of which 11622 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 Periplasmic [NiFeSe] hydrogenase, small subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	277	Total	C	H	N	O	S	0	3	0
			4130	1335	2037	349	389	20			
1	C	278	Total	C	H	N	O	S	0	3	0
			4145	1340	2043	350	392	20			

- Molecule 2 is a protein called Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	B	481	Total	C	H	N	O	S	Se	0	5	0
			7532	2401	3772	654	683	19	3			
2	D	481	Total	C	H	N	O	S	Se	0	5	0
			7530	2401	3770	654	683	19	3			

There are 2 discrepancies between the modelled and reference sequences:

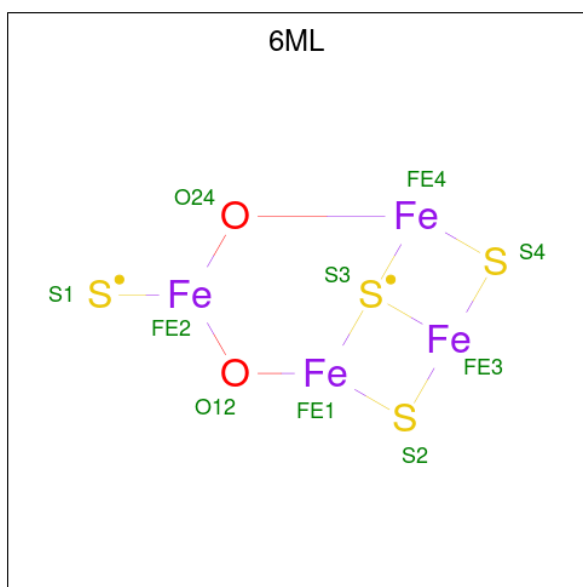
Chain	Residue	Modelled	Actual	Comment	Reference
B	491	ALA	GLY	engineered mutation	UNP Q72AS3
D	491	ALA	GLY	engineered mutation	UNP Q72AS3

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	1
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	1
			8	4	4		

- Molecule 4 is oxygen-damaged SF4 (three-letter code: 6ML) (formula: $\text{Fe}_4\text{O}_2\text{S}_4$).

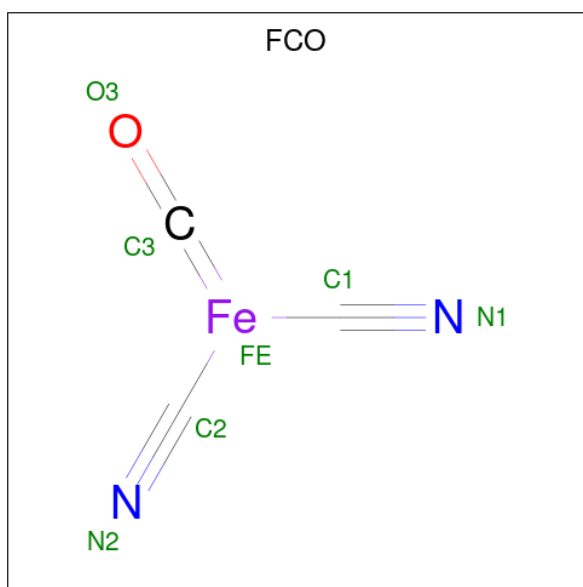


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	O	S	0	1
			10	4	2	4		
4	C	1	Total	Fe	O	S	0	1
			10	4	2	4		

- Molecule 5 is KRYPTON (three-letter code: KR) (formula: Kr) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	Kr	0	0
			6	6		
5	B	5	Total	Kr	0	2
			5	5		
5	C	6	Total	Kr	0	0
			6	6		
5	D	3	Total	Kr	0	0
			3	3		

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C₃FeN₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
6	D	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

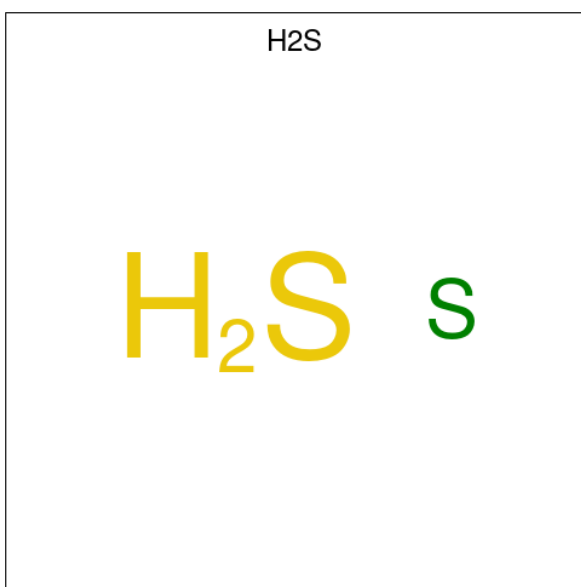
- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ni	0	0
			1	1		
7	D	1	Total	Ni	0	0
			1	1		

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Fe	0	0
			1	1		
8	D	1	Total	Fe	0	0
			1	1		

- Molecule 9 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total S 1 1	0	0
9	D	1	Total S 1 1	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Cl 1 1	0	0
10	D	1	Total Cl 1 1	0	0

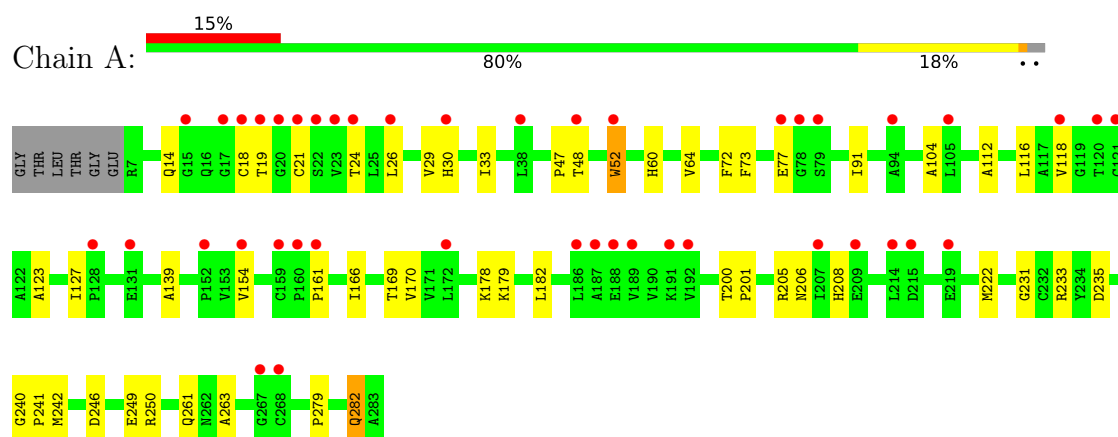
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	6	Total O 6 6	0	0
11	B	9	Total O 9 9	0	0
11	C	11	Total O 11 11	0	0
11	D	12	Total O 12 12	0	0

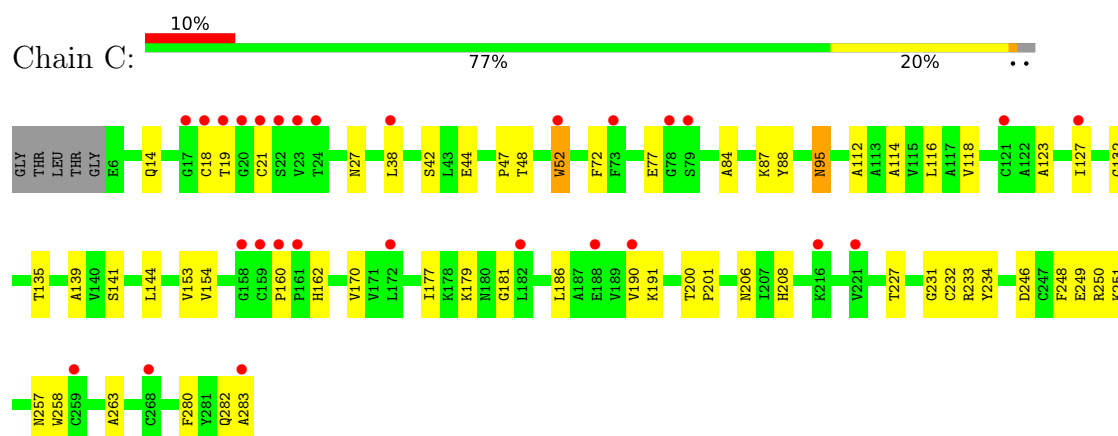
3 Residue-property plots [i](#)

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.

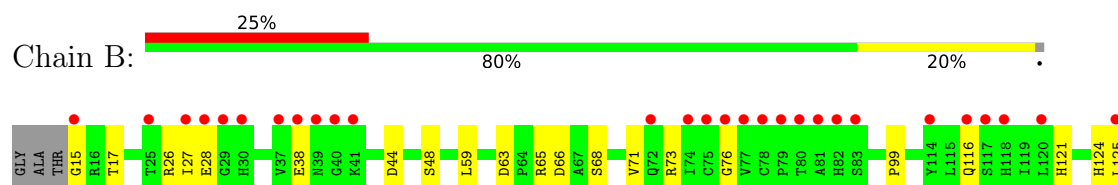
- Molecule 1: Periplasmic [NiFeSe] hydrogenase, small subunit

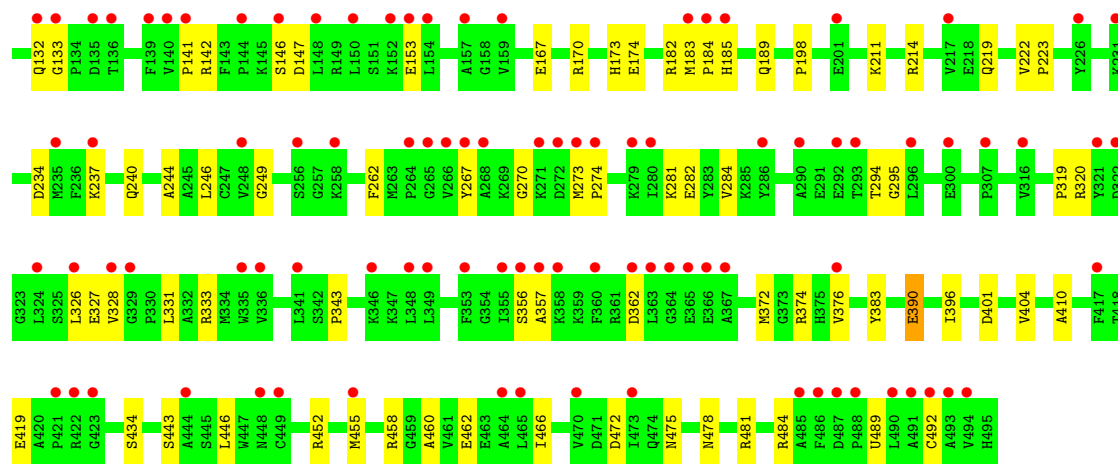


- Molecule 1: Periplasmic [NiFeSe] hydrogenase, small subunit

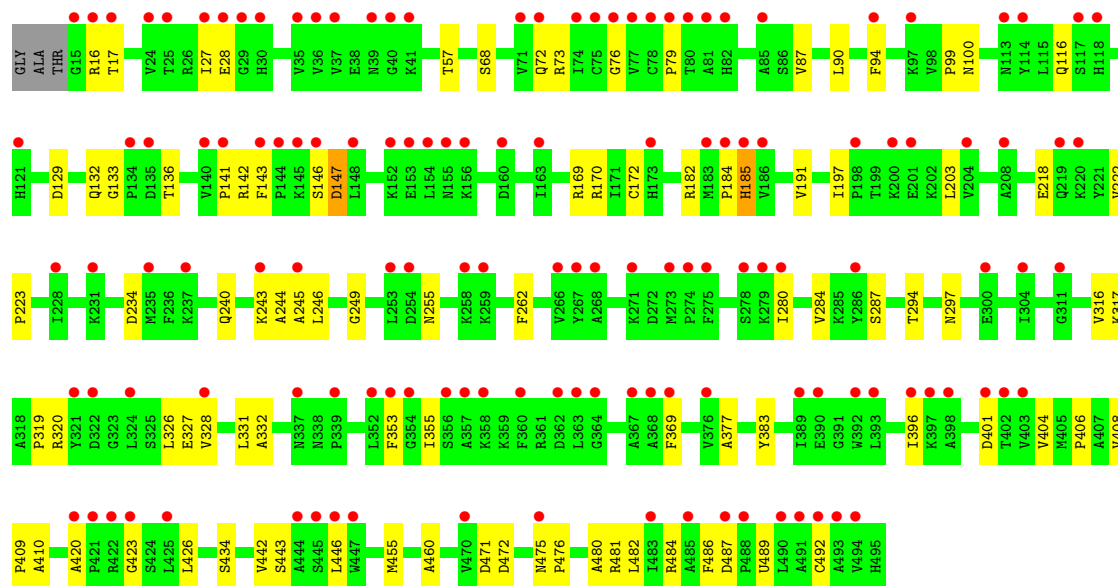
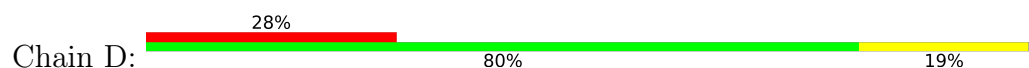


