Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2023 – 12:41 AM EDT

PDB ID	:	4RKD
Title	:	Psychrophilic aromatic amino acids aminotransferase from Psychrobacter sp. B6 cocrystalized with aspartic acid
Authors	:	Bujacz, A.; Rutkiewicz-Krotewicz, M.; Bujacz, G.; Nowakowska-Sapota, K.; Turkiewicz, M.
Deposited on	:	2014-10-12
Resolution	:	2.76 Å(reported)

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

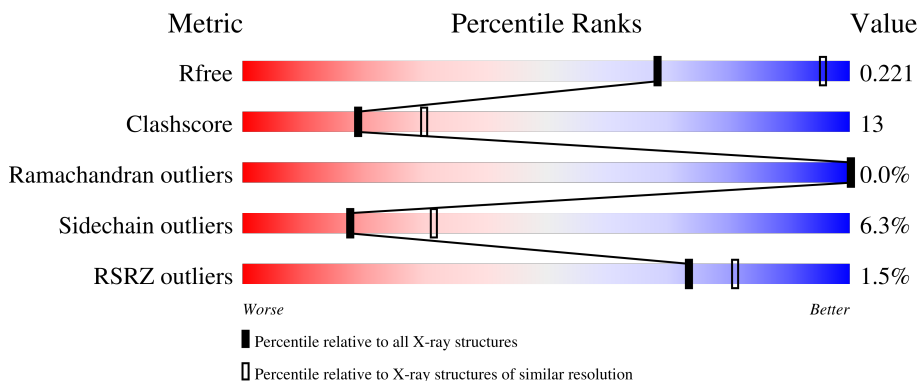|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

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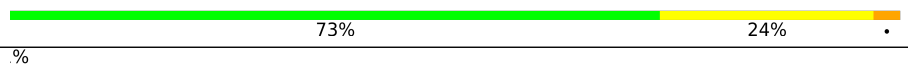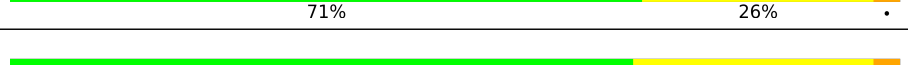*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.76 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	Percentile Ranks	Value
Rfree		0.221
Clashscore		13
Ramachandran outliers		0.0%
Sidechain outliers		6.3%
RSRZ outliers		1.5%

Worse ... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	398	5% 73% 25% •
1	B	398	73% 24% •
1	C	398	% 71% 26% •
1	D	398	70% 27% •

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	398	2% ■ / 70% / 29% •
1	F	398	% ■ / 76% / 21% •
1	G	398	3% ■ / 67% / 31% •
1	H	398	79% / 20% •

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
4	KET	E	404[B]	-	-	X	-
6	PMP	D	401	-	-	X	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 25951 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 Aromatic amino acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total 3115	C 1981	N 520	O 592	S 22	0	2	0
1	B	398	Total 3137	C 1994	N 524	O 597	S 22	0	5	0
1	C	398	Total 3110	C 1977	N 516	O 595	S 22	0	2	0
1	D	398	Total 3101	C 1971	N 516	O 592	S 22	0	0	0
1	E	398	Total 3121	C 1985	N 520	O 594	S 22	0	3	0
1	F	398	Total 3118	C 1981	N 517	O 598	S 22	0	3	0
1	G	398	Total 3117	C 1981	N 522	O 592	S 22	0	2	0
1	H	398	Total 3113	C 1979	N 518	O 594	S 22	0	2	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0
2	G	1	Total 1	Mg 1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).

PLP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	E	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDI N-4-YLMETHYLENE)-AMINO]-SUCCINIC ACID (three-letter code: KET) (formula: $C_{12}H_{16}N_2O_9P$).

KET
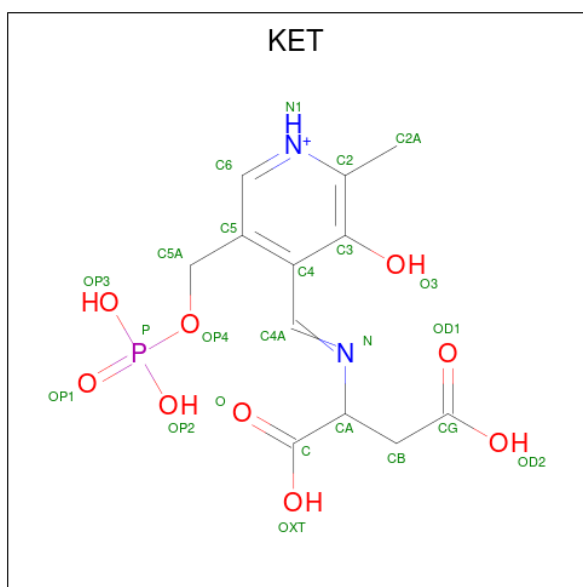
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			24	12	2	9	1		
4	E	1	Total	C	N	O	P	0	1
			24	12	2	9	1		
4	G	1	Total	C	N	O	P	0	0
			24	12	2	9	1		

- Molecule 5 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).

OAA
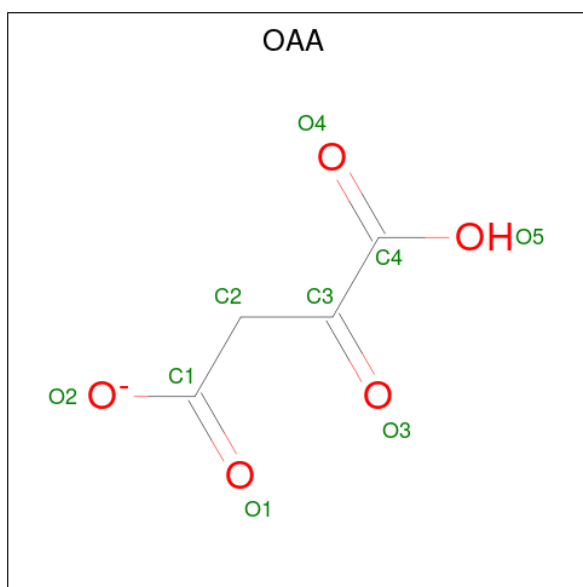
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			9	4	5		

Continued on next page...

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total　C　O 9　　4　5			0	0

- Molecule 6 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).
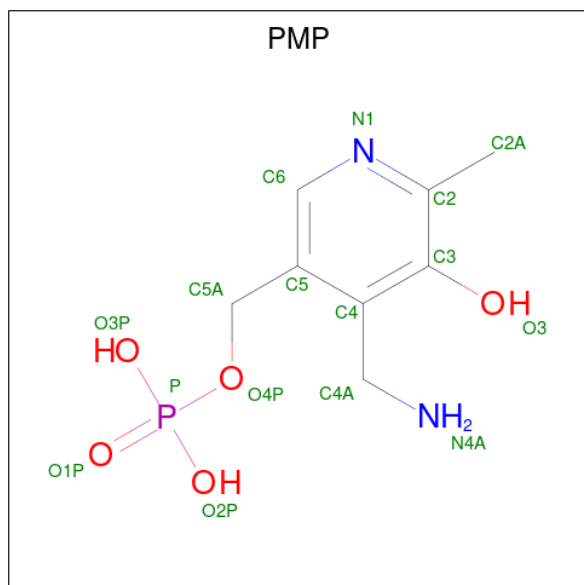
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total 16	C 8	N 2	O 5	P 1	0	0
6	H	1	Total 16	C 8	N 2	O 5	P 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	102	Total 102	O 102	0	0
7	B	142	Total 142	O 142	0	0
7	C	83	Total 83	O 83	0	0
7	D	119	Total 119	O 119	0	0
7	E	84	Total 84	O 84	0	0
7	F	96	Total 96	O 96	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	70	Total 70	O 70	0	0
7	H	122	Total 122	O 122	0	0

3 Residue-property plots ⓘ

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: Aromatic amino acid aminotransferase
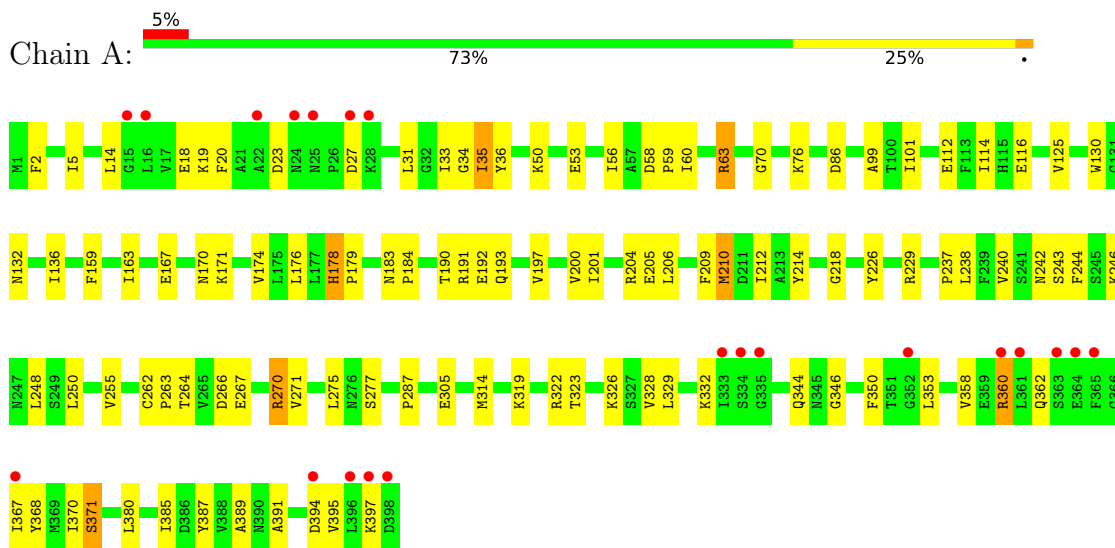
Chain A:

• Molecule 1: Aromatic amino acid aminotransferase

Chain B:

• Molecule 1: Aromatic amino acid aminotransferase

Chain C:

• Molecule 1: Aromatic amino acid aminotransferase

Chain D:

• Molecule 1: Aromatic amino acid aminotransferase

Chain E:
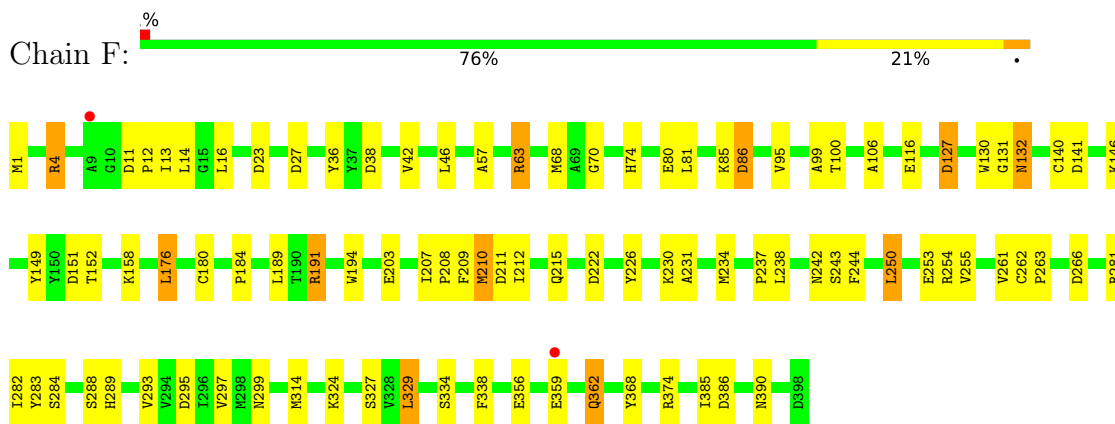
• Molecule 1: Aromatic amino acid aminotransferase

Chain F: 76%   21%

• Molecule 1: Aromatic amino acid aminotransferase

Chain G: 67%   31%

• Molecule 1: Aromatic amino acid aminotransferase
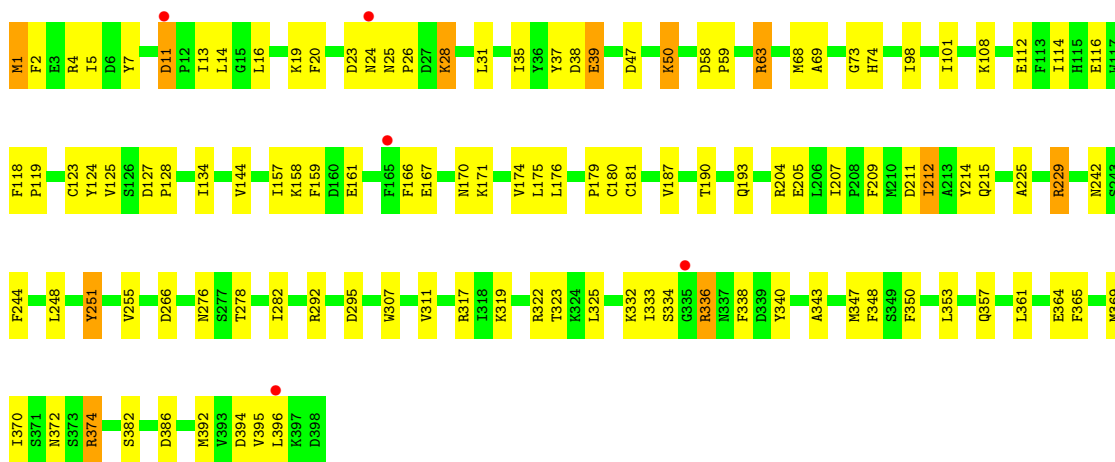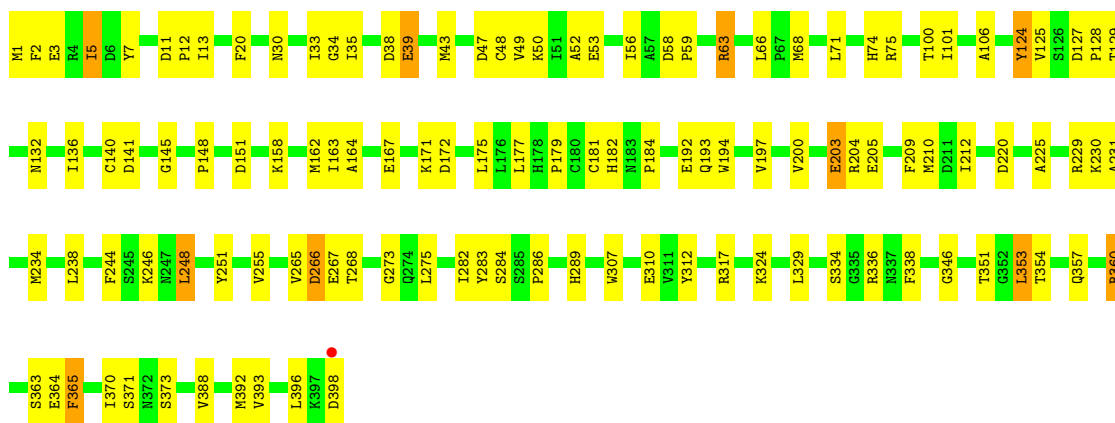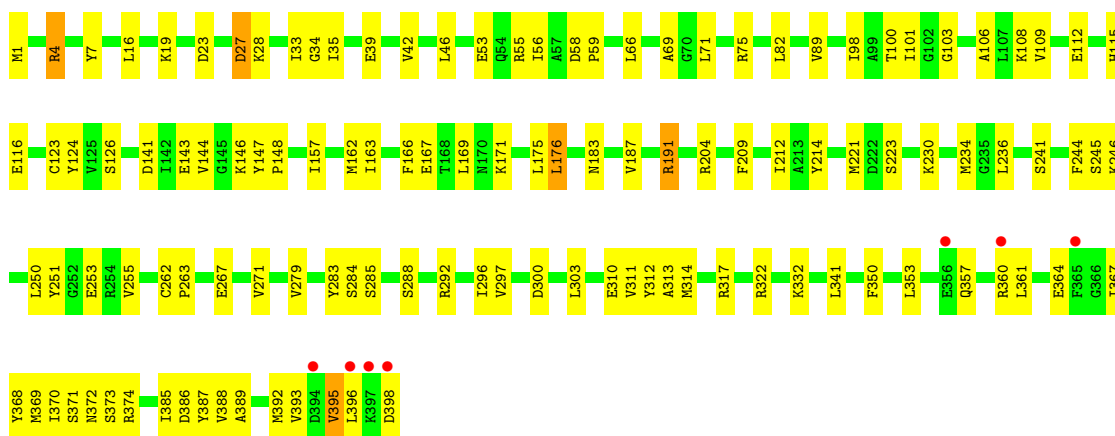

