Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:12 PM BST

PDB ID	:	6YEH
Title	:	Arabidopsis thaliana glutamate dehydrogenase isoform 1 in apo form
Authors	:	Ruszkowski, M.; Grzechowiak, M.; Jaskolski, M.
Deposited on	:	2020-03-24
Resolution	:	2.59 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 following versions of software and data (see references ⓘ) were used in the production of this report:

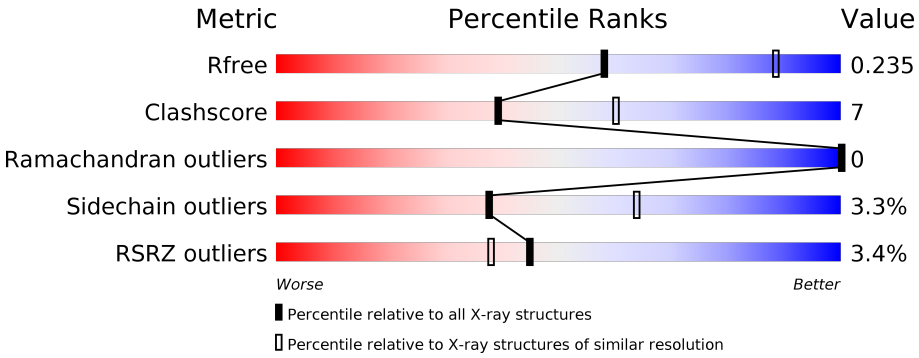
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	414	84% 15%
1	B	414	% 84% 14%
1	C	414	% 80% 18%
1	D	414	2% 76% 21%
1	E	414	7% 76% 22%
1	F	414	10% 78% 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18937 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 Glutamate dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3123	1977	544	588	14			
1	B	409	Total	C	N	O	S	0	0	0
			3115	1973	542	586	14			
1	C	408	Total	C	N	O	S	0	0	0
			3110	1970	541	585	14			
1	D	410	Total	C	N	O	S	0	0	0
			3123	1977	544	588	14			
1	E	410	Total	C	N	O	S	0	0	0
			3123	1977	544	588	14			
1	F	408	Total	C	N	O	S	0	0	0
			3110	1970	541	585	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q43314
A	-1	ASN	-	expression tag	UNP Q43314
A	0	ALA	-	expression tag	UNP Q43314
B	-2	SER	-	expression tag	UNP Q43314
B	-1	ASN	-	expression tag	UNP Q43314
B	0	ALA	-	expression tag	UNP Q43314
C	-2	SER	-	expression tag	UNP Q43314
C	-1	ASN	-	expression tag	UNP Q43314
C	0	ALA	-	expression tag	UNP Q43314
D	-2	SER	-	expression tag	UNP Q43314
D	-1	ASN	-	expression tag	UNP Q43314
D	0	ALA	-	expression tag	UNP Q43314
E	-2	SER	-	expression tag	UNP Q43314
E	-1	ASN	-	expression tag	UNP Q43314
E	0	ALA	-	expression tag	UNP Q43314
F	-2	SER	-	expression tag	UNP Q43314
F	-1	ASN	-	expression tag	UNP Q43314

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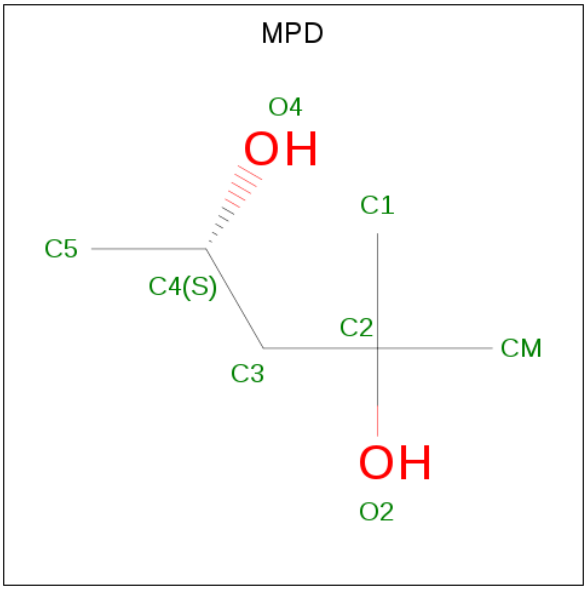
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP Q43314

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	B	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	E	1	Total C O 8 6 2	0	0
2	E	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 8 6 2	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	D	1	Total K 1 1	0	0
3	C	1	Total K 1 1	0	0
3	E	2	Total K 2 2	0	0

- Molecule 4 is water.

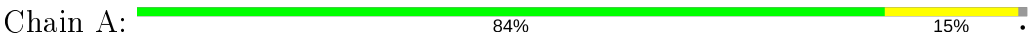
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	30	Total O 30 30	0	0
4	B	25	Total O 25 25	0	0
4	C	27	Total O 27 27	0	0
4	D	20	Total O 20 20	0	0
4	E	18	Total O 18 18	0	0
4	F	19	Total O 19 19	0	0

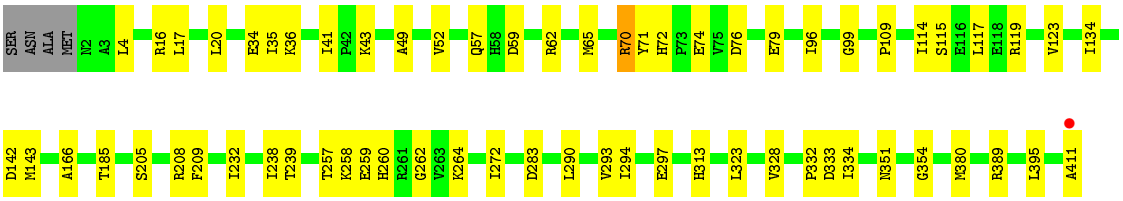
3 Residue-property plots (i)

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: Glutamate dehydrogenase 1

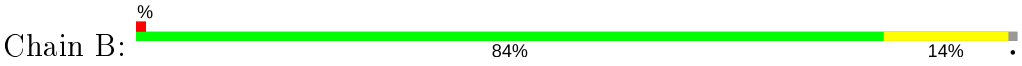
Chain A:

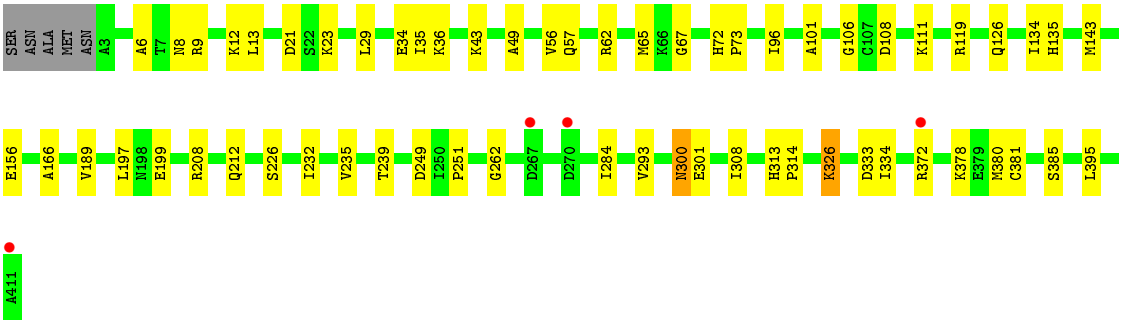




- Molecule 1: Glutamate dehydrogenase 1

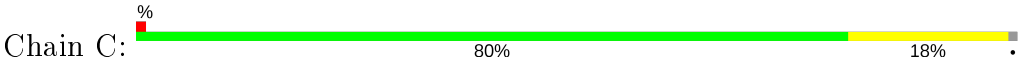
Chain B:

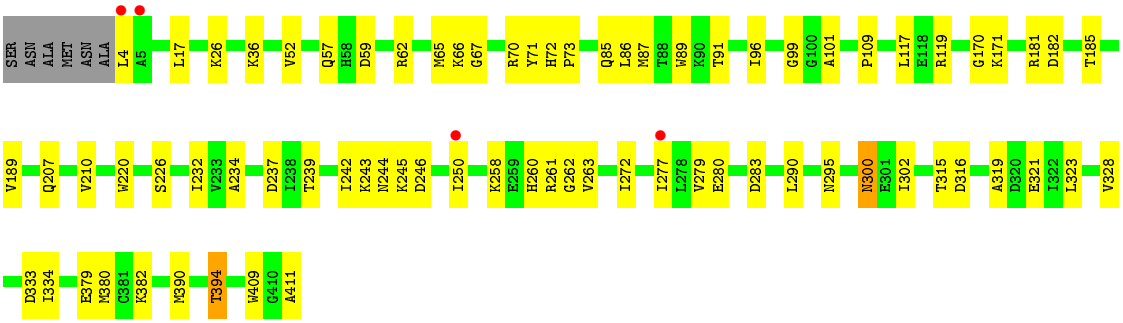




- Molecule 1: Glutamate dehydrogenase 1

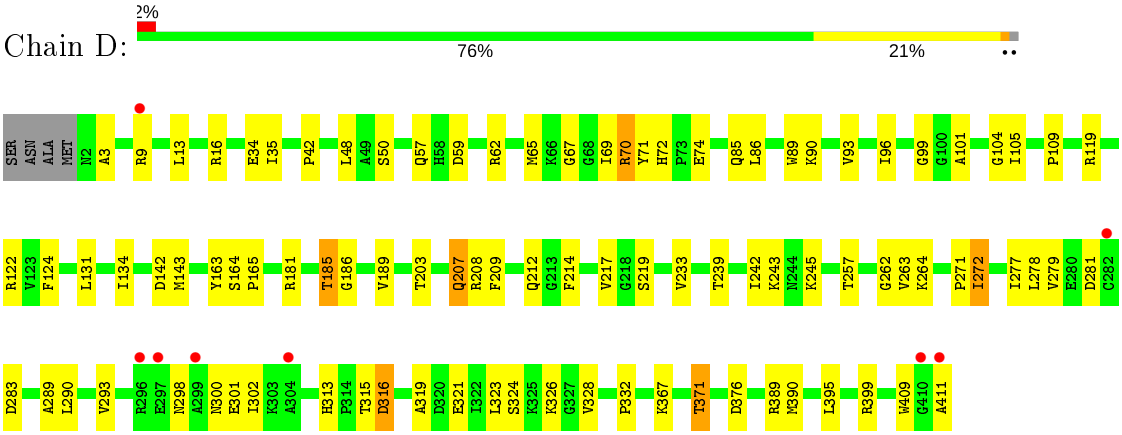
Chain C:





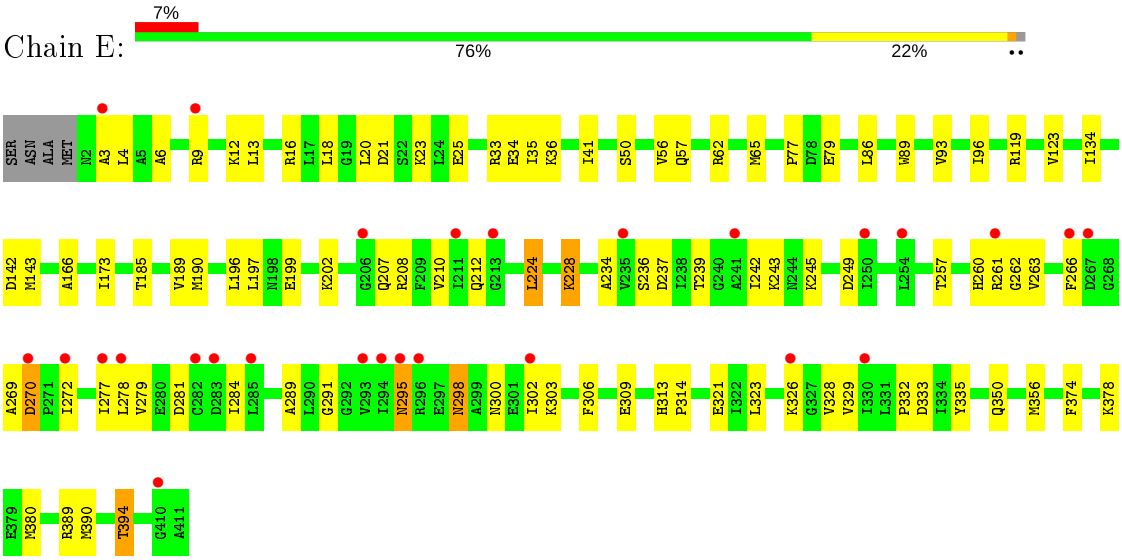
• Molecule 1: Glutamate dehydrogenase 1

Chain D:



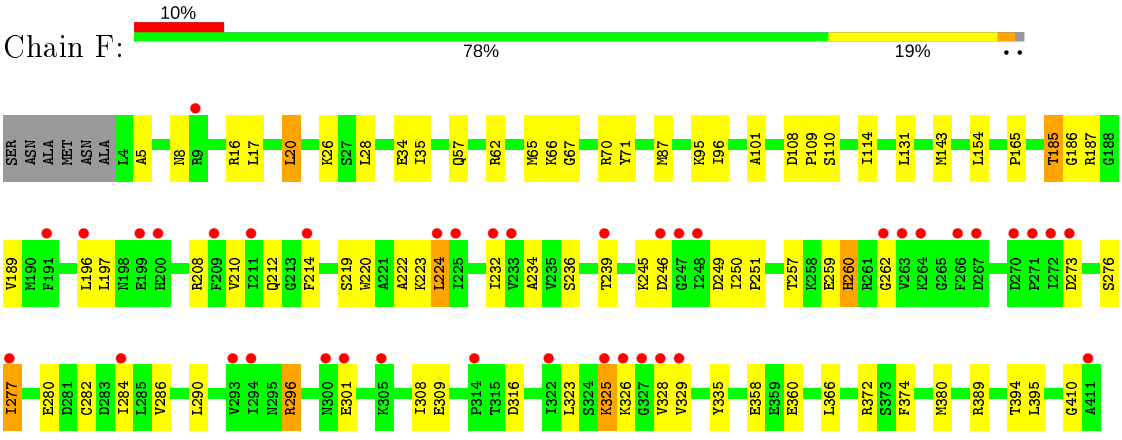
• Molecule 1: Glutamate dehydrogenase 1

Chain E:



• Molecule 1: Glutamate dehydrogenase 1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.57Å 99.17Å 318.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.77 – 2.59 89.77 – 2.59	Depositor EDS
% Data completeness (in resolution range)	74.7 (89.77-2.59) 74.7 (89.77-2.59)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.183 , 0.235 0.183 , 0.235	Depositor DCC
R_{free} test set	1044 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18937	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 3.04% 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

5.1 Standard geometry

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

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	0.39	0/3185	0.54	0/4306
1	B	0.36	0/3177	0.52	0/4295
1	C	0.37	0/3172	0.54	0/4288
1	D	0.36	0/3185	0.51	0/4306
1	E	0.35	0/3185	0.53	0/4306
1	F	0.35	0/3172	0.52	0/4288
All	All	0.36	0/19076	0.53	0/25789

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

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	3123	0	3140	40	0
1	B	3115	0	3134	39	0
1	C	3110	0	3129	47	0
1	D	3123	0	3140	56	0
1	E	3123	0	3140	58	0
1	F	3110	0	3129	52	0
2	A	32	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	0	14	0	0
2	C	16	0	28	2	0
2	D	8	0	14	1	0
2	E	24	0	42	2	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
4	A	30	0	0	0	0
4	B	25	0	0	0	0
4	C	27	0	0	0	0
4	D	20	0	0	0	0
4	E	18	0	0	0	0
4	F	19	0	0	0	0
All	All	18937	0	18966	279	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 7.

