



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:19 AM UTC

PDB ID : 3A5Z / pdb_00003a5z
Title : Crystal structure of Escherichia coli GenX in complex with elongation factor P
Authors : Sumida, T.; Yanagisawa, T.; Ishii, R.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2009-08-17
Resolution : 2.50 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (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

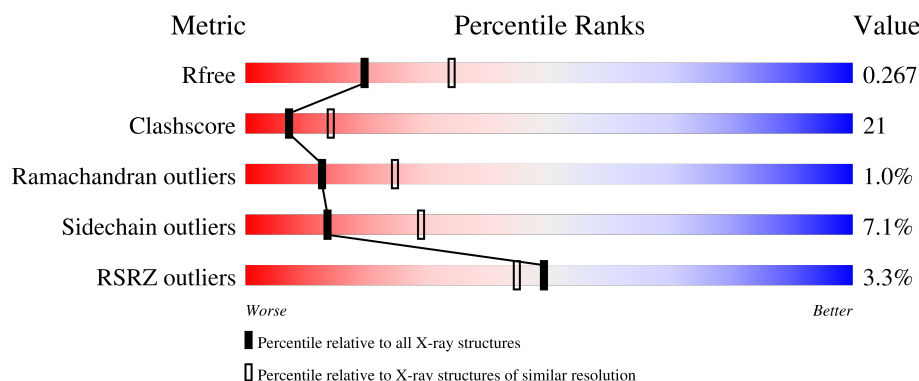
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	328	56% 37% 5%
1	C	328	60% 33% 6%
1	E	328	62% 30% 6%
1	G	328	52% 41% 5%

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Mol	Chain	Length	Quality of chain
2	B	191	
2	D	191	
2	F	191	
2	H	191	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14965 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 Putative lysyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2584	1631	450	487	16			
1	C	324	Total	C	N	O	S	0	0	0
			2590	1634	451	489	16			
1	E	323	Total	C	N	O	S	0	0	0
			2584	1631	450	487	16			
1	G	323	Total	C	N	O	S	0	0	0
			2582	1630	448	487	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP C3SGA2
A	-1	SER	-	expression tag	UNP C3SGA2
A	0	HIS	-	expression tag	UNP C3SGA2
C	-2	GLY	-	expression tag	UNP C3SGA2
C	-1	SER	-	expression tag	UNP C3SGA2
C	0	HIS	-	expression tag	UNP C3SGA2
E	-2	GLY	-	expression tag	UNP C3SGA2
E	-1	SER	-	expression tag	UNP C3SGA2
E	0	HIS	-	expression tag	UNP C3SGA2
G	-2	GLY	-	expression tag	UNP C3SGA2
G	-1	SER	-	expression tag	UNP C3SGA2
G	0	HIS	-	expression tag	UNP C3SGA2

- Molecule 2 is a protein called Elongation factor P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	0	0	0
			1064	680	174	206	4			
2	D	175	Total	C	N	O	S	0	0	0
			1368	873	225	266	4			

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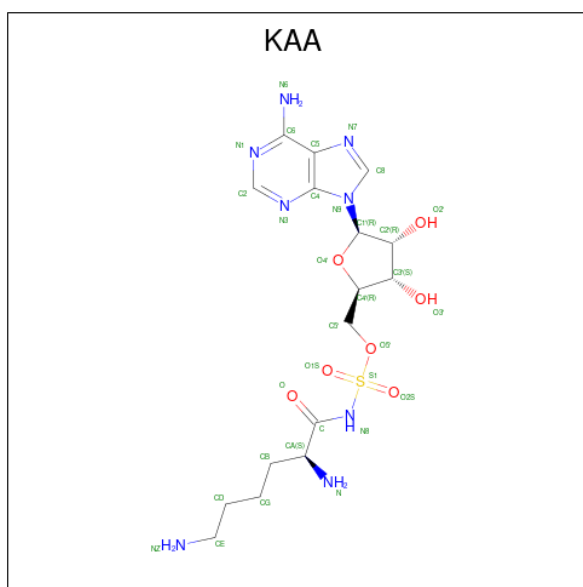
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	59	Total	C	N	O	S	0	0	0
			468	298	82	87	1			
2	H	175	Total	C	N	O	S	0	0	0
			1368	873	225	266	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP C3SGD7
B	-1	SER	-	expression tag	UNP C3SGD7
B	0	HIS	-	expression tag	UNP C3SGD7
D	-2	GLY	-	expression tag	UNP C3SGD7
D	-1	SER	-	expression tag	UNP C3SGD7
D	0	HIS	-	expression tag	UNP C3SGD7
F	-2	GLY	-	expression tag	UNP C3SGD7
F	-1	SER	-	expression tag	UNP C3SGD7
F	0	HIS	-	expression tag	UNP C3SGD7
H	-2	GLY	-	expression tag	UNP C3SGD7
H	-1	SER	-	expression tag	UNP C3SGD7
H	0	HIS	-	expression tag	UNP C3SGD7

- Molecule 3 is 5'-O-[(L-LYSYLAMINO)SULFONYL]ADENOSINE (CCD ID: KAA) (formula: C₁₆H₂₆N₈O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	16	8	7	1		
3	C	1	Total	C	N	O	S	0	0
			32	16	8	7	1		
3	E	1	Total	C	N	O	S	0	0
			32	16	8	7	1		
3	G	1	Total	C	N	O	S	0	0
			32	16	8	7	1		