Chain H: 79%   20%
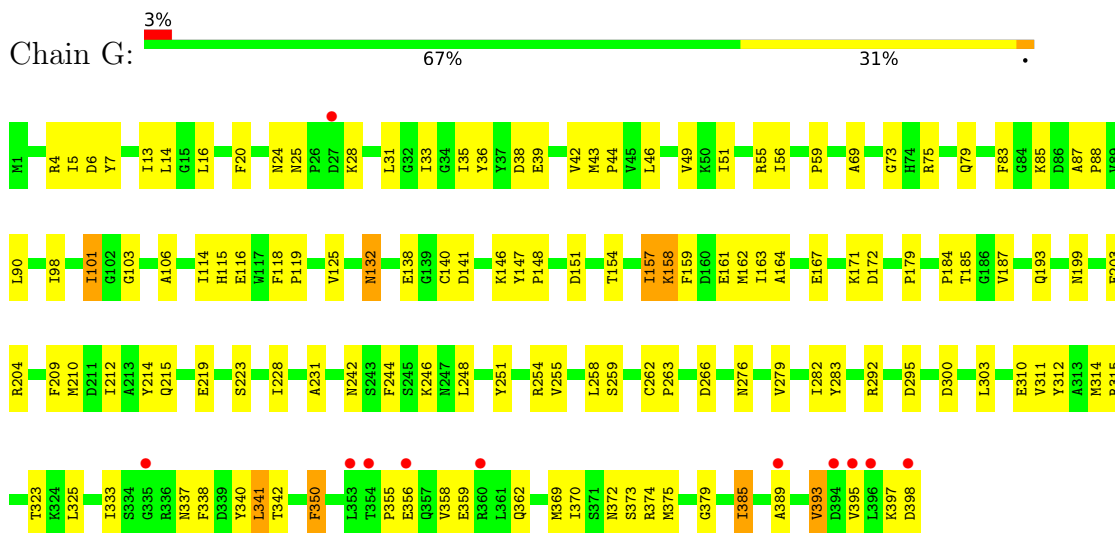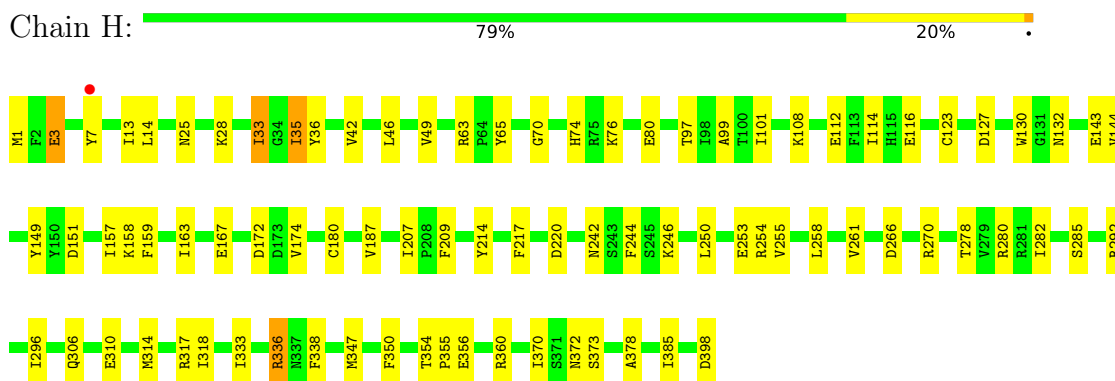
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.25Å 103.23Å 165.78Å 90.00° 98.58° 90.00°	Depositor
Resolution (Å)	45.74 – 2.76 45.61 – 2.76	Depositor EDS
% Data completeness (in resolution range)	97.4 (45.74-2.76) 97.4 (45.61-2.76)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.173 , 0.222 0.173 , 0.221	Depositor DCC
R_{free} test set	3862 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	25951	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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 43.05 % 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 1.8670e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[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: PMP, PLP, OAA, MG, KET

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.84	0/3190	0.97	3/4321 (0.1%)
1	B	0.92	0/3218	1.01	2/4358 (0.0%)
1	C	0.82	0/3185	0.97	4/4316 (0.1%)
1	D	0.98	1/3170 (0.0%)	1.04	3/4296 (0.1%)
1	E	0.83	0/3199	0.93	0/4333
1	F	0.88	0/3193	1.02	8/4328 (0.2%)
1	G	0.78	0/3192	0.93	1/4324 (0.0%)
1	H	0.89	0/3185	0.99	1/4315 (0.0%)
All	All	0.87	1/25532 (0.0%)	0.98	22/34591 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	124	TYR	CE1-CZ	5.30	1.45	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	254	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	C	322	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	F	38	ASP	CB-CG-OD1	5.79	123.51	118.30
1	D	63	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	270	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	F	127	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	F	329	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	C	292	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	H	254	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	157	ILE	CG1-CB-CG2	-5.63	99.01	111.40
1	G	204	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	210	MET	CA-CB-CG	-5.47	104.00	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	31	LEU	CB-CG-CD1	-5.31	101.97	111.00
1	D	248	LEU	CB-CG-CD2	5.31	120.02	111.00
1	B	248	LEU	CB-CG-CD2	5.30	120.02	111.00
1	F	281	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	211	ASP	CB-CG-OD1	5.19	122.97	118.30
1	F	222	ASP	CB-CG-OD1	5.18	122.96	118.30
1	F	176	LEU	CA-CB-CG	-5.15	103.46	115.30
1	A	35	ILE	CG1-CB-CG2	-5.14	100.09	111.40
1	F	254	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	351	THR	CA-CB-CG2	-5.02	105.37	112.40

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	3115	0	3059	85	0
1	B	3137	0	3081	91	0
1	C	3110	0	3044	87	0
1	D	3101	0	3036	92	0
1	E	3121	0	3065	104	0
1	F	3118	0	3047	60	0
1	G	3117	0	3062	94	0
1	H	3113	0	3053	58	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
3	A	15	0	7	1	0
3	B	15	0	6	1	0
3	C	15	0	7	1	0
3	E	15	0	6	1	0
3	F	15	0	6	2	0
4	A	24	0	12	5	0
4	E	24	0	11	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	24	0	12	3	0
5	C	9	0	2	1	0
5	E	9	0	2	0	0
6	D	16	0	11	8	0
6	H	16	0	11	4	0
7	A	102	0	0	5	0
7	B	142	0	0	16	0
7	C	83	0	0	6	0
7	D	119	0	0	5	0
7	E	84	0	0	13	0
7	F	96	0	0	4	0
7	G	70	0	0	5	0
7	H	122	0	0	5	0
All	All	25951	0	24540	646	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 13.

All (646) 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:D:246:LYS:HE3	6:D:401:PMP:N4A	1.44	1.29
1:D:246:LYS:CE	6:D:401:PMP:HNA2	1.56	1.17
1:D:33:ILE:HG13	1:D:35:ILE:HG12	1.37	1.07
1:C:11:ASP:HB2	1:C:14:LEU:HB2	1.32	1.06
1:E:39:GLU:HG2	1:E:317:ARG:HD2	1.38	1.05
1:G:13:ILE:HD12	1:G:14:LEU:H	1.16	1.04
1:F:210:MET:HG3	1:F:238:LEU:HD11	1.40	1.01
1:C:11:ASP:CB	1:C:14:LEU:HB2	1.97	0.95
5:C:403:OAA:H22	6:D:401:PMP:H4A1	1.50	0.94
1:A:167:GLU:HB3	1:A:204:ARG:HH12	1.28	0.94
1:G:246:LYS:HZ1	4:G:402:KET:H4A	1.30	0.92
1:E:221:MET:HB2	7:E:532:HOH:O	1.71	0.89
1:E:191:ARG:HG3	1:E:191:ARG:HH11	1.37	0.89
1:G:246:LYS:NZ	4:G:402:KET:H4A	1.88	0.88
1:A:244:PHE:HB2	1:A:255:VAL:HG23	1.56	0.87
1:D:246:LYS:NZ	6:D:401:PMP:HNA2	1.72	0.87
1:C:23:ASP:O	1:C:28:LYS:HE3	1.74	0.86
1:D:246:LYS:CE	6:D:401:PMP:N4A	2.25	0.86
1:B:64:PRO:HA	7:B:606:HOH:O	1.74	0.86
1:E:39:GLU:HG2	1:E:317:ARG:CD	2.04	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:ILE:HD12	1:G:187:VAL:HG12	1.58	0.85
1:C:190:THR:OG1	1:C:193:GLN:HG3	1.77	0.85
1:C:357:GLN:HE22	1:C:396:LEU:HA	1.40	0.85
1:B:2:PHE:O	1:B:5:ILE:HG12	1.78	0.84
1:A:33:ILE:HD12	1:A:34:GLY:H	1.41	0.84
1:E:4:ARG:HB2	7:E:501:HOH:O	1.77	0.83
1:H:246:LYS:HE2	6:H:401:PMP:H4A2	1.60	0.83
1:G:157:ILE:CD1	1:G:187:VAL:HG12	2.09	0.82
1:B:119:PRO:HB3	7:B:566:HOH:O	1.77	0.82
1:B:132:ASN:O	1:B:136:ILE:HG13	1.79	0.82
1:E:157:ILE:CD1	1:E:187:VAL:HG12	2.10	0.81
1:G:157:ILE:HD12	1:G:187:VAL:CG1	2.10	0.81
1:G:13:ILE:CD1	1:G:14:LEU:H	1.94	0.81
1:A:190:THR:OG1	1:A:193:GLN:HG3	1.81	0.80
1:D:39:GLU:CD	1:D:39:GLU:H	1.83	0.80
1:F:11[A]:ASP:OD1	1:F:12:PRO:HD2	1.81	0.80
1:A:167:GLU:HB3	1:A:204:ARG:NH1	1.95	0.80
1:G:246:LYS:HD3	1:G:251:TYR:HE1	1.45	0.79
1:C:353:LEU:HD11	1:C:361:LEU:HD12	1.64	0.79
1:B:192[A]:GLU:HG2	7:B:543:HOH:O	1.82	0.79
1:G:13:ILE:HD12	1:G:14:LEU:N	1.94	0.79
1:A:167:GLU:HA	1:A:204:ARG:HH11	1.47	0.78
1:G:246:LYS:HD3	1:G:251:TYR:CE1	2.18	0.78
1:F:95:VAL:HG22	1:F:261:VAL:HG22	1.64	0.77
1:D:167:GLU:HA	1:D:167:GLU:OE1	1.85	0.76
1:G:159:PHE:CE2	1:G:193:GLN:HG2	2.20	0.76
1:G:355:PRO:O	1:G:359:GLU:HG3	1.85	0.75
1:B:64:PRO:CA	7:B:606:HOH:O	2.32	0.75
1:A:14:LEU:HD22	7:A:586:HOH:O	1.85	0.74
1:D:246:LYS:HE3	6:D:401:PMP:HNA2	1.04	0.74
1:G:151:ASP:HB2	1:G:158:LYS:HG2	1.68	0.74
1:E:191:ARG:HH11	1:E:191:ARG:CG	2.01	0.73
1:C:174:VAL:HG22	1:C:207:ILE:HB	1.70	0.73
1:C:112:GLU:OE1	1:C:112:GLU:HA	1.88	0.73
1:B:389:ALA:O	1:B:393:VAL:HG23	1.89	0.73
1:C:357:GLN:NE2	1:C:396:LEU:HA	2.03	0.73
1:E:244:PHE:HB2	1:E:255:VAL:HG23	1.70	0.72
1:F:210:MET:CG	1:F:238:LEU:HD11	2.17	0.72
1:G:106:ALA:HB1	1:G:258:LEU:HB2	1.71	0.72
1:A:163:ILE:O	1:A:167:GLU:HG2	1.89	0.72
1:C:11:ASP:HB2	1:C:14:LEU:CB	2.17	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:LYS:O	1:D:172:ASP:HB2	1.90	0.71
1:D:360:ARG:NH2	1:D:364:GLU:OE2	2.23	0.71
1:H:33:ILE:HB	1:H:35:ILE:HD13	1.72	0.71
1:B:157:ILE:HD13	1:B:187:VAL:CG1	2.20	0.71
1:E:4:ARG:HG2	7:E:584:HOH:O	1.91	0.71
1:B:244:PHE:HB2	1:B:255:VAL:HG23	1.71	0.70
1:C:63:ARG:NH2	1:D:53:GLU:OE1	2.23	0.70
1:D:33:ILE:CG1	1:D:35:ILE:HG12	2.21	0.69
1:B:244:PHE:HB2	1:B:255:VAL:CG2	2.22	0.69
1:H:336:ARG:HD2	1:H:338:PHE:CZ	2.27	0.69
1:A:2:PHE:HB3	1:A:5:ILE:HG13	1.74	0.69
1:B:157:ILE:HD13	1:B:187:VAL:HG11	1.74	0.69
1:C:38:ASP:HB2	1:C:39:GLU:OE1	1.93	0.69
1:G:13:ILE:CD1	1:G:14:LEU:N	2.55	0.69
1:D:360:ARG:HG2	1:D:360:ARG:HH21	1.57	0.68
1:F:244:PHE:HB2	1:F:255:VAL:HG23	1.74	0.68
1:E:148:PRO:HG2	1:E:162:MET:HA	1.75	0.68
1:G:246:LYS:CD	1:G:251:TYR:HE1	2.06	0.68
1:E:157:ILE:CD1	1:E:187:VAL:CG1	2.72	0.67
1:A:33:ILE:CD1	1:A:34:GLY:H	2.07	0.67
1:C:25:ASN:OD1	1:C:26:PRO:HD2	1.93	0.67
1:B:220:ASP:OD2	1:B:223:SER:HB2	1.95	0.67
1:B:140:CYS:O	1:B:141:ASP:HB2	1.95	0.67
1:A:101:ILE:HD13	1:B:101:ILE:HD12	1.77	0.66
1:G:101:ILE:HD12	1:H:101:ILE:HD13	1.77	0.66
1:E:157:ILE:HD11	1:E:187:VAL:HG12	1.77	0.66
1:C:179:PRO:HG2	1:C:212:ILE:HB	1.76	0.66
1:E:53:GLU:OE2	1:F:63:ARG:NH1	2.29	0.65
1:E:246[B]:LYS:HE2	4:E:404[B]:KET:N	2.11	0.65
1:A:167:GLU:CA	1:A:204:ARG:HH11	2.10	0.64
1:A:197:VAL:HG12	1:A:201:ILE:HD12	1.78	0.64
1:B:17:VAL:HG13	7:B:554:HOH:O	1.96	0.64
1:E:112:GLU:HA	1:E:112:GLU:OE1	1.97	0.64
1:G:370:ILE:HG13	7:G:552:HOH:O	1.95	0.64
1:E:27:ASP:O	1:E:387:TYR:HE2	1.81	0.64
1:G:311:VAL:HA	1:G:314:MET:HE3	1.79	0.64
1:G:358:VAL:HG12	7:G:545:HOH:O	1.96	0.64
1:H:28:LYS:HE2	7:H:561:HOH:O	1.98	0.64
1:A:53:GLU:HA	1:A:56:ILE:HD12	1.79	0.64
1:G:219:GLU:HG2	1:G:223:SER:CB	2.27	0.64
1:C:370:ILE:N	1:C:370:ILE:HD13	2.12	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:ASP:O	1:E:387:TYR:CE2	2.51	0.63
1:H:246:LYS:HE2	6:H:401:PMP:C4A	2.28	0.63
1:A:171:LYS:HG3	1:A:205:GLU:HB2	1.79	0.63
1:G:214:TYR:CE1	1:G:246:LYS:HG3	2.34	0.63
1:A:370:ILE:N	1:A:370:ILE:HD13	2.14	0.63
1:B:120:GLN:HB2	7:B:628:HOH:O	1.99	0.62
1:A:112:GLU:OE1	1:A:112:GLU:HA	1.97	0.62
1:A:328:VAL:O	1:A:332:LYS:HG3	2.00	0.62
1:C:353:LEU:HD11	1:C:361:LEU:CD1	2.29	0.62
1:B:4[A]:ARG:HH11	1:B:4[A]:ARG:HB3	1.64	0.62
1:A:237:PRO:HB3	1:B:1:MET:HG2	1.82	0.62
1:B:322:ARG:HD3	1:B:341:LEU:O	2.00	0.62
1:E:33:ILE:HD12	1:E:34:GLY:H	1.65	0.62
1:E:367:ILE:HG12	1:E:388:VAL:HG22	1.82	0.62
7:C:506:HOH:O	1:D:289:HIS:HB2	1.99	0.62
1:D:38:ASP:HB2	1:D:39:GLU:OE1	2.00	0.61
1:B:157:ILE:CD1	1:B:187:VAL:CG1	2.77	0.61
1:A:59:PRO:HA	7:A:567:HOH:O	1.99	0.61
1:H:151:ASP:HB2	1:H:158:LYS:HG2	1.82	0.61
1:B:46:LEU:HD21	1:B:314:MET:CE	2.30	0.61
1:D:246:LYS:HZ1	6:D:401:PMP:HNA2	1.44	0.61
1:G:199:ASN:O	1:G:203:GLU:HG3	2.00	0.61
1:E:246[B]:LYS:HE2	4:E:404[B]:KET:C4A	2.30	0.61
1:E:360[B]:ARG:HE	1:E:395:VAL:HG23	1.64	0.61
1:A:63:ARG:NH2	1:B:53:GLU:OE1	2.25	0.60
1:A:319:LYS:O	1:A:323:THR:HG23	2.01	0.60
1:E:148:PRO:O	1:E:162:MET:HB2	2.01	0.60
1:E:246[B]:LYS:CE	4:E:404[B]:KET:O	2.49	0.60
1:H:114:ILE:HD13	1:H:174:VAL:HG21	1.84	0.60
1:B:157:ILE:CD1	1:B:187:VAL:HG12	2.32	0.60
1:G:325:LEU:HD12	1:G:389:ALA:HB2	1.83	0.60
1:C:101:ILE:HD13	1:D:101:ILE:HD12	1.84	0.59
1:A:191:ARG:HD3	1:A:226:TYR:CE1	2.37	0.59
1:B:64:PRO:CB	7:B:606:HOH:O	2.50	0.59
1:F:211:ASP:OD2	3:F:401:PLP:N1	2.36	0.59
1:G:7:TYR:OH	1:H:266:ASP:OD1	2.20	0.59
1:B:46:LEU:HD21	1:B:314:MET:HE1	1.85	0.59
1:E:246[B]:LYS:HZ3	4:E:404[B]:KET:CA	2.16	0.59
1:C:2:PHE:HB3	1:C:5:ILE:HD12	1.83	0.59
1:B:360:ARG:NH1	1:B:395:VAL:HA	2.18	0.58
1:D:193:GLN:O	1:D:197:VAL:HG23	2.04	0.58

