



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:14 PM UTC

PDB ID : 6YEH / pdb_00006yeh
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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

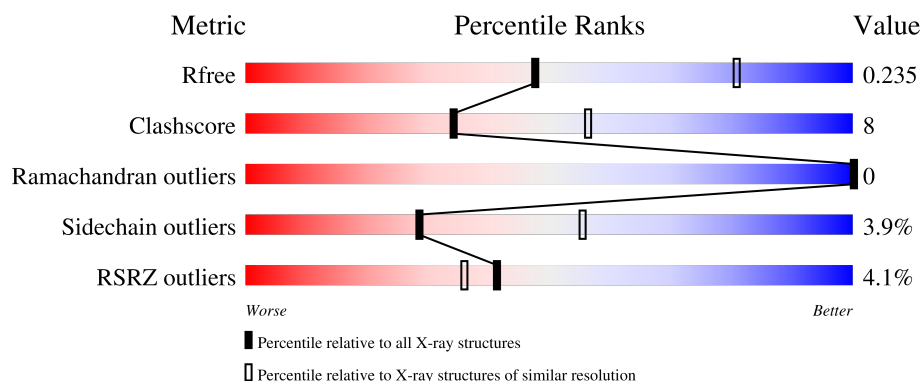
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	414	82% 16% .
1	B	414	84% 15% .
1	C	414	3% 79% 18% ..
1	D	414	2% 76% 21% ..
1	E	414	6% 76% 21% ..

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Mol	Chain	Length	Quality of chain
1	F	414	11% 77% 20% ..

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:

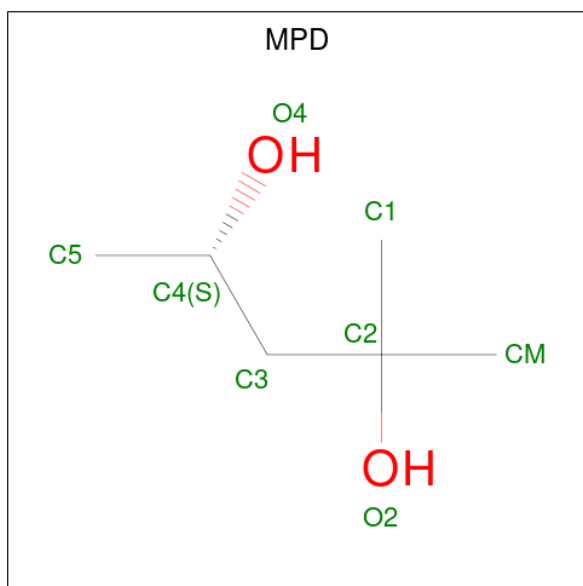
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q43314
A	-1	ASN	-	expression tag	UNP Q43314
A	0	ALA	-	expression tag	UNP Q43314
B	-2	SER	-	expression tag	UNP Q43314
B	-1	ASN	-	expression tag	UNP Q43314
B	0	ALA	-	expression tag	UNP Q43314
C	-2	SER	-	expression tag	UNP Q43314
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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

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

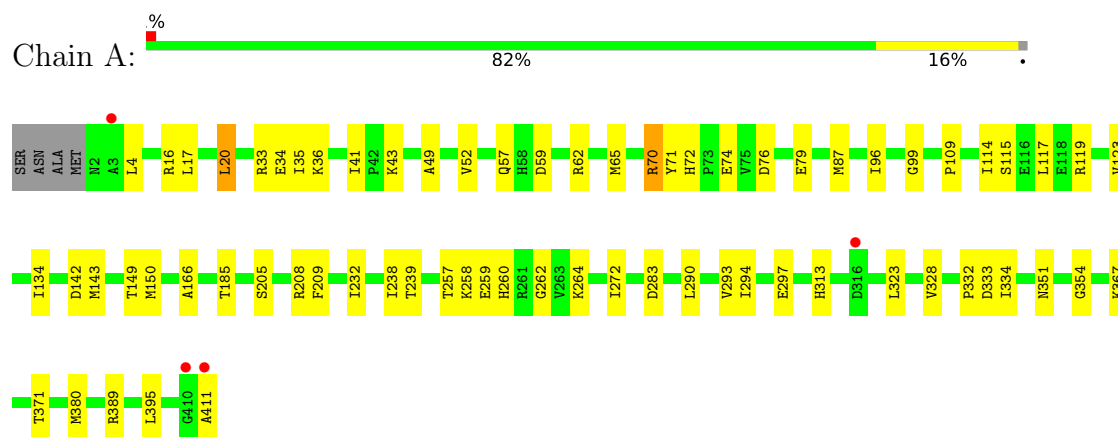
- Molecule 4 is water.

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

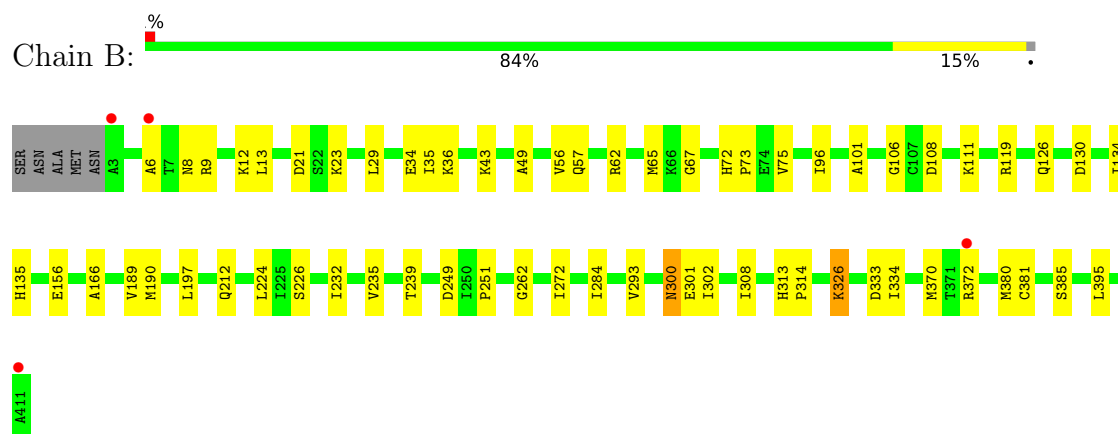
3 Residue-property plots [i](#)

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.