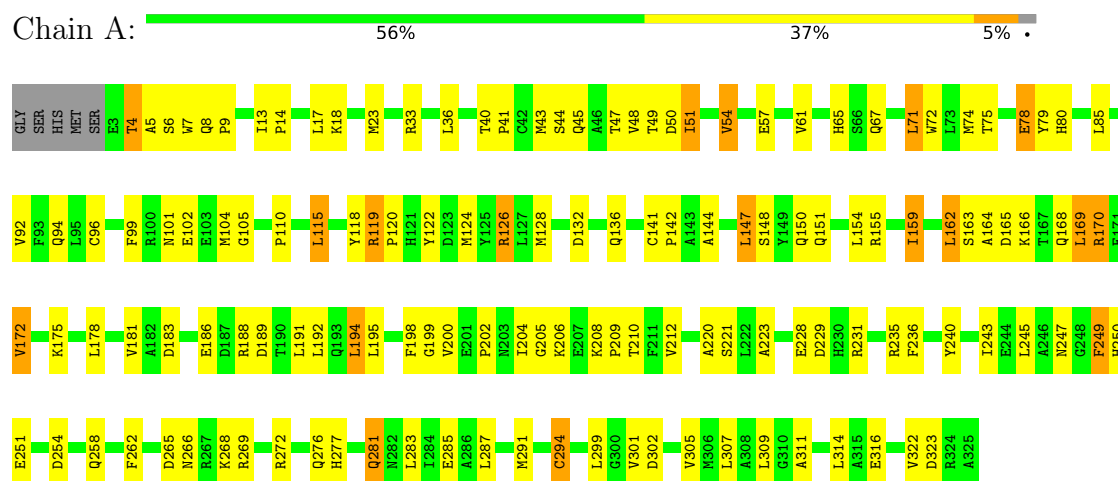
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	4	Total	O	0	0
			4	4		
4	C	56	Total	O	0	0
			56	56		
4	D	13	Total	O	0	0
			13	13		
4	E	62	Total	O	0	0
			62	62		
4	F	2	Total	O	0	0
			2	2		
4	G	29	Total	O	0	0
			29	29		
4	H	11	Total	O	0	0
			11	11		

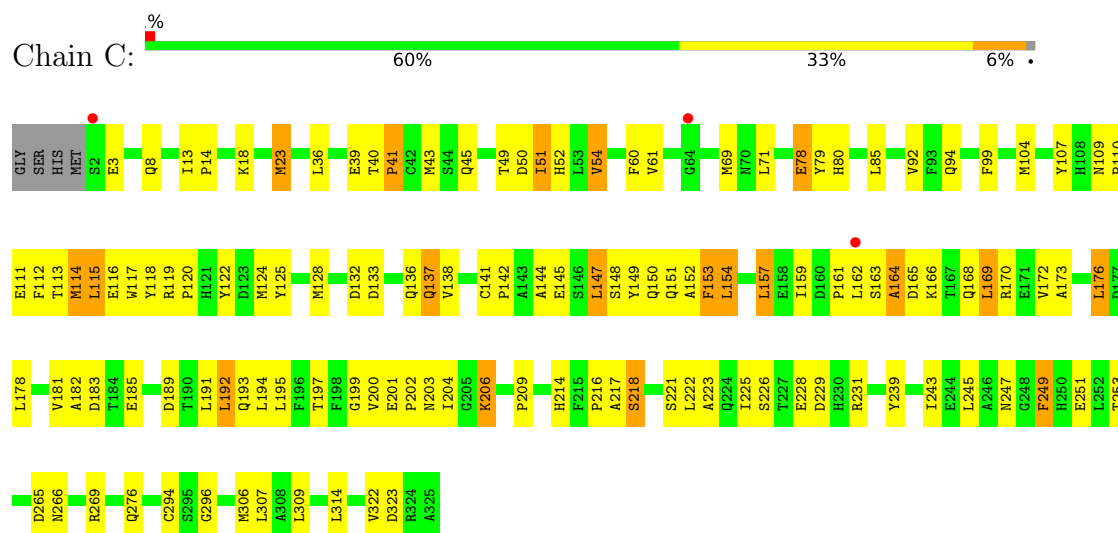
3 Residue-property plots

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: Putative lysyl-tRNA synthetase