- Molecule 2: Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing





- Molecule 2: Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.72Å 97.02Å 121.32Å 90.00° 104.66° 90.00°	Depositor
Resolution (Å)	39.12 – 2.20 39.12 – 2.20	Depositor EDS
% Data completeness (in resolution range)	46.5 (39.12-2.20) 46.5 (39.12-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.226 , 0.275 0.226 , 0.274	Depositor DCC
R_{free} test set	1684 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23485	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6786e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 6ML, FCO, SF4, H2S, CL, FE2, KR, SEC, NI

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	0.30	0/2157	0.52	0/2931
1	C	0.29	0/2166	0.52	0/2943
2	B	0.29	0/3852	0.54	0/5206
2	D	0.31	0/3852	0.55	0/5206
All	All	0.30	0/12027	0.54	0/16286

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2093	2037	2030	34	2
1	C	2102	2043	2036	39	1
2	B	3760	3772	3761	59	1
2	D	3760	3770	3761	71	2
3	A	24	0	0	1	0
3	C	24	0	0	1	0
4	A	10	0	0	2	0
4	C	10	0	0	2	0
5	A	6	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5	0	0	1	0
5	C	6	0	0	4	0
5	D	3	0	0	0	0
6	B	7	0	0	1	0
6	D	7	0	0	3	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	1	0	0	1	0
9	D	1	0	0	1	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	A	6	0	0	0	0
11	B	9	0	0	3	0
11	C	11	0	0	1	0
11	D	12	0	0	4	0
All	All	11863	11622	11588	189	3

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 8.

All (189) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:489[A]:SEC:SE	6:D:501:FCO:C1	2.72	0.88
2:B:489[A]:SEC:SE	6:B:501:FCO:C1	2.71	0.88
2:D:486:PHE:O	11:D:601:HOH:O	2.05	0.75
2:D:169:ARG:NH1	11:D:602:HOH:O	2.20	0.72
2:B:189:GLN:O	11:B:602:HOH:O	2.08	0.72
2:B:66:ASP:OD2	11:B:601:HOH:O	2.07	0.71
2:D:94:PHE:CD2	2:D:191:VAL:HG21	2.25	0.71
2:B:214:ARG:NH2	2:B:390:GLU:OE1	2.23	0.70
2:B:282:GLU:OE2	11:B:603:HOH:O	2.12	0.68
1:C:18:CYS:O	2:D:76:GLY:N	2.25	0.67
1:C:21[B]:CYS:N	4:C:304[B]:6ML:S1	2.69	0.66
1:C:132:GLY:O	2:D:57:THR:OG1	2.10	0.66
2:D:94:PHE:CD1	2:D:409:PRO:HD2	2.32	0.65
2:D:240:GLN:HA	2:D:369:PHE:O	1.97	0.65
1:A:19:THR:HG22	1:A:19:THR:O	1.98	0.63
2:B:357:ALA:HB1	2:B:362:ASP:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:PHE:O	11:C:401:HOH:O	2.16	0.62
2:D:94:PHE:CE1	2:D:408:VAL:HA	2.35	0.61
2:D:94:PHE:HE1	2:D:408:VAL:HA	1.66	0.61
3:A:302:SF4:S2	2:B:182:ARG:NH1	2.74	0.60
1:C:19:THR:HG22	1:C:19:THR:O	2.02	0.58
2:D:203:LEU:HD21	2:D:396:ILE:HG21	1.86	0.58
2:B:333:ARG:NH1	2:B:419:GLU:OE1	2.31	0.56
1:C:123:ALA:O	1:C:139:ALA:HB1	2.05	0.56
1:C:21[B]:CYS:SG	1:C:118:VAL:HG12	2.46	0.56
2:D:203:LEU:CD2	2:D:396:ILE:HG21	2.36	0.56
1:C:177:ILE:O	1:C:181:GLY:N	2.39	0.56
1:C:234:TYR:CE2	1:C:283:ALA:HB1	2.41	0.55
2:D:94:PHE:CD1	2:D:409:PRO:CD	2.89	0.55
2:B:234:ASP:N	2:B:234:ASP:OD1	2.39	0.55
2:D:489[C]:SEC:CB	9:D:504:H2S:S	2.95	0.55
2:B:472:ASP:OD2	2:B:475:ASN:ND2	2.37	0.54
2:B:410:ALA:HA	2:B:434:SER:OG	2.08	0.54
2:B:28:GLU:O	2:B:489[A]:SEC:HA	2.09	0.53
2:D:94:PHE:CE1	2:D:409:PRO:HD2	2.43	0.53
2:D:443:SER:OG	2:D:492:CYS:O	2.19	0.53
2:B:170:ARG:NH1	2:B:174:GLU:OE2	2.42	0.53
2:D:280:ILE:O	2:D:297:ASN:ND2	2.38	0.53
2:B:489[C]:SEC:CB	9:B:504:H2S:S	2.98	0.52
1:C:42:SER:OG	1:C:44:GLU:OE2	2.28	0.52
2:D:28:GLU:HB3	2:D:489[A]:SEC:CB	2.40	0.52
2:D:99:PRO:HD3	2:D:404:VAL:HG13	1.90	0.52
2:B:237:LYS:C	2:B:240:GLN:HE22	2.14	0.51
1:A:21[B]:CYS:SG	1:A:118:VAL:HG12	2.50	0.51
1:A:170:VAL:HG21	5:A:307:KR:KR	2.70	0.51
2:D:443:SER:O	2:D:446:LEU:HB3	2.10	0.51
2:B:249:GLY:HA2	2:B:262:PHE:O	2.11	0.50
2:B:267:TYR:OH	2:B:270:GLY:HA2	2.10	0.50
1:A:19:THR:HA	1:A:77:GLU:OE2	2.11	0.50
2:B:15:GLY:O	2:B:38:GLU:HA	2.11	0.50
2:B:284:VAL:HG22	2:B:294:THR:HB	1.94	0.50
2:D:249:GLY:HA2	2:D:262:PHE:O	2.11	0.50
1:C:48:THR:HG23	2:D:27:ILE:O	2.10	0.50
1:A:231:GLY:O	1:A:233:ARG:NH1	2.40	0.50
2:D:129:ASP:HB3	2:D:481:ARG:HG2	1.94	0.50
2:B:99:PRO:HD3	2:B:404:VAL:HG13	1.94	0.49
1:C:170:VAL:HG21	5:C:308:KR:KR	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ASP:OD2	2:B:65:ARG:NH2	2.39	0.49
2:B:458:ARG:HD2	2:B:462:GLU:HB3	1.94	0.49
1:A:18:CYS:O	2:B:76:GLY:N	2.45	0.49
1:A:123:ALA:O	1:A:139:ALA:HB1	2.12	0.49
1:A:21[A]:CYS:HB3	1:A:118:VAL:HG12	1.94	0.48
1:C:72:PHE:CE1	1:C:112:ALA:HB2	2.48	0.48
2:B:331:LEU:HD22	2:B:374:ARG:HG2	1.96	0.48
2:B:443:SER:OG	2:B:492:CYS:O	2.25	0.48
1:A:29:VAL:O	1:A:30:HIS:HD2	1.98	0.47
2:D:410:ALA:HA	2:D:434:SER:OG	2.14	0.47
1:C:52:TRP:HB2	2:D:141:PRO:O	2.15	0.47
1:A:14:GLN:OE1	1:A:47:PRO:HG2	2.15	0.47
2:D:353:PHE:HB3	2:D:355:ILE:HD12	1.96	0.47
1:A:200:THR:N	1:A:201:PRO:CD	2.78	0.47
2:B:121:HIS:NE2	2:B:484:ARG:O	2.45	0.47
1:C:206:ASN:OD1	1:C:208:HIS:N	2.47	0.47
1:C:114:ALA:HB3	5:C:307:KR:KR	2.75	0.47
1:A:73:PHE:CE1	5:A:306:KR:KR	3.29	0.47
3:C:302:SF4:S2	2:D:182:ARG:NH1	2.88	0.47
2:D:245:ALA:HB1	2:D:332:ALA:HB1	1.97	0.46
1:C:27:ASN:HA	2:D:170:ARG:HG3	1.98	0.46
1:A:73:PHE:CD1	5:A:306:KR:KR	3.30	0.46
2:D:246:LEU:HB2	2:D:326:LEU:HD13	1.96	0.46
2:B:167:GLU:OE1	2:B:170:ARG:NE	2.39	0.46
4:C:304[B]:6ML:S1	4:C:304[B]:6ML:S2	3.14	0.46
2:D:284:VAL:HG22	2:D:294:THR:HB	1.97	0.46
2:D:218:GLU:HG2	2:D:383:TYR:CE1	2.50	0.46
1:A:21[B]:CYS:N	4:A:304[B]:6ML:S1	2.89	0.46
1:C:19:THR:HA	1:C:77:GLU:OE2	2.16	0.45
1:C:14:GLN:OE1	1:C:47:PRO:HG2	2.16	0.45
2:D:331:LEU:N	2:D:377:ALA:HB1	2.31	0.45
2:D:116:GLN:HB2	2:D:172:CYS:CB	2.46	0.45
2:D:184:PRO:O	2:D:185:HIS:HB2	2.17	0.45
2:D:331:LEU:HA	2:D:377:ALA:HB1	1.98	0.45
2:B:219:GLN:O	2:B:223:PRO:HG2	2.16	0.45
2:B:443:SER:O	2:B:446:LEU:HB3	2.17	0.45
2:D:317:LYS:NZ	11:D:604:HOH:O	2.31	0.45
1:A:48:THR:O	2:B:26:ARG:HA	2.17	0.45
2:B:273[A]:MET:HB2	2:B:274:PRO:HD2	1.99	0.45
2:D:319:PRO:O	2:D:320:ARG:NH1	2.36	0.45
1:A:72:PHE:CE1	1:A:112:ALA:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LEU:HD11	2:B:71:VAL:HG12	1.99	0.45
2:D:234:ASP:N	2:D:234:ASP:OD1	2.50	0.45
2:B:28:GLU:OE1	2:B:489[C]:SEC:SE	2.85	0.45
1:A:205:ARG:HH22	1:A:249:GLU:CD	2.21	0.44
2:B:319:PRO:O	2:B:320:ARG:NH1	2.41	0.44
2:D:146:SER:O	2:D:147:ASP:HB3	2.17	0.44
2:D:244:ALA:O	2:D:327:GLU:HG2	2.18	0.44
1:A:166:ILE:O	1:A:169:THR:N	2.51	0.44
1:C:162:HIS:NE2	1:C:251:LYS:O	2.51	0.44
2:D:353:PHE:HB3	2:D:355:ILE:CD1	2.47	0.44
2:D:482:LEU:C	2:D:482:LEU:HD13	2.38	0.44
1:C:248:PHE:CD1	1:C:249:GLU:N	2.85	0.44
1:A:91:ILE:HD11	1:A:104:ALA:HB2	2.00	0.44
2:B:121:HIS:O	2:B:125:LEU:HB2	2.17	0.44
1:C:38:LEU:CD2	2:D:136:THR:HG21	2.47	0.44
1:C:144:LEU:HD12	1:C:153:VAL:HG21	1.99	0.43
1:A:52:TRP:CZ3	2:B:141:PRO:HB2	2.54	0.43
1:C:246:ASP:OD1	1:C:250:ARG:NE	2.48	0.43
1:A:206:ASN:OD1	1:A:208:HIS:N	2.51	0.43
2:B:343:PRO:HD2	2:B:383:TYR:CZ	2.53	0.43
1:A:48:THR:HG23	2:B:27:ILE:O	2.17	0.43
2:B:184:PRO:O	2:B:185:HIS:HB2	2.18	0.43
1:A:246:ASP:OD1	1:A:250:ARG:NE	2.45	0.43
4:A:304[B]:6ML:S1	4:A:304[B]:6ML:S2	3.16	0.43
1:C:88:TYR:CG	1:C:135:THR:HG22	2.54	0.43
2:B:222:VAL:HB	2:B:223:PRO:HD3	2.01	0.43
1:C:116:LEU:HD23	1:C:154:VAL:HB	2.00	0.43
2:D:222:VAL:HB	2:D:223:PRO:HD3	2.01	0.43
2:D:331:LEU:CA	2:D:377:ALA:HB1	2.48	0.43
1:C:200:THR:N	1:C:201:PRO:CD	2.82	0.43
2:D:487:ASP:OD2	11:D:603:HOH:O	2.21	0.43
2:B:146:SER:O	2:B:147:ASP:HB3	2.18	0.43
2:D:100:ASN:OD1	2:D:255:ASN:ND2	2.49	0.43
2:D:132:GLN:OE1	2:D:142:ARG:HD3	2.19	0.43
2:B:44:ASP:OD1	2:B:452:ARG:NH2	2.52	0.42
2:B:478:ASN:OD1	2:B:481:ARG:NH1	2.49	0.42
1:A:24:THR:HG21	1:A:161:PRO:O	2.19	0.42
2:B:244:ALA:O	2:B:327:GLU:HG2	2.19	0.42
2:B:198:PRO:HG2	2:B:396:ILE:HD11	2.01	0.42
1:C:84:ALA:O	1:C:87:LYS:HG3	2.19	0.42
1:C:227:THR:CG2	2:D:197:ILE:HG13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:489[A]:SEC:SE	6:D:501:FCO:N1	3.01	0.42
2:D:404:VAL:HG23	2:D:406:PRO:HD3	2.00	0.42
2:B:132:GLN:OE1	2:B:142:ARG:HD3	2.19	0.42
1:C:127:ILE:HD12	2:D:73:ARG:HG2	2.00	0.42
1:C:154:VAL:HG23	5:C:310:KR:KR	2.80	0.42
1:A:116:LEU:HD23	1:A:154:VAL:HB	2.02	0.42
2:B:173:HIS:CD2	2:B:183:MET:HG2	2.55	0.42
2:B:458:ARG:NH2	2:B:466:ILE:HG13	2.34	0.42
1:C:154:VAL:CG2	5:C:310:KR:KR	3.29	0.42
1:C:257:ASN:OD1	1:C:258:TRP:N	2.50	0.42
2:D:316:VAL:CG1	2:D:446:LEU:HD12	2.50	0.42
2:D:129:ASP:OD1	2:D:484:ARG:NH1	2.52	0.42
2:D:326:LEU:O	2:D:460:ALA:HB2	2.20	0.42
2:D:480:ALA:O	2:D:484:ARG:HG3	2.20	0.42
2:B:28:GLU:HB3	2:B:489[B]:SEC:SE	2.70	0.42
2:B:246:LEU:HB3	2:B:328:VAL:HG12	2.02	0.42
1:C:52:TRP:CZ3	2:D:141:PRO:HB2	2.55	0.42
2:D:420:ALA:HB1	6:D:501:FCO:N2	2.35	0.42
2:B:326:LEU:O	2:B:460:ALA:HB2	2.20	0.41
1:C:95:ASN:OD1	1:C:95:ASN:N	2.54	0.41
2:B:124:HIS:HB3	5:B:508[B]:KR:KR	2.81	0.41
1:C:160:PRO:HG3	2:D:184:PRO:HD2	2.02	0.41
1:C:231:GLY:O	1:C:233:ARG:NH1	2.50	0.41
2:D:472:ASP:OD2	2:D:475:ASN:ND2	2.45	0.41
1:C:186:LEU:O	1:C:190:VAL:HG23	2.20	0.41
1:A:116:LEU:CD2	1:A:154:VAL:HB	2.51	0.41
2:D:243:LYS:HA	2:D:369:PHE:CD2	2.56	0.41
1:A:240:GLY:N	1:A:241:PRO:CD	2.83	0.41
2:B:244:ALA:HB1	2:B:326:LEU:CD2	2.50	0.41
2:D:328:VAL:HB	2:D:423:GLY:HA3	2.02	0.41
1:C:232:CYS:SG	1:C:233:ARG:N	2.93	0.41
2:D:143:PHE:O	2:D:146:SER:OG	2.39	0.41
2:B:281:LYS:HD3	2:B:295:GLY:O	2.21	0.41
2:D:72:GLN:HB3	2:D:79:PRO:HB2	2.02	0.41
2:D:87:VAL:HA	2:D:90:LEU:HD12	2.03	0.41
1:A:26:LEU:HD23	1:A:33:ILE:HG12	2.03	0.41
1:A:279:PRO:HB2	1:A:282:GLN:HG3	2.02	0.41
1:A:60:HIS:O	1:A:64:VAL:HG23	2.20	0.40
2:B:28:GLU:HB3	2:B:489[A]:SEC:CB	2.52	0.40
2:D:284:VAL:O	2:D:284:VAL:HG23	2.21	0.40
2:D:409:PRO:O	2:D:434:SER:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:HD12	2:B:73:ARG:HG2	2.02	0.40
1:A:222:MET:HG3	1:A:235:ASP:OD2	2.21	0.40
2:B:147:ASP:O	2:B:481:ARG:NH2	2.54	0.40
2:B:372:MET:O	2:B:376:VAL:HG23	2.20	0.40
2:D:143:PHE:CZ	2:D:476:PRO:HD2	2.56	0.40
2:D:28:GLU:O	2:D:489[A]:SEC:HA	2.22	0.40
2:D:426:LEU:HG	2:D:442:VAL:HB	2.04	0.40
1:A:60:HIS:ND1	2:B:141:PRO:HG3	2.37	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LYS:O	2:D:16:ARG:NH1[2_545]	1.72	0.48
1:A:178:LYS:O	2:D:16:ARG:HH12[2_545]	1.37	0.23
2:B:153:GLU:OE1	1:C:191:LYS:NZ[1_655]	2.09	0.11