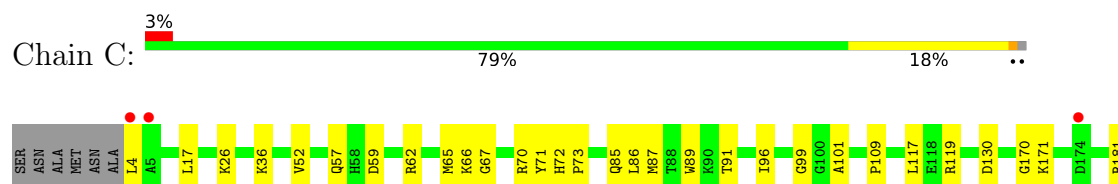
- Molecule 1: Glutamate dehydrogenase 1

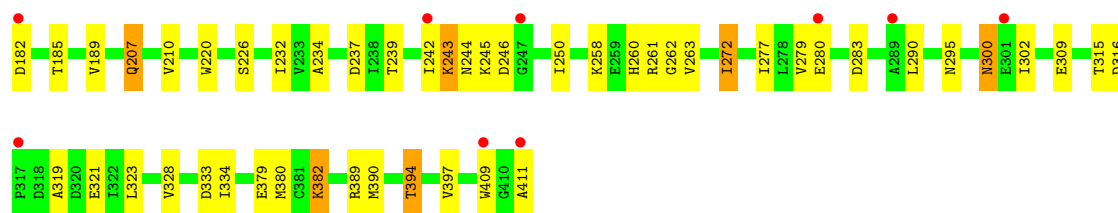


- Molecule 1: Glutamate dehydrogenase 1

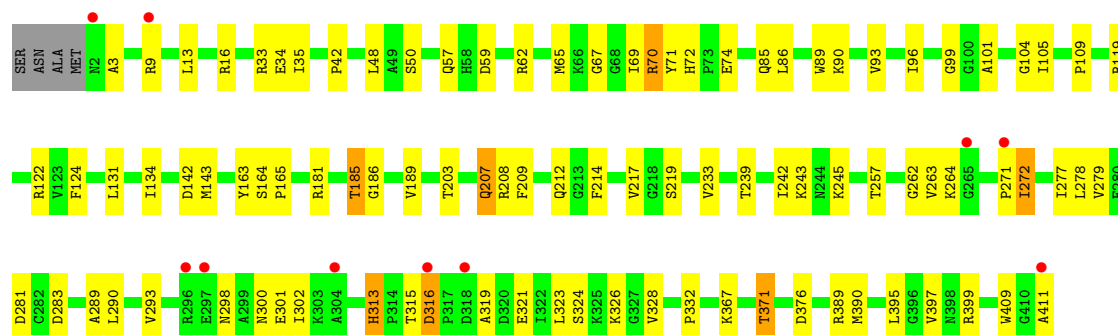
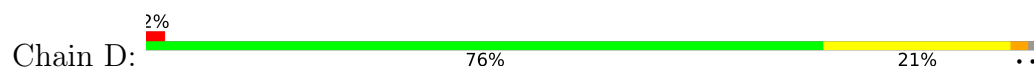


- Molecule 1: Glutamate dehydrogenase 1

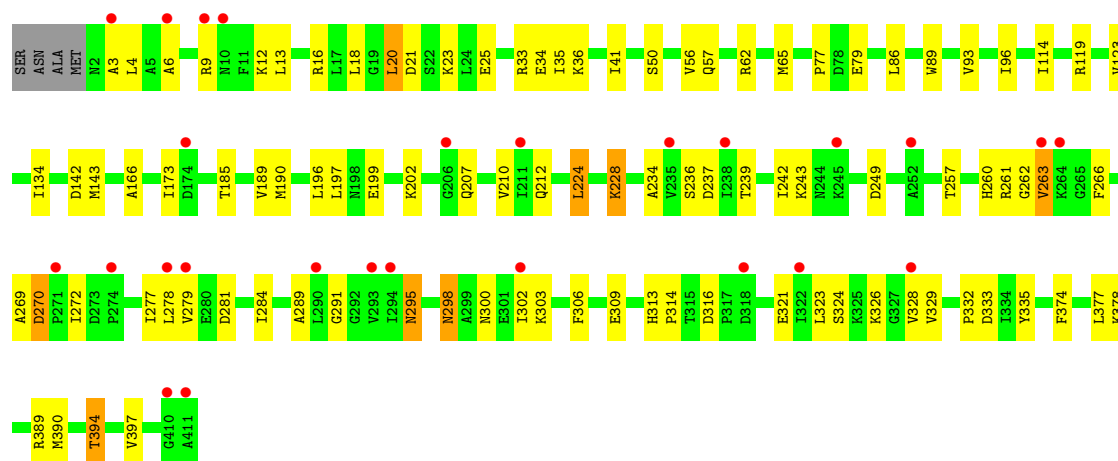
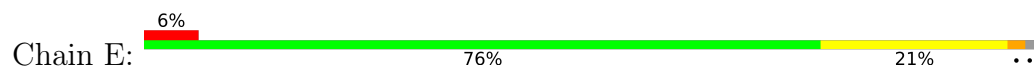




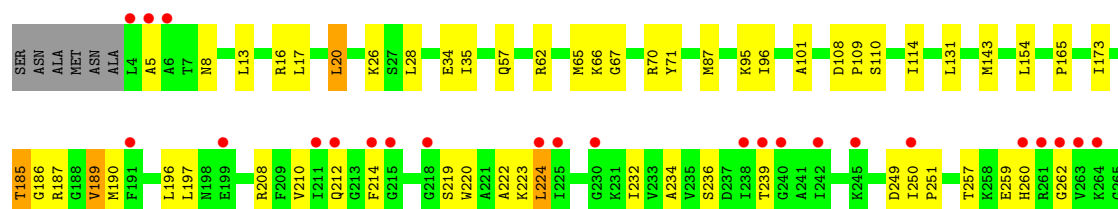
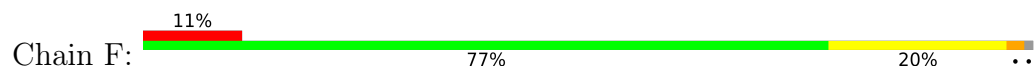
● Molecule 1: Glutamate dehydrogenase 1