All (279) 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:E:199:GLU:HG3	1:E:378:LYS:HE2	1.65	0.78
1:E:3:ALA:HB3	1:E:313:HIS:HB3	1.64	0.78
1:E:210:VAL:HG13	1:E:234:ALA:HB3	1.70	0.73
1:D:9:ARG:HH12	1:D:13:LEU:HD12	1.55	0.72
1:F:16:ARG:NH1	1:F:20:LEU:O	2.25	0.70
1:D:277:ILE:HG23	1:D:278:LEU:HD22	1.75	0.69
1:B:119:ARG:HH21	1:D:411:ALA:HB1	1.61	0.66
1:A:134:ILE:HD12	1:A:166:ALA:HB3	1.77	0.65
1:D:3:ALA:HB3	1:D:313:HIS:HB3	1.77	0.65
1:E:243:LYS:HB2	1:E:272:ILE:HD13	1.79	0.64
1:A:293:VAL:HG23	1:A:294:ILE:HD12	1.77	0.64
1:C:380:MET:HE2	1:C:394:THR:HB	1.78	0.64
1:E:62:ARG:NH2	1:E:96:ILE:O	2.31	0.64
1:C:171:LYS:O	1:C:181:ARG:NH1	2.29	0.64
1:C:36:LYS:HG3	1:D:34:GLU:HB2	1.79	0.64
1:D:239:THR:HG21	1:D:262:GLY:HA3	1.82	0.62
1:F:236:SER:HB3	1:F:277:ILE:HG21	1.80	0.62
1:B:62:ARG:NH2	1:B:96:ILE:O	2.33	0.62
1:E:41:ILE:HG22	1:E:123:VAL:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ASN:HD22	2:A:503:MPD:H51	1.64	0.62
1:C:411:ALA:HB1	1:E:119:ARG:HE	1.65	0.61
1:B:134:ILE:HD12	1:B:166:ALA:HB3	1.81	0.61
1:C:62:ARG:NH2	1:C:96:ILE:O	2.33	0.61
1:E:323:LEU:HB3	1:E:328:VAL:HB	1.82	0.61
1:C:36:LYS:HE3	1:C:52:VAL:HG11	1.81	0.61
1:A:36:LYS:HE2	1:A:52:VAL:HG11	1.82	0.61
1:E:298:ASN:OD1	1:E:298:ASN:N	2.33	0.61
1:E:89:TRP:O	1:E:93:VAL:HG23	2.00	0.61
1:E:12:LYS:HG3	1:E:25:GLU:OE2	2.01	0.61
1:B:34:GLU:HG2	1:B:56:VAL:HG22	1.83	0.60
1:D:62:ARG:NH2	1:D:96:ILE:O	2.34	0.60
1:F:360:GLU:H	1:F:360:GLU:CD	2.04	0.60
1:C:210:VAL:HG13	1:C:234:ALA:HB3	1.82	0.60
1:F:239:THR:HG21	1:F:262:GLY:HA3	1.83	0.60
1:C:185:THR:O	1:C:189:VAL:HG23	2.01	0.59
1:D:239:THR:O	1:D:264:LYS:HD2	2.01	0.59
1:E:134:ILE:HD12	1:E:166:ALA:HB3	1.84	0.59
1:C:171:LYS:O	1:C:181:ARG:NH2	2.34	0.58
1:A:72:HIS:CE1	1:A:74:GLU:HB2	2.39	0.58
1:D:300:ASN:HA	1:D:326:LYS:HE3	1.85	0.58
1:D:35:ILE:HD13	1:D:131:LEU:HD13	1.86	0.58
1:D:323:LEU:HB3	1:D:328:VAL:HB	1.85	0.57
1:B:57:GLN:HB3	1:B:65:MET:SD	2.44	0.57
1:B:380:MET:HG3	1:B:395:LEU:HB2	1.86	0.57
1:F:62:ARG:NH2	1:F:96:ILE:O	2.37	0.57
1:E:277:ILE:HG23	1:E:278:LEU:HD22	1.86	0.57
1:A:115:SER:OG	1:A:119:ARG:NH2	2.38	0.57
1:A:36:LYS:NZ	1:B:34:GLU:OE1	2.33	0.56
1:A:16:ARG:NH1	1:A:20:LEU:O	2.38	0.56
1:D:243:LYS:HE3	1:D:272:ILE:HG21	1.87	0.56
1:E:332:PRO:HG3	1:E:389:ARG:HA	1.87	0.56
1:F:296:ARG:H	1:F:296:ARG:HE	1.53	0.56
1:D:367:LYS:O	1:D:371:THR:OG1	2.23	0.56
1:E:197:LEU:HD13	1:E:207:GLN:HE22	1.71	0.55
1:A:239:THR:O	1:A:264:LYS:HD2	2.05	0.55
1:B:21:ASP:OD1	1:B:23:LYS:N	2.33	0.55
1:D:243:LYS:HB2	1:D:272:ILE:HG12	1.88	0.55
1:F:108:ASP:OD1	1:F:110:SER:OG	2.24	0.55
1:F:309:GLU:OE2	1:F:389:ARG:NH2	2.40	0.55
1:D:208:ARG:NH2	1:D:281:ASP:OD2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:THR:HG21	1:E:262:GLY:HA3	1.89	0.54
1:C:302:ILE:HD12	1:C:323:LEU:HD21	1.89	0.54
1:D:186:GLY:O	1:D:189:VAL:HG22	2.07	0.54
1:A:117:LEU:HD13	2:A:501:MPD:H53	1.90	0.54
1:C:59:ASP:O	1:C:99:GLY:HA3	2.08	0.54
1:E:309:GLU:OE1	1:E:389:ARG:NH2	2.30	0.54
1:C:243:LYS:HG3	1:C:244:ASN:N	2.23	0.54
1:D:42:PRO:O	1:D:119:ARG:NH1	2.41	0.54
1:A:34:GLU:OE1	1:B:36:LYS:HE2	2.08	0.54
1:D:316:ASP:N	1:D:316:ASP:OD1	2.37	0.53
1:E:237:ASP:OD2	1:E:263:VAL:HG23	2.07	0.53
1:E:33:ARG:HG2	1:E:35:ILE:HD11	1.90	0.53
1:F:20:LEU:HD21	1:F:28:LEU:HD12	1.90	0.53
1:B:126:GLN:NE2	1:B:156:GLU:OE2	2.37	0.53
1:D:93:VAL:HG13	1:D:395:LEU:HD23	1.88	0.53
1:F:325:LYS:O	1:F:326:LYS:HG2	2.09	0.53
1:B:134:ILE:HG22	1:B:135:HIS:CE1	2.44	0.53
1:F:186:GLY:O	1:F:189:VAL:HG22	2.08	0.53
1:D:332:PRO:HG3	1:D:389:ARG:HA	1.91	0.53
1:C:300:ASN:N	1:C:300:ASN:OD1	2.37	0.52
1:E:50:SER:HB2	1:F:26:LYS:HE3	1.91	0.52
1:D:321:GLU:HA	1:D:324:SER:HB3	1.92	0.52
1:C:277:ILE:O	1:C:280:GLU:HG2	2.09	0.52
1:D:242:ILE:HA	1:D:271:PRO:HA	1.91	0.52
1:E:302:ILE:HD12	1:E:323:LEU:HD21	1.92	0.52
1:F:220:TRP:O	1:F:224:LEU:HD22	2.09	0.52
1:B:301:GLU:OE1	1:B:301:GLU:N	2.43	0.52
1:E:6:ALA:O	1:E:9:ARG:HB3	2.09	0.52
1:C:390:MET:O	1:C:394:THR:OG1	2.28	0.51
1:E:57:GLN:HB3	1:E:65:MET:SD	2.50	0.51
1:E:212:GLN:OE1	1:E:278:LEU:HD11	2.10	0.51
1:B:199:GLU:OE2	1:B:378:LYS:NZ	2.35	0.51
1:C:379:GLU:O	1:C:382:LYS:HG3	2.10	0.51
1:D:279:VAL:HG13	1:D:301:GLU:O	2.11	0.51
1:E:295:ASN:ND2	1:E:298:ASN:OD1	2.41	0.51
1:B:226:SER:HB3	1:B:232:ILE:CD1	2.41	0.51
1:E:190:MET:SD	1:E:228:LYS:HD2	2.51	0.51
1:F:187:ARG:HD2	1:F:366:LEU:HD23	1.93	0.51
1:A:62:ARG:NH2	1:A:96:ILE:O	2.43	0.51
1:D:185:THR:HB	1:D:217:VAL:HG22	1.92	0.51
1:D:89:TRP:O	1:D:93:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LYS:HD2	1:A:49:ALA:HB2	1.93	0.51
1:A:57:GLN:HB3	1:A:65:MET:SD	2.51	0.51
1:C:57:GLN:HB3	1:C:65:MET:SD	2.51	0.50
1:D:376:ASP:OD2	1:D:399:ARG:NH2	2.35	0.50
1:E:350:GLN:HB3	1:E:356:MET:HE2	1.93	0.50
1:A:34:GLU:HB2	1:B:36:LYS:HB2	1.92	0.50
1:D:70:ARG:HG2	1:D:142:ASP:CG	2.31	0.50
1:D:212:GLN:OE1	1:D:278:LEU:HD21	2.12	0.50
1:A:142:ASP:OD1	1:A:143:MET:N	2.38	0.50
1:F:57:GLN:HB3	1:F:65:MET:SD	2.52	0.50
1:F:214:PHE:CE1	1:F:219:SER:HA	2.47	0.50
1:B:372:ARG:NH2	1:F:358:GLU:OE2	2.45	0.49
1:D:134:ILE:HD11	1:D:164:SER:HB3	1.94	0.49
1:E:390:MET:O	1:E:394:THR:OG1	2.28	0.49
1:E:34:GLU:HG2	1:E:56:VAL:HG22	1.92	0.49
1:D:257:THR:HG21	1:D:263:VAL:HG12	1.93	0.49
1:E:35:ILE:HD12	1:F:35:ILE:HD12	1.93	0.49
1:B:313:HIS:N	1:B:314:PRO:HD3	2.27	0.49
1:A:354:GLY:HA2	2:A:503:MPD:HM3	1.94	0.49
1:F:154:LEU:CD1	1:F:165:PRO:HA	2.43	0.49
1:F:67:GLY:HA3	1:F:101:ALA:O	2.13	0.49
1:C:239:THR:HG21	1:C:262:GLY:HA3	1.94	0.49
1:C:315:THR:HG23	1:C:319:ALA:HB3	1.95	0.49
1:A:71:TYR:HB3	1:A:109:PRO:HG3	1.95	0.49
1:A:380:MET:HE3	1:A:395:LEU:HD13	1.95	0.49
1:C:71:TYR:HB3	1:C:109:PRO:HG3	1.94	0.49
2:C:502:MPD:H4	2:C:502:MPD:HM1	1.67	0.48
1:E:300:ASN:O	1:E:326:LYS:HE3	2.14	0.48
1:F:16:ARG:HA	1:F:16:ARG:NE	2.28	0.48
1:E:16:ARG:NE	1:E:16:ARG:HA	2.28	0.48
1:F:245:LYS:NZ	1:F:246:ASP:OD1	2.40	0.48
1:E:21:ASP:OD1	1:E:23:LYS:N	2.43	0.48
1:C:237:ASP:OD1	1:C:263:VAL:HG22	2.13	0.48
1:E:335:TYR:OH	1:E:374:PHE:HB2	2.13	0.48
1:A:35:ILE:HD12	1:B:35:ILE:HD12	1.96	0.48
1:A:411:ALA:HB1	1:C:119:ARG:HE	1.79	0.48
1:A:297:GLU:OE1	1:A:297:GLU:N	2.42	0.48
1:D:72:HIS:CE1	1:D:74:GLU:HB2	2.48	0.48
1:D:13:LEU:HD22	1:D:390:MET:SD	2.54	0.47
1:D:59:ASP:O	1:D:99:GLY:HA3	2.15	0.47
1:F:277:ILE:HA	1:F:280:GLU:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:LYS:HD3	1:F:372:ARG:HE	1.80	0.47
1:E:36:LYS:HB2	1:F:34:GLU:HB2	1.96	0.47
1:F:249:ASP:OD1	1:F:251:PRO:HD2	2.14	0.47
1:F:35:ILE:HG21	1:F:131:LEU:HD13	1.97	0.47
1:A:209:PHE:HB2	1:A:232:ILE:HD13	1.97	0.47