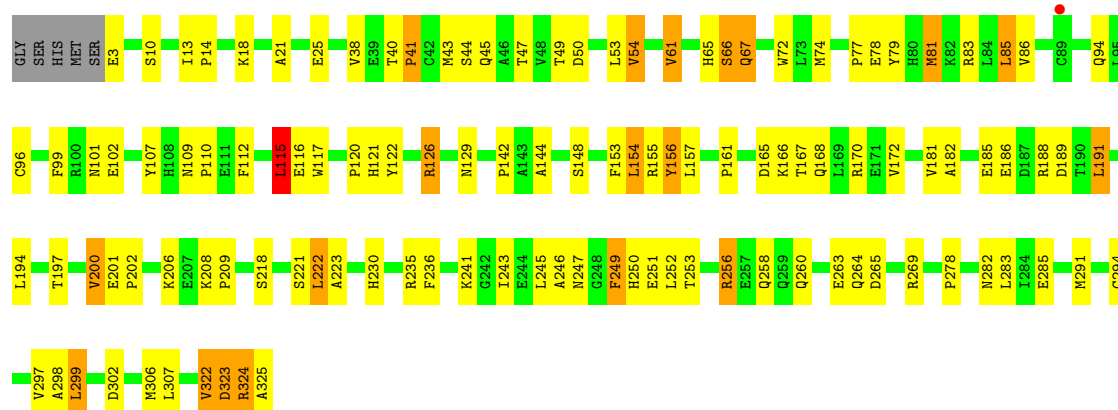


• Molecule 1: Putative lysyl-tRNA synthetase

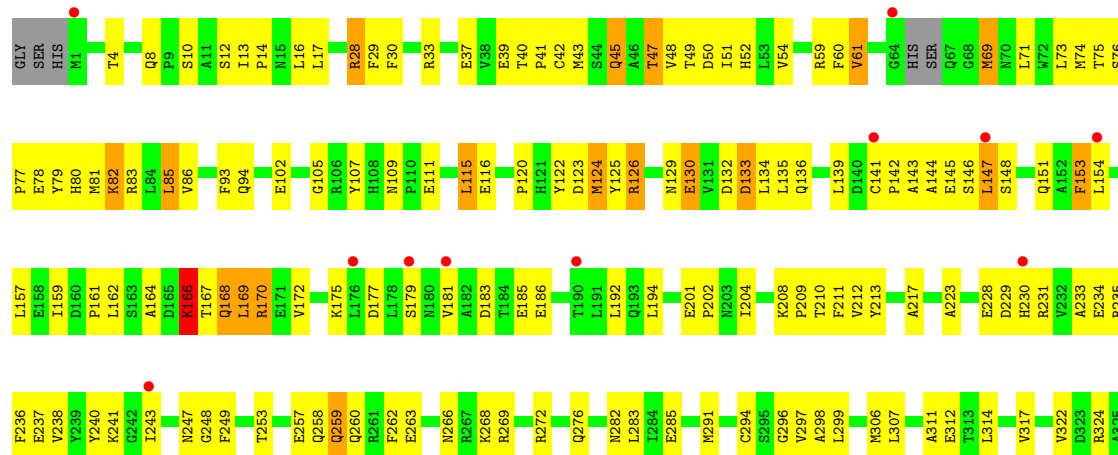


• Molecule 1: Putative lysyl-tRNA synthetase

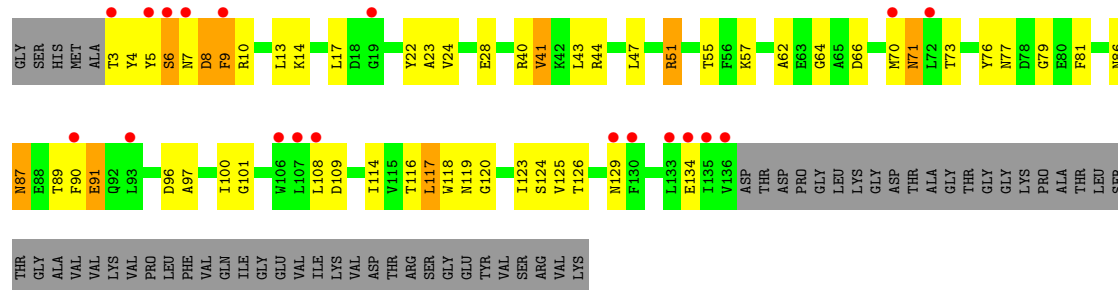
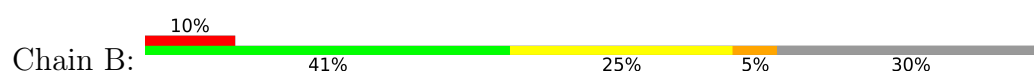




• Molecule 1: Putative lysyl-tRNA synthetase

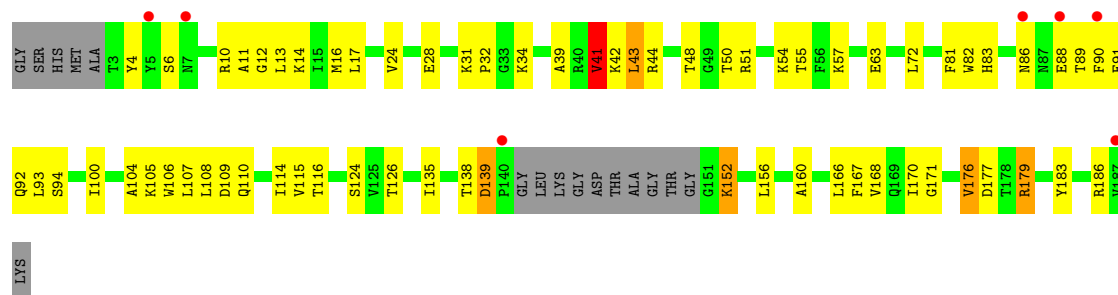


• Molecule 2: Elongation factor P

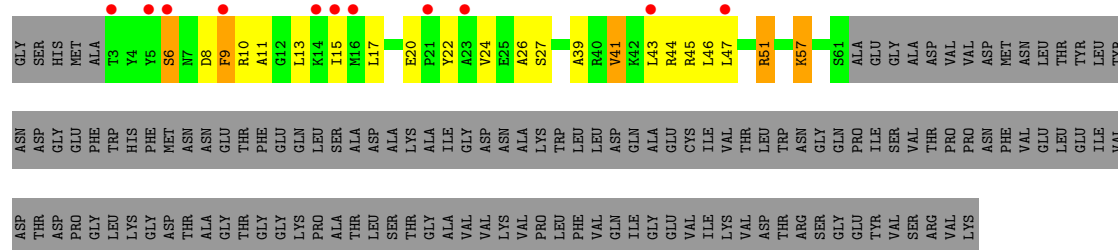


• Molecule 2: Elongation factor P

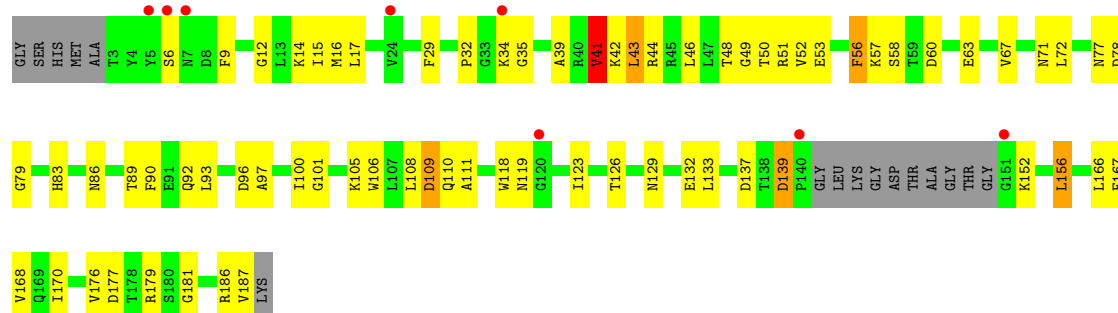




• Molecule 2: Elongation factor P



• Molecule 2: Elongation factor P



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.93Å 102.96Å 119.94Å 90.00° 99.40° 90.00°	Depositor
Resolution (Å)	45.68 – 2.50 45.68 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.7 (45.68-2.50) 93.8 (45.68-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.268 0.225 , 0.267	Depositor DCC
R_{free} test set	4162 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14965	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.10% 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: KAA