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	278/283 (98%)	257 (92%)	19 (7%)	2 (1%)	22	22
1	C	279/283 (99%)	256 (92%)	22 (8%)	1 (0%)	34	37
2	B	483/484 (100%)	450 (93%)	32 (7%)	1 (0%)	47	55
2	D	483/484 (100%)	452 (94%)	28 (6%)	3 (1%)	25	26
All	All	1523/1534 (99%)	1415 (93%)	101 (7%)	7 (0%)	29	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	LEU
1	C	263	ALA
2	D	185	HIS
1	A	263	ALA
2	B	133	GLY
2	D	133	GLY
2	D	147	ASP

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	225/226 (100%)	221 (98%)	4 (2%)	59	72
1	C	226/226 (100%)	221 (98%)	5 (2%)	52	65
2	B	396/392 (101%)	386 (98%)	10 (2%)	47	60
2	D	396/392 (101%)	390 (98%)	6 (2%)	65	78
All	All	1243/1236 (101%)	1218 (98%)	25 (2%)	55	69

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	TRP
1	A	179	LYS
1	A	261	GLN
1	A	282	GLN
2	B	17	THR
2	B	48[A]	SER
2	B	48[B]	SER
2	B	68	SER
2	B	116	GLN
2	B	211	LYS
2	B	356	SER
2	B	390	GLU
2	B	401	ASP
2	B	455	MET
1	C	52	TRP

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Mol	Chain	Res	Type
1	C	95	ASN
1	C	141	SER
1	C	179	LYS
1	C	282	GLN
2	D	17	THR
2	D	68	SER
2	D	287	SER
2	D	401	ASP
2	D	455	MET
2	D	471	ASP

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

Mol	Chain	Res	Type
1	A	30	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 26 are monoatomic and 2 are modelled with single atom - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	6ML	A	304[B]	1	0,12,12	-	-	-		
3	SF4	C	301	1	0,12,12	-	-	-		
6	FCO	D	501	2	0,6,6	-	-	-		
6	FCO	B	501	2	0,6,6	-	-	-		
3	SF4	A	302	1	0,12,12	-	-	-		
3	SF4	C	302	1	0,12,12	-	-	-		
3	SF4	C	303[A]	1	0,12,12	-	-	-		
4	6ML	C	304[B]	1	0,12,12	-	-	-		
3	SF4	A	301	1	0,12,12	-	-	-		
3	SF4	A	303[A]	1	0,12,12	-	-	-		

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	6ML	A	304[B]	1	-	-	0/2/3/3
3	SF4	C	301	1	-	-	0/6/5/5
3	SF4	A	302	1	-	-	0/6/5/5
3	SF4	C	302	1	-	-	0/6/5/5
3	SF4	C	303[A]	1	-	-	0/6/5/5
4	6ML	C	304[B]	1	-	-	0/2/3/3
3	SF4	A	301	1	-	-	0/6/5/5
3	SF4	A	303[A]	1	-	-	0/6/5/5

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.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304[B]	6ML	2	0
6	D	501	FCO	3	0
6	B	501	FCO	1	0
3	A	302	SF4	1	0
3	C	302	SF4	1	0
4	C	304[B]	6ML	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	277/283 (97%)	0.86	43 (15%) 2 1	27, 39, 57, 76	1 (0%)
1	C	278/283 (98%)	0.79	28 (10%) 7 6	21, 39, 57, 69	2 (0%)
2	B	480/484 (99%)	1.27	121 (25%) 0 0	22, 45, 67, 78	3 (0%)
2	D	480/484 (99%)	1.40	136 (28%) 0 0	23, 48, 65, 84	2 (0%)
All	All	1515/1534 (98%)	1.15	328 (21%) 0 0	21, 43, 65, 84	8 (0%)