1:E:212:GLN:HE21	1:E:289:ALA:HB3	1.79	0.47
1:F:208:ARG:NH1	1:F:282:CYS:HA	2.29	0.47
1:A:323:LEU:HB3	1:A:328:VAL:HB	1.96	0.47
1:D:212:GLN:HE21	1:D:289:ALA:HB3	1.79	0.46
1:C:295:ASN:HA	1:C:316:ASP:OD1	2.15	0.46
1:F:286:VAL:HG22	1:F:308:ILE:HB	1.96	0.46
1:F:66:LYS:O	1:F:87:MET:HG2	2.15	0.46
1:F:301:GLU:N	1:F:301:GLU:OE1	2.49	0.46
1:A:72:HIS:HE1	1:A:74:GLU:HB2	1.81	0.46
1:D:85:GLN:HG2	1:D:89:TRP:NE1	2.29	0.46
1:B:326:LYS:HB2	1:B:326:LYS:HE3	1.69	0.46
1:C:226:SER:HB3	1:C:232:ILE:CD1	2.46	0.46
1:E:18:LEU:HD21	1:E:394:THR:HG22	1.97	0.46
1:F:210:VAL:HG12	1:F:234:ALA:HB3	1.97	0.46
1:F:223:LYS:HA	1:F:250:ILE:HG21	1.98	0.46
1:C:26:LYS:HE2	1:D:50:SER:HB2	1.98	0.46
1:C:333:ASP:OD1	1:C:334:ILE:N	2.49	0.46
1:A:17:LEU:HD23	1:A:17:LEU:HA	1.86	0.45
1:A:4:LEU:HD13	1:A:313:HIS:NE2	2.31	0.45
1:C:272:ILE:HD13	1:C:280:GLU:OE2	2.16	0.45
1:E:202:LYS:HD3	1:E:207:GLN:OE1	2.15	0.45
1:E:291:GLY:HA2	1:E:314:PRO:HA	1.98	0.45
1:D:69:ILE:HG23	1:D:104:GLY:HA2	1.99	0.45
1:D:185:THR:O	1:D:189:VAL:HG13	2.16	0.45
1:F:323:LEU:HD22	1:F:328:VAL:HG11	1.98	0.45
1:A:208:ARG:NH1	1:A:283:ASP:OD1	2.49	0.45
1:E:190:MET:HE2	1:E:224:LEU:HB3	1.97	0.45
1:A:333:ASP:OD1	1:A:334:ILE:N	2.49	0.45
1:C:182:ASP:OD2	1:C:220:TRP:NE1	2.43	0.45
1:D:57:GLN:HB3	1:D:65:MET:SD	2.57	0.45
1:B:333:ASP:OD1	1:B:334:ILE:N	2.48	0.45
1:C:279:VAL:HG12	1:C:279:VAL:O	2.17	0.45
1:D:142:ASP:OD1	1:D:143:MET:N	2.38	0.45
1:E:16:ARG:NH2	1:E:25:GLU:OE1	2.23	0.45
1:F:185:THR:O	1:F:189:VAL:HG13	2.17	0.45
1:A:238:ILE:H	1:A:238:ILE:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ASN:HA	1:B:326:LYS:HE2	1.97	0.45
1:D:302:ILE:HD12	1:D:323:LEU:HD21	1.99	0.44
1:D:105:ILE:HD11	1:D:124:PHE:HB2	1.98	0.44
1:D:315:THR:HG23	1:D:319:ALA:HB3	1.99	0.44
1:A:36:LYS:HG3	2:A:504:MPD:H31	2.00	0.44
1:A:70:ARG:HG2	1:A:143:MET:HB3	1.99	0.44
1:E:196:LEU:HD11	1:E:329:VAL:HG11	1.99	0.44
1:E:4:LEU:HD21	1:E:79:GLU:HG3	1.99	0.44
1:E:224:LEU:O	1:E:228:LYS:HG2	2.18	0.44
1:B:43:LYS:HD2	1:B:49:ALA:HB2	1.99	0.44
1:C:17:LEU:HA	1:C:17:LEU:HD23	1.87	0.44
1:F:71:TYR:HB3	1:F:109:PRO:HG3	2.00	0.44
1:D:67:GLY:HA3	1:D:101:ALA:O	2.18	0.44
1:F:335:TYR:OH	1:F:374:PHE:HB2	2.18	0.44
1:F:380:MET:HG3	1:F:395:LEU:HB2	2.00	0.44
1:B:249:ASP:OD1	1:B:251:PRO:HD2	2.18	0.44
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.82	0.43
1:D:208:ARG:NH1	1:D:283:ASP:OD1	2.51	0.43
1:D:90:LYS:NZ	2:D:502:MPD:O4	2.30	0.43
1:F:197:LEU:HD21	1:F:284:ILE:HD11	2.01	0.43
1:A:59:ASP:O	1:A:99:GLY:HA3	2.18	0.43
1:C:170:GLY:HA2	1:C:181:ARG:HD2	2.01	0.43
1:F:5:ALA:HA	1:F:8:ASN:HD22	1.83	0.43
1:C:323:LEU:HB3	1:C:328:VAL:HB	2.00	0.43
1:E:333:ASP:N	1:E:333:ASP:OD1	2.51	0.43
1:E:380:MET:HE2	1:E:394:THR:HB	2.01	0.43
1:D:122:ARG:NE	1:F:410:GLY:HA2	2.33	0.43
1:F:154:LEU:HD12	1:F:165:PRO:HA	2.00	0.43
1:F:273:ASP:HB3	1:F:276:SER:OG	2.19	0.43
1:F:197:LEU:HD11	1:F:284:ILE:HD11	2.00	0.43
1:F:290:LEU:HA	1:F:290:LEU:HD23	1.86	0.43
1:C:260:HIS:O	1:C:261:ARG:HB2	2.18	0.42
1:B:189:VAL:HG13	1:B:308:ILE:HG21	2.00	0.42
1:E:185:THR:O	1:E:189:VAL:HG23	2.19	0.42
1:F:259:GLU:HG3	1:F:260:HIS:ND1	2.34	0.42
1:B:67:GLY:HA3	1:B:101:ALA:O	2.19	0.42
1:B:226:SER:HB3	1:B:232:ILE:HD11	2.01	0.42
1:B:8:ASN:O	1:B:12:LYS:HG3	2.19	0.42
1:C:91:THR:HG22	1:C:96:ILE:HD11	2.01	0.42
1:F:222:ALA:HB1	1:F:250:ILE:HD12	2.00	0.42
1:A:259:GLU:HG2	1:A:260:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ILE:HD12	1:B:232:ILE:H	1.83	0.42
1:C:171:LYS:O	1:C:181:ARG:CZ	2.67	0.42
1:B:29:LEU:HA	1:B:29:LEU:HD23	1.91	0.42
1:B:72:HIS:CG	1:B:73:PRO:HD2	2.55	0.42
1:C:66:LYS:O	1:C:87:MET:HG2	2.19	0.42
1:C:409:TRP:CE2	1:D:48:LEU:HD11	2.54	0.42
1:E:266:PHE:HD2	1:E:269:ALA:HB3	1.84	0.42
1:B:143:MET:HB2	1:B:143:MET:HE2	1.95	0.42
1:D:214:PHE:CE1	1:D:219:SER:HA	2.55	0.42
1:E:16:ARG:NH1	1:E:20:LEU:O	2.53	0.42
1:B:72:HIS:O	1:B:106:GLY:HA2	2.20	0.42
1:C:72:HIS:CG	1:C:73:PRO:HD2	2.55	0.42
1:E:77:PRO:HA	2:E:504:MPD:HM1	2.02	0.42
1:F:65:MET:HB3	1:F:101:ALA:HB2	2.01	0.42
1:D:163:TYR:CD2	1:D:165:PRO:HD3	2.54	0.42
1:C:4:LEU:HA	1:C:4:LEU:HD13	1.93	0.41
1:B:134:ILE:HG22	1:B:135:HIS:ND1	2.34	0.41
1:C:207:GLN:HG3	1:C:283:ASP:HB2	2.02	0.41
1:C:85:GLN:HG2	1:C:89:TRP:NE1	2.35	0.41
1:C:210:VAL:HG21	1:C:280:GLU:HB2	2.03	0.41
1:D:86:LEU:HD12	1:D:86:LEU:HA	1.94	0.41
1:F:17:LEU:HD23	1:F:17:LEU:HA	1.94	0.41
1:F:232:ILE:HD12	1:F:232:ILE:H	1.85	0.41
1:B:134:ILE:HD13	1:B:134:ILE:HA	1.86	0.41
1:B:381:CYS:O	1:B:385:SER:N	2.53	0.41
1:E:260:HIS:O	1:E:261:ARG:HB2	2.21	0.41
1:E:212:GLN:NE2	1:E:289:ALA:HB3	2.35	0.41
1:A:41:ILE:HG22	1:A:123:VAL:HG21	2.01	0.41
1:D:290:LEU:HD23	1:D:290:LEU:HA	1.92	0.41
1:B:108:ASP:OD2	1:B:111:LYS:HE2	2.20	0.41
1:B:197:LEU:HD11	1:B:284:ILE:HD11	2.02	0.41
1:A:332:PRO:HG3	1:A:389:ARG:HA	2.02	0.41
1:B:239:THR:HG21	1:B:262:GLY:HA3	2.02	0.41
1:C:67:GLY:HA3	1:C:101:ALA:O	2.20	0.41
1:E:142:ASP:OD1	1:E:143:MET:N	2.47	0.41
1:C:232:ILE:HD13	1:C:250:ILE:HG13	2.02	0.41
1:E:281:ASP:HA	1:E:303:LYS:HB2	2.02	0.41
2:E:503:MPD:H4	2:E:503:MPD:HM1	1.83	0.41
1:D:207:GLN:HG3	1:D:283:ASP:HB2	2.03	0.41
1:D:71:TYR:HB3	1:D:109:PRO:HG3	2.03	0.41
1:E:284:ILE:HG12	1:E:306:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:LEU:HD11	1:F:329:VAL:HG11	2.02	0.41
1:F:212:GLN:HG3	1:F:277:ILE:HD13	2.03	0.41
1:B:6:ALA:O	1:B:9:ARG:HB3	2.22	0.41
1:E:270:ASP:N	1:E:270:ASP:OD1	2.52	0.41
1:E:306:PHE:CD1	1:E:329:VAL:HB	2.56	0.41
1:A:380:MET:HE3	1:A:380:MET:HB2	1.96	0.40
1:C:290:LEU:HA	1:C:290:LEU:HD12	1.80	0.40
1:C:17:LEU:HD12	1:C:390:MET:HG3	2.03	0.40
1:C:117:LEU:HD22	2:C:503:MPD:H53	2.03	0.40
1:D:257:THR:HG22	1:D:263:VAL:HA	2.02	0.40
1:A:76:ASP:HB3	1:A:79:GLU:HB3	2.03	0.40
1:E:13:LEU:HD23	1:E:13:LEU:C	2.41	0.40
1:A:239:THR:HG21	1:A:262:GLY:HA3	2.03	0.40
1:D:209:PHE:O	1:D:233:VAL:HG22	2.22	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	408/414 (99%)	400 (98%)	8 (2%)	0	100	100
1	B	407/414 (98%)	403 (99%)	4 (1%)	0	100	100
1	C	406/414 (98%)	397 (98%)	9 (2%)	0	100	100
1	D	408/414 (99%)	398 (98%)	10 (2%)	0	100	100
1	E	408/414 (99%)	396 (97%)	12 (3%)	0	100	100
1	F	406/414 (98%)	396 (98%)	10 (2%)	0	100	100
All	All	2443/2484 (98%)	2390 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	330/333 (99%)	323 (98%)	7 (2%)	53	77
1	B	329/333 (99%)	322 (98%)	7 (2%)	53	77
1	C	329/333 (99%)	320 (97%)	9 (3%)	44	71
1	D	330/333 (99%)	317 (96%)	13 (4%)	32	58
1	E	330/333 (99%)	314 (95%)	16 (5%)	25	49
1	F	329/333 (99%)	316 (96%)	13 (4%)	31	57
All	All	1977/1998 (99%)	1912 (97%)	65 (3%)	38	64