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	0.51	0/2641	0.97	11/3578 (0.3%)
1	C	0.47	0/2647	0.96	10/3586 (0.3%)
1	E	0.50	1/2641 (0.0%)	1.00	13/3578 (0.4%)
1	G	0.44	0/2637	0.92	5/3570 (0.1%)
2	B	0.37	0/1088	0.90	3/1476 (0.2%)
2	D	0.41	0/1396	0.85	3/1895 (0.2%)
2	F	0.36	0/476	0.95	2/637 (0.3%)
2	H	0.39	0/1396	0.88	3/1895 (0.2%)
All	All	0.46	1/14922 (0.0%)	0.94	50/20215 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	81	MET	SD-CE	-5.13	1.66	1.79

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ILE	N-CA-C	9.49	120.30	110.62
2	F	41	VAL	N-CA-C	7.55	118.68	108.11
1	E	250	HIS	N-CA-C	-7.35	97.28	108.67
2	F	57	LYS	N-CA-C	-6.95	100.19	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	GLU	N-CA-C	6.95	120.46	110.10
1	A	172	VAL	N-CA-C	-6.89	102.21	111.44
1	E	249	PHE	N-CA-C	6.81	118.54	108.60
2	D	57	LYS	N-CA-C	-6.64	100.65	110.48
2	B	41	VAL	N-CA-C	6.63	117.46	108.17
1	E	148	SER	N-CA-C	-6.63	101.59	110.55
1	G	82	LYS	N-CA-C	-6.63	103.98	111.14
1	A	250	HIS	N-CA-C	-6.55	98.52	108.67
1	E	121	HIS	N-CA-C	6.44	120.72	112.86
1	A	249	PHE	N-CA-C	6.32	117.75	108.14
2	D	41	VAL	N-CA-C	6.17	118.35	108.85
2	B	57	LYS	N-CA-C	-6.16	101.82	110.50
1	A	78	GLU	N-CA-C	6.15	121.52	111.37
1	G	75	THR	N-CA-C	-6.13	105.28	112.89
1	E	115	LEU	N-CA-C	-5.99	98.75	108.52
1	G	134	LEU	N-CA-C	-5.98	104.84	111.36
1	E	78	GLU	N-CA-C	5.93	121.09	111.37
1	G	52	HIS	N-CA-C	5.91	120.49	113.16
1	A	6	SER	N-CA-C	5.88	119.27	111.75
1	C	52	HIS	N-CA-C	5.80	119.98	113.02
1	C	78	GLU	N-CA-C	5.78	118.04	111.11
1	C	249	PHE	N-CA-C	5.76	117.01	108.60
1	E	109	ASN	CA-C-N	5.71	126.10	119.47
1	E	109	ASN	C-N-CA	5.71	126.10	119.47
1	C	145	GLU	N-CA-C	-5.69	102.04	110.46
2	H	83	HIS	N-CA-C	5.57	118.70	109.46
1	G	322	VAL	N-CA-C	5.57	116.96	110.62
1	E	156	TYR	N-CA-C	5.55	120.11	113.23
1	C	138	VAL	N-CA-C	5.52	117.02	111.00
1	E	41	PRO	N-CA-C	5.50	119.95	111.21
1	C	41	PRO	N-CA-C	5.42	119.83	111.21
1	A	294	CYS	N-CA-C	5.33	116.38	108.60
2	B	64	GLY	N-CA-C	-5.29	105.85	111.93
1	A	75	THR	N-CA-C	-5.26	106.37	112.89
2	D	83	HIS	N-CA-C	5.25	117.80	109.24
1	E	251	GLU	N-CA-C	5.24	117.48	110.35
2	H	15	ILE	N-CA-C	5.22	117.38	108.86
2	H	41	VAL	N-CA-C	5.21	116.22	108.46
1	A	245	LEU	N-CA-C	5.13	119.54	113.12
1	E	197	THR	N-CA-C	5.13	117.77	111.82
1	A	4	THR	N-CA-C	5.12	121.29	113.61
1	C	51	ILE	N-CA-C	5.08	119.91	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	200	VAL	N-CA-C	5.06	116.24	111.48
1	A	251	GLU	N-CA-C	5.06	117.57	110.23
1	C	54	VAL	CA-C-N	5.00	125.44	120.14
1	C	54	VAL	C-N-CA	5.00	125.44	120.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2584	0	2522	109	0
1	C	2590	0	2527	106	0
1	E	2584	0	2522	101	0
1	G	2582	0	2526	132	0
2	B	1064	0	1028	46	0
2	D	1368	0	1344	62	0
2	F	468	0	475	16	0
2	H	1368	0	1344	53	0
3	A	32	0	26	2	0
3	C	32	0	26	2	0
3	E	32	0	26	1	0
3	G	32	0	26	7	0
4	A	52	0	0	2	0
4	B	4	0	0	1	0
4	C	56	0	0	0	0
4	D	13	0	0	1	0
4	E	62	0	0	4	0
4	F	2	0	0	0	0
4	G	29	0	0	0	0
4	H	11	0	0	1	0
All	All	14965	0	14392	605	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 21.