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:CB	1:A:204:ARG:NH1	2.65	0.58
1:C:212:ILE:HG23	1:C:212:ILE:O	2.03	0.58
1:E:66:LEU:CD1	1:E:288:SER:HB2	2.32	0.58
1:D:230:LYS:O	1:D:234:MET:HG3	2.04	0.58
1:E:322:ARG:HD3	1:E:341:LEU:O	2.03	0.58
1:A:218:GLY:O	1:A:319:LYS:NZ	2.37	0.58
1:C:353:LEU:HD22	1:C:357:GLN:HB3	1.86	0.58
1:D:39:GLU:HG3	1:D:317:ARG:HD2	1.86	0.58
1:E:357:GLN:NE2	1:E:396:LEU:HA	2.19	0.58
1:G:184:PRO:HB3	1:G:374:ARG:HD3	1.84	0.58
1:F:130:TRP:CH2	1:F:132:ASN:HB3	2.39	0.58
1:H:76:LYS:O	1:H:80:GLU:HG3	2.04	0.58
1:D:124:TYR:HA	1:D:145:GLY:O	2.03	0.58
1:F:230:LYS:O	1:F:234:MET:HG3	2.04	0.58
1:A:19:LYS:HD3	1:A:368:TYR:HE2	1.68	0.57
1:D:184:PRO:HG3	7:D:578:HOH:O	2.03	0.57
1:E:246[B]:LYS:NZ	4:E:404[B]:KET:N	2.52	0.57
1:G:140:CYS:O	1:G:141:ASP:HB2	2.03	0.57
1:G:340:TYR:CE1	1:G:341:LEU:HD23	2.39	0.57
1:B:196:THR:HA	7:B:550:HOH:O	2.05	0.57
1:F:151:ASP:HB2	1:F:158:LYS:HG2	1.86	0.57
1:C:16:LEU:HA	1:C:19:LYS:HB3	1.86	0.57
1:C:124:TYR:HB2	1:C:175:LEU:CD2	2.34	0.57
1:C:158:LYS:HB3	1:C:161[B]:GLU:HB2	1.85	0.57
1:G:56:ILE:HD11	1:G:292:ARG:HB2	1.86	0.57
1:E:300:ASP:HB3	1:E:303:LEU:HB2	1.87	0.57
1:G:333:ILE:HG12	1:G:397:LYS:HD3	1.87	0.57
1:H:36:TYR:CZ	1:H:314:MET:HG2	2.39	0.57
1:A:159:PHE:CE2	1:A:193:GLN:HB3	2.40	0.57
1:A:167:GLU:CA	1:A:204:ARG:NH1	2.68	0.57
1:D:329:LEU:HD12	1:D:393:VAL:HG23	1.87	0.56
1:E:372:ASN:O	1:E:373:SER:OG	2.16	0.56
7:G:567:HOH:O	1:H:132:ASN:HB2	2.05	0.56
1:B:220:ASP:OD2	1:B:223:SER:CB	2.52	0.56
1:G:310:GLU:O	1:G:314:MET:HE3	2.04	0.56
1:E:370:ILE:HD13	1:E:370:ILE:N	2.20	0.56
1:G:87:ALA:HB1	1:G:88:PRO:HD2	1.87	0.56
1:H:296:ILE:HA	7:H:588:HOH:O	2.06	0.56
1:A:322:ARG:NH1	1:A:346:GLY:O	2.39	0.56
1:E:46:LEU:HD21	1:E:314:MET:CE	2.36	0.56
1:G:75:ARG:O	1:G:79:GLN:HG3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PRO:HG2	1:A:212:ILE:HB	1.87	0.56
1:C:353:LEU:HD23	1:C:396:LEU:HD21	1.87	0.56
1:A:167:GLU:HA	1:A:204:ARG:NH1	2.20	0.56
1:C:16:LEU:O	1:C:20:PHE:N	2.38	0.56
1:G:163:ILE:O	1:G:167:GLU:HG2	2.06	0.56
1:A:246[B]:LYS:NZ	4:A:403[B]:KET:O	2.25	0.55
1:C:35:ILE:HG12	1:C:251:TYR:CE1	2.41	0.55
1:D:171:LYS:HD2	1:D:205:GLU:OE1	2.06	0.55
1:D:273:GLY:HA3	7:D:582:HOH:O	2.07	0.55
1:E:176:LEU:HB3	7:E:508:HOH:O	2.06	0.55
1:E:389:ALA:O	1:E:393:VAL:HG23	2.06	0.55
1:A:244:PHE:HB3	1:A:248:LEU:HD12	1.89	0.55
1:E:1:MET:HG2	1:F:237:PRO:HB3	1.87	0.55
1:A:326:LYS:CE	7:A:580:HOH:O	2.53	0.55
1:G:103:GLY:N	4:G:402:KET:OP1	2.40	0.55
1:G:148:PRO:O	1:G:162:MET:HB2	2.05	0.55
1:G:258:LEU:HD12	1:G:259:SER:H	1.71	0.55
1:C:244:PHE:HB3	1:C:248:LEU:HD12	1.89	0.55
1:G:159:PHE:O	1:G:163:ILE:HG12	2.07	0.55
1:G:369:MET:HG2	1:G:375:MET:HB2	1.89	0.55
1:B:357:GLN:HB3	1:B:395:VAL:CG1	2.36	0.54
1:E:55:ARG:NH1	7:E:517:HOH:O	2.26	0.54
1:E:245:SER:HB3	1:E:251:TYR:HA	1.89	0.54
1:E:246[B]:LYS:NZ	4:E:404[B]:KET:CA	2.70	0.54
1:A:367:ILE:CD1	1:A:391:ALA:CB	2.85	0.54
1:B:10:GLY:HA2	7:B:598:HOH:O	2.06	0.54
1:C:134:ILE:HG12	1:C:144:VAL:HG11	1.89	0.54
1:E:53:GLU:CD	1:F:63:ARG:HH12	2.09	0.54
1:G:266:ASP:OD1	1:H:7:TYR:OH	2.22	0.54
1:B:184:PRO:HB2	1:B:350:PHE:HE2	1.72	0.54
1:C:69:ALA:CB	1:C:98:ILE:HG22	2.37	0.54
1:F:127:ASP:O	1:F:149:TYR:HB3	2.08	0.54
1:C:73:GLY:HA3	1:C:295:ASP:OD1	2.08	0.54
1:D:265:VAL:O	1:D:268:THR:HB	2.08	0.54
1:E:253:GLU:OE1	1:F:63:ARG:HD2	2.08	0.54
1:G:69:ALA:CB	1:G:98:ILE:HG22	2.38	0.54
1:E:191:ARG:HG3	1:E:191:ARG:NH1	2.16	0.54
1:G:69:ALA:O	1:G:75:ARG:HD2	2.07	0.53
1:G:312:TYR:HB3	1:G:315:ARG:NH2	2.22	0.53
1:B:184:PRO:HB2	1:B:350:PHE:CE2	2.43	0.53
1:D:52:ALA:O	1:D:56:ILE:HG13	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246[B]:LYS:CE	4:E:404[B]:KET:N	2.72	0.53
1:H:255:VAL:HG12	7:H:621:HOH:O	2.08	0.53
1:G:244:PHE:O	1:G:248:LEU:HB2	2.08	0.53
1:D:192:GLU:CD	1:D:192:GLU:H	2.11	0.53
1:A:362:GLN:HB3	1:A:368:TYR:CZ	2.44	0.53
1:C:125:VAL:HG12	1:C:176:LEU:HD23	1.91	0.53
7:E:577:HOH:O	1:F:1:MET:HE1	2.09	0.53
1:G:5:ILE:O	1:H:270:ARG:HD3	2.08	0.53
1:B:360:ARG:NH2	1:B:364:GLU:OE2	2.42	0.53
1:D:11:ASP:OD1	1:D:12:PRO:HD2	2.08	0.53
1:D:388:VAL:O	1:D:392:MET:HG3	2.08	0.53
1:C:174:VAL:CG2	1:C:207:ILE:HB	2.38	0.53
1:A:27:ASP:HB3	1:A:387:TYR:CE2	2.44	0.53
1:B:4[A]:ARG:HB3	1:B:4[A]:ARG:NH1	2.24	0.53
1:C:180:CYS:SG	1:C:181:CYS:SG	3.05	0.53
1:E:7:TYR:OH	1:F:266:ASP:OD1	2.20	0.53
1:F:386:ASP:O	1:F:390:ASN:ND2	2.42	0.52
1:A:31:LEU:HD21	1:A:380:LEU:HD23	1.91	0.52
1:B:80:GLU:OE1	1:B:85[B]:LYS:HE2	2.09	0.52
1:E:357:GLN:HE22	1:E:396:LEU:HD23	1.74	0.52
1:B:100:THR:HB	7:B:505:HOH:O	2.09	0.52
1:D:364:GLU:HB2	1:D:365:PHE:CD2	2.44	0.52
1:E:66:LEU:HD11	1:E:288:SER:HB2	1.90	0.52
1:C:212:ILE:CD1	1:C:215:GLN:HB2	2.39	0.52
1:G:161:GLU:O	1:G:164:ALA:HB3	2.09	0.52
1:B:8:TYR:CD1	1:B:9:ALA:N	2.78	0.52
1:B:13:ILE:HG13	1:B:14:LEU:N	2.24	0.52
1:C:39:GLU:H	1:C:39:GLU:CD	2.11	0.52
1:D:164:ALA:O	1:D:167:GLU:HB2	2.10	0.52
1:E:163:ILE:O	1:E:167:GLU:HG2	2.09	0.52
1:F:212:ILE:CD1	1:F:215:GLN:HB2	2.40	0.52
1:D:360:ARG:NH2	1:D:360:ARG:HG2	2.25	0.52
1:B:157:ILE:HD13	1:B:187:VAL:HG12	1.91	0.52
1:B:315:ARG:O	1:B:319:LYS:HG3	2.09	0.52
1:C:124:TYR:HB2	1:C:175:LEU:HD23	1.92	0.52
1:D:49:VAL:O	1:D:53:GLU:HG3	2.09	0.52
1:D:181:CYS:HB3	1:D:346:GLY:HA3	1.92	0.52
1:E:183:ASN:HD22	4:E:404[B]:KET:H2A1	1.75	0.52
1:F:189:LEU:HD12	1:F:194:TRP:CZ2	2.45	0.52
1:H:70:GLY:HA3	1:H:99:ALA:HB3	1.92	0.52
1:E:246[B]:LYS:HZ3	4:E:404[B]:KET:HA	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:354:THR:HB	1:H:355:PRO:HD2	1.92	0.51
1:A:266:ASP:OD1	1:B:7:TYR:OH	2.26	0.51
1:A:19:LYS:HD3	1:A:368:TYR:CE2	2.45	0.51
1:B:21:ALA:HB2	7:B:554:HOH:O	2.11	0.51
1:C:317:ARG:HD2	7:C:535:HOH:O	2.10	0.51
1:B:64:PRO:HB3	7:B:606:HOH:O	2.11	0.51
1:E:296:ILE:HG22	1:E:297:VAL:N	2.24	0.51
1:H:333:ILE:HG22	1:H:333:ILE:O	2.09	0.51
1:H:97:THR:HA	1:H:258:LEU:O	2.10	0.51
1:H:127:ASP:O	1:H:149:TYR:HB3	2.09	0.51
1:C:157:ILE:HD11	1:C:187:VAL:HG12	1.91	0.51
1:E:191:ARG:CG	1:E:191:ARG:NH1	2.71	0.51
1:E:283:TYR:O	1:E:284:SER:HB2	2.09	0.51
1:F:130:TRP:CZ3	1:F:132:ASN:HB3	2.46	0.51
1:B:184:PRO:HG3	7:B:544:HOH:O	2.10	0.51
1:H:3:GLU:CD	1:H:3:GLU:H	2.15	0.51
1:G:333:ILE:HG22	1:G:333:ILE:O	2.11	0.50
1:D:47:ASP:N	1:D:310:GLU:OE1	2.44	0.50
1:B:371:SER:C	1:B:373:SER:H	2.14	0.50
1:E:171:LYS:HE2	7:E:563:HOH:O	2.10	0.50
1:H:372:ASN:O	1:H:373:SER:OG	2.28	0.50
1:B:360:ARG:O	1:B:364:GLU:HB2	2.10	0.50
1:C:167:GLU:HA	1:C:204:ARG:HE	1.76	0.50
1:F:329:LEU:HD23	1:F:338:PHE:CE1	2.47	0.50
1:G:31:LEU:HD13	1:G:375:MET:HG3	1.94	0.50
1:C:47:ASP:HA	1:C:50:LYS:HE2	1.93	0.50
1:C:336:ARG:HG2	1:C:338:PHE:CZ	2.46	0.50
1:D:181:CYS:HB3	7:D:508:HOH:O	2.12	0.50
1:E:360[B]:ARG:NH2	1:E:364:GLU:OE2	2.44	0.50
1:F:4:ARG:HG2	7:F:578:HOH:O	2.11	0.50
1:G:385:ILE:HG13	1:G:385:ILE:O	2.11	0.50
1:A:171:LYS:HE3	1:A:205:GLU:OE2	2.12	0.50
1:C:348:PHE:CD2	1:C:374:ARG:HD2	2.47	0.50
1:G:20:PHE:CZ	1:G:28:LYS:HG3	2.47	0.50
1:A:114:ILE:HD13	1:A:174:VAL:HG21	1.94	0.50
1:C:158:LYS:HB3	1:C:161[A]:GLU:HB2	1.93	0.50
1:C:214:TYR:N	7:C:518:HOH:O	2.43	0.50
1:G:39:GLU:CD	1:G:39:GLU:H	2.14	0.50
1:H:46:LEU:HB2	1:H:49:VAL:HG23	1.93	0.50
1:E:46:LEU:HD21	1:E:314:MET:HE1	1.94	0.49
1:C:336:ARG:CG	1:C:338:PHE:CZ	2.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:LYS:O	1:C:323:THR:HG23	2.12	0.49
1:D:39:GLU:HB3	7:D:529:HOH:O	2.11	0.49
1:H:360:ARG:HH12	1:H:398:ASP:HA	1.78	0.49
1:D:371:SER:C	1:D:373:SER:H	2.15	0.49
1:G:244:PHE:HB2	1:G:255:VAL:HG23	1.93	0.49
1:C:370:ILE:HB	1:C:372:ASN:OD1	2.11	0.49
1:G:46:LEU:O	1:G:49:VAL:N	2.38	0.49
1:H:123:CYS:O	1:H:144:VAL:HA	2.12	0.49
1:H:292:ARG:O	1:H:296:ILE:HG13	2.12	0.49
1:C:1:MET:N	1:D:267:GLU:OE1	2.46	0.49
1:F:191:ARG:HD3	7:F:568:HOH:O	2.13	0.49
1:F:250:LEU:HD13	1:F:253:GLU:HB2	1.94	0.49
1:H:130:TRP:CZ2	1:H:132:ASN:HB3	2.48	0.49
1:D:212:ILE:HG23	1:D:212:ILE:O	2.13	0.49
1:C:7:TYR:OH	1:D:266:ASP:OD2	2.27	0.49
1:E:361:LEU:HG	1:E:367:ILE:HB	1.95	0.49
1:G:159:PHE:CZ	1:G:193:GLN:HG2	2.48	0.49
1:H:13:ILE:HG12	1:H:370:ILE:HD12	1.94	0.49
1:A:243:SER:OG	4:A:403[B]:KET:OP3	2.25	0.48
1:E:221:MET:CE	1:E:311:VAL:HG11	2.43	0.48
1:F:80:GLU:OE2	1:F:85:LYS:HG3	2.13	0.48
1:H:157:ILE:HG22	1:H:159:PHE:N	2.28	0.48
1:A:130:TRP:NE1	4:A:403[B]:KET:HB2	2.28	0.48
1:E:360[B]:ARG:CZ	1:E:364:GLU:OE2	2.60	0.48
1:H:25:ASN:O	1:H:28:LYS:HG2	2.12	0.48
1:H:214:TYR:HH	6:H:401:PMP:HO3	1.60	0.48
1:D:220:ASP:HB2	1:D:312:TYR:OH	2.13	0.48
1:F:140:CYS:O	1:F:141:ASP:HB2	2.13	0.48
1:C:278:THR:O	1:C:282:ILE:HG13	2.13	0.48
1:A:125:VAL:HG12	1:A:176:LEU:HD23	1.96	0.48
1:D:231:ALA:HB3	1:D:238:LEU:HD22	1.96	0.48
1:F:68:MET:HG2	1:F:284:SER:O	2.13	0.48
1:E:279:VAL:HG13	1:E:283:TYR:CE2	2.49	0.48
1:H:217:PHE:CE1	1:H:347:MET:HE1	2.47	0.48
1:C:39:GLU:HB3	7:C:577:HOH:O	2.13	0.48
1:D:151:ASP:HB2	1:D:158:LYS:HG2	1.95	0.48
1:D:364:GLU:HB2	1:D:365:PHE:CE2	2.49	0.48
1:E:246[B]:LYS:HE3	4:E:404[B]:KET:O	2.14	0.48
1:H:306:GLN:O	1:H:310:GLU:HG3	2.14	0.48
1:B:180:CYS:SG	1:B:181:CYS:SG	3.10	0.48
1:E:392:MET:O	1:E:396:LEU:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:337:ASN:OD1	1:G:338:PHE:N	2.47	0.48
1:H:163:ILE:O	1:H:167:GLU:HG2	2.14	0.48
1:A:33:ILE:CG1	1:A:34:GLY:N	2.76	0.47
1:A:353:LEU:HB3	1:A:358:VAL:HG23	1.95	0.47
1:A:367:ILE:CD1	1:A:391:ALA:HB3	2.44	0.47
1:C:190:THR:HG1	1:C:193:GLN:HG3	1.76	0.47
1:C:225:ALA:O	1:C:229:ARG:HG3	2.14	0.47
1:D:100:THR:HG21	1:D:106:ALA:HA	1.97	0.47
1:D:171:LYS:HG3	1:D:205:GLU:HB2	1.97	0.47
1:D:282:ILE:HG22	1:D:283:TYR:HD1	1.79	0.47
1:E:353:LEU:HD21	1:E:396:LEU:HG	1.96	0.47
1:G:282:ILE:HG23	1:H:108:LYS:HG2	1.95	0.47
1:D:203:GLU:HG3	1:D:204:ARG:HG2	1.96	0.47
1:B:249:SER:HB3	7:B:525:HOH:O	2.14	0.47
1:C:20:PHE:CE1	1:C:28:LYS:HB2	2.49	0.47
1:C:69:ALA:HB1	1:C:98:ILE:HG22	1.96	0.47
3:C:402:PLP:H5A1	7:C:574:HOH:O	2.14	0.47
1:B:157:ILE:HD11	1:B:187:VAL:HG12	1.95	0.47
1:H:347:MET:HE3	1:H:347:MET:HB2	1.80	0.47
1:B:71:LEU:HA	1:B:72:PRO:HD2	1.77	0.47
1:C:212:ILE:HD13	1:C:215:GLN:HB2	1.97	0.47
1:C:244:PHE:HB2	1:C:255:VAL:HG23	1.96	0.47
1:C:251:TYR:CD2	1:C:251:TYR:N	2.80	0.47
1:D:244:PHE:O	1:D:248:LEU:HB2	2.15	0.47
1:E:16:LEU:HA	1:E:16:LEU:HD12	1.75	0.47
1:H:244:PHE:HB2	1:H:255:VAL:HG23	1.97	0.47
1:D:20:PHE:CE1	1:D:30:ASN:HB2	2.49	0.47
1:H:112:GLU:OE1	1:H:112:GLU:HA	2.15	0.47
1:D:177:LEU:HB2	1:D:210:MET:HG2	1.97	0.47
1:E:369:MET:HB3	1:E:374:ARG:O	2.14	0.47
1:H:370:ILE:HB	1:H:372:ASN:OD1	2.14	0.47
1:F:212:ILE:HD11	1:F:215:GLN:HB2	1.96	0.46
1:A:132:ASN:O	1:A:136:ILE:HG13	2.15	0.46
1:C:58:ASP:HA	1:C:59:PRO:HA	1.86	0.46
1:C:214:TYR:CD1	1:C:347:MET:HE3	2.50	0.46
1:H:46:LEU:HB2	1:H:49:VAL:CG2	2.45	0.46
1:B:157:ILE:HD13	1:B:157:ILE:N	2.31	0.46
1:D:244:PHE:HB3	1:D:248:LEU:HB2	1.96	0.46
1:G:31:LEU:HD23	1:G:379:GLY:HA3	1.96	0.46
1:G:228:ILE:O	1:G:231:ALA:HB3	2.16	0.46
1:E:157:ILE:HD12	1:E:187:VAL:HG11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ARG:HD3	1:B:5:ILE:O	2.15	0.46
1:H:278:THR:O	1:H:282:ILE:HG13	2.16	0.46
1:A:171:LYS:HG3	1:A:205:GLU:CB	2.46	0.46
1:D:71:LEU:O	1:D:75:ARG:HG3	2.15	0.46
1:A:33:ILE:HG13	1:A:34:GLY:N	2.30	0.46
1:C:357:GLN:NE2	1:C:395:VAL:O	2.41	0.46
1:F:36:TYR:CE2	1:F:314:MET:HG2	2.51	0.46
1:G:159:PHE:CD2	1:G:193:GLN:HG2	2.50	0.46
1:G:171:LYS:O	1:G:172:ASP:HB2	2.16	0.46