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	114	ILE
1	A	185	THR
1	A	205	SER
1	A	257	THR
1	A	258	LYS
1	A	272	ILE
1	B	13	LEU
1	B	208	ARG
1	B	212	GLN
1	B	235	VAL
1	B	293	VAL
1	B	300	ASN
1	B	326	LYS
1	C	70	ARG
1	C	86	LEU
1	C	242	ILE
1	C	245	LYS
1	C	246	ASP
1	C	258	LYS
1	C	300	ASN
1	C	321	GLU

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Mol	Chain	Res	Type
1	C	394	THR
1	D	16	ARG
1	D	70	ARG
1	D	181	ARG
1	D	185	THR
1	D	203	THR
1	D	207	GLN
1	D	245	LYS
1	D	272	ILE
1	D	293	VAL
1	D	298	ASN
1	D	316	ASP
1	D	371	THR
1	D	409	TRP
1	E	86	LEU
1	E	173	ILE
1	E	208	ARG
1	E	224	LEU
1	E	228	LYS
1	E	236	SER
1	E	242	ILE
1	E	245	LYS
1	E	249	ASP
1	E	257	THR
1	E	270	ASP
1	E	279	VAL
1	E	295	ASN
1	E	298	ASN
1	E	321	GLU
1	E	394	THR
1	F	20	LEU
1	F	70	ARG
1	F	114	ILE
1	F	143	MET
1	F	185	THR
1	F	224	LEU
1	F	257	THR
1	F	260	HIS
1	F	277	ILE
1	F	296	ARG
1	F	316	ASP
1	F	325	LYS

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Mol	Chain	Res	Type
1	F	394	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	207	GLN
1	B	212	GLN
1	B	384	HIS
1	C	207	GLN
1	D	207	GLN
1	D	256	HIS
1	D	298	ASN
1	D	300	ASN
1	E	207	GLN
1	E	384	HIS
1	F	398	ASN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	$\#\|Z\|>2$
2	MPD	D	502	-	7,7,7	0.29	0	9,10,10	0.36	0
2	MPD	A	502	-	7,7,7	0.29	0	9,10,10	0.45	0
2	MPD	C	502	-	7,7,7	0.26	0	9,10,10	0.42	0
2	MPD	E	503	-	7,7,7	0.21	0	9,10,10	0.78	0
2	MPD	B	501	-	7,7,7	0.32	0	9,10,10	0.43	0
2	MPD	C	503	-	7,7,7	0.34	0	9,10,10	0.32	0
2	MPD	A	503	-	7,7,7	0.38	0	9,10,10	0.63	0
2	MPD	A	504	-	7,7,7	0.29	0	9,10,10	0.94	1 (11%)
2	MPD	E	501	-	7,7,7	0.35	0	9,10,10	0.49	0
2	MPD	E	504	-	7,7,7	0.26	0	9,10,10	0.36	0
2	MPD	A	501	-	7,7,7	0.37	0	9,10,10	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	D	502	-	-	0/5/5/5	-
2	MPD	A	502	-	-	0/5/5/5	-
2	MPD	C	502	-	-	0/5/5/5	-
2	MPD	E	503	-	-	1/5/5/5	-
2	MPD	B	501	-	-	0/5/5/5	-
2	MPD	C	503	-	-	3/5/5/5	-
2	MPD	A	503	-	-	2/5/5/5	-
2	MPD	A	504	-	-	0/5/5/5	-
2	MPD	E	501	-	-	2/5/5/5	-
2	MPD	E	504	-	-	0/5/5/5	-
2	MPD	A	501	-	-	1/5/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	504	MPD	CM-C2-C1	-2.43	105.50	110.57