All (605) 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:G:82:LYS:HD2	1:G:291:MET:HE1	1.36	1.07
1:A:124:MET:HG2	1:A:128:MET:HE2	1.36	1.07
2:B:116:THR:HB	2:B:124:SER:HB3	1.48	0.95
1:C:124:MET:HG2	1:C:128:MET:HE2	1.48	0.95
1:C:206:LYS:H	1:C:206:LYS:HD2	1.28	0.94
2:F:44:ARG:HE	2:F:51:ARG:HH12	1.03	0.94
1:E:243:ILE:HD13	1:E:307:LEU:HD21	1.50	0.93
1:G:33:ARG:HH21	1:G:33:ARG:HG3	1.35	0.91
1:G:28:ARG:HE	1:G:28:ARG:HA	1.36	0.90
1:C:247:ASN:HD22	3:C:991:KAA:HN8	1.12	0.89
1:A:102:GLU:HG3	1:C:61:VAL:HG13	1.53	0.89
2:B:44:ARG:HG3	2:B:51:ARG:NH1	1.89	0.88
1:C:197:THR:HG21	2:D:32:PRO:HG3	1.57	0.87
1:G:144:ALA:HB2	1:G:209:PRO:HB2	1.56	0.87
1:E:61:VAL:HG22	1:G:102:GLU:HG2	1.59	0.85
1:G:159:ILE:HG13	1:G:172:VAL:HG21	1.58	0.85
2:B:71:ASN:HD22	2:B:71:ASN:H	1.24	0.85
2:F:44:ARG:NE	2:F:51:ARG:HH12	1.75	0.84
1:C:206:LYS:HD2	1:C:206:LYS:N	1.91	0.84
2:F:44:ARG:HE	2:F:51:ARG:NH1	1.75	0.84
2:D:139:ASP:O	2:D:152:LYS:HE3	1.76	0.84
1:E:110:PRO:HG2	1:E:322:VAL:HG11	1.58	0.83
1:G:124:MET:HE1	1:G:213:TYR:HB2	1.59	0.83
1:C:159:ILE:HG13	1:C:172:VAL:HG21	1.62	0.81
1:G:235:ARG:HA	1:G:249:PHE:HB3	1.63	0.81
1:C:104:MET:HE1	1:C:322:VAL:HG21	1.64	0.80
1:A:166:LYS:HB3	1:A:170:ARG:HH22	1.47	0.80
1:G:181:VAL:HG13	1:G:194:LEU:HD21	1.63	0.80
1:C:206:LYS:H	1:C:206:LYS:CD	1.90	0.80
1:A:281:GLN:H	1:A:281:GLN:CD	1.89	0.79
1:E:40:THR:HB	1:E:41:PRO:HD2	1.65	0.79
1:A:159:ILE:HG13	1:A:172:VAL:HG21	1.62	0.79
1:G:40:THR:H	1:G:94:GLN:HE22	1.29	0.79
1:G:266:ASN:HB3	1:G:276:GLN:HE21	1.46	0.78
2:B:100:ILE:HG22	2:B:125:VAL:HG21	1.66	0.78
1:G:120:PRO:HA	1:G:294:CYS:HB3	1.64	0.78
1:A:122:TYR:CD2	1:A:126:ARG:HG2	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:ILE:HD13	1:G:307:LEU:HD21	1.66	0.76
1:A:18:LYS:HE3	1:A:309:LEU:HD22	1.68	0.76
1:E:299:LEU:C	1:E:299:LEU:HD12	2.11	0.76
2:H:100:ILE:HD12	2:H:101:GLY:N	2.01	0.75
1:A:181:VAL:HG13	1:A:194:LEU:HD11	1.68	0.75
2:B:71:ASN:H	2:B:71:ASN:ND2	1.83	0.75
2:H:129:ASN:HB3	2:H:179:ARG:HH21	1.51	0.75
1:C:176:LEU:HD13	1:C:178:LEU:HD12	1.69	0.75
1:G:4:THR:HB	1:G:8:GLN:NE2	2.02	0.75
1:G:141:CYS:HB2	1:G:142:PRO:HD2	1.67	0.75
2:D:86:ASN:HB3	2:D:88:GLU:OE1	1.87	0.75
1:C:40:THR:H	1:C:94:GLN:HE22	1.35	0.74
1:A:110:PRO:HG2	1:A:322:VAL:HG11	1.69	0.74
1:C:204:ILE:HA	1:C:206:LYS:HE3	1.70	0.74
1:G:60:PHE:HD1	1:G:69:MET:HE2	1.51	0.74
2:D:41:VAL:HG22	2:D:43:LEU:HD11	1.70	0.74
1:G:130:GLU:HA	1:G:133:ASP:OD1	1.87	0.74
2:B:71:ASN:HD22	2:B:71:ASN:N	1.84	0.73
1:G:33:ARG:HG3	1:G:33:ARG:NH2	2.03	0.73
1:C:147:LEU:HD12	1:C:152:ALA:HB2	1.70	0.73
2:D:177:ASP:OD2	2:D:179:ARG:HD3	1.89	0.72
1:E:222:LEU:HD22	1:E:258:GLN:HE22	1.55	0.72
2:B:89:THR:O	2:B:90:PHE:HB2	1.89	0.71
1:G:28:ARG:HE	1:G:28:ARG:CA	2.01	0.71
2:D:16:MET:O	2:D:17:LEU:HD12	1.90	0.71
1:A:144:ALA:HB2	1:A:209:PRO:HG2	1.73	0.71
1:E:81:MET:HE1	1:E:116:GLU:HB3	1.71	0.71
2:B:100:ILE:HD12	2:B:101:GLY:N	2.05	0.70
1:C:165:ASP:H	1:C:168:GLN:NE2	1.88	0.70
1:C:189:ASP:OD2	1:C:218:SER:HB3	1.92	0.70
1:G:241:LYS:HD2	1:G:307:LEU:HD22	1.71	0.70