1:A:214:TYR:CE1	1:A:246[B]:LYS:HG2	2.51	0.46
1:G:69:ALA:HB1	1:G:98:ILE:HG22	1.97	0.46
1:A:322:ARG:HH21	1:A:344:GLN:HB2	1.81	0.46
1:A:360:ARG:HE	1:A:360:ARG:HB2	1.48	0.46
1:B:286:PRO:HG3	7:B:504:HOH:O	2.15	0.46
1:E:246[B]:LYS:NZ	4:E:404[B]:KET:HA	2.30	0.46
1:G:179:PRO:HG3	1:G:210:MET:HG2	1.98	0.46
1:G:311:VAL:HA	1:G:314:MET:CE	2.43	0.46
1:A:5:ILE:HD12	1:B:113:PHE:CZ	2.51	0.46
1:A:370:ILE:HG22	1:A:371:SER:N	2.31	0.46
1:G:38:ASP:HB2	1:G:39:GLU:OE1	2.16	0.46
1:G:79:GLN:O	1:G:83:PHE:HD2	1.99	0.46
1:H:250:LEU:HA	1:H:250:LEU:HD12	1.53	0.46
1:A:237:PRO:CB	1:B:1:MET:HG2	2.46	0.45
1:D:194:TRP:HA	1:D:194:TRP:CE3	2.51	0.45
6:D:401:PMP:H4A2	6:D:401:PMP:O4P	2.16	0.45
7:E:571:HOH:O	1:F:57:ALA:HB2	2.16	0.45
1:F:295:ASP:OD1	1:F:299:ASN:ND2	2.47	0.45
1:B:39:GLU:HB3	1:B:317:ARG:HD2	1.96	0.45
1:B:248:LEU:HD23	1:B:307:TRP:CD1	2.51	0.45
1:D:182:HIS:HE1	1:D:184:PRO:HD2	1.80	0.45
1:D:354:THR:HG23	1:D:357:GLN:OE1	2.16	0.45
1:E:123:CYS:O	1:E:144:VAL:HA	2.15	0.45
1:B:212:ILE:HG23	1:B:212:ILE:O	2.15	0.45
1:C:68:MET:HE3	1:C:276:ASN:HB3	1.99	0.45
1:C:214:TYR:HB2	7:C:518:HOH:O	2.14	0.45
1:C:361:LEU:HG	1:C:395:VAL:HG21	1.98	0.45
1:A:328:VAL:HG11	1:A:389:ALA:HB1	1.99	0.45
1:B:104:SER:OG	3:B:401:PLP:O3P	2.22	0.45
1:D:2:PHE:O	1:D:5:ILE:HB	2.17	0.45
1:D:66:LEU:HD22	1:D:286:PRO:O	2.16	0.45
1:H:149:TYR:O	1:H:157:ILE:HA	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:TYR:CE2	1:B:314:MET:HG2	2.52	0.45
1:D:365:PHE:CD2	1:D:365:PHE:N	2.84	0.45
1:G:51:ILE:O	1:G:55:ARG:HG3	2.17	0.45
1:A:163:ILE:HG23	1:A:200:VAL:HG21	1.98	0.45
1:C:266:ASP:OD1	1:D:7:TYR:OH	2.28	0.45
1:D:35:ILE:HG21	1:D:43:MET:CE	2.46	0.45
1:D:127:ASP:HA	1:D:128:PRO:HA	1.84	0.45
1:E:115:HIS:ND1	7:E:506:HOH:O	2.34	0.45
1:B:358:VAL:HA	1:B:361:LEU:HD12	1.98	0.45
1:G:262:CYS:HA	1:G:263:PRO:HD2	1.79	0.45
7:G:548:HOH:O	1:H:116:GLU:HG3	2.16	0.45
1:A:238:LEU:HG	1:A:240:VAL:HG23	1.99	0.45
1:B:89:VAL:HG22	1:B:95:VAL:HG23	1.98	0.45
1:F:207:ILE:HA	1:F:208:PRO:HD3	1.76	0.45
1:G:219:GLU:HG2	1:G:223:SER:HB3	1.98	0.45
1:D:225:ALA:O	1:D:229:ARG:HG3	2.17	0.44
1:H:1:MET:N	1:H:3:GLU:OE1	2.40	0.44
1:B:157:ILE:CD1	1:B:157:ILE:N	2.80	0.44
1:C:123:CYS:O	1:C:144:VAL:HA	2.16	0.44
1:C:340:TYR:HA	1:C:343:ALA:HB3	1.99	0.44
1:G:79:GLN:HB3	1:G:90:LEU:HD21	1.99	0.44
1:H:360:ARG:HD3	7:H:613:HOH:O	2.16	0.44
1:E:56:ILE:HA	1:E:292:ARG:NH1	2.32	0.44
4:A:403[B]:KET:OP4	4:A:403[B]:KET:H4A	2.18	0.44
1:D:192:GLU:CD	1:D:192:GLU:N	2.70	0.44
1:F:324:LYS:O	1:F:327:SER:HB2	2.17	0.44
1:A:130:TRP:CH2	1:A:132:ASN:HB3	2.52	0.44
1:A:214:TYR:OH	3:A:402[A]:PLP:O3	2.33	0.44
1:B:128:PRO:HG2	1:B:184:PRO:HG2	1.99	0.44
1:D:20:PHE:CZ	1:D:30:ASN:HB2	2.53	0.44
1:D:370:ILE:HD13	1:D:370:ILE:N	2.31	0.44
1:E:100:THR:HG21	1:E:106:ALA:HA	2.00	0.44
1:E:112:GLU:O	1:E:116[B]:GLU:HG2	2.18	0.44
1:E:124:TYR:CE2	1:E:169:LEU:HD22	2.52	0.44
1:G:212:ILE:HD11	1:G:215:GLN:HG3	2.00	0.44
1:C:157:ILE:HG22	1:C:159:PHE:N	2.32	0.44
1:F:13:ILE:HD11	7:F:591:HOH:O	2.16	0.44
1:H:130:TRP:CH2	1:H:132:ASN:HB3	2.53	0.44
1:A:183:ASN:OD1	1:A:184:PRO:HA	2.17	0.44
1:B:23:ASP:OD1	1:B:368:TYR:OH	2.25	0.44
1:C:325:LEU:HD11	1:C:392:MET:CE	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:300:ASP:HB3	1:G:303:LEU:HB2	2.00	0.44
1:H:246:LYS:HE2	6:H:401:PMP:N4A	2.32	0.44
1:A:263:PRO:HB2	1:A:264:THR:HG23	2.00	0.44
1:A:326:LYS:HE3	7:A:580:HOH:O	2.14	0.44
1:F:289:HIS:O	1:F:293:VAL:HG23	2.18	0.44
1:A:191:ARG:HD3	1:A:226:TYR:CZ	2.53	0.44
1:B:283:TYR:O	1:B:284:SER:HB2	2.18	0.44
1:C:244:PHE:O	1:C:248:LEU:HB2	2.17	0.44
1:D:33:ILE:HD12	1:D:34:GLY:H	1.83	0.44
1:D:35:ILE:CG2	1:D:43:MET:CE	2.95	0.44
1:D:171:LYS:HG3	1:D:205:GLU:CB	2.48	0.44
1:F:36:TYR:CD2	1:F:314:MET:HE1	2.52	0.44
1:E:19:LYS:HD3	1:E:368:TYR:HE2	1.83	0.43
1:E:23:ASP:O	1:E:28:LYS:HE2	2.18	0.43
1:E:370:ILE:HG22	1:E:371:SER:N	2.33	0.43
1:F:243:SER:OG	3:F:401:PLP:O3P	2.22	0.43
1:A:192:GLU:CD	1:A:192:GLU:H	2.22	0.43
1:A:271:VAL:O	1:A:275:LEU:HG	2.18	0.43
1:B:171:LYS:O	1:B:172:ASP:HB2	2.19	0.43
1:C:127:ASP:HA	1:C:128:PRO:HA	1.75	0.43
1:D:35:ILE:CG2	1:D:43:MET:HE2	2.49	0.43
1:E:143:GLU:HG2	7:E:562:HOH:O	2.18	0.43
1:E:166:PHE:CE1	1:E:175:LEU:HD22	2.54	0.43
1:E:263:PRO:HD3	7:E:554:HOH:O	2.18	0.43
1:F:262:CYS:HA	1:F:263:PRO:HD3	1.85	0.43
1:C:108:LYS:HE2	1:D:282:ILE:HG12	2.00	0.43
1:C:171:LYS:HE3	1:C:205:GLU:HB3	1.99	0.43
1:D:336:ARG:HB3	1:D:338:PHE:CE2	2.53	0.43
1:B:190:THR:HG23	1:B:193:GLN:OE1	2.19	0.43
1:C:364:GLU:HG2	1:C:365:PHE:CD2	2.54	0.43
1:E:126:SER:HA	1:E:147:TYR:CE2	2.54	0.43
1:A:27:ASP:O	1:A:387:TYR:HE2	2.02	0.43
1:D:39:GLU:CD	1:D:39:GLU:N	2.58	0.43
1:G:114:ILE:O	1:G:115:HIS:C	2.56	0.43
1:B:46:LEU:HD21	1:B:314:MET:HE3	1.99	0.43
1:D:68:MET:HG2	1:D:284:SER:O	2.18	0.43
1:D:140:CYS:O	1:D:141:ASP:HB2	2.19	0.43
1:E:58:ASP:HA	1:E:59:PRO:HA	1.72	0.43
1:A:36:TYR:CZ	1:A:314:MET:HG2	2.54	0.43
1:D:163:ILE:HG23	1:D:200:VAL:HG21	2.01	0.43
1:G:20:PHE:CE1	1:G:28:LYS:HG3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:PRO:HB2	1:E:267:GLU:OE2	2.18	0.43
1:F:11[A]:ASP:OD1	1:F:12:PRO:CD	2.62	0.43
1:G:258:LEU:HD12	1:G:259:SER:N	2.34	0.43
1:A:170:ASN:O	1:A:206:LEU:HD23	2.19	0.43
1:E:230:LYS:O	1:E:234:MET:HG3	2.18	0.43
1:G:51:ILE:HG21	1:G:303:LEU:HD21	2.01	0.43
1:A:130:TRP:HE1	4:A:403[B]:KET:HB2	1.84	0.42
1:C:175:LEU:HD23	1:C:175:LEU:HA	1.68	0.42
1:C:307:TRP:O	1:C:311:VAL:HG23	2.19	0.42
1:D:353:LEU:HD12	1:D:396:LEU:HD21	2.01	0.42
1:E:250:LEU:HD12	1:E:250:LEU:HA	1.88	0.42
1:G:279:VAL:HG13	1:G:283:TYR:CE2	2.54	0.42
1:H:253:GLU:HA	1:H:253:GLU:OE2	2.19	0.42
1:B:37:TYR:O	1:B:317:ARG:NH2	2.52	0.42
1:F:283:TYR:O	1:F:284:SER:HB2	2.19	0.42
1:G:323:THR:HG22	1:G:342:THR:HG21	2.01	0.42
1:H:261:VAL:HG12	7:H:597:HOH:O	2.18	0.42
1:H:318:ILE:HD11	1:H:378:ALA:HB2	2.00	0.42
1:B:130:TRP:O	1:B:133:HIS:HB2	2.19	0.42
1:B:236:LEU:HD23	1:B:236:LEU:HA	1.78	0.42
1:C:118:PHE:N	1:C:119:PRO:CD	2.81	0.42
1:E:103:GLY:HA3	3:E:402[A]:PLP:H5A2	2.01	0.42
1:E:332:LYS:HD3	7:E:525:HOH:O	2.18	0.42
1:F:231:ALA:HB3	1:F:238:LEU:HD22	2.01	0.42
1:B:116:GLU:HB3	1:B:117:TRP:CD1	2.55	0.42
1:B:164:ALA:O	1:B:167:GLU:HB2	2.19	0.42
1:E:157:ILE:HD12	1:E:187:VAL:CG1	2.49	0.42
1:E:221:MET:HE1	1:E:311:VAL:HG11	2.00	0.42
1:F:385:ILE:HG23	1:F:386:ASP:N	2.34	0.42
1:C:24:ASN:ND2	1:F:86:ASP:OD1	2.53	0.42
1:E:46:LEU:HD21	1:E:314:MET:HE2	2.01	0.42
1:G:36:TYR:CD2	1:G:36:TYR:C	2.92	0.42
1:G:43:MET:HA	1:G:44:PRO:HD3	1.91	0.42
1:B:370:ILE:H	1:B:370:ILE:HG12	1.70	0.42
1:E:221:MET:HG2	1:E:312:TYR:OH	2.20	0.42
1:F:184:PRO:CB	1:F:374:ARG:HD3	2.49	0.42
1:G:118:PHE:N	1:G:119:PRO:HD3	2.35	0.42
1:G:147:TYR:HA	1:G:148:PRO:HD3	1.88	0.42
1:B:321:MET:CE	7:B:605:HOH:O	2.67	0.42
4:E:404[B]:KET:C4A	4:E:404[B]:KET:OP4	2.67	0.42
1:B:157:ILE:CD1	1:B:187:VAL:HG11	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:276:ASN:HD22	1:G:276:ASN:H	1.68	0.42
1:B:382:SER:HA	1:B:385:ILE:HG22	2.02	0.42
1:D:71:LEU:HA	1:D:71:LEU:HD23	1.77	0.42
1:G:4[A]:ARG:NH1	1:G:4[A]:ARG:HB2	2.35	0.42
1:B:192[A]:GLU:HA	1:B:192[A]:GLU:OE1	2.20	0.42
1:D:148:PRO:O	1:D:162:MET:HB2	2.20	0.42
1:F:191:ARG:HH21	1:F:226:TYR:HB2	1.85	0.42
1:D:132:ASN:O	1:D:136:ILE:HG13	2.20	0.41
1:E:214:TYR:OH	4:E:404[B]:KET:O3	2.29	0.41
1:A:58:ASP:HA	1:A:59:PRO:HA	1.82	0.41
1:A:179:PRO:HG3	1:A:210:MET:HB3	2.02	0.41
1:C:166:PHE:CE1	1:C:175:LEU:HD13	2.55	0.41
1:F:184:PRO:HB3	1:F:374:ARG:HD3	2.02	0.41
1:G:132:ASN:HD22	1:G:132:ASN:HA	1.75	0.41
1:H:172:ASP:O	1:H:207:ILE:HD12	2.19	0.41
1:B:353:LEU:HD23	1:B:361:LEU:HD11	2.02	0.41
1:C:25:ASN:OD1	1:C:26:PRO:CD	2.67	0.41
1:E:357:GLN:HE21	1:E:396:LEU:HA	1.85	0.41
1:F:131:GLY:HA2	7:F:575:HOH:O	2.19	0.41
1:H:36:TYR:CD2	1:H:36:TYR:C	2.93	0.41
1:A:178:HIS:N	1:A:178:HIS:CD2	2.88	0.41
1:C:50:LYS:HE2	1:C:50:LYS:HB2	1.67	0.41
1:E:267:GLU:O	1:E:271:VAL:HG23	2.20	0.41
1:F:132:ASN:HD22	1:F:132:ASN:HA	1.64	0.41
1:G:138:GLU:HG2	7:G:528:HOH:O	2.20	0.41
1:G:151:ASP:CB	1:G:158:LYS:HG2	2.45	0.41
1:G:248:LEU:HD23	1:G:248:LEU:HA	1.88	0.41
1:A:27:ASP:O	1:A:387:TYR:CE2	2.73	0.41
1:F:23:ASP:OD1	1:F:368:TYR:OH	2.37	0.41
1:C:114:ILE:HD13	1:C:174:VAL:HG21	2.03	0.41
1:D:58:ASP:HA	1:D:59:PRO:HA	1.96	0.41
1:G:372:ASN:O	1:G:373:SER:OG	2.34	0.41
1:A:287:PRO:HG3	1:B:287:PRO:HG3	2.01	0.41
1:B:179:PRO:HG2	1:B:212:ILE:HB	2.03	0.41
1:D:246:LYS:HD3	1:D:251:TYR:HE1	1.86	0.41
1:E:98:ILE:HD11	1:E:109:VAL:HG11	2.03	0.41
1:E:310:GLU:O	1:E:313:ALA:HB3	2.20	0.41
1:F:46:LEU:HD21	1:F:314:MET:HE3	2.03	0.41
1:A:159:PHE:HE2	1:A:193:GLN:HB3	1.84	0.41
1:C:2:PHE:CB	1:C:5:ILE:HD12	2.49	0.41
1:F:70:GLY:HA3	1:F:99:ALA:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:TYR:CE2	1:H:314:MET:HG2	2.56	0.41
1:A:5:ILE:CG2	1:B:274:GLN:HG3	2.51	0.41
1:A:277:SER:HB2	1:B:8:TYR:CD1	2.55	0.41
1:B:105:GLY:O	1:B:109:VAL:HG23	2.21	0.41
1:B:176:LEU:HA	1:B:176:LEU:HD12	1.76	0.41
1:D:74:HIS:CD2	1:D:74:HIS:C	2.94	0.41
1:D:275:LEU:HD23	1:D:275:LEU:HA	1.96	0.41
1:E:69:ALA:O	1:E:75:ARG:HD2	2.21	0.41
1:E:71:LEU:O	1:E:75:ARG:HG3	2.21	0.41
1:E:108:LYS:HE2	1:F:282:ILE:HG12	2.02	0.41
1:E:157:ILE:CD1	1:E:187:VAL:HG11	2.51	0.41
1:E:236:LEU:HD23	1:E:236:LEU:HA	1.89	0.41
1:F:81:LEU:HA	1:F:81:LEU:HD12	1.87	0.41
1:F:356:GLU:O	1:F:359[B]:GLU:HG3	2.21	0.41
1:H:385:ILE:HD12	1:H:385:ILE:HA	1.72	0.41
1:A:76:LYS:HE3	7:A:540:HOH:O	2.21	0.41
1:C:353:LEU:CD1	1:C:361:LEU:HD12	2.44	0.41
1:D:48:CYS:SG	1:D:307:TRP:HB2	2.61	0.41
1:D:125:VAL:HB	1:D:129:THR:HG21	2.03	0.41
1:E:244:PHE:HB2	1:E:255:VAL:CG2	2.46	0.41
1:F:288:SER:O	1:F:289:HIS:C	2.58	0.41
1:G:333:ILE:HD12	1:G:393:VAL:HG22	2.02	0.41
1:B:53:GLU:OE2	1:B:289:HIS:NE2	2.39	0.40
1:B:125:VAL:HG12	1:B:176:LEU:HD23	2.03	0.40
1:E:82:LEU:HD23	1:E:82:LEU:HA	1.72	0.40
1:A:267:GLU:OE1	1:B:2:PHE:N	2.50	0.40
1:E:19:LYS:HD3	1:E:368:TYR:CE2	2.56	0.40
1:E:284:SER:HB3	7:E:550:HOH:O	2.20	0.40
1:F:74:HIS:CD2	1:F:74:HIS:C	2.94	0.40
1:H:157:ILE:CD1	1:H:187:VAL:HG12	2.50	0.40
1:B:112:GLU:HG2	1:B:140:CYS:SG	2.61	0.40
1:D:177:LEU:O	1:D:179:PRO:HD3	2.21	0.40
1:D:317:ARG:HH11	1:D:317:ARG:HG2	1.86	0.40
1:F:100:THR:HG21	1:F:106:ALA:HA	2.02	0.40
1:G:254:ARG:NH1	1:H:65:TYR:HE2	2.18	0.40
1:A:70:GLY:HA3	1:A:99:ALA:HB3	2.04	0.40
1:C:336:ARG:HG3	1:C:338:PHE:CZ	2.57	0.40
1:D:100:THR:HB	7:D:503:HOH:O	2.22	0.40
1:F:293:VAL:O	1:F:297:VAL:HG23	2.21	0.40
1:G:24:ASN:HD22	1:G:24:ASN:HA	1.72	0.40
1:G:25:ASN:O	1:G:28:LYS:HD3	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:TYR:O	1:C:317:ARG:NH2	2.54	0.40
1:D:255:VAL:HG23	1:D:255:VAL:O	2.22	0.40
1:E:106:ALA:HB3	1:E:241:SER:HB2	2.03	0.40
1:E:246[A]:LYS:HG3	1:E:251:TYR:HE1	1.86	0.40
1:G:73:GLY:HA3	1:G:295:ASP:OD1	2.22	0.40
1:G:185:THR:HA	1:G:350:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/398 (100%)	377 (95%)	21 (5%)	0	100	100
1	B	401/398 (101%)	383 (96%)	18 (4%)	0	100	100
1	C	398/398 (100%)	374 (94%)	23 (6%)	1 (0%)	41	60
1	D	396/398 (100%)	377 (95%)	19 (5%)	0	100	100
1	E	399/398 (100%)	373 (94%)	26 (6%)	0	100	100
1	F	399/398 (100%)	380 (95%)	19 (5%)	0	100	100
1	G	398/398 (100%)	372 (94%)	26 (6%)	0	100	100
1	H	398/398 (100%)	371 (93%)	27 (7%)	0	100	100
All	All	3187/3184 (100%)	3007 (94%)	179 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	333	ILE