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	503	MPD	O2-C2-C3-C4
2	E	503	MPD	CM-C2-C3-C4
2	C	503	MPD	C1-C2-C3-C4
2	C	503	MPD	CM-C2-C3-C4
2	A	503	MPD	C2-C3-C4-C5
2	E	501	MPD	C2-C3-C4-C5
2	A	503	MPD	C2-C3-C4-O4
2	E	501	MPD	C2-C3-C4-O4
2	A	501	MPD	C2-C3-C4-O4

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	502	MPD	1	0
2	C	502	MPD	1	0
2	E	503	MPD	1	0
2	C	503	MPD	1	0
2	A	503	MPD	2	0
2	A	504	MPD	1	0
2	E	504	MPD	1	0
2	A	501	MPD	1	0

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, 95^{th} 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	410/414 (99%)	-0.13	1 (0%) 95 95	17, 34, 63, 104	0
1	B	409/414 (98%)	0.00	4 (0%) 82 80	20, 45, 92, 143	0
1	C	408/414 (98%)	0.04	4 (0%) 82 80	20, 47, 96, 131	0
1	D	410/414 (99%)	0.10	8 (1%) 65 60	22, 48, 104, 128	0
1	E	410/414 (99%)	0.38	27 (6%) 18 13	22, 59, 144, 182	0
1	F	408/414 (98%)	0.42	40 (9%) 7 5	25, 61, 135, 170	0
All	All	2455/2484 (98%)	0.14	84 (3%) 45 38	17, 46, 117, 182	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	ALA	4.9
1	E	410	GLY	4.9
1	B	411	ALA	4.6
1	F	262	GLY	4.5
1	F	328	VAL	4.5
1	F	214	PHE	4.4
1	E	270	ASP	4.3
1	D	9	ARG	4.2
1	F	277	ILE	4.1
1	F	300	ASN	4.0
1	F	266	PHE	3.9
1	F	224	LEU	3.7
1	F	294	ILE	3.6
1	F	200	HIS	3.6
1	E	272	ILE	3.6
1	F	411	ALA	3.3
1	E	294	ILE	3.3
1	F	329	VAL	3.3
1	F	211	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	273	ASP	3.1
1	C	5	ALA	3.1
1	F	233	VAL	3.1
1	F	199	GLU	3.1
1	F	305	LYS	2.8
1	F	325	LYS	2.8
1	F	263	VAL	2.8
1	F	246	ASP	2.8
1	F	225	ILE	2.8
1	F	293	VAL	2.7
1	F	209	PHE	2.7
1	F	267	ASP	2.7
1	E	206	GLY	2.7
1	D	411	ALA	2.7
1	F	270	ASP	2.7
1	E	277	ILE	2.7
1	E	250	ILE	2.6
1	E	235	VAL	2.6
1	F	271	PRO	2.6
1	E	267	ASP	2.6
1	E	330	ILE	2.6
1	F	247	GLY	2.5
1	E	241	ALA	2.5
1	E	302	ILE	2.5
1	E	9	ARG	2.5
1	D	282	CYS	2.4
1	E	266	PHE	2.4
1	F	264	LYS	2.4
1	E	254	LEU	2.4
1	F	314	PRO	2.4
1	D	296	ARG	2.4
1	E	283	ASP	2.4
1	E	282	CYS	2.4
1	F	9	ARG	2.3
1	F	239	THR	2.3
1	B	267	ASP	2.3
1	F	248	ILE	2.3
1	E	293	VAL	2.3
1	F	272	ILE	2.3
1	C	4	LEU	2.3
1	B	372	ARG	2.3
1	E	296	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	304	ALA	2.3
1	E	326	LYS	2.3
1	E	285	LEU	2.2
1	C	277	ILE	2.2
1	D	410	GLY	2.2
1	F	301	GLU	2.2
1	E	295	ASN	2.1
1	F	191	PHE	2.1
1	D	297	GLU	2.1
1	C	250	ILE	2.1
1	E	3	ALA	2.1
1	B	270	ASP	2.1
1	F	284	ILE	2.1
1	F	327	GLY	2.1
1	E	261	ARG	2.1
1	E	211	ILE	2.1
1	F	232	ILE	2.1
1	F	196	LEU	2.1
1	D	299	ALA	2.0
1	E	278	LEU	2.0
1	F	326	LYS	2.0
1	E	213	GLY	2.0
1	F	322	ILE	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, 95^{th} 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.

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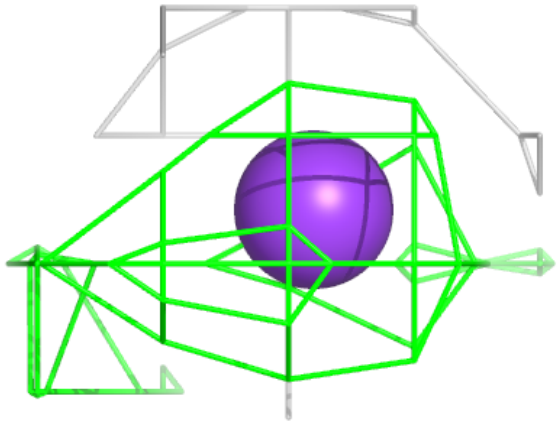
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

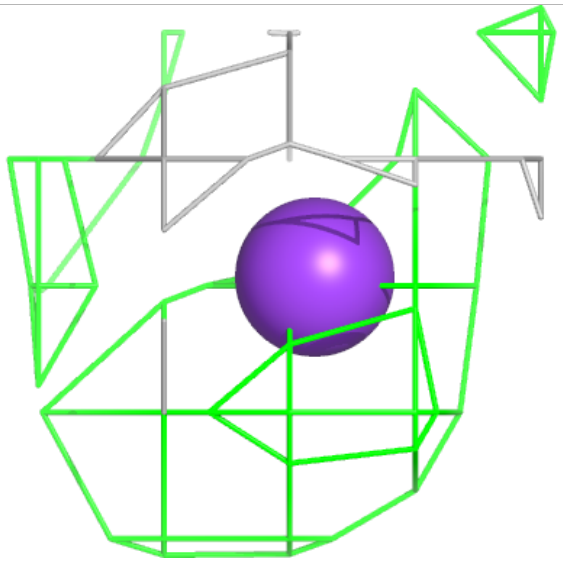
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MPD	A	504	8/8	0.75	0.31	56,62,66,68	0
2	MPD	E	501	8/8	0.86	0.20	59,63,74,76	0
2	MPD	A	503	8/8	0.88	0.35	57,61,69,73	0
2	MPD	D	502	8/8	0.89	0.27	56,60,69,71	0
2	MPD	A	501	8/8	0.90	0.23	45,49,52,54	0
2	MPD	E	503	8/8	0.93	0.26	45,47,56,60	0
2	MPD	C	503	8/8	0.94	0.28	58,63,65,67	0
2	MPD	E	504	8/8	0.95	0.19	55,57,60,61	0
2	MPD	B	501	8/8	0.95	0.26	39,46,51,53	0
2	MPD	A	502	8/8	0.96	0.27	53,57,59,63	0
2	MPD	C	502	8/8	0.96	0.18	37,42,49,54	0
3	K	A	506	1/1	0.97	0.19	47,47,47,47	0
3	K	E	505	1/1	0.98	0.17	39,39,39,39	0
3	K	D	501	1/1	0.98	0.15	30,30,30,30	0
3	K	A	505	1/1	0.98	0.26	44,44,44,44	0
3	K	C	501	1/1	0.99	0.14	39,39,39,39	0
3	K	E	502	1/1	0.99	0.17	40,40,40,40	0

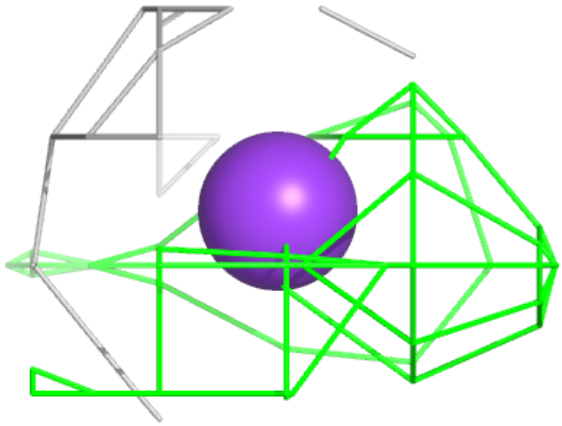
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around K A 506:

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

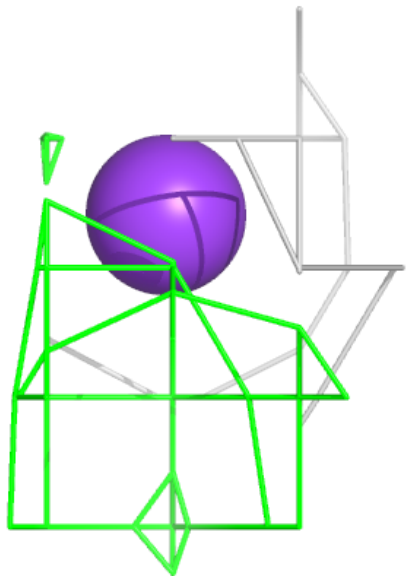


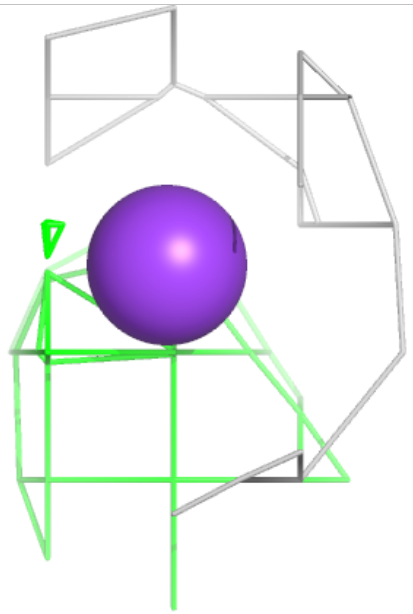


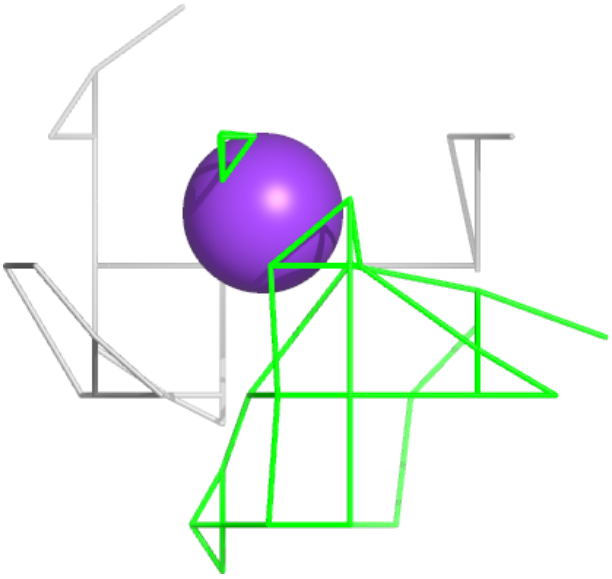


Electron density around K E 505:

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

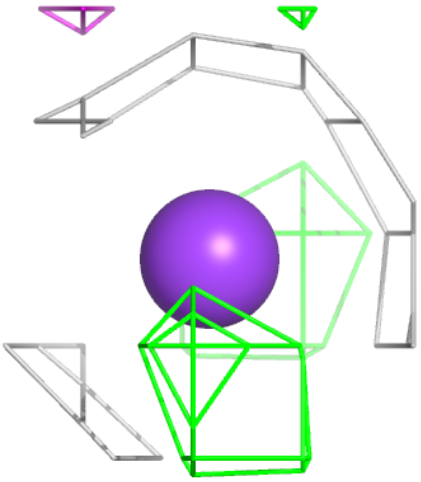


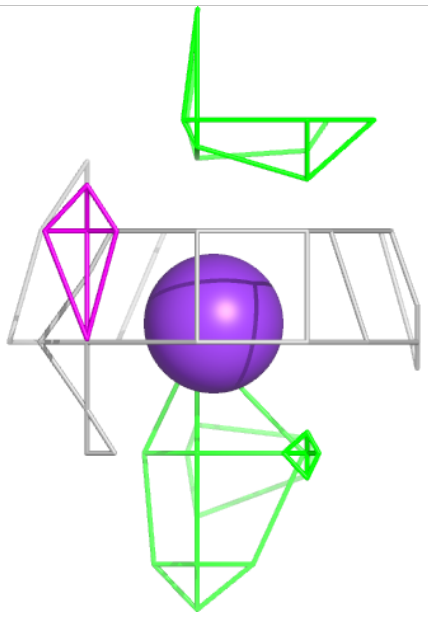


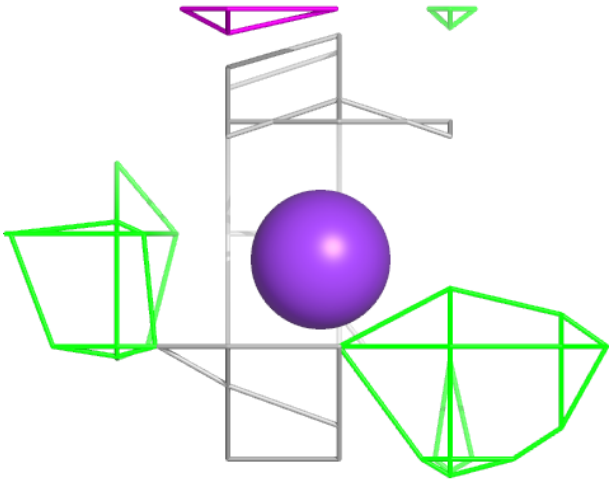


Electron density around K D 501:

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

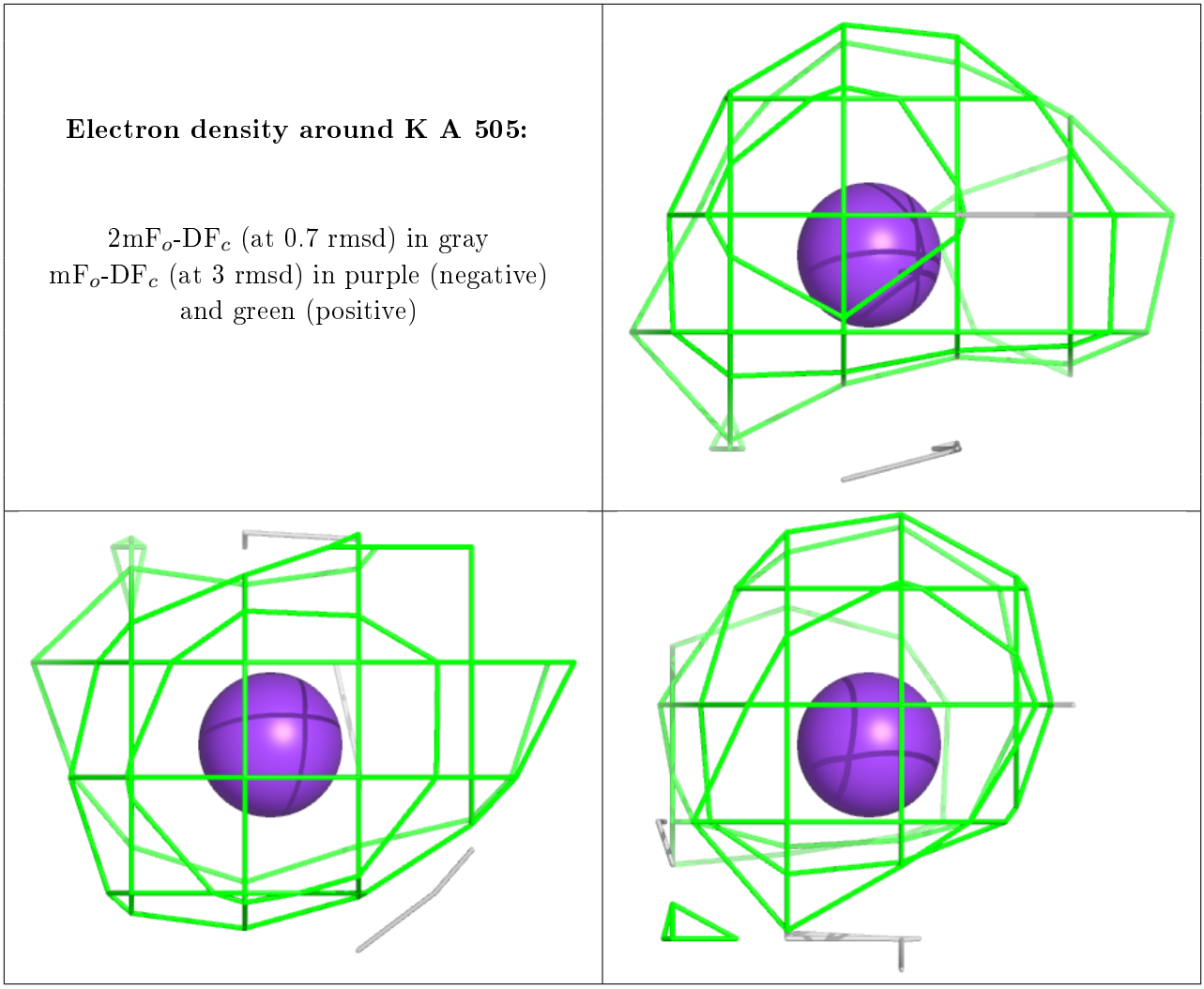






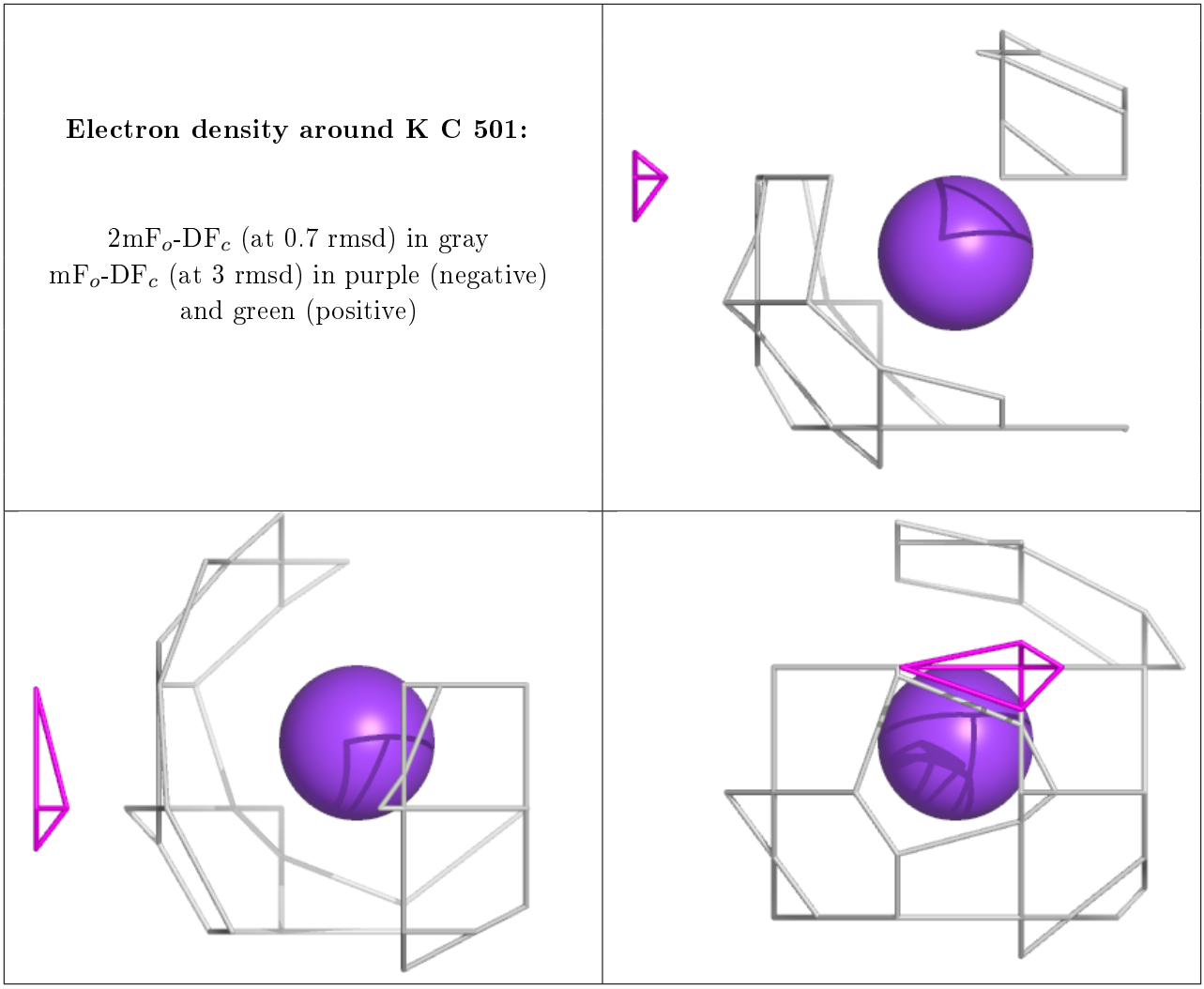
Electron density around K A 505:

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



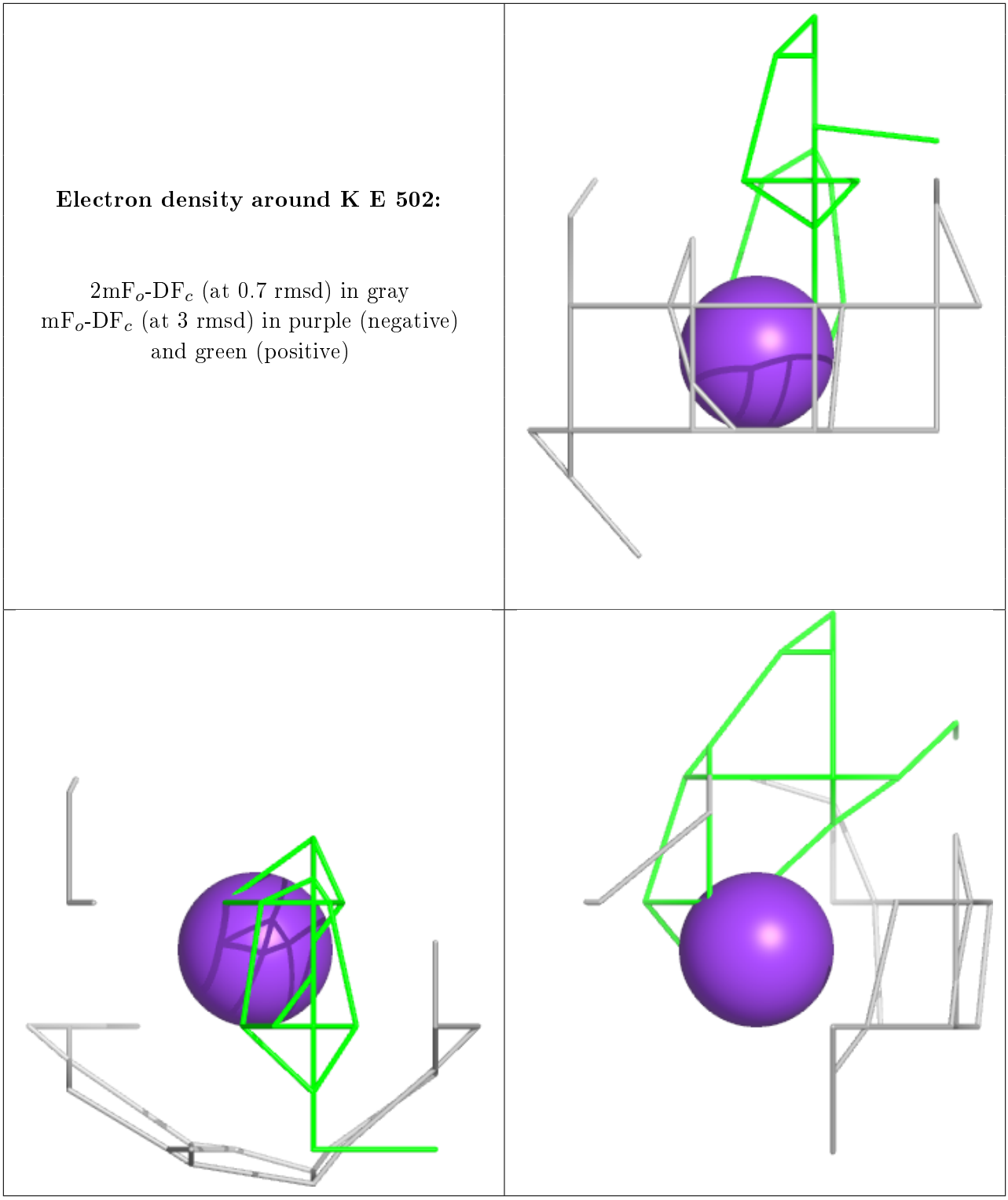
Electron density around K C 501:

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



Electron density around K E 502:

$2mF_o$-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

There are no such residues in this entry.