2:H:44:ARG:NH1	2:H:51:ARG:HD3	2.07	0.70
1:G:211:PHE:CE1	1:G:238:VAL:HG22	2.27	0.69
1:A:148:SER:OG	1:A:151:GLN:HG2	1.92	0.69
1:A:166:LYS:HB3	1:A:170:ARG:NH2	2.07	0.69
2:H:44:ARG:HH12	2:H:51:ARG:HH21	1.40	0.69
1:A:229:ASP:OD1	1:A:231:ARG:HD3	1.93	0.69
1:G:169:LEU:HD21	1:G:192:LEU:HD13	1.74	0.69
1:A:166:LYS:HA	1:A:169:LEU:CD2	2.24	0.68
1:G:306:MET:HG3	1:G:311:ALA:HB3	1.76	0.68
2:B:24:VAL:HA	2:B:43:LEU:HD23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:109:ASP:O	2:H:110:GLN:HB2	1.94	0.68
1:E:66:SER:HB3	1:E:67:GLN:HE22	1.58	0.67
1:G:268:LYS:O	1:G:272:ARG:HG3	1.94	0.67
2:H:52:VAL:HG22	2:H:53:GLU:N	2.10	0.67
1:C:60:PHE:HD1	1:C:69:MET:HE2	1.59	0.67
2:D:109:ASP:O	2:D:110:GLN:HB2	1.95	0.67
2:H:16:MET:O	2:H:17:LEU:HD12	1.95	0.67
1:E:66:SER:HB3	1:E:67:GLN:NE2	2.10	0.66
2:D:88:GLU:CD	2:D:89:THR:H	2.02	0.66
1:A:247:ASN:HD22	3:A:990:KAA:HN8	1.43	0.66
1:C:40:THR:H	1:C:94:GLN:NE2	1.92	0.66
2:D:89:THR:O	2:D:90:PHE:HB2	1.94	0.66
1:G:122:TYR:CD2	1:G:126:ARG:HB3	2.30	0.66
1:C:78:GLU:HG3	1:C:118:TYR:OH	1.96	0.66
1:G:28:ARG:HA	1:G:28:ARG:NE	2.08	0.66
1:G:164:ALA:HB1	1:G:168:GLN:HB3	1.77	0.65
2:D:44:ARG:HH12	2:D:51:ARG:CZ	2.08	0.65
1:A:13:ILE:HB	1:A:14:PRO:HD3	1.79	0.65
1:E:77:PRO:HB2	1:E:81:MET:HE2	1.79	0.65
1:C:247:ASN:ND2	3:C:991:KAA:HN8	1.92	0.65
2:D:89:THR:HG22	2:D:91:GLU:OE1	1.96	0.65
1:G:40:THR:H	1:G:94:GLN:NE2	1.94	0.65
1:E:61:VAL:CG2	1:G:102:GLU:HG2	2.27	0.65
1:A:141:CYS:HB2	1:A:142:PRO:HD2	1.79	0.64
1:E:44:SER:HB3	1:E:74:MET:HE3	1.79	0.64
2:B:77:ASN:ND2	2:B:79:GLY:H	1.95	0.64
1:E:241:LYS:O	1:E:243:ILE:HD12	1.97	0.64
1:G:33:ARG:HD3	1:G:130:GLU:OE1	1.98	0.64
1:G:148:SER:OG	1:G:151:GLN:HG2	1.97	0.64
1:A:166:LYS:HA	1:A:169:LEU:HD21	1.80	0.63
2:D:82:TRP:CD2	2:D:100:ILE:HG13	2.33	0.63
1:G:10:SER:HB3	1:G:324:ARG:HD2	1.80	0.63
1:C:23:MET:HE1	1:C:113:THR:HG21	1.80	0.63
2:B:87:ASN:N	2:B:87:ASN:HD22	1.95	0.63
1:C:165:ASP:H	1:C:168:GLN:HE21	1.46	0.63
2:D:72:LEU:HD12	2:D:115:VAL:HG21	1.80	0.63
2:B:17:LEU:HB2	2:B:22:TYR:CE1	2.34	0.62
1:C:18:LYS:HD2	1:C:309:LEU:HD22	1.81	0.62
1:G:124:MET:CE	1:G:213:TYR:HB2	2.29	0.62
1:C:147:LEU:HD12	1:C:152:ALA:CB	2.29	0.62
1:C:109:ASN:HB2	1:C:314:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LEU:HD21	1:C:192:LEU:HD13	1.80	0.62
2:H:97:ALA:HA	2:H:100:ILE:HD11	1.82	0.62
2:F:9:PHE:HD2	2:F:41:VAL:HG21	1.65	0.62
1:E:189:ASP:OD1	1:E:218:SER:HB2	1.99	0.61
2:D:41:VAL:HG22	2:D:43:LEU:CD1	2.31	0.61
1:A:266:ASN:HB3	1:A:276:GLN:HE21	1.66	0.61
2:H:48:THR:O	2:H:50:THR:HG23	2.01	0.61
1:C:125:TYR:HA	1:C:128:MET:HE3	1.83	0.60
1:C:265:ASP:O	1:C:269:ARG:HG3	2.02	0.60
1:A:243:ILE:HG13	1:A:307:LEU:HD11	1.84	0.60
1:G:136:GLN:OE1	1:G:143:ALA:HA	2.02	0.60
1:A:291:MET:HE3	1:A:294:CYS:SG	2.41	0.60
2:D:50:THR:HG22	2:D:51:ARG:O	2.00	0.60
1:A:240:TYR:HD2	1:A:307:LEU:HD23	1.67	0.60
1:C:173:ALA:O	1:C:176:LEU:HD12	2.01	0.60
2:D:88:GLU:CG	2:D:89:THR:N	2.65	0.60
1:A:57:GLU:HG2	1:A:72:TRP:CZ3	2.37	0.59
1:C:182:ALA:O	1:C:185:GLU:HB3	2.02	0.59