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	363	LEU	12.8
1	A	21[A]	CYS	9.2
2	D	259	LYS	8.7
2	D	135	ASP	7.5
2	B	353	PHE	7.1
1	A	191	LYS	6.9
2	D	368	ALA	6.6
2	D	75	CYS	6.6
2	B	40	GLY	6.5
2	B	150	LEU	6.4
2	D	358	LYS	6.4
2	B	75	CYS	6.4
2	B	273[A]	MET	6.3
1	A	18	CYS	6.3
2	D	78	CYS	6.2
1	A	20	GLY	6.2
2	B	140	VAL	5.9
2	B	492	CYS	5.8
2	D	492	CYS	5.8
2	D	273[A]	MET	5.8
2	B	268	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
2	D	201	GLU	5.6
1	C	18	CYS	5.6
1	A	17	GLY	5.5
2	D	153	GLU	5.5
2	B	78	CYS	5.5
2	B	135	ASP	5.4
1	C	221	VAL	5.4
2	D	357	ALA	5.4
2	D	397	LYS	5.3
2	B	360	PHE	5.3
2	D	140	VAL	5.3
2	B	358	LYS	5.2
2	B	237	LYS	5.2
2	D	488	PRO	5.1
2	D	364	GLY	5.1
2	B	363	LEU	5.0
2	D	40	GLY	4.9
2	D	143	PHE	4.9
1	A	172	LEU	4.9
2	D	204	VAL	4.8
2	D	322	ASP	4.8
1	A	23	VAL	4.7
1	C	283	ALA	4.7
1	C	21[A]	CYS	4.6
2	B	76	GLY	4.6
2	D	29	GLY	4.6
1	A	30	HIS	4.6
1	C	20	GLY	4.6
2	B	77	VAL	4.5
2	D	271	LYS	4.5
2	B	491	ALA	4.5
1	C	17	GLY	4.5
2	D	74	ILE	4.5
2	D	403	VAL	4.5
2	D	163	ILE	4.5
2	D	152	LYS	4.5
1	A	22[A]	SER	4.5
2	B	266	VAL	4.5
2	B	157	ALA	4.5
2	D	160	ASP	4.4
1	A	94	ALA	4.4
2	B	39	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	186	LEU	4.4
2	D	79	PRO	4.4
2	D	493	ALA	4.4
1	A	188	GLU	4.4
2	D	253	LEU	4.3
2	B	357	ALA	4.3
2	B	470	VAL	4.3
2	D	321	TYR	4.3
2	D	490[A]	LEU	4.3
2	D	491	ALA	4.3
2	B	488	PRO	4.2
1	A	207	ILE	4.2
1	A	19	THR	4.2
2	D	27	ILE	4.2
1	C	23	VAL	4.2
2	B	271	LYS	4.1
2	B	74	ILE	4.1
2	D	352	LEU	4.1
2	B	366	GLU	4.1
2	B	274	PRO	4.1
2	D	141	PRO	4.0
2	D	444	ALA	4.0
2	B	132	GLN	4.0
2	B	265	GLY	4.0
2	D	254	ASP	4.0
2	B	290	ALA	4.0
2	B	421	PRO	4.0
2	D	200	LYS	4.0
2	D	184	PRO	3.9
1	A	121	CYS	3.9
2	B	141	PRO	3.9
2	B	154	LEU	3.9
2	B	473	ILE	3.9
2	D	36	VAL	3.9
2	B	148	LEU	3.9
2	B	29	GLY	3.8
1	A	215	ASP	3.8
2	B	493	ALA	3.8
2	B	349	LEU	3.8
2	D	422	ARG	3.7
2	D	37	VAL	3.7
2	B	346	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	367	ALA	3.7
2	D	185	HIS	3.7
1	A	268	CYS	3.7
2	B	133	GLY	3.7
2	D	360	PHE	3.7
2	B	235	MET	3.7
2	D	266	VAL	3.7
2	D	41	LYS	3.6
2	D	258	LYS	3.6
2	B	272	ASP	3.6
2	B	300	GLU	3.6
1	C	19	THR	3.6
1	C	160	PRO	3.6
2	B	27	ILE	3.6
2	B	267	TYR	3.6
2	B	41	LYS	3.5
2	D	220	LYS	3.5
2	D	487	ASP	3.5
1	A	159	CYS	3.5
2	D	77	VAL	3.5
2	D	423	GLY	3.5
2	B	487	ASP	3.5
2	D	328	VAL	3.5
1	C	159	CYS	3.5
2	B	117	SER	3.5
1	A	209	GLU	3.5
2	D	245	ALA	3.5
2	B	185	HIS	3.5
2	D	274	PRO	3.4
1	A	24	THR	3.4
2	D	447	TRP	3.4
2	B	79	PRO	3.4
2	D	154	LEU	3.4
2	D	275	PHE	3.4
2	D	280	ILE	3.4
2	D	446	LEU	3.3
2	D	324	LEU	3.3
1	C	22[A]	SER	3.2
2	B	159	VAL	3.2
1	C	24	THR	3.2
1	A	187	ALA	3.2
2	B	422	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	134	PRO	3.2
1	A	214	LEU	3.2
2	D	421	PRO	3.2
2	D	76	GLY	3.1
2	D	118	HIS	3.1
2	D	393	LEU	3.1
2	D	369	PHE	3.1
1	C	172	LEU	3.1
1	A	219	GLU	3.1
2	B	365	GLU	3.1
1	A	48	THR	3.1
2	D	304	ILE	3.1
2	B	201	GLU	3.1
2	D	231	LYS	3.0
2	D	356	SER	3.0
2	D	16	ARG	3.0
2	D	311	GLY	3.0
2	B	231	LYS	3.0
2	D	82	HIS	3.0
2	D	228	ILE	3.0
2	D	445	SER	3.0
2	B	324	LEU	3.0
2	B	139	PHE	3.0
1	C	158	GLY	3.0
2	D	17	THR	3.0
2	D	494	VAL	3.0
2	D	117	SER	2.9
1	A	52	TRP	2.9
2	B	184	PRO	2.9
2	B	490[A]	LEU	2.9
2	D	396	ILE	2.9
2	D	94	PHE	2.9
2	B	328	VAL	2.9
2	D	114	TYR	2.9
2	D	279	LYS	2.9
2	B	153	GLU	2.9
2	B	364	GLY	2.9
2	B	307	PRO	2.9
2	D	278	SER	2.9
2	B	125	LEU	2.8
1	A	160	PRO	2.8
2	D	39	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	420	ALA	2.8
1	C	188	GLU	2.8
2	D	81	ALA	2.8
2	B	321	TYR	2.8
2	B	286	TYR	2.8
2	D	146	SER	2.8
2	B	280	ILE	2.8
2	D	267	TYR	2.8
2	B	444	ALA	2.7
2	B	494	VAL	2.7
1	A	38	LEU	2.7
2	B	256	SER	2.7
1	C	121	CYS	2.7
2	D	121	HIS	2.7
1	A	78	GLY	2.7
1	C	161	PRO	2.7
2	B	367	ALA	2.7
2	D	237	LYS	2.7
2	B	30	HIS	2.7
2	B	118	HIS	2.7
2	B	25	THR	2.7
2	B	486	PHE	2.7
2	B	28	GLU	2.6
2	B	322	ASP	2.6
2	B	293	THR	2.6
2	D	353	PHE	2.6
2	D	198	PRO	2.6
2	D	392	TRP	2.6
2	D	398	ALA	2.6
2	D	28	GLU	2.6
1	A	79	SER	2.6
1	A	189	VAL	2.6
2	B	226	TYR	2.6
2	D	401	ASP	2.6
1	A	152	PRO	2.6
1	A	192	VAL	2.6
2	B	38	GLU	2.6
2	B	114	TYR	2.6
2	D	173	HIS	2.6
2	B	183	MET	2.6
2	D	24	VAL	2.6
2	D	25	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	348	LEU	2.5
2	B	136	THR	2.5
2	B	144	PRO	2.5
2	B	292	GLU	2.5
2	D	243	LYS	2.5
1	C	52	TRP	2.5
2	D	376	VAL	2.5
2	B	355	ILE	2.5
2	D	475	ASN	2.5
2	D	425	LEU	2.5
1	A	15	GLY	2.5
1	C	127	ILE	2.4
2	B	146	SER	2.4
2	B	258	LYS	2.4
2	B	329	GLY	2.4
1	A	77	GLU	2.4
2	D	362	ASP	2.4
2	D	148	LEU	2.4
2	D	15	GLY	2.4
1	A	120	THR	2.4
1	C	78	GLY	2.4
2	B	423	GLY	2.4
1	A	161	PRO	2.4
2	D	300	GLU	2.4
1	C	182	LEU	2.3
2	B	264	PRO	2.3
2	D	485	ALA	2.3
2	B	455	MET	2.3
1	A	105	LEU	2.3
2	D	235	MET	2.3
2	B	449	CYS	2.3
2	B	465	LEU	2.3
2	B	279	LYS	2.3
2	D	71	VAL	2.3
2	D	337	ASN	2.3
2	B	83	SER	2.3
2	D	219	GLN	2.3
1	C	216	LYS	2.3
2	B	120	LEU	2.3
2	B	296	LEU	2.3
2	D	156	LYS	2.3
2	D	85	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	155	ASN	2.2
2	B	81	ALA	2.2
1	A	128	PRO	2.2
1	A	154	VAL	2.2
2	B	248	VAL	2.2
2	B	336	VAL	2.2
2	B	335	TRP	2.2
2	D	208	ALA	2.2
2	B	341	LEU	2.2
2	B	362	ASP	2.2
2	D	183	MET	2.2
1	C	259	CYS	2.2
2	D	30	HIS	2.2
2	B	72	GLN	2.2
2	D	286	TYR	2.2
2	D	470	VAL	2.2
2	B	15	GLY	2.2
2	B	356	SER	2.2
2	B	448	ASN	2.2
1	C	38	LEU	2.2
2	D	389	ILE	2.1
1	A	26	LEU	2.1
1	A	118	VAL	2.1
2	B	217	VAL	2.1
2	D	35	VAL	2.1
2	B	152	LYS	2.1
1	C	268	CYS	2.1
2	D	80	THR	2.1
2	D	97	LYS	2.1
1	C	73	PHE	2.1
1	C	79	SER	2.1
2	D	113	ASN	2.1
2	B	316	VAL	2.1
2	D	145	LYS	2.1
2	D	390	GLU	2.1
2	B	485	ALA	2.1
2	D	186	VAL	2.1
2	D	483	ILE	2.1
2	B	116	GLN	2.1
1	A	267	GLY	2.1
2	D	354	GLY	2.1
2	B	417	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	402	THR	2.0
2	B	464	ALA	2.0
1	A	131	GLU	2.0
2	D	72	GLN	2.0
2	D	339	PRO	2.0
2	B	326	LEU	2.0
2	D	268	ALA	2.0
2	D	144	PRO	2.0
1	C	190	VAL	2.0
2	B	37	VAL	2.0
2	B	82	HIS	2.0
2	B	376	VAL	2.0
2	B	80	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
5	KR	C	307	1/1	0.93	0.13	42,42,42,42	1
5	KR	B	508[B]	1/1	0.94	0.24	36,36,36,36	1
5	KR	C	308	1/1	0.94	0.06	51,51,51,51	1
5	KR	D	508	1/1	0.94	0.06	53,53,53,53	1
5	KR	D	506	1/1	0.95	0.09	58,58,58,58	1
3	SF4	A	303[A]	8/8	0.96	0.24	25,29,34,38	8
9	H2S	D	504	1/1	0.96	0.67	38,38,38,38	1
5	KR	A	306	1/1	0.97	0.07	58,58,58,58	1
5	KR	A	307	1/1	0.97	0.08	45,45,45,45	1
5	KR	A	309	1/1	0.97	0.11	46,46,46,46	1

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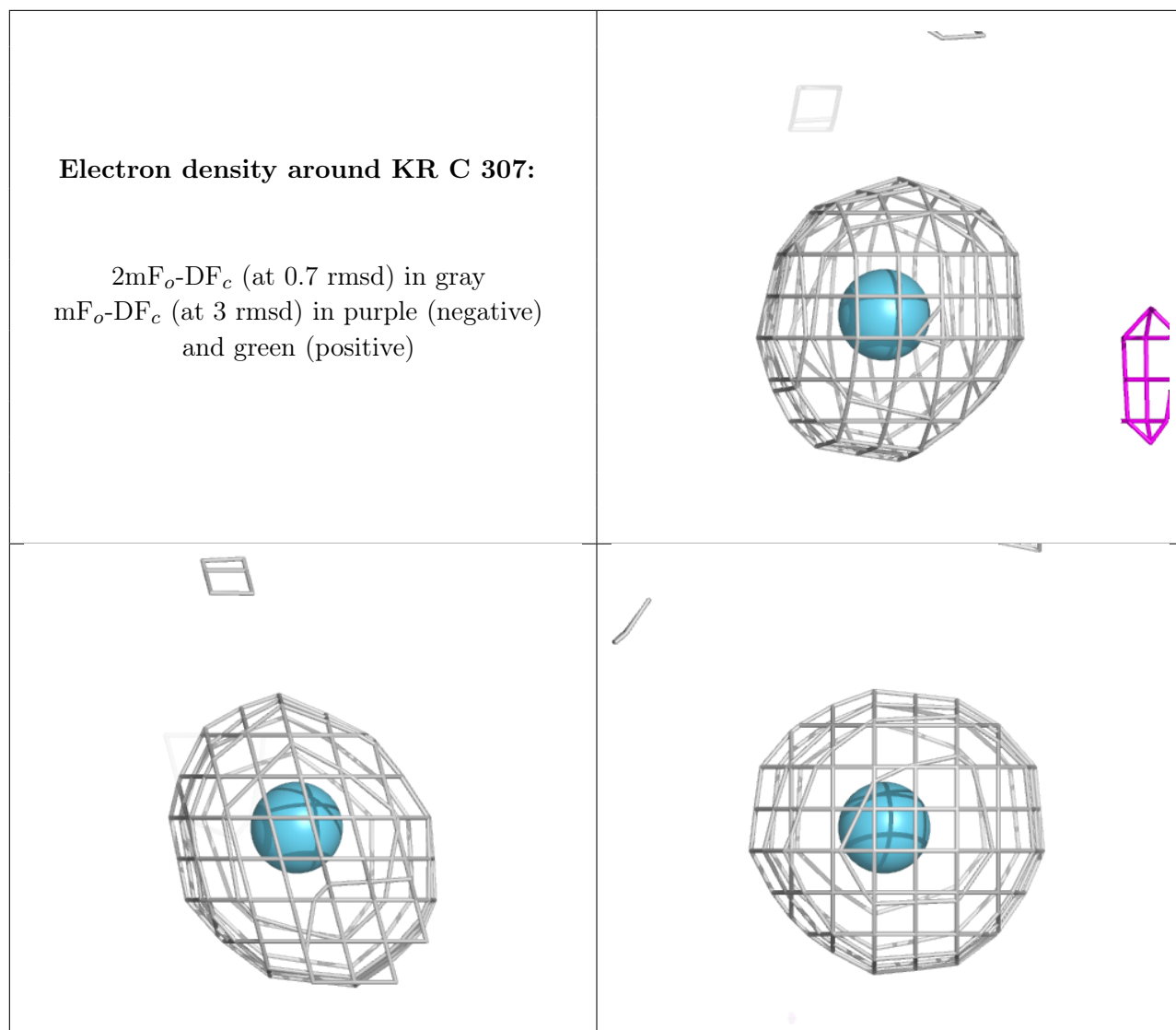
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	KR	B	506	1/1	0.97	0.07	43,43,43,43	1
3	SF4	A	302	8/8	0.97	0.20	24,30,34,41	0
5	KR	B	509	1/1	0.97	0.09	45,45,45,45	1
5	KR	B	510	1/1	0.97	0.11	93,93,93,93	0
3	SF4	A	301	8/8	0.97	0.10	25,41,51,55	0
3	SF4	C	301	8/8	0.97	0.11	40,47,56,63	0
3	SF4	C	302	8/8	0.97	0.20	25,31,37,50	0
5	KR	D	507	1/1	0.97	0.07	43,43,43,43	1
3	SF4	C	303[A]	8/8	0.97	0.24	21,24,27,29	8
6	FCO	D	501	7/7	0.97	0.36	20,33,37,39	0
7	NI	D	502	1/1	0.97	0.23	22,22,22,22	1
4	6ML	A	304[B]	10/10	0.97	0.25	25,29,37,39	10
4	6ML	C	304[B]	10/10	0.98	0.25	21,23,28,29	10
5	KR	A	310	1/1	0.98	0.17	36,36,36,36	1
5	KR	C	306	1/1	0.98	0.05	48,48,48,48	1
6	FCO	B	501	7/7	0.98	0.35	21,30,34,41	0
5	KR	A	305	1/1	0.98	0.05	57,57,57,57	1
5	KR	A	308	1/1	0.98	0.08	52,52,52,52	1
5	KR	C	309	1/1	0.98	0.08	52,52,52,52	1
5	KR	C	305	1/1	0.99	0.04	59,59,59,59	1
7	NI	B	502	1/1	0.99	0.24	23,23,23,23	1
5	KR	C	310	1/1	0.99	0.10	39,39,39,39	1
8	FE2	B	503	1/1	0.99	0.08	22,22,22,22	0
8	FE2	D	503	1/1	0.99	0.14	23,23,23,23	0
9	H2S	B	504	1/1	0.99	0.34	31,31,31,31	0
5	KR	B	507[A]	1/1	0.99	0.07	40,40,40,40	1
10	CL	B	505	1/1	0.99	0.22	29,29,29,29	0
10	CL	D	505	1/1	0.99	0.11	37,37,37,37	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.