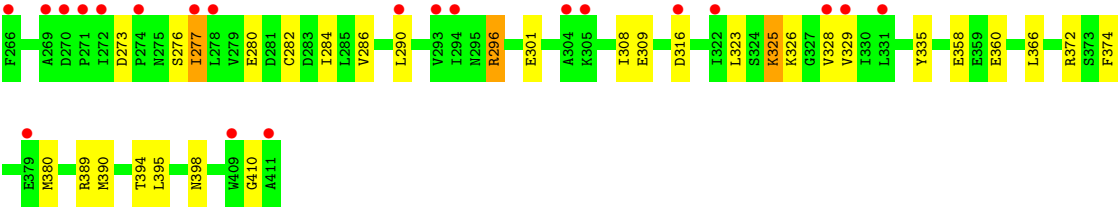


● Molecule 1: Glutamate dehydrogenase 1



● Molecule 1: Glutamate dehydrogenase 1





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.183 , 0.235 0.184 , 0.235	Depositor DCC
R_{free} test set	1045 reflections (1.13%)	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 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: MPD, K

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	0.32	0/3185	0.54	0/4306
1	B	0.29	0/3177	0.51	0/4295
1	C	0.31	0/3172	0.54	0/4288
1	D	0.29	0/3185	0.49	0/4306
1	E	0.28	0/3185	0.50	0/4306
1	F	0.27	0/3172	0.50	0/4288
All	All	0.29	0/19076	0.51	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 [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	3123	0	3140	43	0
1	B	3115	0	3134	40	0
1	C	3110	0	3129	49	0
1	D	3123	0	3140	57	0
1	E	3123	0	3140	58	0
1	F	3110	0	3129	54	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	2	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	287	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 8.

All (287) 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
2:D:502:MPD:HO4	2:D:502:MPD:HO2	1.32	0.74
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:F:360:GLU:H	1:F:360:GLU:CD	2.04	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:ILE:HG22	1:E:123:VAL:HG21	1.82	0.62
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:89:TRP:O	1:E:93:VAL:HG23	2.00	0.61
1:E:298:ASN:N	1:E:298:ASN:OD1	2.33	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:C:380:MET:HE2	1:C:394:THR:HB	1.83	0.60
1:A:36:LYS:NZ	1:B:34:GLU:OE1	2.33	0.60
1:D:62:ARG:NH2	1:D:96:ILE:O	2.34	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:A:380:MET:HE3	1:A:395:LEU:HD13	1.84	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:16:ARG:NH1	1:A:20:LEU:O	2.38	0.56
1:F:13:LEU:HD23	1:F:390:MET:HE3	1.87	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:F:190:MET:HE2	1:F:224:LEU:HB3	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:380:MET:HE1	1:F:398:ASN:HD22	1.71	0.55
1:D:70:ARG:HG2	1:D:142:ASP:CG	2.31	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
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:OD1	1:D:316:ASP:N	2.37	0.53
1:E:33:ARG:HG2	1:E:35:ILE:HD11	1.90	0.53
1:E:237:ASP:OD2	1:E:263:VAL:HG23	2.07	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:OD1	1:C:300:ASN:N	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:N	1:B:301:GLU:OE1	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:89:TRP:O	1:D:93:VAL:HG23	2.11	0.51
1:D:185:THR:HB	1:D:217:VAL:HG22	1.92	0.51
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:A:34:GLU:HB2	1:B:36:LYS:HB2	1.92	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:34:GLU:HG2	1:E:56:VAL:HG22	1.92	0.49
1:E:390:MET:O	1:E:394:THR:OG1	2.28	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:C:71:TYR:HB3	1:C:109:PRO:HG3	1.94	0.49
2:C:502:MPD:HM1	2:C:502:MPD:H4	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: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

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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:F:277:ILE:HA	1:F:280:GLU:HG2	1.95	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:A:367:LYS:O	1:A:371:THR:OG1	2.26	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:66:LYS:O	1:F:87:MET:HG2	2.15	0.46
1:F:286:VAL:HG22	1:F:308:ILE:HB	1.96	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:E:13:LEU:C	1:E:13:LEU:HD23	2.41	0.46
1:A:17:LEU:HD23	1:A:17:LEU:HA	1.86	0.45
1:B:190:MET:HE2	1:B:224:LEU:HB3	1.98	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:A:238:ILE:H	1.81	0.45
1:B:300:ASN:HA	1:B:326:LYS:HE2	1.97	0.45
1:B:370:MET:HE2	1:B:370:MET:HB3	1.83	0.44
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:4:LEU:HD21	1:E:79:GLU:HG3	1.99	0.44
1:E:196:LEU:HD11	1:E:329:VAL:HG11	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:HD23	1:C:17:LEU:HA	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:90:LYS:NZ	2:D:502:MPD:O4	2.30	0.43
1:D:208:ARG:NH1	1:D:283:ASP:OD1	2.51	0.43
1:A:33:ARG:HH22	1:B:130:ASP:CG	2.26	0.43
1:C:130:ASP:CG	1:D:33:ARG:HH22	2.26	0.43
1:E:324:SER:C	1:E:326:LYS:H	2.26	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: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:197:LEU:HD11	1:F:284:ILE:HD11	2.00	0.43
1:F:273:ASP:HB3	1:F:276:SER:OG	2.19	0.43
1:F:290:LEU:HD23	1:F:290:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ASN:O	1:B:12:LYS:HG3	2.19	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: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
1:B:232:ILE:H	1:B:232:ILE:HD12	1.83	0.42
1:C:171:LYS:O	1:C:181:ARG:CZ	2.67	0.42
1:A:149:THR:HB	1:A:150:MET:HE2	2.02	0.42
1:B:29:LEU:HD23	1:B:29:LEU:HA	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:309:GLU:CD	1:C:389:ARG:HH22	2.28	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: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:HD13	1:C:4:LEU:HA	1.93	0.41
1:B:134:ILE:HG22	1:B:135:HIS:ND1	2.34	0.41
1:C:85:GLN:HG2	1:C:89:TRP:NE1	2.35	0.41
1:C:207:GLN:HG3	1:C:283:ASP:HB2	2.02	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:212:GLN:NE2	1:E:289:ALA:HB3	2.35	0.41
1:E:260:HIS:O	1:E:261:ARG:HB2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ASP:OD1	1:E:143:MET:N	2.47	0.41
1:E:377:LEU:C	1:E:377:LEU:HD23	2.46	0.41
1:A:87:MET:HE2	1:A:87:MET:HB2	1.93	0.41
1:C:232:ILE:HD13	1:C:250:ILE:HG13	2.02	0.41
1:D:71:TYR:HB3	1:D:109:PRO:HG3	2.03	0.41
1:D:207:GLN:HG3	1:D:283:ASP:HB2	2.03	0.41
1:E:281:ASP:HA	1:E:303:LYS:HB2	2.02	0.41
1:E:284:ILE:HG12	1:E:306:PHE:HB2	2.02	0.41
1:E:295:ASN:HA	1:E:316:ASP:CG	2.45	0.41
2:E:503:MPD:HM1	2:E:503:MPD:H4	1.83	0.41
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:OD1	1:E:270:ASP:N	2.52	0.41
1:E:306:PHE:CD1	1:E:329:VAL:HB	2.56	0.41
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:C:290:LEU:HD12	1:C:290:LEU:HA	1.80	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: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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	322 (98%)	8 (2%)	43	70
1	B	329/333 (99%)	320 (97%)	9 (3%)	39	67
1	C	329/333 (99%)	315 (96%)	14 (4%)	26	51
1	D	330/333 (99%)	315 (96%)	15 (4%)	24	50
1	E	330/333 (99%)	312 (94%)	18 (6%)	19	41
1	F	329/333 (99%)	315 (96%)	14 (4%)	26	51
All	All	1977/1998 (99%)	1899 (96%)	78 (4%)	28	55