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	339/337 (101%)	315 (93%)	24 (7%)	14	26
1	B	342/337 (102%)	322 (94%)	20 (6%)	20	35
1	C	339/337 (101%)	313 (92%)	26 (8%)	13	22
1	D	337/337 (100%)	319 (95%)	18 (5%)	22	38
1	E	340/337 (101%)	319 (94%)	21 (6%)	18	32
1	F	340/337 (101%)	319 (94%)	21 (6%)	18	32
1	G	339/337 (101%)	314 (93%)	25 (7%)	13	24
1	H	339/337 (101%)	321 (95%)	18 (5%)	22	38
All	All	2715/2696 (101%)	2542 (94%)	173 (6%)	18	31

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	20	PHE
1	A	23	ASP
1	A	35	ILE
1	A	50	LYS
1	A	60	ILE
1	A	63	ARG
1	A	86	ASP
1	A	116	GLU
1	A	178	HIS
1	A	209	PHE
1	A	229	ARG
1	A	242	ASN
1	A	250	LEU
1	A	262	CYS
1	A	305	GLU
1	A	329	LEU
1	A	350	PHE
1	A	360	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	371	SER
1	A	385	ILE
1	A	394	ASP
1	A	395	VAL
1	A	397	LYS
1	B	4[A]	ARG
1	B	4[B]	ARG
1	B	13	ILE
1	B	24	ASN
1	B	39	GLU
1	B	120	GLN
1	B	132	ASN
1	B	143	GLU
1	B	146	LYS
1	B	152	THR
1	B	157	ILE
1	B	209	PHE
1	B	219	GLU
1	B	250	LEU
1	B	251	TYR
1	B	353	LEU
1	B	360	ARG
1	B	370	ILE
1	B	371	SER
1	B	398	ASP
1	C	1	MET
1	C	4	ARG
1	C	11	ASP
1	C	13	ILE
1	C	28	LYS
1	C	39	GLU
1	C	50	LYS
1	C	63	ARG
1	C	74	HIS
1	C	116	GLU
1	C	170	ASN
1	C	209	PHE
1	C	212	ILE
1	C	229	ARG
1	C	242	ASN
1	C	251	TYR
1	C	332	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	334	SER
1	C	336	ARG
1	C	350	PHE
1	C	369	MET
1	C	374	ARG
1	C	382[A]	SER
1	C	382[B]	SER
1	C	386	ASP
1	C	394	ASP
1	D	1	MET
1	D	3	GLU
1	D	5	ILE
1	D	13	ILE
1	D	39	GLU
1	D	50	LYS
1	D	63	ARG
1	D	175	LEU
1	D	203	GLU
1	D	209	PHE
1	D	266	ASP
1	D	324	LYS
1	D	334	SER
1	D	353	LEU
1	D	360	ARG
1	D	363	SER
1	D	365	PHE
1	D	398	ASP
1	E	4	ARG
1	E	27	ASP
1	E	35	ILE
1	E	42	VAL
1	E	89	VAL
1	E	101	ILE
1	E	141	ASP
1	E	146	LYS
1	E	176	LEU
1	E	191	ARG
1	E	204	ARG
1	E	209	PHE
1	E	212	ILE
1	E	223	SER
1	E	262	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	285	SER
1	E	350	PHE
1	E	385	ILE
1	E	386	ASP
1	E	395	VAL
1	E	398	ASP
1	F	4	ARG
1	F	14	LEU
1	F	16	LEU
1	F	27	ASP
1	F	42	VAL
1	F	63	ARG
1	F	86	ASP
1	F	116	GLU
1	F	132	ASN
1	F	146	LYS
1	F	152	THR
1	F	176	LEU
1	F	180	CYS
1	F	191	ARG
1	F	203	GLU
1	F	209	PHE
1	F	210	MET
1	F	242	ASN
1	F	250	LEU
1	F	334	SER
1	F	362	GLN
1	G	6	ASP
1	G	16	LEU
1	G	33	ILE
1	G	35	ILE
1	G	42	VAL
1	G	59	PRO
1	G	85	LYS
1	G	101	ILE
1	G	116	GLU
1	G	125	VAL
1	G	132	ASN
1	G	146	LYS
1	G	154	THR
1	G	157	ILE
1	G	158	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	209	PHE
1	G	242	ASN
1	G	341	LEU
1	G	350	PHE
1	G	356	GLU
1	G	362	GLN
1	G	385	ILE
1	G	393	VAL
1	G	395	VAL
1	G	398	ASP
1	H	3	GLU
1	H	14	LEU
1	H	33	ILE
1	H	35	ILE
1	H	42	VAL
1	H	63	ARG
1	H	74	HIS
1	H	143	GLU
1	H	180	CYS
1	H	209	PHE
1	H	220	ASP
1	H	242	ASN
1	H	280	ARG
1	H	285	SER
1	H	317	ARG
1	H	336	ARG
1	H	350	PHE
1	H	356	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	178	HIS
1	B	24	ASN
1	B	132	ASN
1	B	304	HIS
1	C	304	HIS
1	C	357	GLN
1	C	362	GLN
1	D	24	ASN
1	D	362	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	120	GLN
1	E	304	HIS
1	E	345	ASN
1	F	24	ASN
1	F	79	GLN
1	F	132	ASN
1	G	24	ASN
1	G	132	ASN
1	G	276	ASN
1	G	306	GLN
1	G	345	ASN
1	H	24	ASN
1	H	132	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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
3	PLP	F	401	1	15,15,16	4.05	3 (20%)	20,22,23	2.23	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	PLP	B	401	1	15,15,16	3.41	3 (20%)	20,22,23	2.71	10 (50%)
3	PLP	A	402[A]	1	15,15,16	3.49	3 (20%)	20,22,23	1.75	7 (35%)
4	KET	E	404[B]	-	23,24,24	1.18	1 (4%)	30,34,34	3.52	7 (23%)
5	OAA	E	403	-	8,8,8	2.69	1 (12%)	9,10,10	1.57	2 (22%)
4	KET	A	403[B]	-	23,24,24	1.04	1 (4%)	30,34,34	1.66	5 (16%)
4	KET	G	402	-	23,24,24	1.34	3 (13%)	30,34,34	2.97	7 (23%)
3	PLP	C	402	1	15,15,16	4.14	4 (26%)	20,22,23	2.82	8 (40%)
5	OAA	C	403	-	8,8,8	2.47	1 (12%)	9,10,10	1.69	2 (22%)
6	PMP	H	401	-	16,16,16	3.92	3 (18%)	21,23,23	1.91	6 (28%)
6	PMP	D	401	-	16,16,16	2.84	3 (18%)	21,23,23	1.78	4 (19%)
3	PLP	E	402[A]	1	15,15,16	3.35	4 (26%)	20,22,23	1.71	4 (20%)