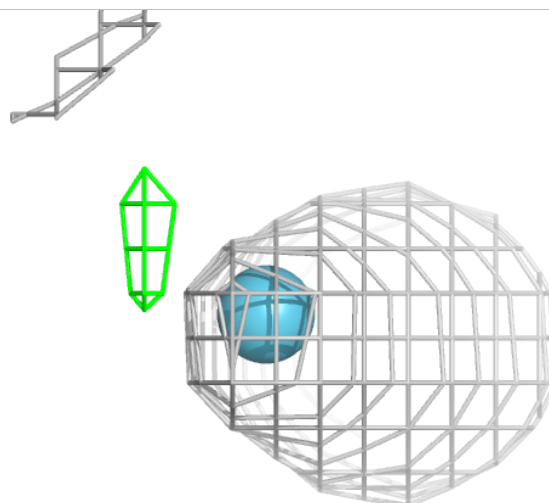
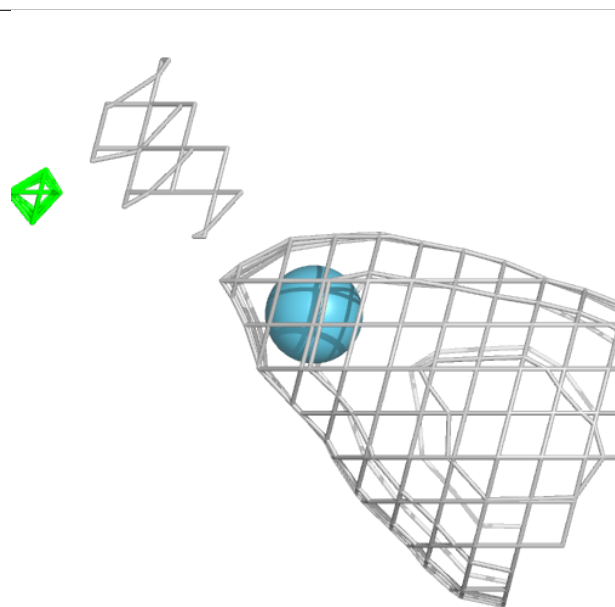
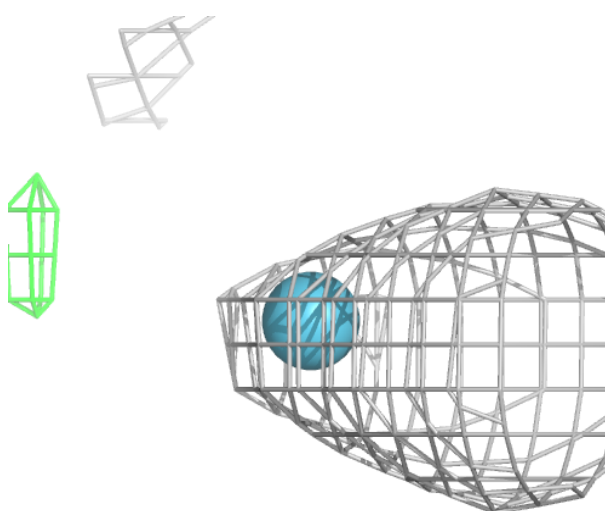
Electron density around KR C 307:

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



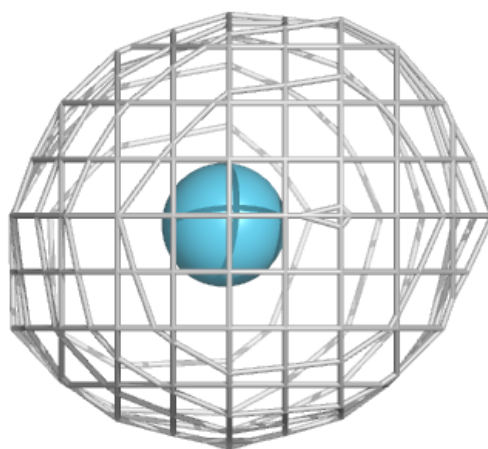
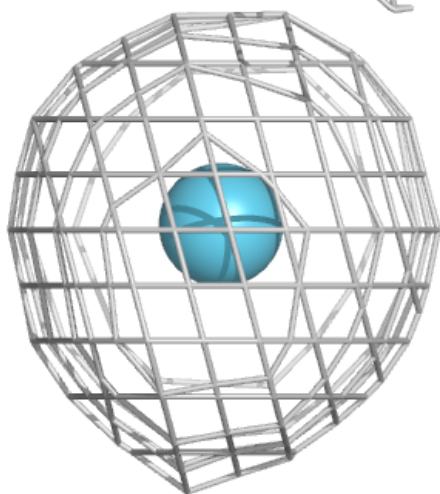
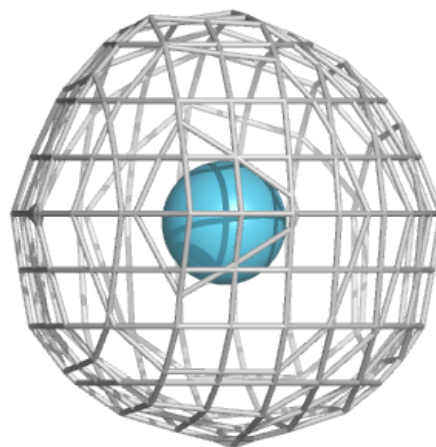
Electron density around KR B 508 (B):

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



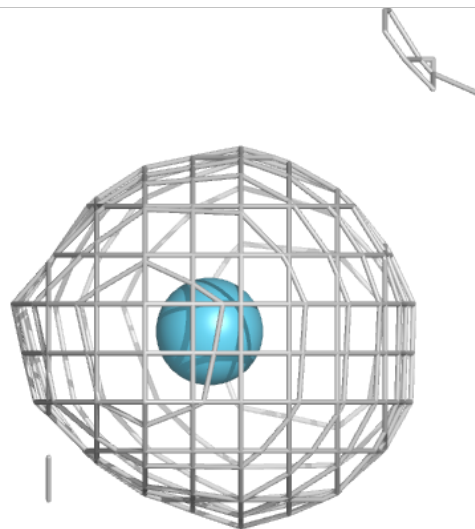
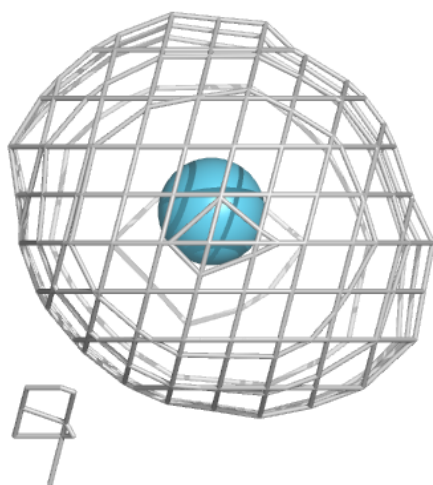
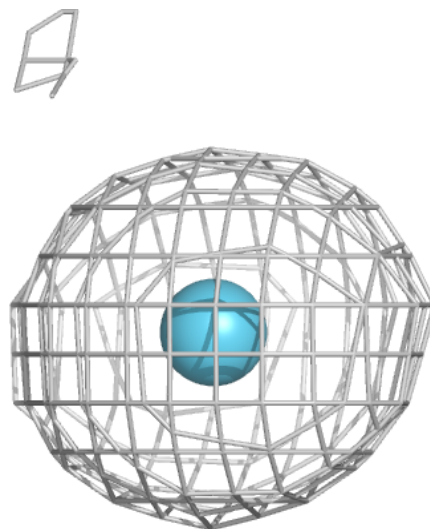
Electron density around KR C 308:

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



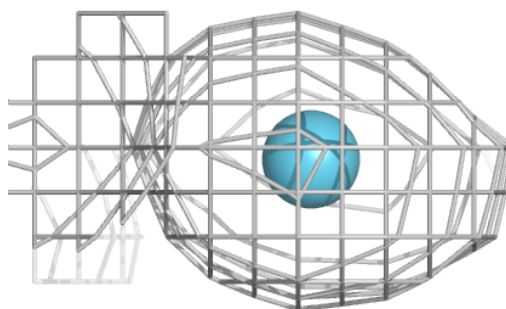
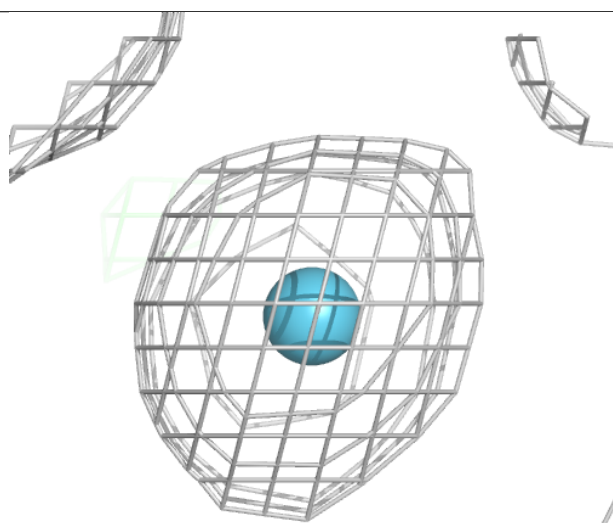
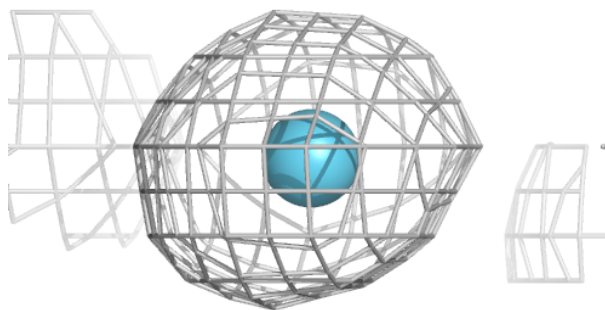
Electron density around KR D 508:

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



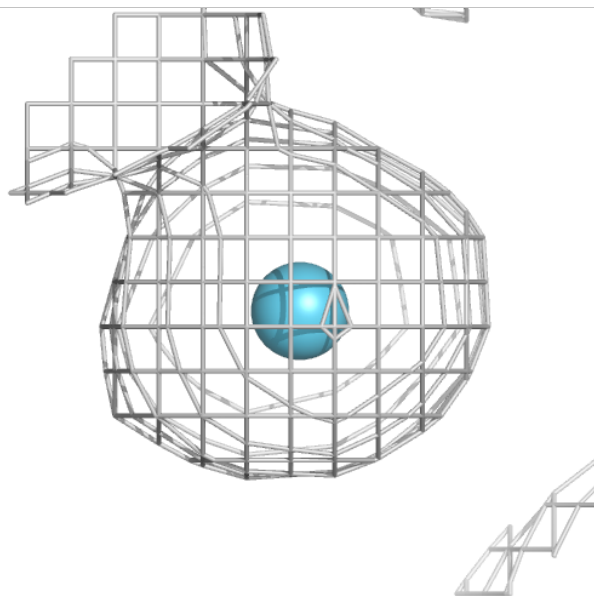
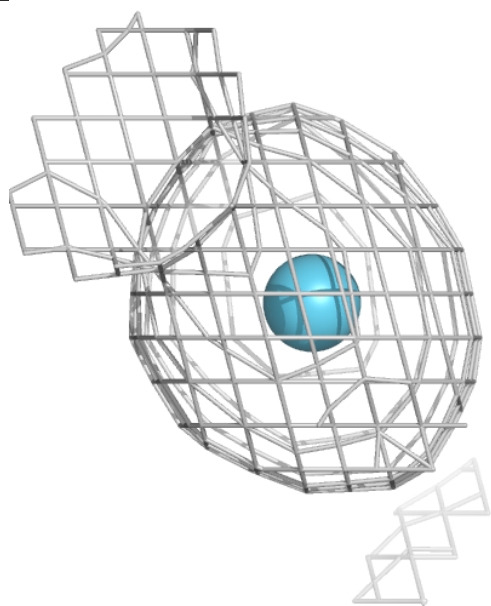
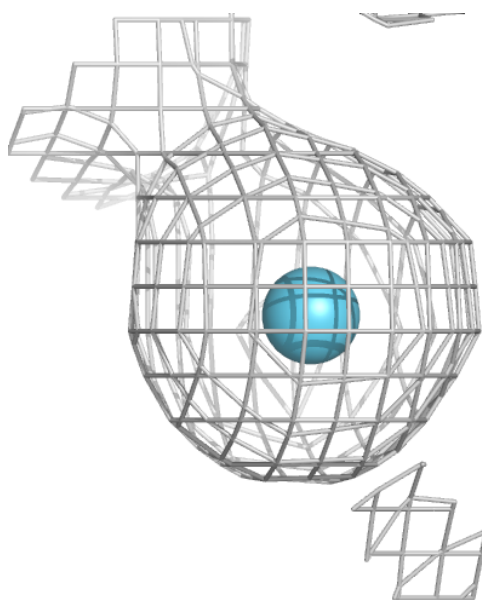
Electron density around KR D 506:

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



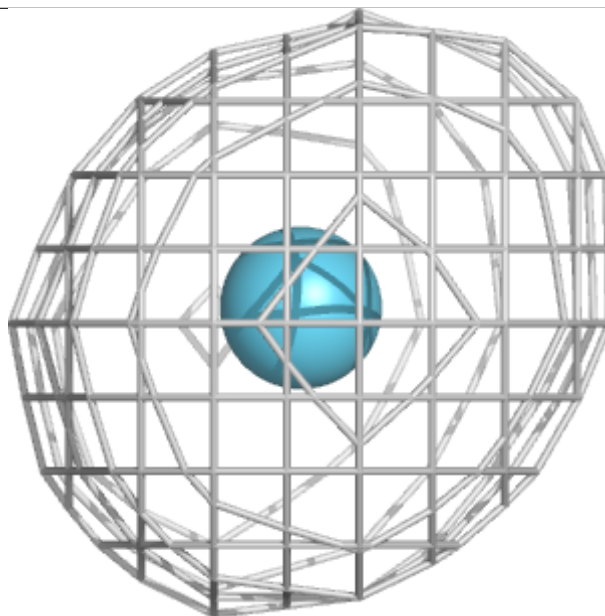
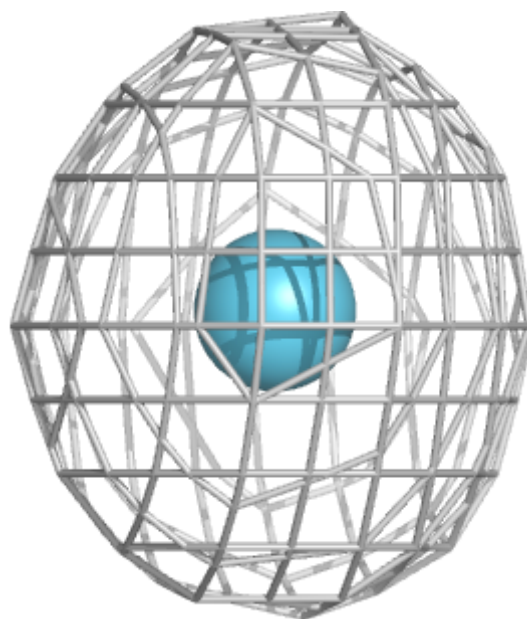
Electron density around KR A 306:

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



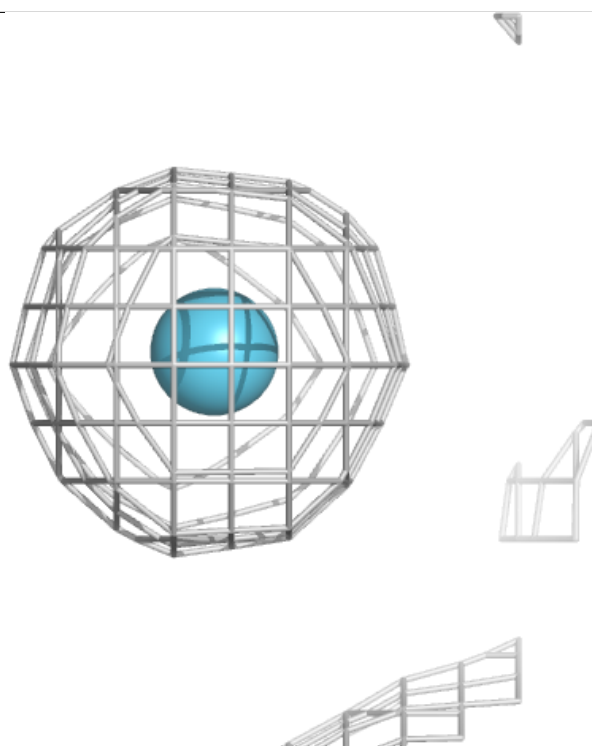
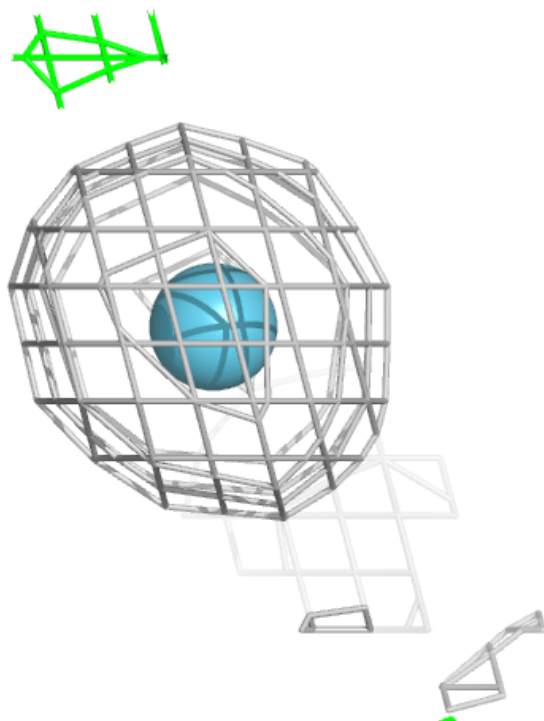
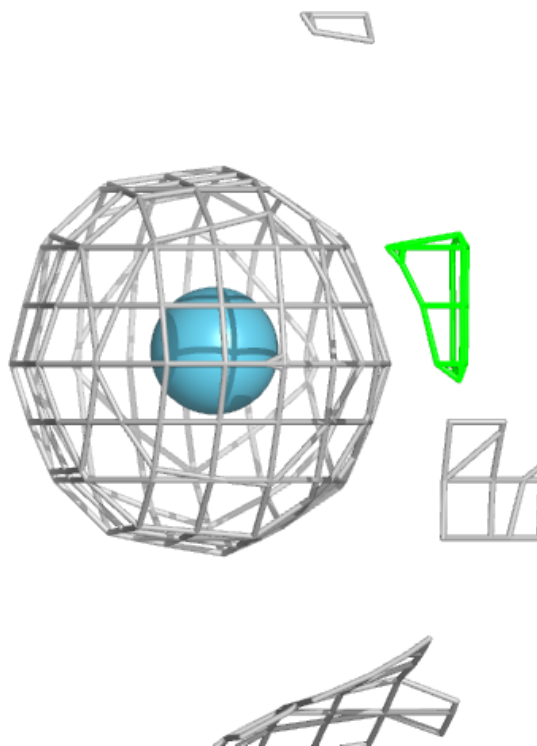
Electron density around KR A 307:

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



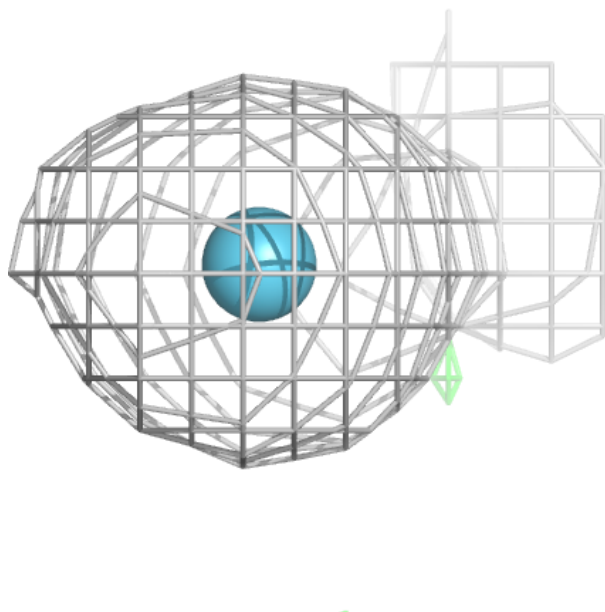
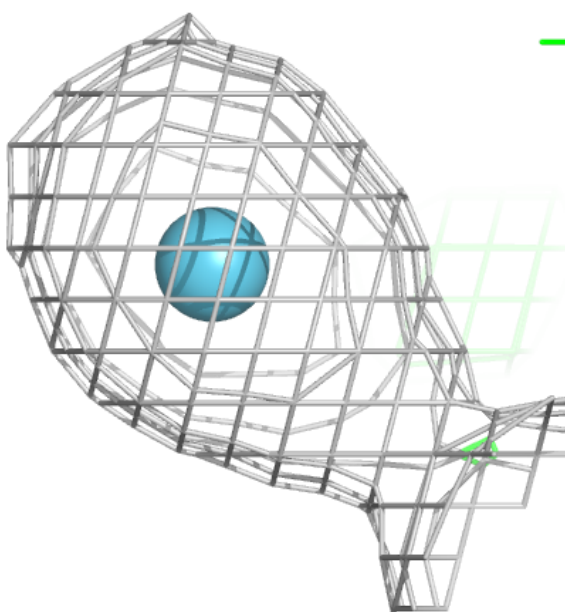
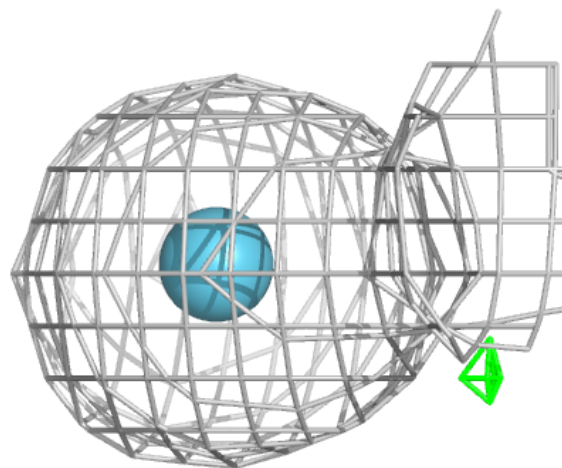
Electron density around KR A 309:

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



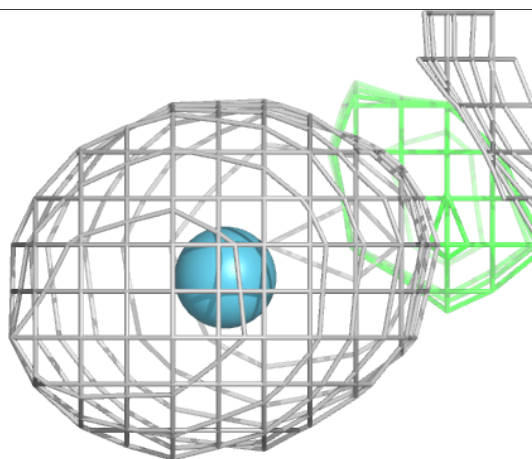
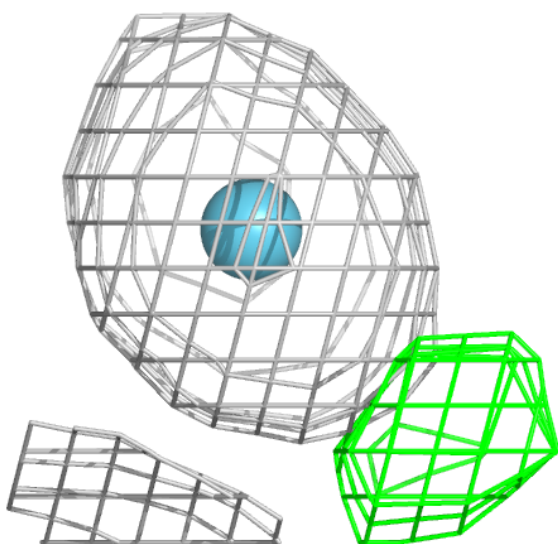
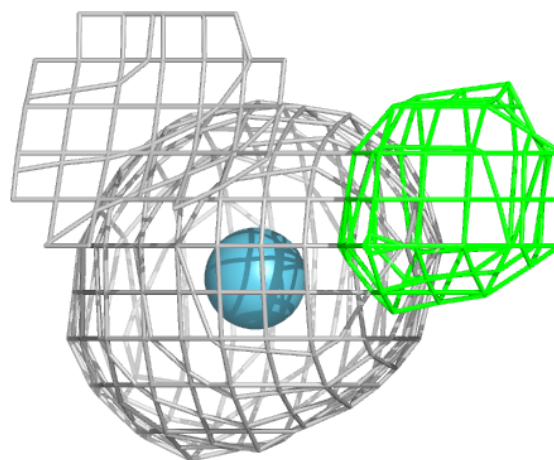
Electron density around KR B 506:

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



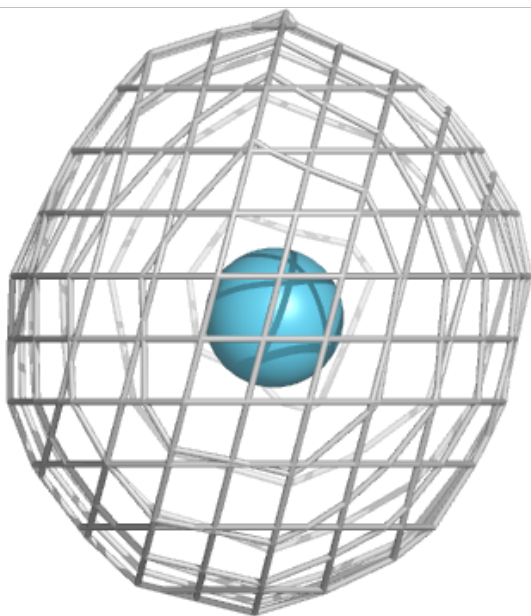
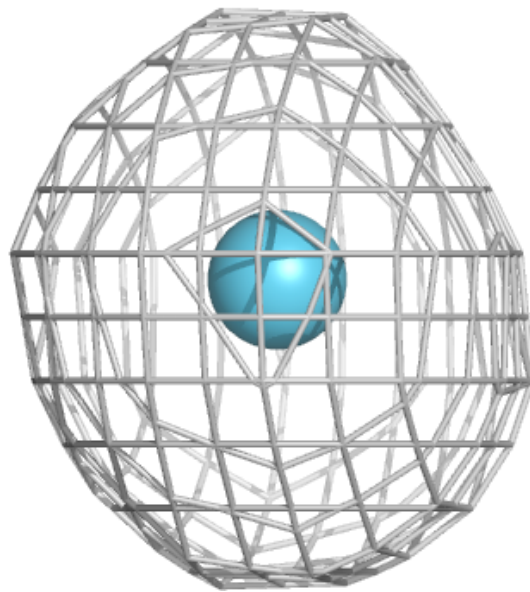
Electron density around KR B 509:

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



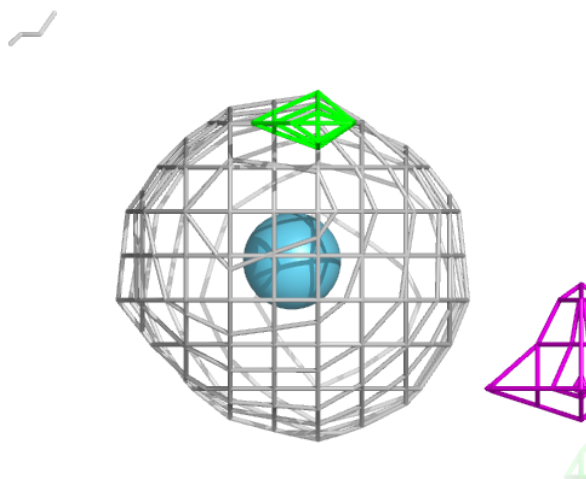
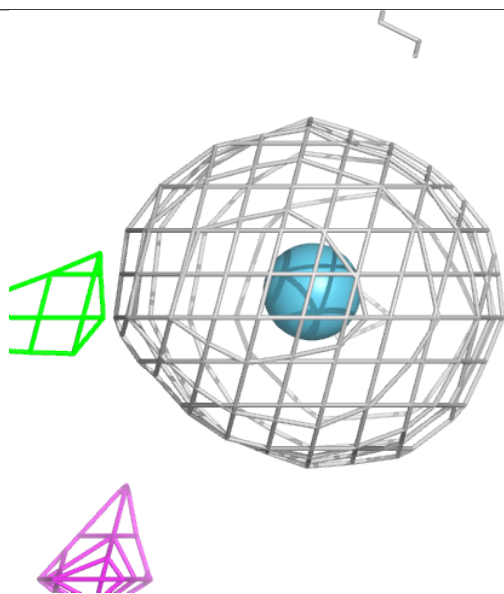
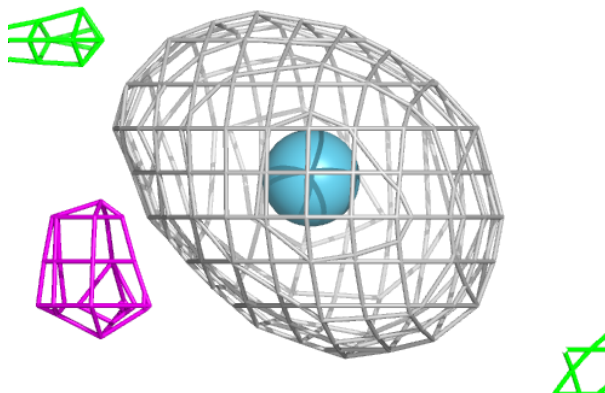
Electron density around KR B 510:

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



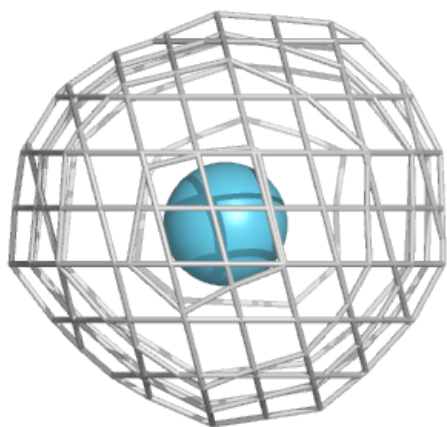
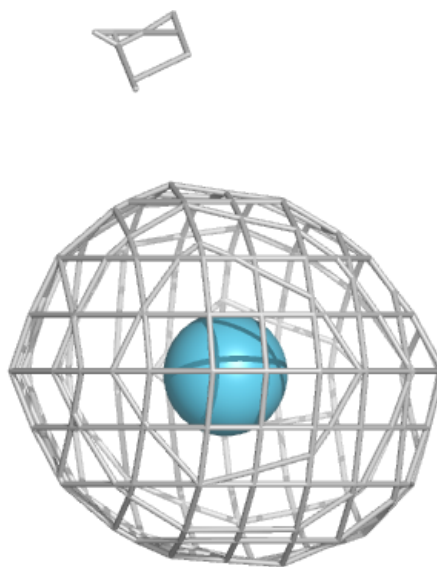
Electron density around KR D 507:

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



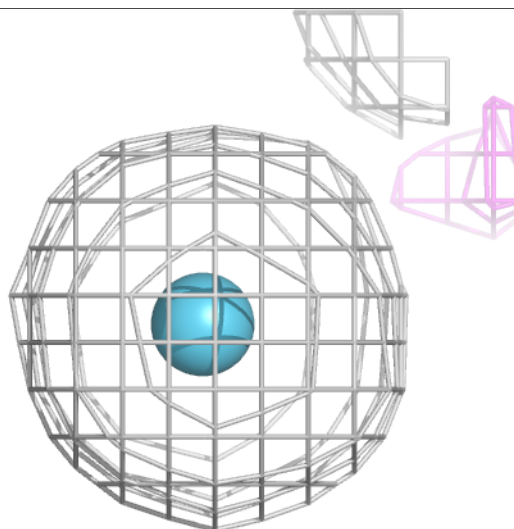
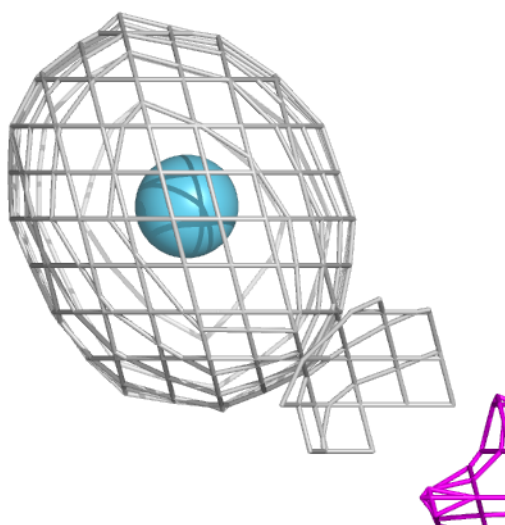
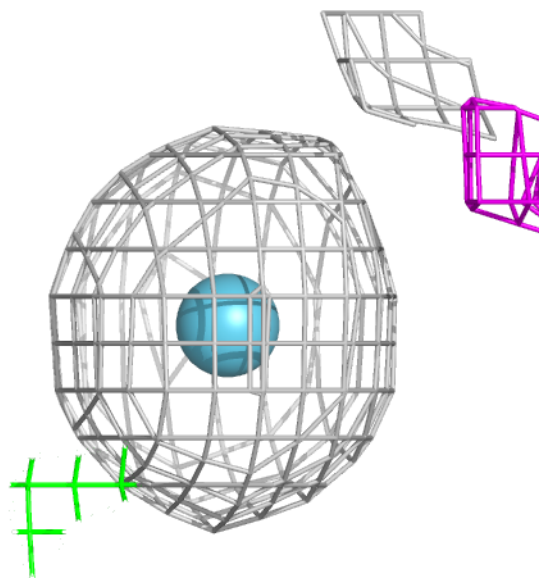
Electron density around KR A 310:

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



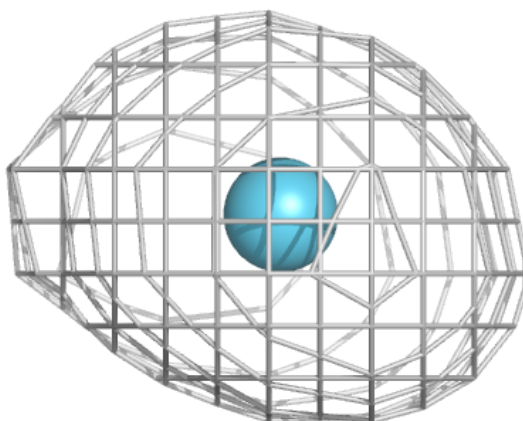
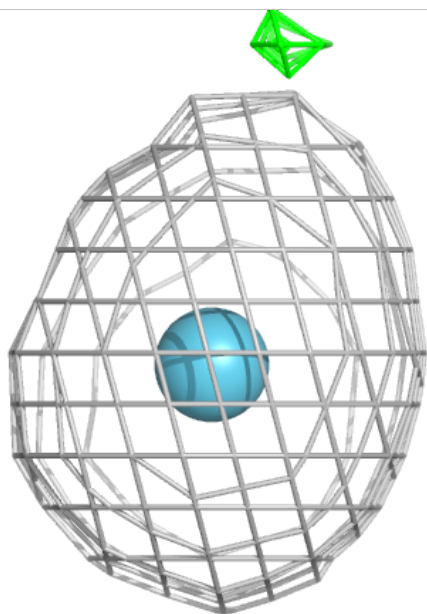
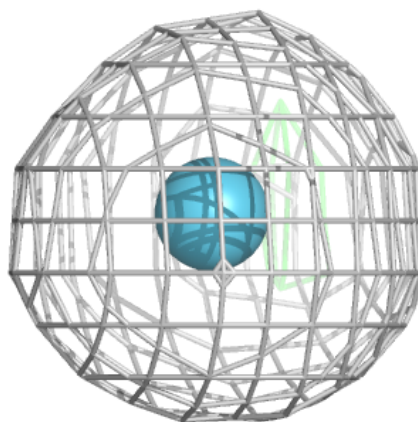
Electron density around KR C 306:

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



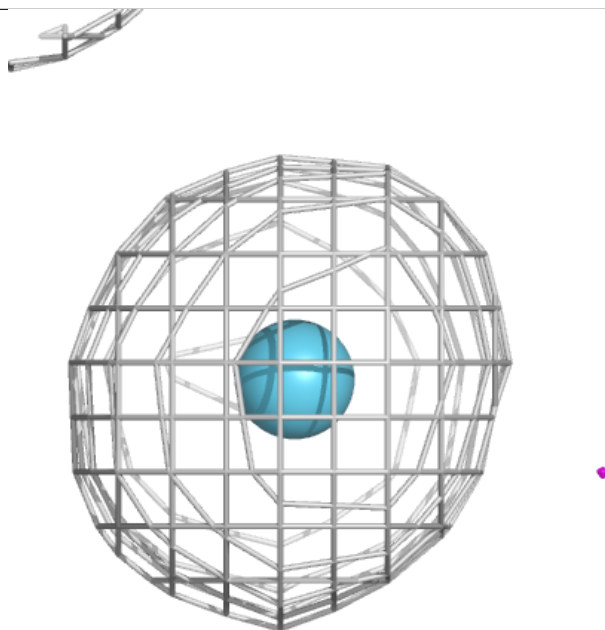
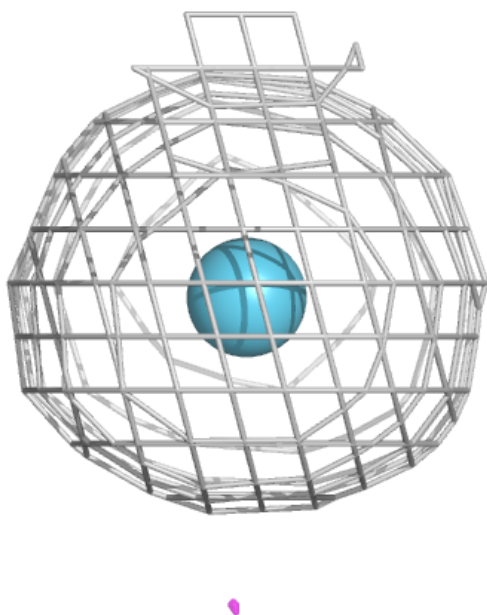
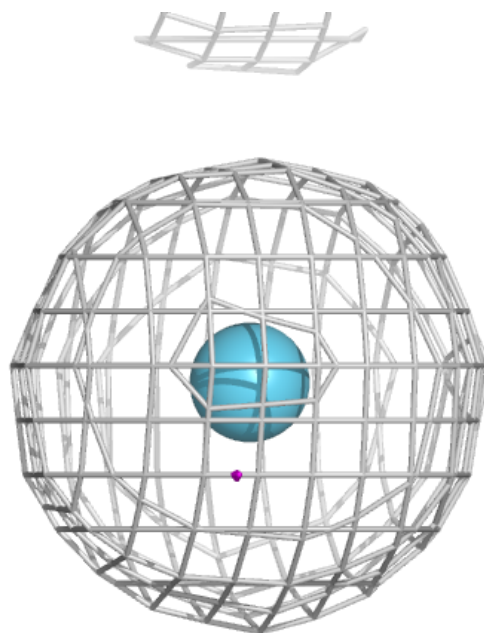
Electron density around KR A 305:

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



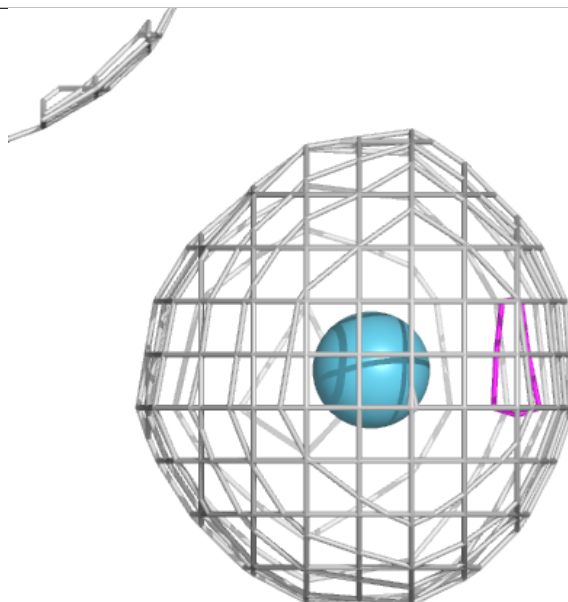
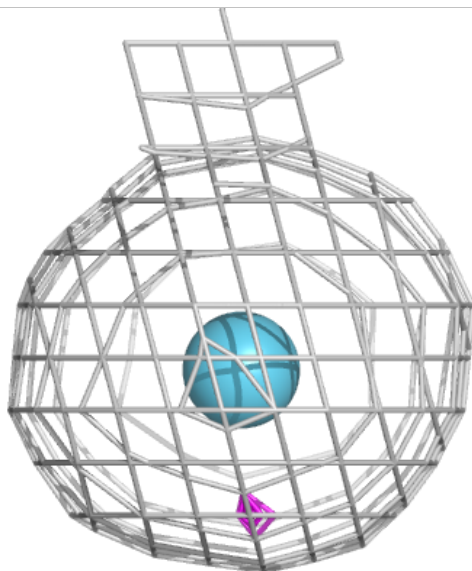
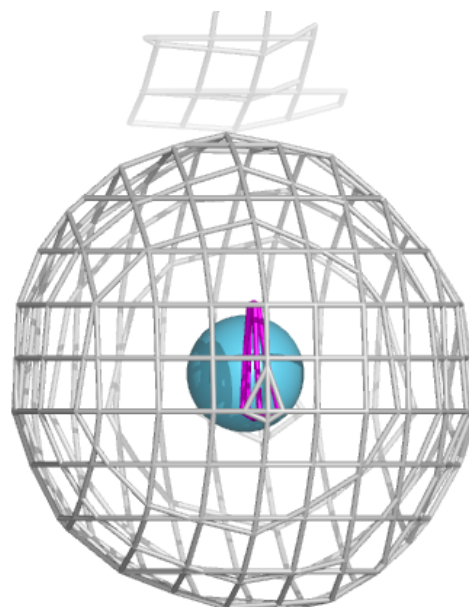
Electron density around KR A 308:

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



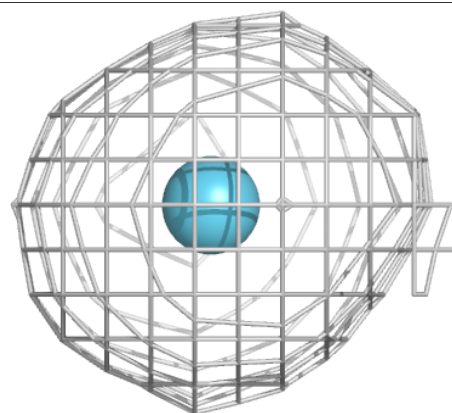
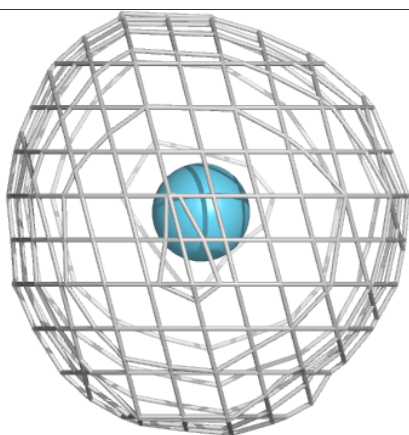
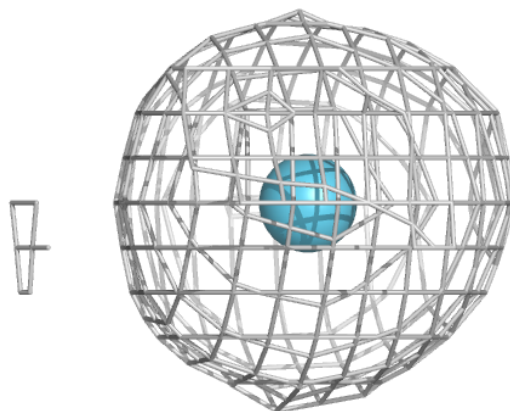
Electron density around KR C 309:

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



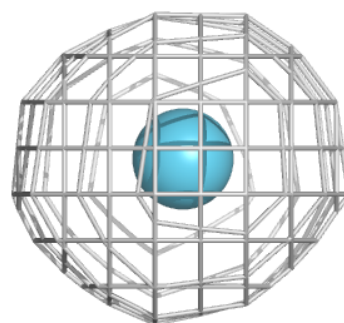
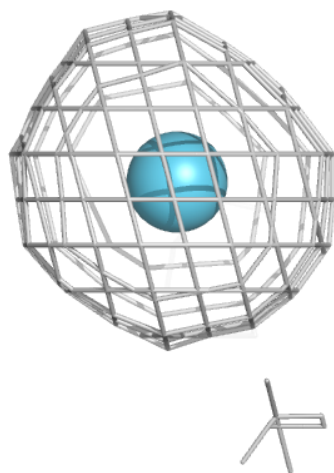
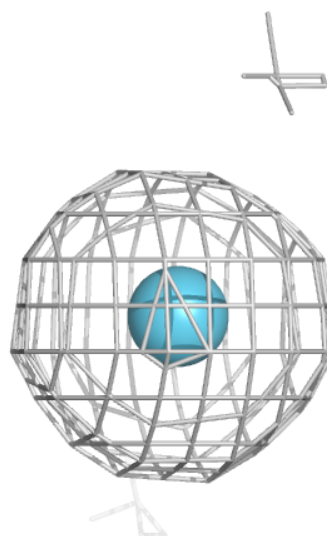
Electron density around KR C 305:

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



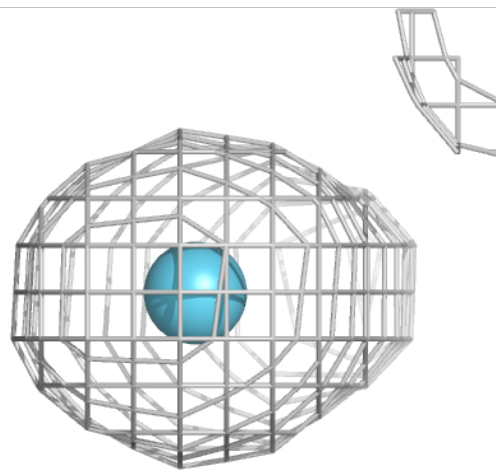
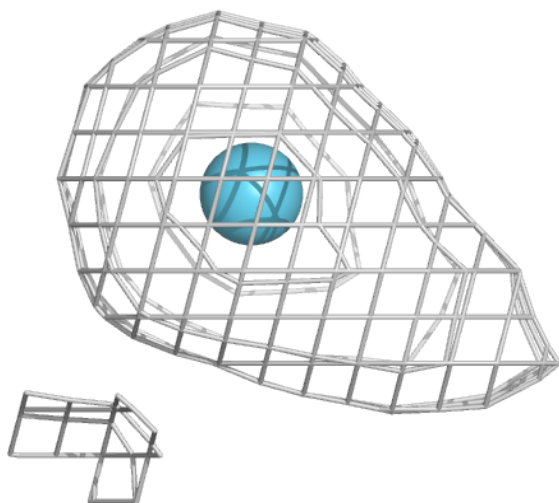
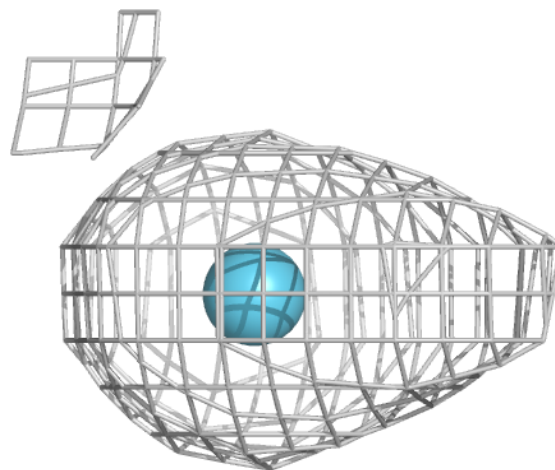
Electron density around KR C 310:

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



Electron density around KR B 507 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 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.