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
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	75	VAL

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Mol	Chain	Res	Type
1	B	212	GLN
1	B	235	VAL
1	B	272	ILE
1	B	293	VAL
1	B	300	ASN
1	B	302	ILE
1	B	326	LYS
1	C	70	ARG
1	C	86	LEU
1	C	207	GLN
1	C	242	ILE
1	C	243	LYS
1	C	245	LYS
1	C	246	ASP
1	C	258	LYS
1	C	272	ILE
1	C	300	ASN
1	C	321	GLU
1	C	382	LYS
1	C	394	THR
1	C	397	VAL
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	313	HIS
1	D	316	ASP
1	D	371	THR
1	D	397	VAL
1	D	409	TRP
1	E	20	LEU
1	E	86	LEU
1	E	114	ILE
1	E	173	ILE
1	E	224	LEU
1	E	228	LYS

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Mol	Chain	Res	Type
1	E	236	SER
1	E	242	ILE
1	E	249	ASP
1	E	257	THR
1	E	263	VAL
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	E	397	VAL
1	F	20	LEU
1	F	70	ARG
1	F	114	ILE
1	F	143	MET
1	F	173	ILE
1	F	185	THR
1	F	189	VAL
1	F	224	LEU
1	F	257	THR
1	F	277	ILE
1	F	296	ARG
1	F	316	ASP
1	F	325	LYS
1	F	394	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	198	ASN
1	A	212	GLN
1	A	353	GLN
1	B	207	GLN
1	B	212	GLN
1	B	216	ASN
1	B	300	ASN
1	B	384	HIS
1	C	57	GLN
1	C	198	ASN
1	C	207	GLN

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Mol	Chain	Res	Type
1	C	260	HIS
1	C	398	ASN
1	D	207	GLN
1	D	260	HIS
1	D	298	ASN
1	E	126	GLN
1	E	200	HIS
1	E	207	GLN
1	E	384	HIS
1	F	57	GLN
1	F	198	ASN
1	F	398	ASN

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 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	E	501	-	7,7,7	0.38	0	9,10,10	0.46	0
2	MPD	E	503	-	7,7,7	0.26	0	9,10,10	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MPD	A	501	-	7,7,7	0.40	0	9,10,10	0.35	0
2	MPD	A	503	-	7,7,7	0.42	0	9,10,10	0.61	0
2	MPD	C	503	-	7,7,7	0.37	0	9,10,10	0.33	0
2	MPD	D	502	-	7,7,7	0.32	0	9,10,10	0.35	0
2	MPD	A	502	-	7,7,7	0.33	0	9,10,10	0.43	0
2	MPD	C	502	-	7,7,7	0.30	0	9,10,10	0.40	0
2	MPD	E	504	-	7,7,7	0.29	0	9,10,10	0.35	0
2	MPD	B	501	-	7,7,7	0.36	0	9,10,10	0.42	0
2	MPD	A	504	-	7,7,7	0.30	0	9,10,10	0.90	1 (11%)

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	E	501	-	-	2/5/5/5	-
2	MPD	E	503	-	-	2/5/5/5	-
2	MPD	A	501	-	-	1/5/5/5	-
2	MPD	A	503	-	-	1/5/5/5	-
2	MPD	C	503	-	-	3/5/5/5	-
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	504	-	-	0/5/5/5	-
2	MPD	B	501	-	-	1/5/5/5	-
2	MPD	A	504	-	-	0/5/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	504	MPD	CM-C2-C1	-2.29	105.50	110.63

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	503	MPD	C1-C2-C3-C4
2	C	503	MPD	CM-C2-C3-C4