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
3	PLP	F	401	1	-	2/6/6/8	0/1/1/1
3	PLP	B	401	1	-	3/6/6/8	0/1/1/1
3	PLP	A	402[A]	1	-	2/6/6/8	0/1/1/1
4	KET	E	404[B]	-	-	11/19/19/19	0/1/1/1
5	OAA	E	403	-	-	3/8/8/8	-
4	KET	A	403[B]	-	-	8/19/19/19	0/1/1/1
4	KET	G	402	-	-	7/19/19/19	0/1/1/1
3	PLP	C	402	1	-	3/6/6/8	0/1/1/1
5	OAA	C	403	-	-	5/8/8/8	-
6	PMP	H	401	-	-	7/8/8/8	0/1/1/1
6	PMP	D	401	-	-	4/8/8/8	0/1/1/1
3	PLP	E	402[A]	1	-	5/6/6/8	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	401	PMP	C3-C2	12.12	1.53	1.40
3	F	401	PLP	C5-C4	11.96	1.53	1.40
3	B	401	PLP	C3-C2	10.81	1.51	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	PLP	C3-C2	10.18	1.51	1.40
3	C	402	PLP	C5-C4	9.53	1.51	1.40
3	A	402[A]	PLP	C3-C2	9.10	1.50	1.40
3	A	402[A]	PLP	C5-C4	8.60	1.50	1.40
3	E	402[A]	PLP	C5-C4	8.38	1.49	1.40
3	E	402[A]	PLP	C3-C2	8.33	1.49	1.40
3	F	401	PLP	C3-C2	7.97	1.48	1.40
6	D	401	PMP	C3-C4	7.06	1.50	1.40
3	C	402	PLP	C3-C4	6.95	1.54	1.40
5	E	403	OAA	C3-C4	-6.94	1.44	1.53
6	H	401	PMP	C5-C4	6.79	1.50	1.40
6	H	401	PMP	C3-C4	6.68	1.50	1.40
6	D	401	PMP	C5-C4	6.48	1.49	1.40
5	C	403	OAA	C3-C4	-6.32	1.45	1.53
6	D	401	PMP	C3-C2	5.76	1.46	1.40
3	F	401	PLP	C3-C4	5.67	1.51	1.40
3	B	401	PLP	C5-C4	5.61	1.46	1.40
3	A	402[A]	PLP	C3-C4	4.69	1.49	1.40
3	E	402[A]	PLP	C3-C4	4.09	1.48	1.40
3	B	401	PLP	C3-C4	3.59	1.47	1.40
4	G	402	KET	C4-C5	-3.31	1.37	1.42
4	G	402	KET	CA-C	-2.89	1.48	1.52
4	A	403[B]	KET	CA-C	-2.82	1.48	1.52
3	C	402	PLP	C2-N1	2.33	1.38	1.33
4	E	404[B]	KET	C4-C4A	2.25	1.50	1.46
3	E	402[A]	PLP	P-O3P	-2.25	1.46	1.54
4	G	402	KET	OD2-CG	-2.13	1.23	1.30

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	404[B]	KET	CA-N-C4A	15.25	139.33	117.31
4	G	402	KET	CA-N-C4A	11.26	133.57	117.31
4	E	404[B]	KET	C4-C4A-N	8.62	142.16	123.01
4	G	402	KET	C4-C4A-N	-7.80	105.69	123.01
3	B	401	PLP	C6-C5-C4	6.77	123.48	118.16
3	C	402	PLP	C6-C5-C4	6.64	123.38	118.16
3	F	401	PLP	O4P-C5A-C5	5.60	120.02	109.35
4	G	402	KET	OP4-P-OP1	-5.53	90.96	106.47
4	A	403[B]	KET	CB-CA-C	-5.28	99.62	110.35
6	D	401	PMP	O4P-C5A-C5	5.01	118.89	109.35
3	B	401	PLP	O3P-P-O4P	-4.89	93.71	106.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	PLP	C3-C4-C5	-4.77	113.58	118.74
3	F	401	PLP	C3-C4-C5	-4.67	113.69	118.74
3	C	402	PLP	O2P-P-O4P	-4.49	94.79	106.73
3	C	402	PLP	C4A-C4-C3	4.29	127.77	120.50
3	B	401	PLP	C3-C4-C5	-4.11	114.31	118.74
6	H	401	PMP	C2A-C2-C3	4.05	125.89	120.89
3	B	401	PLP	C5A-C5-C6	3.93	125.83	119.37
3	E	402[A]	PLP	C4A-C4-C5	3.91	124.97	120.94
4	A	403[B]	KET	CA-N-C4A	3.88	122.91	117.31
3	F	401	PLP	C5A-C5-C6	-3.48	113.64	119.37
4	E	404[B]	KET	C5A-C5-C6	-3.46	113.68	119.37
3	A	402[A]	PLP	C5A-C5-C6	-3.44	113.71	119.37
3	F	401	PLP	O3P-P-O2P	3.35	120.44	107.64
6	H	401	PMP	C6-C5-C4	3.33	120.47	118.12
4	E	404[B]	KET	C-CA-N	3.24	115.09	108.67
3	C	402	PLP	O3-C3-C4	3.18	126.48	118.10
4	E	404[B]	KET	C3-C4-C5	-3.11	115.87	118.26
3	A	402[A]	PLP	C3-C4-C5	-3.06	115.44	118.74
6	H	401	PMP	O3-C3-C2	3.01	124.04	117.49
6	H	401	PMP	O3P-P-O2P	2.98	119.01	107.64
5	C	403	OAA	O1-C1-C2	-2.94	113.48	122.08
6	D	401	PMP	C6-N1-C2	2.83	124.41	119.17
3	F	401	PLP	O3-C3-C4	2.76	125.38	118.10
3	B	401	PLP	C4A-C4-C3	2.75	125.16	120.50
6	H	401	PMP	C6-N1-C2	2.75	124.25	119.17
5	E	403	OAA	O3-C3-C2	2.71	124.51	120.58
4	G	402	KET	C-CA-N	2.71	114.04	108.67
3	E	402[A]	PLP	C5A-C5-C6	-2.69	114.94	119.37
3	B	401	PLP	O3P-P-O2P	2.68	117.89	107.64
4	E	404[B]	KET	OP3-P-OP4	-2.66	99.67	106.73
6	D	401	PMP	C3-C4-C5	-2.65	116.18	118.72
4	G	402	KET	C5A-C5-C6	2.63	123.69	119.37
6	D	401	PMP	O2P-P-O4P	-2.52	100.02	106.73
3	C	402	PLP	C6-N1-C2	2.47	123.73	119.17
3	C	402	PLP	O2P-P-O1P	2.46	120.32	110.68
5	C	403	OAA	O4-C4-C3	-2.46	118.44	121.72
3	B	401	PLP	O3-C3-C2	2.45	122.83	117.49
3	A	402[A]	PLP	C6-C5-C4	2.40	120.04	118.16
3	A	402[A]	PLP	C4A-C4-C5	2.39	123.40	120.94
3	B	401	PLP	O3P-P-O1P	2.37	119.95	110.68
4	G	402	KET	OP3-P-OP1	2.31	119.74	110.68
3	E	402[A]	PLP	C3-C4-C5	-2.30	116.25	118.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	402[A]	PLP	C6-N1-C2	2.29	123.41	119.17
4	G	402	KET	OP3-P-OP2	2.29	116.39	107.64
4	A	403[B]	KET	C2A-C2-C3	2.27	123.69	120.89
3	B	401	PLP	C2A-C2-C3	-2.26	118.10	120.89
5	E	403	OAA	O4-C4-C3	-2.24	118.72	121.72
4	E	404[B]	KET	OP4-C5A-C5	2.24	113.61	109.35
3	C	402	PLP	C4A-C4-C5	-2.23	118.64	120.94
3	A	402[A]	PLP	O4P-C5A-C5	2.21	113.55	109.35
4	A	403[B]	KET	OD1-CG-CB	-2.20	115.75	122.80
6	H	401	PMP	C3-C4-C5	-2.19	116.62	118.72
3	A	402[A]	PLP	C6-N1-C2	2.17	123.19	119.17
3	B	401	PLP	O4P-P-O1P	-2.09	100.62	106.47
4	A	403[B]	KET	C5A-C5-C6	-2.07	115.97	119.37
3	A	402[A]	PLP	C2A-C2-C3	2.01	123.37	120.89