1:E:61:VAL:HG22	1:G:102:GLU:CG	2.30	0.59
1:A:120:PRO:HA	1:A:294:CYS:HB3	1.83	0.59
1:A:162:LEU:HB3	1:A:231:ARG:NH2	2.17	0.59
1:C:203:ASN:O	1:C:206:LYS:HE3	2.01	0.59
1:C:217:ALA:HB1	1:C:225:ILE:HD12	1.84	0.59
1:E:247:ASN:HD22	3:E:992:KAA:HN8	1.50	0.59
1:G:237:GLU:HG2	1:G:247:ASN:HA	1.82	0.59
1:E:186:GLU:O	1:E:186:GLU:HG3	2.02	0.59
1:A:44:SER:HB3	1:A:74:MET:HE3	1.85	0.59
2:D:88:GLU:HG2	2:D:89:THR:N	2.16	0.59
2:H:129:ASN:HB3	2:H:179:ARG:NH2	2.17	0.59
1:C:223:ALA:HB2	1:C:249:PHE:CG	2.38	0.58
1:E:265:ASP:O	1:E:269:ARG:HG3	2.03	0.58
1:A:162:LEU:HB3	1:A:231:ARG:HH21	1.67	0.58
1:E:107:TYR:CE1	1:E:306:MET:HE1	2.38	0.58
1:A:166:LYS:HE2	1:A:186:GLU:O	2.04	0.58
1:A:181:VAL:O	1:A:181:VAL:HG22	2.04	0.58
2:B:97:ALA:HA	2:B:100:ILE:HD11	1.86	0.58
1:E:74:MET:HA	1:E:74:MET:HE2	1.85	0.58
1:E:253:THR:HG22	1:E:291:MET:HE2	1.86	0.57
2:H:139:ASP:O	2:H:152:LYS:HE2	2.03	0.57
1:E:102:GLU:HG2	1:G:61:VAL:HG22	1.85	0.57
1:E:44:SER:HB3	1:E:74:MET:CE	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PRO:HG2	1:A:208:LYS:HB3	1.86	0.57
1:E:43:MET:HE2	1:G:111:GLU:HB3	1.86	0.57
1:A:265:ASP:O	1:A:269:ARG:HG3	2.05	0.57
1:A:44:SER:HB3	1:A:74:MET:CE	2.35	0.57
2:D:88:GLU:OE1	2:D:88:GLU:N	2.36	0.57
1:E:77:PRO:CG	1:E:81:MET:HE2	2.35	0.57
1:E:116:GLU:HG3	1:E:298:ALA:HB2	1.85	0.57
2:F:24:VAL:HA	2:F:43:LEU:HD23	1.87	0.57
1:E:230:HIS:HB2	4:E:353:HOH:O	2.05	0.57
1:C:120:PRO:HA	1:C:294:CYS:HB3	1.85	0.56
1:C:144:ALA:HB2	1:C:209:PRO:HB2	1.87	0.56
2:D:12:GLY:O	2:D:14:LYS:HE3	2.04	0.56
1:E:235:ARG:HA	1:E:249:PHE:HB3	1.87	0.56
1:G:154:LEU:HD23	1:G:159:ILE:C	2.30	0.56
1:A:126:ARG:HD2	4:A:335:HOH:O	2.03	0.56
1:G:107:TYR:CD1	1:G:306:MET:HE1	2.40	0.56
1:E:246:ALA:HB2	1:E:299:LEU:HB2	1.86	0.56
1:A:150:GLN:HG3	1:A:162:LEU:HD22	1.88	0.56
1:C:229:ASP:OD1	1:C:231:ARG:HB2	2.06	0.56
1:G:161:PRO:HG2	1:G:162:LEU:CD1	2.36	0.56
2:H:32:PRO:HG2	2:H:35:GLY:HA3	1.86	0.56
1:C:189:ASP:O	1:C:193:GLN:HG3	2.06	0.56
2:B:9:PHE:HD2	2:B:41:VAL:HG21	1.71	0.56
2:D:11:ALA:HA	2:D:24:VAL:O	2.06	0.56
1:G:161:PRO:HG2	1:G:162:LEU:HD13	1.87	0.56
1:A:51:ILE:HD11	1:A:268:LYS:HD2	1.89	0.55
1:C:166:LYS:HG2	1:C:170:ARG:HH22	1.71	0.55
1:E:156:TYR:O	1:E:157:LEU:HD23	2.05	0.55
1:E:181:VAL:HG23	1:E:194:LEU:HD21	1.87	0.55
1:E:223:ALA:HB2	1:E:249:PHE:CG	2.41	0.55
2:H:152:LYS:HE3	2:H:166:LEU:HA	1.87	0.55
2:D:105:LYS:HB2	2:D:160:ALA:HB2	1.89	0.55
1:G:78:GLU:OE2	3:G:993:KAA:NZ	2.40	0.55
1:G:185:GLU:HA	1:G:185:GLU:OE1	2.06	0.55
2:D:43:LEU:HD12	2:D:43:LEU:N	2.21	0.55
1:G:60:PHE:CD1	1:G:69:MET:HE2	2.38	0.55
1:A:132:ASP:CG	1:A:136:GLN:HE21	2.15	0.55
1:A:200:VAL:O	1:A:204:ILE:HG12	2.06	0.55
1:A:235:ARG:HA	1:A:249:PHE:HB3	1.88	0.54
2:B:8:ASP:O	2:B:10:ARG:HG2	2.07	0.54
1:G:247:ASN:O	3:G:993:KAA:HD2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:133:LEU:HD12	2:H:156:LEU:HD23	1.89	0.54
1:G:145:GLU:O	1:G:145:GLU:HG3	2.06	0.54
1:G:40:THR:HB	1:G:41:PRO:HD2	1.88	0.54
1:G:146:SER:O	1:G:147:LEU:HD12	2.08	0.54
1:A:102:GLU:HA	1:C:61:VAL:O	2.07	0.54