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

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	503	MPD	1	0
2	A	501	MPD	1	0
2	A	503	MPD	2	0
2	C	503	MPD	1	0
2	D	502	MPD	2	0
2	C	502	MPD	1	0
2	E	504	MPD	1	0
2	A	504	MPD	1	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	410/414 (99%)	-0.30	4 (0%) 79 76	17, 34, 63, 104	0
1	B	409/414 (98%)	-0.08	4 (0%) 79 76	20, 45, 92, 143	0
1	C	408/414 (98%)	0.03	12 (2%) 53 48	20, 47, 96, 130	0
1	D	410/414 (99%)	0.09	10 (2%) 59 54	22, 48, 104, 128	0
1	E	410/414 (99%)	0.38	26 (6%) 26 20	22, 59, 144, 182	0
1	F	408/414 (98%)	0.53	45 (11%) 10 8	25, 61, 135, 170	0
All	All	2455/2484 (98%)	0.11	101 (4%) 41 36	17, 46, 117, 182	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	ALA	5.7
1	F	290	LEU	4.8
1	F	411	ALA	4.7
1	C	5	ALA	4.6
1	F	238	ILE	4.5
1	B	411	ALA	4.4
1	F	214	PHE	4.2
1	E	3	ALA	4.2
1	D	411	ALA	4.2
1	F	277	ILE	4.1
1	B	3	ALA	4.1
1	F	6	ALA	3.7
1	F	211	ILE	3.7
1	F	278	LEU	3.5
1	A	3	ALA	3.5
1	D	9	ARG	3.4
1	E	9	ARG	3.2
1	D	265	GLY	3.2
1	E	271	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	316	ASP	3.1
1	E	294	ILE	3.1
1	E	290	LEU	3.0
1	F	4	LEU	3.0
1	F	294	ILE	3.0
1	F	272	ILE	2.9
1	B	372	ARG	2.8
1	F	322	ILE	2.8
1	A	410	GLY	2.8
1	E	302	ILE	2.8
1	F	270	ASP	2.8
1	F	305	LYS	2.8
1	F	271	PRO	2.8
1	C	4	LEU	2.7
1	F	328	VAL	2.7
1	F	304	ALA	2.7
1	B	6	ALA	2.7
1	E	278	LEU	2.7
1	F	263	VAL	2.6
1	F	261	ARG	2.6
1	F	212	GLN	2.6
1	F	240	GLY	2.5
1	F	218	GLY	2.5
1	F	5	ALA	2.5
1	F	239	THR	2.5
1	F	215	GLY	2.5
1	F	199	GLU	2.5
1	E	274	PRO	2.5
1	E	263	VAL	2.5
1	D	316	ASP	2.4
1	F	266	PHE	2.4
1	F	293	VAL	2.4
1	E	6	ALA	2.4
1	F	224	LEU	2.4
1	F	191	PHE	2.4
1	C	280	GLU	2.4
1	F	331	LEU	2.4
1	E	235	VAL	2.4
1	E	238	ILE	2.3
1	F	329	VAL	2.3
1	E	252	ALA	2.3
1	E	410	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	411	ALA	2.3
1	F	245	LYS	2.3
1	A	316	ASP	2.3
1	E	279	VAL	2.3
1	C	247	GLY	2.2
1	E	206	GLY	2.2
1	D	271	PRO	2.2
1	E	245	LYS	2.2
1	F	269	ALA	2.2
1	F	260	HIS	2.2
1	F	262	GLY	2.2
1	C	242	ILE	2.2
1	E	174	ASP	2.2
1	E	322	ILE	2.2
1	C	409	TRP	2.2
1	F	409	TRP	2.2
1	E	411	ALA	2.1
1	C	317	PRO	2.1
1	F	264	LYS	2.1
1	E	10	ASN	2.1
1	D	296	ARG	2.1
1	C	301	GLU	2.1
1	F	250	ILE	2.1
1	C	182	ASP	2.1
1	D	318	ASP	2.1
1	E	318	ASP	2.1
1	E	293	VAL	2.1
1	E	328	VAL	2.1
1	D	304	ALA	2.1
1	D	2	ASN	2.1
1	E	211	ILE	2.1
1	F	225	ILE	2.1
1	F	379	GLU	2.0
1	E	264	LYS	2.0
1	F	242	ILE	2.0
1	C	289	ALA	2.0
1	D	297	GLU	2.0
1	F	230	GLY	2.0
1	C	174	ASP	2.0
1	F	274	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

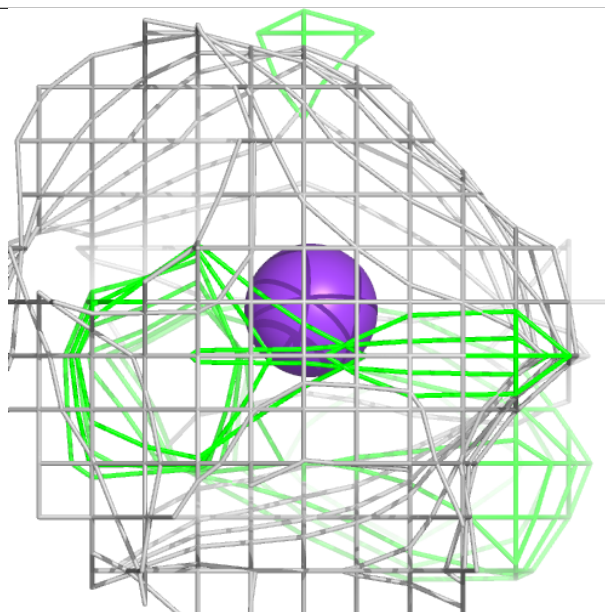
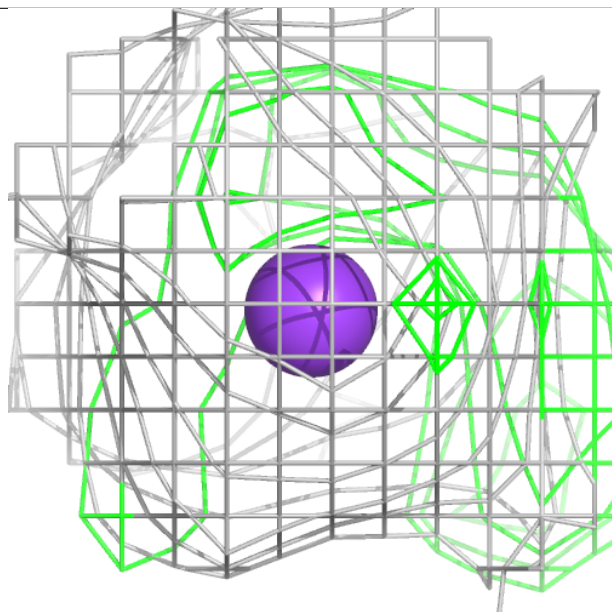
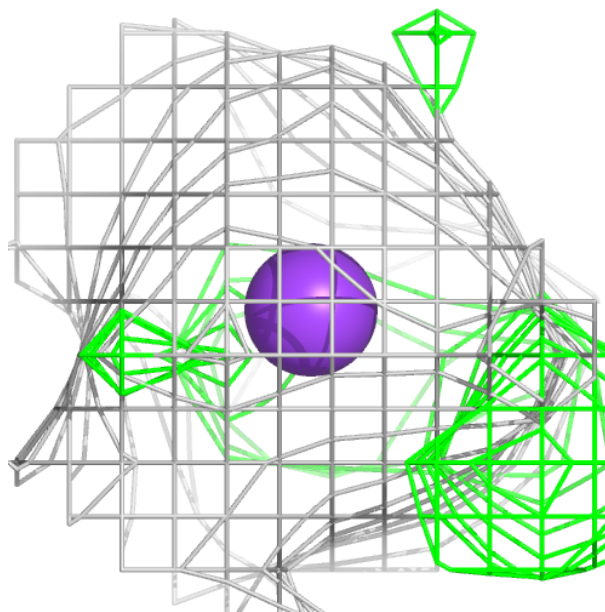
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MPD	A	504	8/8	0.65	0.26	56,62,66,68	0
2	MPD	E	501	8/8	0.77	0.18	59,63,74,76	0
2	MPD	A	501	8/8	0.82	0.18	45,49,52,54	0
2	MPD	D	502	8/8	0.86	0.16	56,60,69,71	0
2	MPD	E	504	8/8	0.88	0.15	55,57,60,61	0
2	MPD	C	503	8/8	0.89	0.15	58,63,65,67	0
2	MPD	A	503	8/8	0.90	0.20	57,61,69,73	0
2	MPD	B	501	8/8	0.93	0.11	39,46,51,53	0
2	MPD	A	502	8/8	0.95	0.12	53,57,59,63	0
2	MPD	E	503	8/8	0.95	0.15	45,47,56,60	0
2	MPD	C	502	8/8	0.95	0.10	37,42,49,54	0
3	K	A	506	1/1	0.96	0.12	47,47,47,47	0
3	K	D	501	1/1	0.97	0.06	30,30,30,30	0
3	K	E	502	1/1	0.97	0.09	40,40,40,40	0
3	K	E	505	1/1	0.97	0.08	39,39,39,39	0
3	K	C	501	1/1	0.98	0.04	39,39,39,39	0
3	K	A	505	1/1	0.98	0.17	44,44,44,44	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.