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402[A]	PLP	C4-C5-C5A-O4P
3	A	402[A]	PLP	C6-C5-C5A-O4P
3	B	401	PLP	C5A-O4P-P-O1P
3	B	401	PLP	C5A-O4P-P-O2P
3	B	401	PLP	C5A-O4P-P-O3P
3	C	402	PLP	C5A-O4P-P-O1P
3	C	402	PLP	C5A-O4P-P-O2P
3	C	402	PLP	C5A-O4P-P-O3P
3	E	402[A]	PLP	C4-C5-C5A-O4P
3	E	402[A]	PLP	C6-C5-C5A-O4P
3	E	402[A]	PLP	C5A-O4P-P-O2P
3	E	402[A]	PLP	C5A-O4P-P-O3P
3	F	401	PLP	C4-C5-C5A-O4P
3	F	401	PLP	C6-C5-C5A-O4P
4	A	403[B]	KET	C5A-OP4-P-OP2
4	A	403[B]	KET	C5A-OP4-P-OP3
4	A	403[B]	KET	N-CA-CB-CG
4	E	404[B]	KET	C4-C4A-N-CA
4	E	404[B]	KET	C4-C5-C5A-OP4
4	E	404[B]	KET	C6-C5-C5A-OP4
4	E	404[B]	KET	C5A-OP4-P-OP1
4	E	404[B]	KET	C5A-OP4-P-OP3
4	E	404[B]	KET	CB-CA-N-C4A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	402	KET	C-CA-N-C4A
4	G	402	KET	N-CA-CB-CG
4	G	402	KET	C-CA-CB-CG
5	C	403	OAA	C1-C2-C3-O3
5	C	403	OAA	C2-C3-C4-O5
5	E	403	OAA	C1-C2-C3-O3
5	E	403	OAA	C2-C3-C4-O5
6	D	401	PMP	C4-C5-C5A-O4P
6	D	401	PMP	C6-C5-C5A-O4P
6	H	401	PMP	C3-C4-C4A-N4A
6	H	401	PMP	C5-C4-C4A-N4A
6	H	401	PMP	C4-C5-C5A-O4P
6	H	401	PMP	C6-C5-C5A-O4P
6	H	401	PMP	C5A-O4P-P-O2P
6	H	401	PMP	C5A-O4P-P-O3P
4	A	403[B]	KET	C-CA-CB-CG
4	G	402	KET	C3-C4-C4A-N
3	E	402[A]	PLP	C5A-O4P-P-O1P
4	A	403[B]	KET	C5A-OP4-P-OP1
6	H	401	PMP	C5A-O4P-P-O1P
6	D	401	PMP	C5-C4-C4A-N4A
4	A	403[B]	KET	C6-C5-C5A-OP4
4	A	403[B]	KET	OXT-C-CA-N
4	G	402	KET	OXT-C-CA-N
4	G	402	KET	O-C-CA-N
4	A	403[B]	KET	C4-C5-C5A-OP4
4	E	404[B]	KET	CA-CB-CG-OD1
4	E	404[B]	KET	CA-CB-CG-OD2
4	E	404[B]	KET	C-CA-N-C4A
5	C	403	OAA	O3-C3-C4-O4
5	C	403	OAA	C2-C3-C4-O4
5	C	403	OAA	O3-C3-C4-O5
4	E	404[B]	KET	C3-C4-C4A-N
4	G	402	KET	C5-C4-C4A-N
4	E	404[B]	KET	C5A-OP4-P-OP2
6	D	401	PMP	C3-C4-C4A-N4A
5	E	403	OAA	O1-C1-C2-C3

There are no ring outliers.

11 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	PLP	2	0
3	B	401	PLP	1	0
3	A	402[A]	PLP	1	0
4	E	404[B]	KET	13	0
4	A	403[B]	KET	5	0
4	G	402	KET	3	0
3	C	402	PLP	1	0
5	C	403	OAA	1	0
6	H	401	PMP	4	0
6	D	401	PMP	8	0
3	E	402[A]	PLP	1	0

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

Ligand KET E 404 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand KET A 403 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand KET G 402

Bond lengths

Bond angles

Torsions

Rings
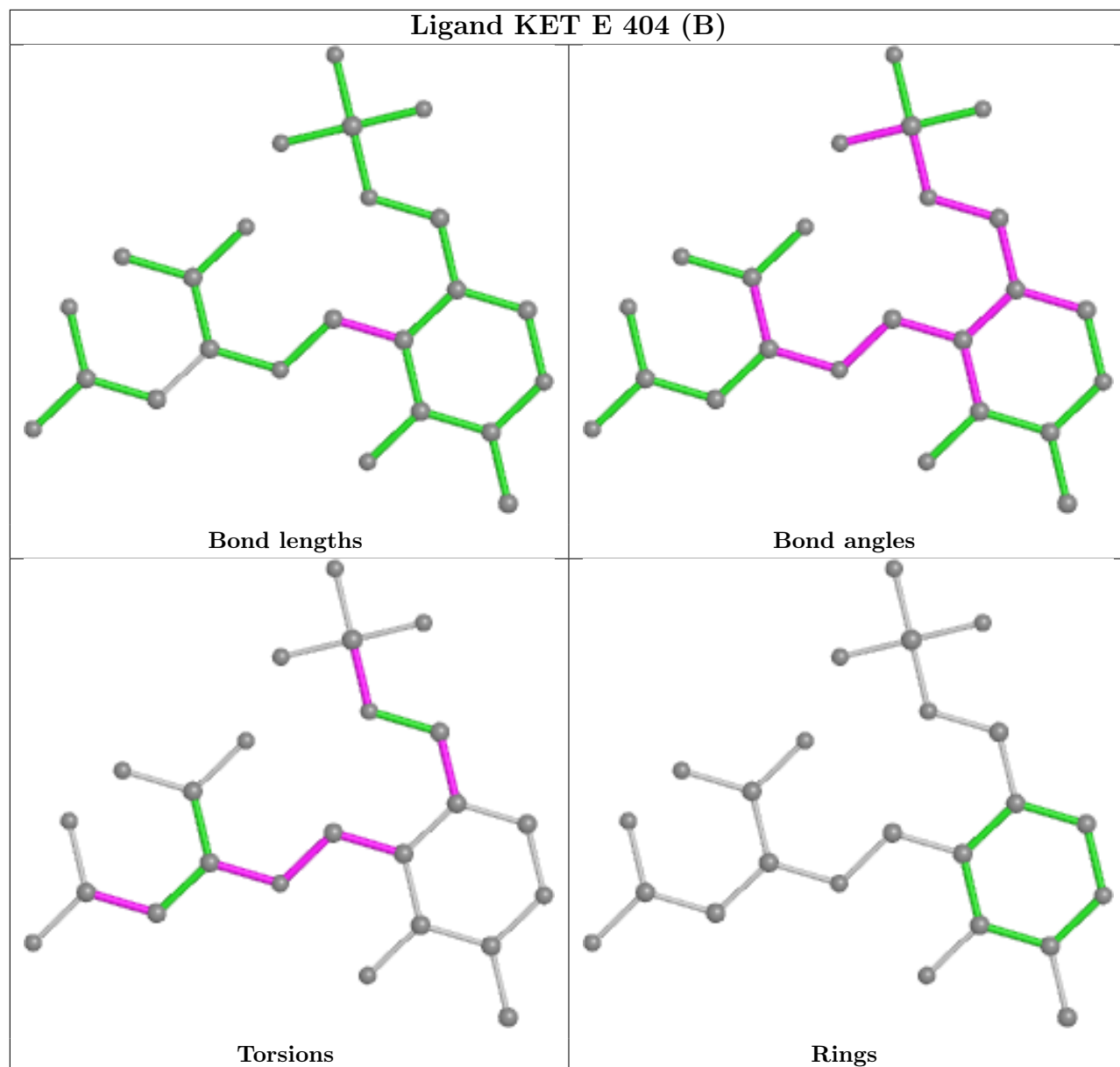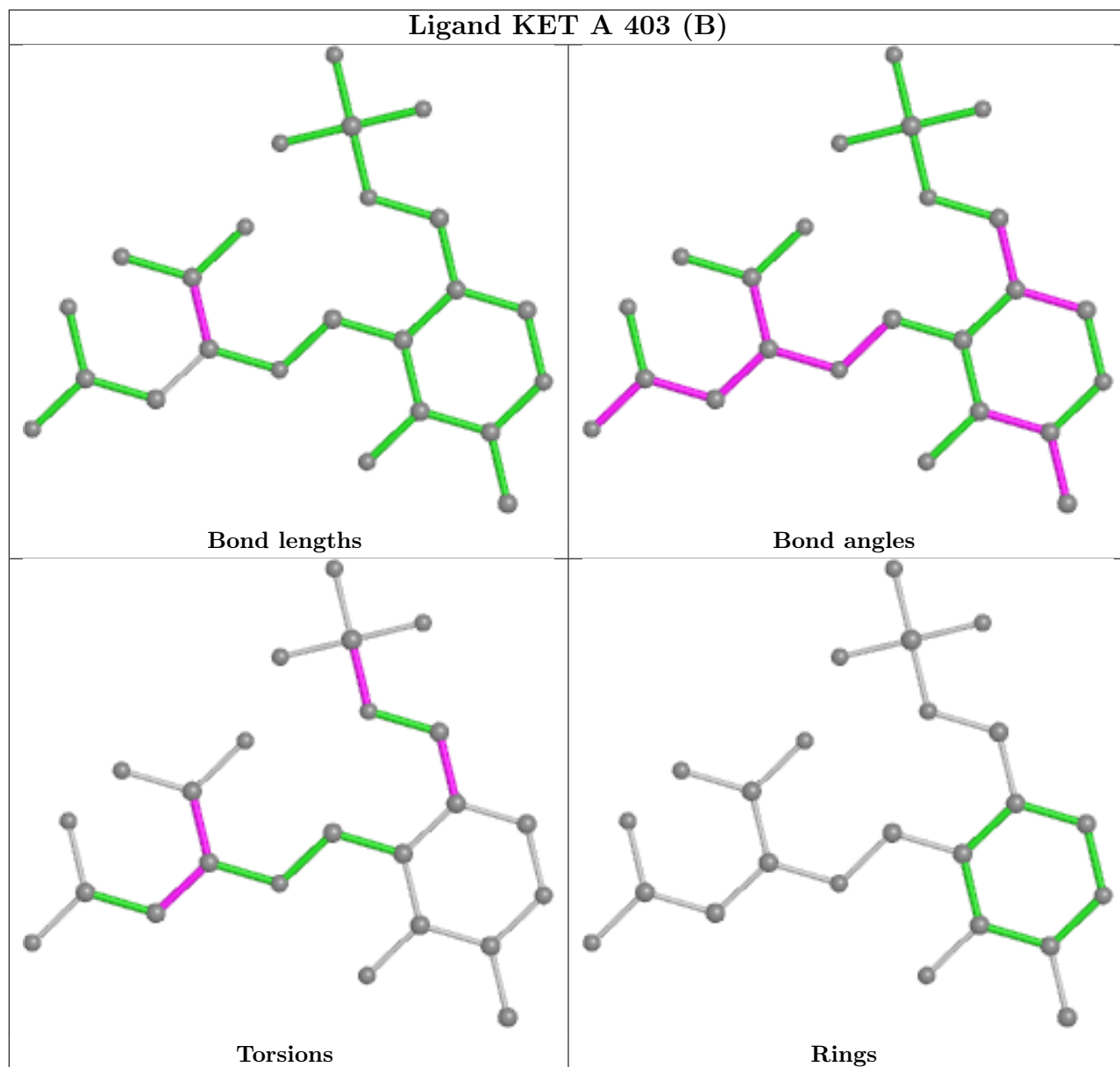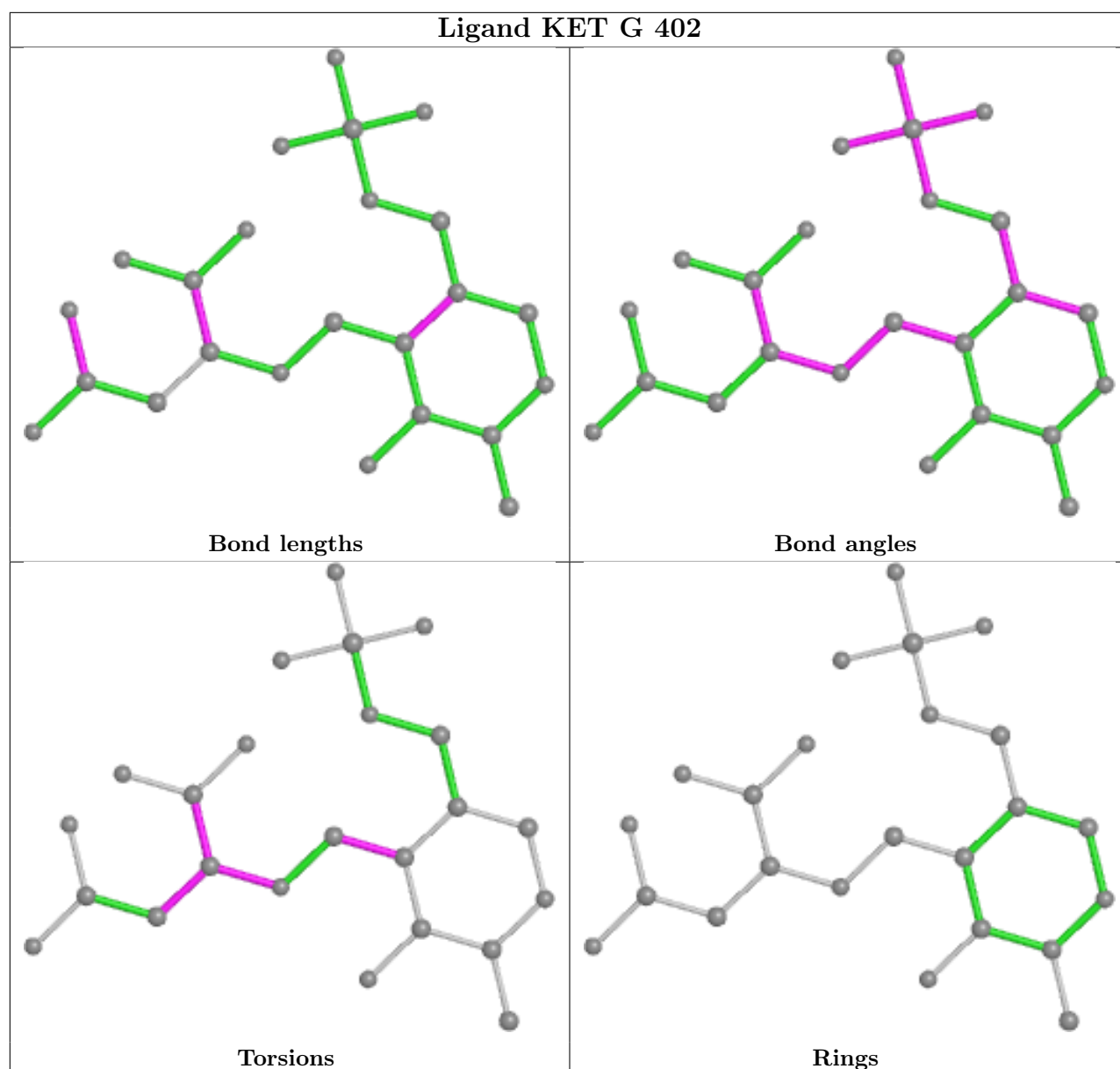
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	398/398 (100%)	-0.23	21 (5%)	26	31	18, 36, 94, 128	0
1	B	398/398 (100%)	-0.48	1 (0%)	94	96	16, 31, 64, 114	0
1	C	398/398 (100%)	-0.21	5 (1%)	77	84	22, 42, 86, 130	0
1	D	398/398 (100%)	-0.56	1 (0%)	94	96	17, 29, 55, 99	0
1	E	398/398 (100%)	-0.36	7 (1%)	68	76	19, 37, 89, 123	0
1	F	398/398 (100%)	-0.47	2 (0%)	91	94	21, 34, 63, 94	0
1	G	398/398 (100%)	-0.29	11 (2%)	53	62	19, 45, 85, 112	0
1	H	398/398 (100%)	-0.52	1 (0%)	94	96	15, 31, 66, 93	0
All	All	3184/3184 (100%)	-0.39	49 (1%)	73	81	15, 35, 78, 130	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	398	ASP	4.4
1	A	16	LEU	4.2
1	A	24	ASN	4.2
1	A	335	GLY	4.2
1	C	335	GLY	3.9
1	A	394	ASP	3.6
1	A	397	LYS	3.6
1	A	365	PHE	3.4
1	A	364	GLU	3.2
1	A	27	ASP	3.2
1	A	360	ARG	3.2
1	E	360[A]	ARG	3.1
1	A	334	SER	3.1
1	E	398	ASP	3.1
1	A	15	GLY	3.1
1	A	333	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	397	LYS	3.0
1	A	28	LYS	2.9
1	A	396	LEU	2.9
1	A	22	ALA	2.8
1	G	398	ASP	2.8
1	F	359[A]	GLU	2.7
1	E	394	ASP	2.7
1	A	352	GLY	2.7
1	C	24	ASN	2.7
1	A	361	LEU	2.6
1	E	396	LEU	2.6
1	G	396	LEU	2.6
1	B	24	ASN	2.6
1	G	394	ASP	2.5
1	G	335	GLY	2.4
1	A	25	ASN	2.4
1	D	398	ASP	2.4
1	A	367	ILE	2.4
1	G	354	THR	2.3
1	C	396	LEU	2.3
1	F	9	ALA	2.2
1	G	395	VAL	2.2
1	E	356	GLU	2.2
1	E	365	PHE	2.2
1	G	27	ASP	2.1
1	H	7	TYR	2.1
1	G	389	ALA	2.1
1	A	363	SER	2.1
1	C	11	ASP	2.1
1	G	356	GLU	2.1
1	C	165	PHE	2.1
1	G	353	LEU	2.0
1	G	360	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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(Å^2)	Q<0.9
5	OAA	C	403	9/9	0.87	0.31	26,28,31,32	9
5	OAA	E	403	9/9	0.89	0.34	20,24,27,27	9
4	KET	E	404[B]	24/24	0.95	0.26	24,38,42,44	24
4	KET	A	403[B]	24/24	0.97	0.15	9,12,13,14	24
2	MG	A	401	1/1	0.97	0.04	15,15,15,15	0
2	MG	G	401	1/1	0.97	0.08	19,19,19,19	0
3	PLP	E	402[A]	15/16	0.97	0.21	30,61,71,71	15
3	PLP	A	402[A]	15/16	0.98	0.12	34,39,43,50	15
3	PLP	C	402	15/16	0.98	0.13	21,35,46,48	0
4	KET	G	402	24/24	0.98	0.17	27,45,90,102	0
2	MG	C	401	1/1	0.98	0.09	25,25,25,25	0
3	PLP	F	401	15/16	0.98	0.11	21,25,30,30	0
6	PMP	H	401	16/16	0.98	0.11	22,29,35,36	0
3	PLP	B	401	15/16	0.99	0.12	18,26,35,38	0
6	PMP	D	401	16/16	0.99	0.12	19,28,34,35	0
2	MG	E	401	1/1	0.99	0.09	13,13,13,13	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.
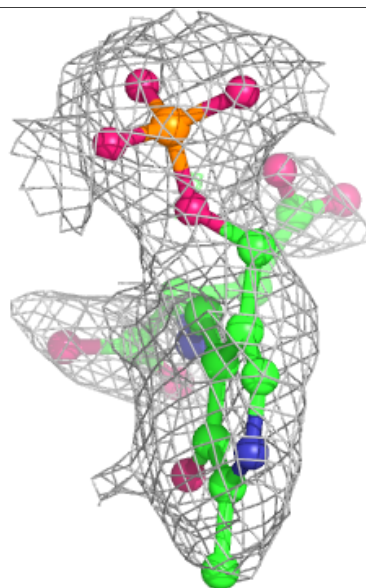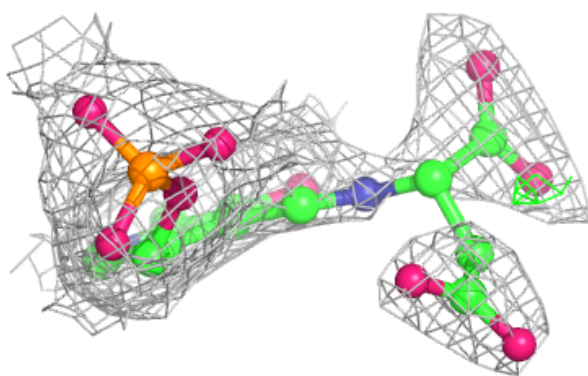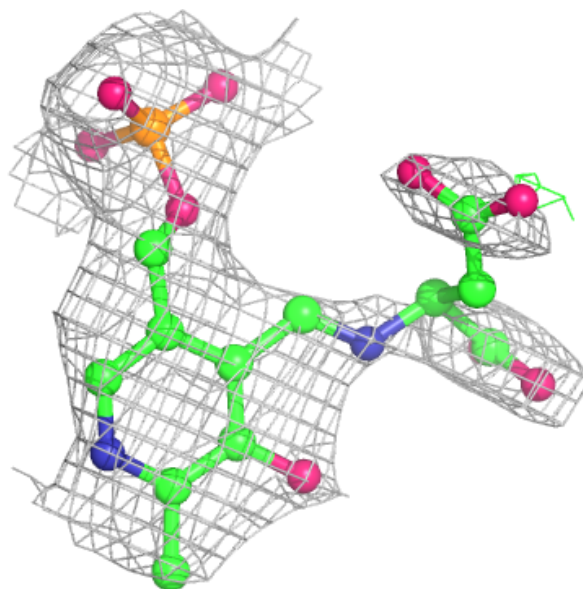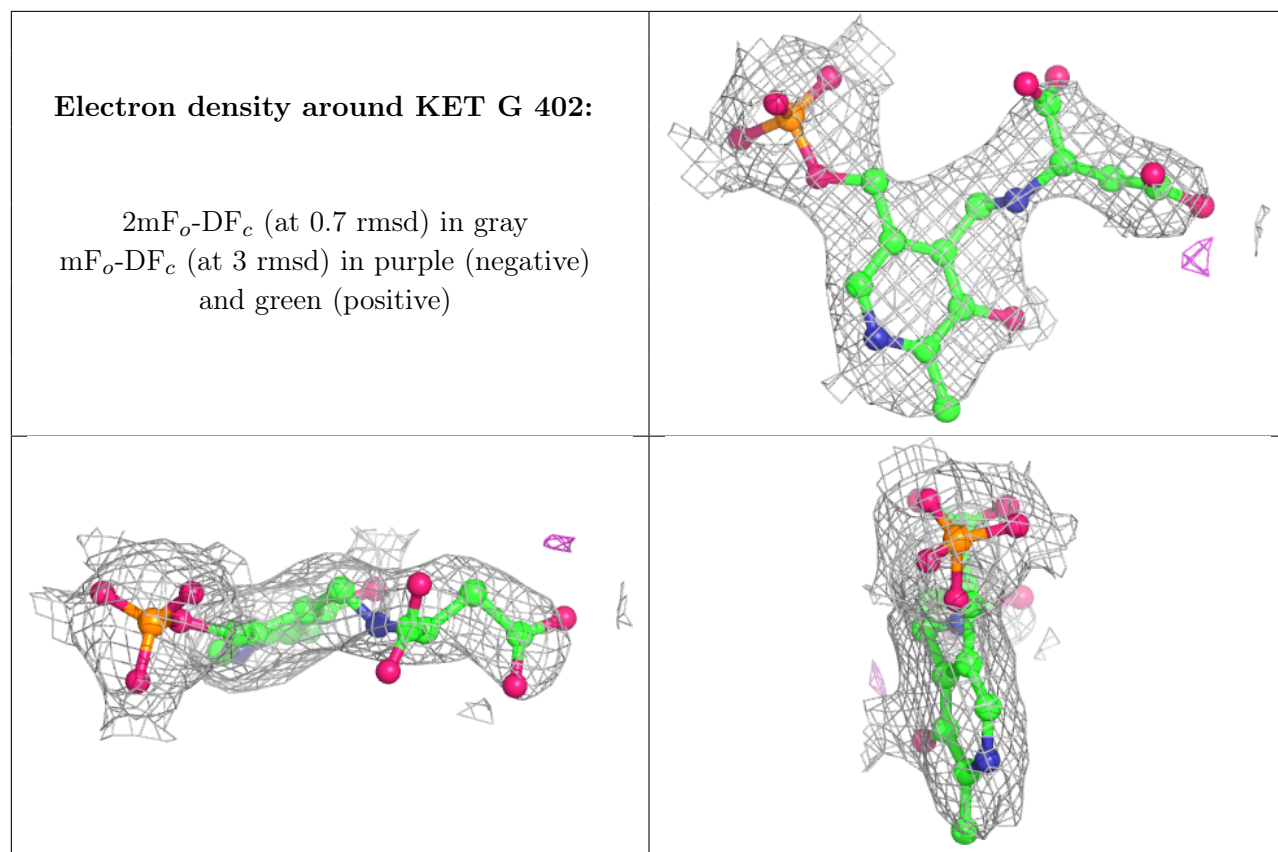
Electron density around KET E 404 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
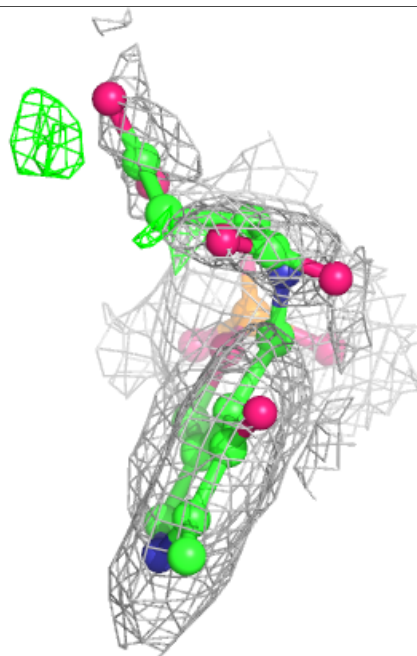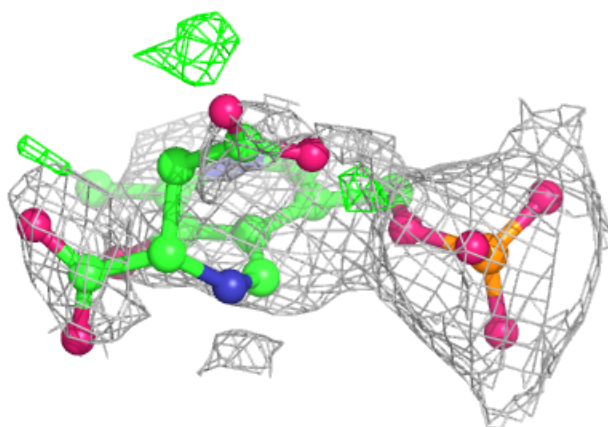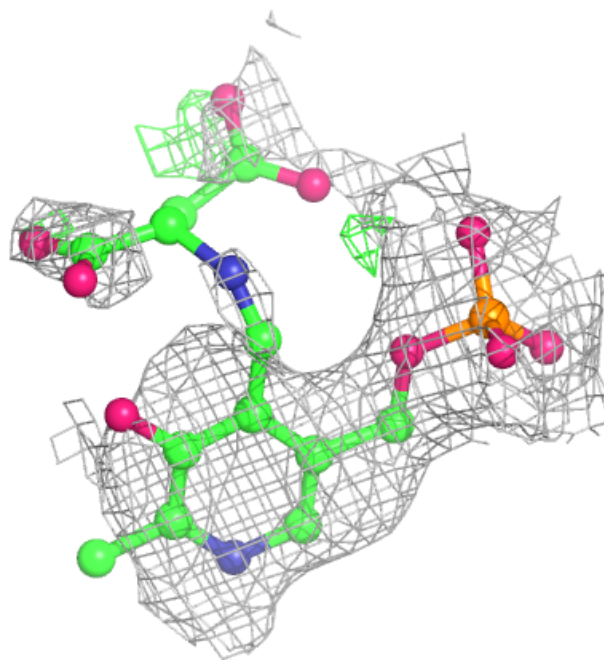
Electron density around KET A 403 (B):

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

Electron density around KET G 402:

$2mF_o$-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.