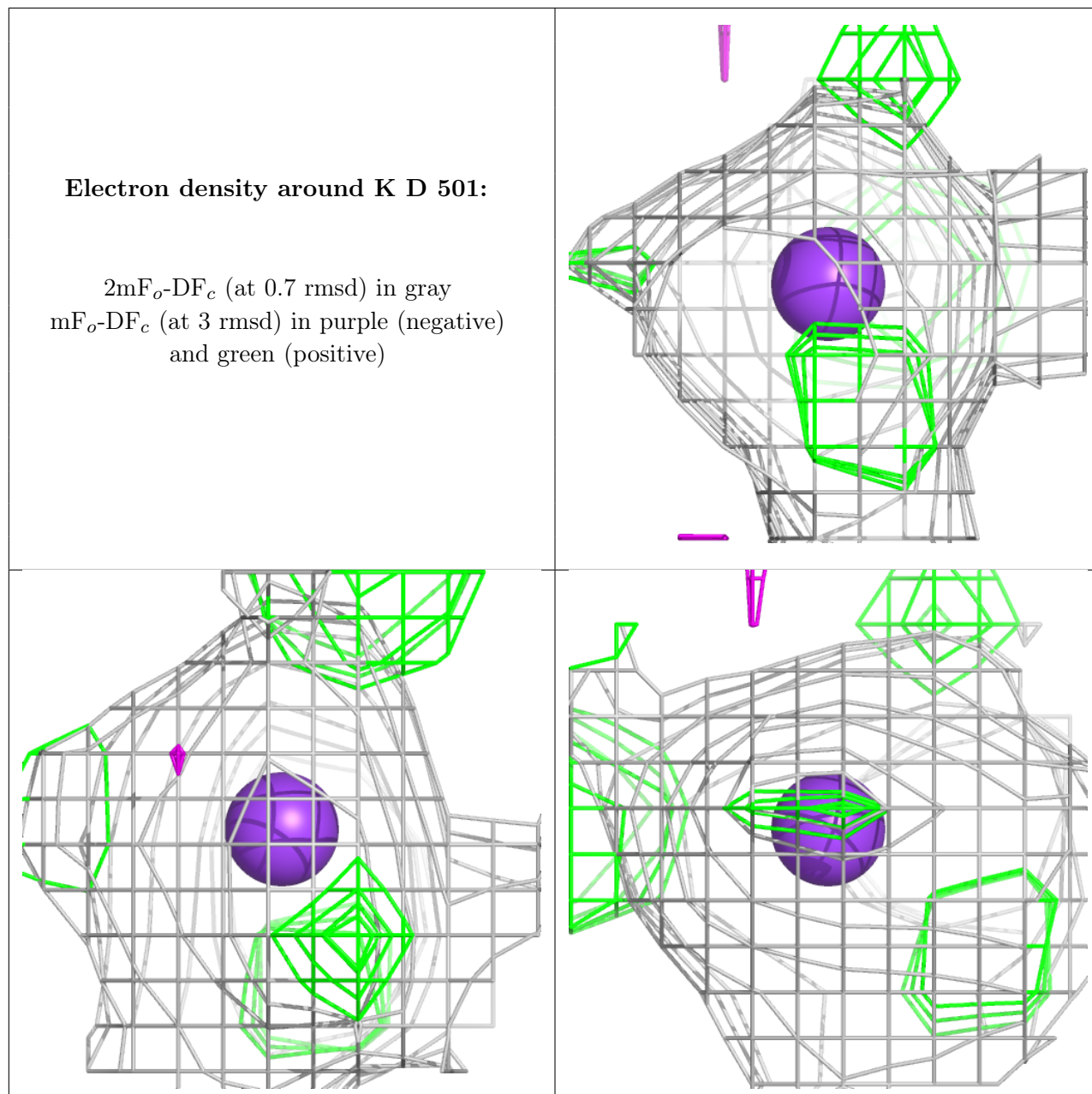
Electron density around K A 506:

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



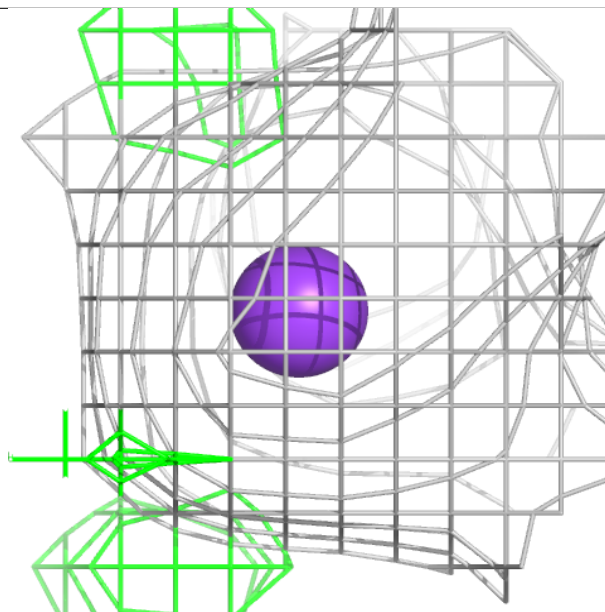
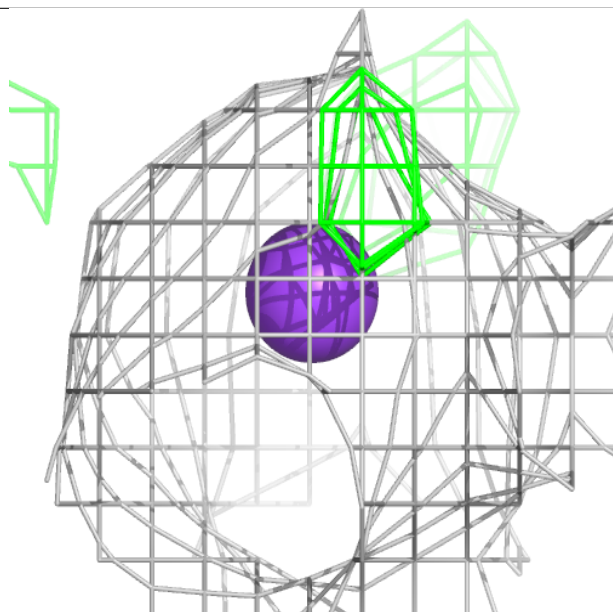
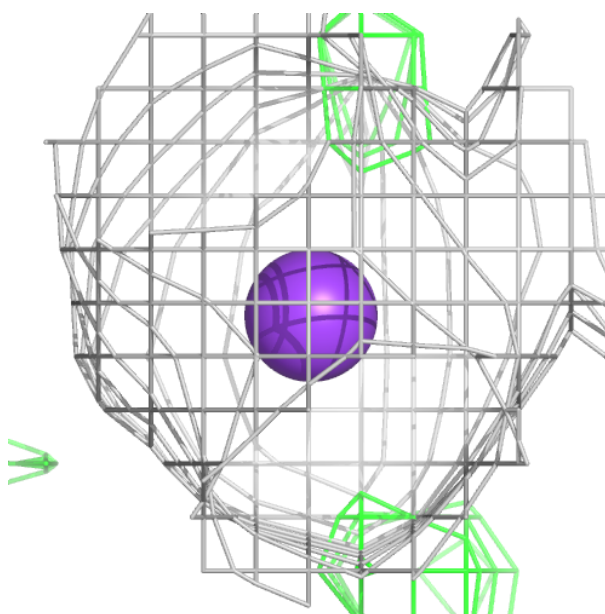
Electron density around K D 501:

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



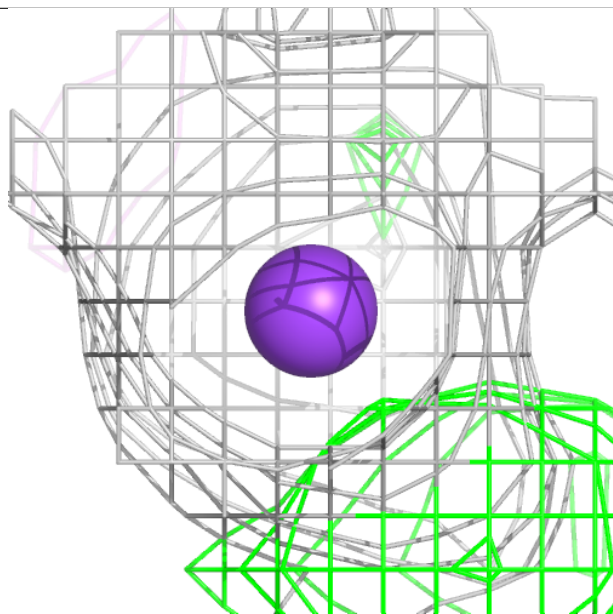
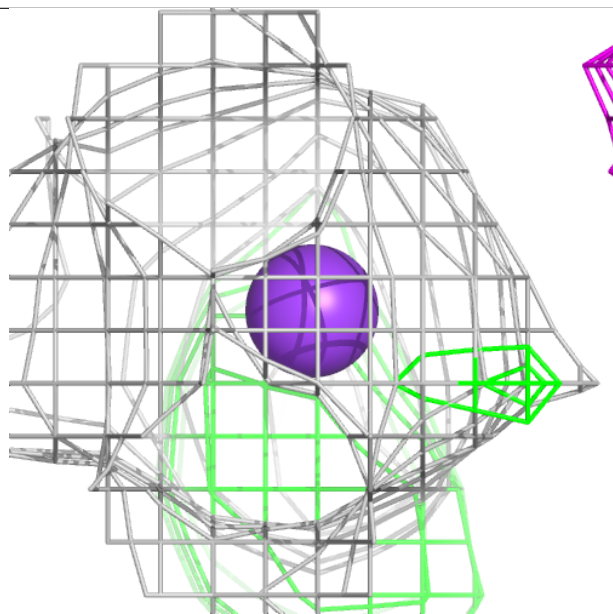
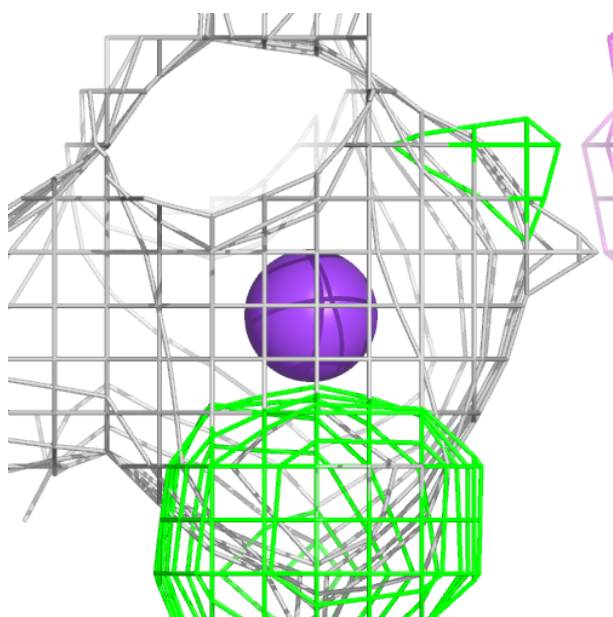
Electron density around K E 502:

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



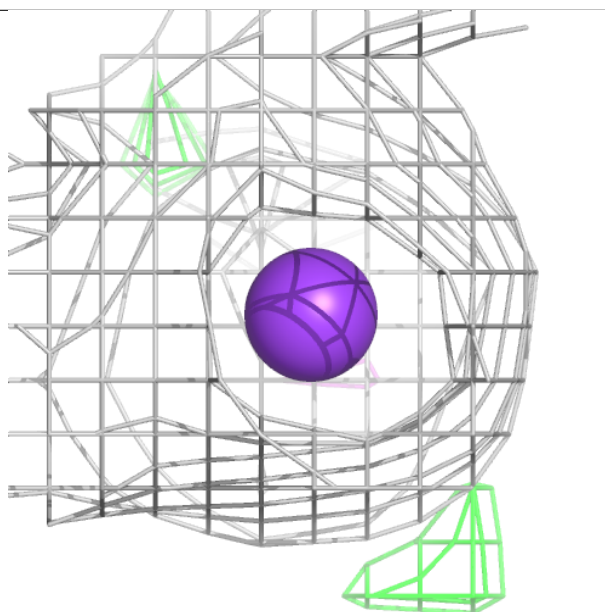
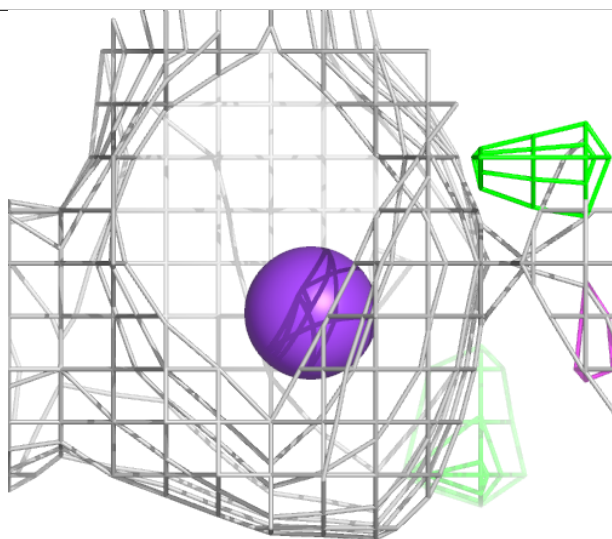
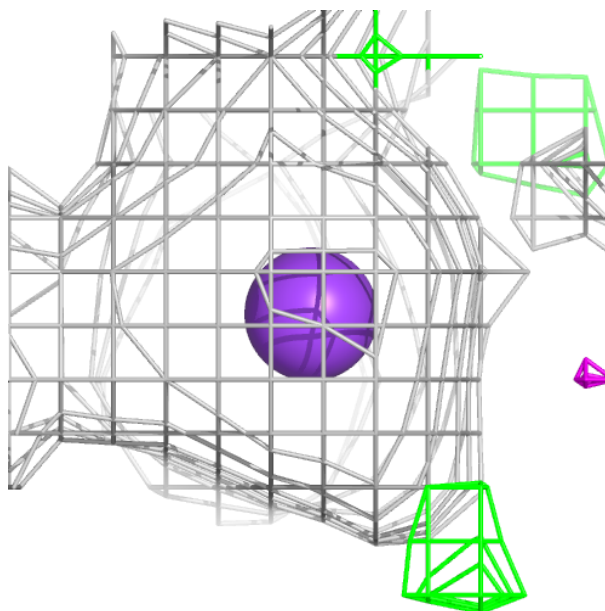
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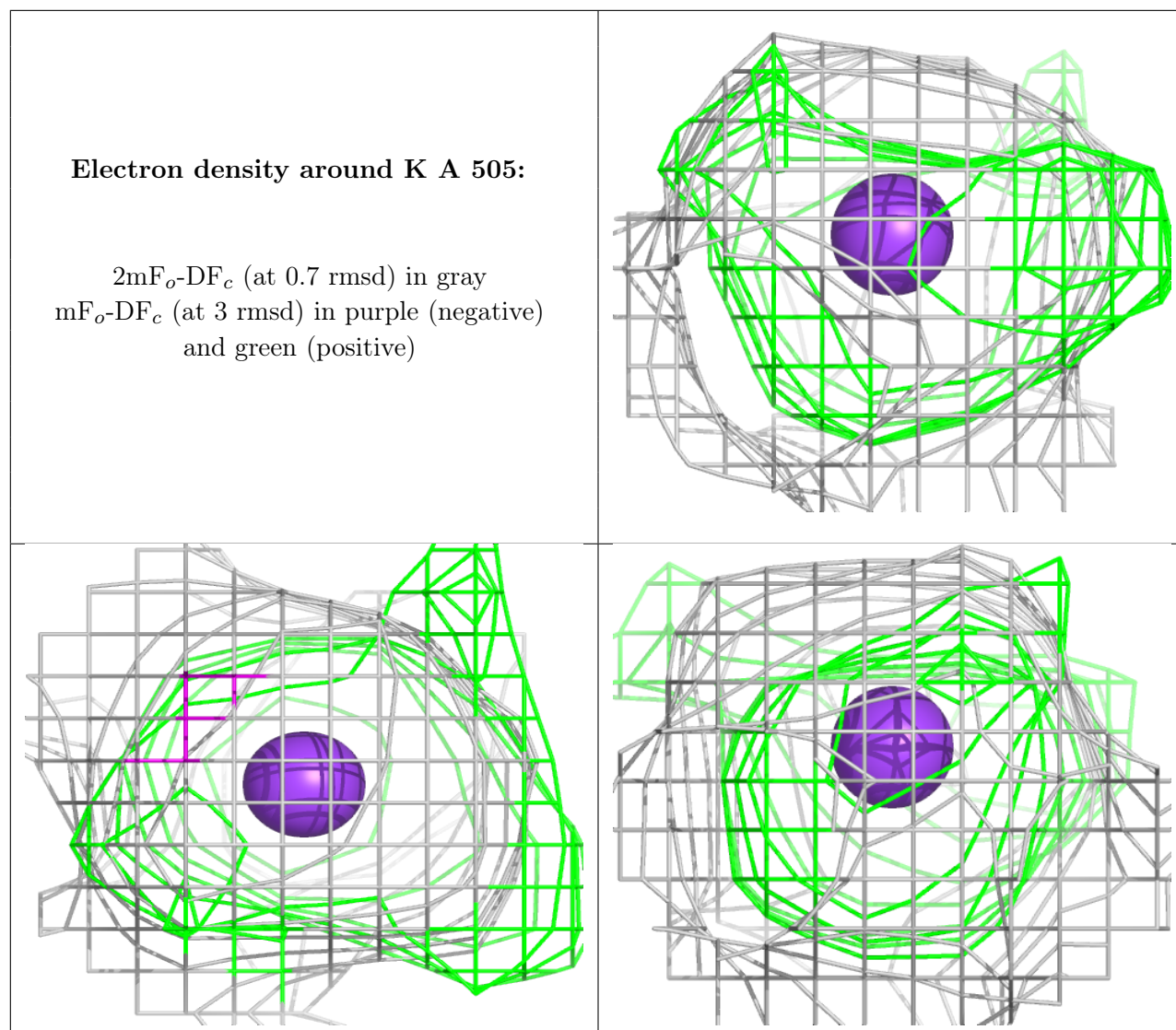
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.