1:E:54:VAL:HG22	1:E:101:ASN:HB3	1.90	0.54
2:D:108:LEU:O	2:D:109:ASP:C	2.51	0.54
1:E:77:PRO:CB	1:E:81:MET:HE2	2.38	0.54
1:A:191:LEU:O	1:A:195:LEU:HD13	2.07	0.54
1:E:221:SER:C	1:E:222:LEU:HD23	2.33	0.54
2:H:137:ASP:HA	2:H:170:ILE:HD11	1.88	0.54
1:G:201:GLU:HB2	1:G:202:PRO:HD3	1.89	0.54
1:A:40:THR:HB	1:A:41:PRO:HD2	1.89	0.54
1:G:181:VAL:CG1	1:G:194:LEU:HD21	2.37	0.54
1:A:202:PRO:O	1:A:206:LYS:HE3	2.07	0.54
2:B:89:THR:HG22	2:B:91:GLU:OE1	2.08	0.53
1:E:181:VAL:HG23	1:E:182:ALA:N	2.23	0.53
1:G:249:PHE:CE1	3:G:993:KAA:HE2	2.43	0.53
1:A:240:TYR:CD2	1:A:307:LEU:HD23	2.42	0.53
1:C:40:THR:HB	1:C:41:PRO:HD2	1.90	0.53
2:D:44:ARG:NH1	2:D:51:ARG:HD3	2.23	0.53
1:E:263:GLU:OE1	1:E:263:GLU:HA	2.07	0.53
2:H:52:VAL:CG2	2:H:53:GLU:N	2.70	0.53
1:G:204:ILE:HB	1:G:210:THR:HG21	1.90	0.53
2:D:44:ARG:HH12	2:D:51:ARG:NE	2.06	0.53
1:C:141:CYS:HB2	1:C:142:PRO:HD2	1.90	0.53
1:E:122:TYR:CE2	1:E:126:ARG:HD2	2.43	0.53
1:G:259:GLN:O	1:G:263:GLU:HG3	2.07	0.53
1:A:178:LEU:HD13	1:A:194:LEU:HD22	1.91	0.53
1:G:135:LEU:O	1:G:139:LEU:HB2	2.09	0.53
1:A:41:PRO:HG2	1:A:80:HIS:CE1	2.44	0.53
1:G:179:SER:HB3	1:G:183:ASP:OD1	2.09	0.53
2:H:34:LYS:HG2	2:H:34:LYS:O	2.09	0.53
2:H:42:LYS:HG2	2:H:53:GLU:HG2	1.91	0.53
1:E:299:LEU:C	1:E:299:LEU:CD1	2.80	0.53
1:C:150:GLN:O	1:C:154:LEU:HD22	2.08	0.52
1:C:226:SER:HB3	1:C:229:ASP:O	2.09	0.52
1:C:132:ASP:O	1:C:136:GLN:HG3	2.10	0.52
1:E:201:GLU:HB2	1:E:202:PRO:HD3	1.90	0.52
1:C:169:LEU:HD21	1:C:192:LEU:CD1	2.39	0.52
1:C:197:THR:HG21	2:D:32:PRO:CG	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:THR:HG22	2:D:51:ARG:N	2.25	0.52
2:D:106:TRP:CZ3	2:D:176:VAL:HG21	2.45	0.52
2:F:17:LEU:HB2	2:F:22:TYR:CE1	2.44	0.52
1:G:59:ARG:HH21	1:G:59:ARG:HG3	1.74	0.52
1:A:194:LEU:HD23	1:A:198:PHE:HD1	1.75	0.52
1:E:77:PRO:HG2	1:E:81:MET:HE2	1.89	0.52
1:G:12:SER:HB2	1:G:14:PRO:HD2	1.90	0.52
1:A:283:LEU:O	1:A:287:LEU:HG	2.10	0.52
2:B:73:THR:HG21	2:B:87:ASN:HD21	1.74	0.52
1:G:306:MET:HA	1:G:317:VAL:HG11	1.92	0.52
1:G:59:ARG:HG3	1:G:59:ARG:NH2	2.25	0.52
1:G:60:PHE:HD1	1:G:69:MET:CE	2.22	0.52
1:A:119:ARG:HG2	1:A:122:TYR:CD2	2.44	0.52
1:C:18:LYS:HD2	1:C:309:LEU:CD2	2.40	0.52
2:D:88:GLU:CG	2:D:89:THR:H	2.23	0.52
2:D:139:ASP:O	2:D:152:LYS:CE	2.53	0.51
1:G:47:THR:OG1	1:G:48:VAL:N	2.43	0.51
2:H:43:LEU:N	2:H:43:LEU:HD12	2.25	0.51
1:A:49:THR:O	1:A:50:ASP:C	2.53	0.51
1:A:148:SER:H	1:A:151:GLN:CG	2.22	0.51
2:B:100:ILE:CG2	2:B:125:VAL:HG21	2.39	0.51
1:G:247:ASN:HD22	3:G:993:KAA:HN8	1.59	0.51
1:A:147:LEU:O	1:A:212:VAL:HA	2.09	0.51
1:C:107:TYR:CD1	1:C:306:MET:HE1	2.46	0.51
1:E:112:PHE:HB2	1:E:302:ASP:OD2	2.10	0.51
1:A:223:ALA:HB2	1:A:249:PHE:CG	2.45	0.51
1:E:77:PRO:HG2	1:E:81:MET:CE	2.40	0.51
1:G:78:GLU:O	1:G:82:LYS:HG2	2.10	0.51
1:A:99:PHE:N	1:A:99:PHE:CD1	2.78	0.51
2:B:70:MET:HE3	2:B:86:ASN:ND2	2.25	0.51
1:G:217:ALA:HA	1:G:233:ALA:HB2	1.92	0.51
1:G:296:GLY:O	3:G:993:KAA:HE1	2.11	0.51
2:B:3:THR:HA	2:B:62:ALA:O	2.11	0.51
2:D:44:ARG:HH21	2:D:44:ARG:HG3	1.76	0.51
1:E:252:LEU:HD23	1:E:258:GLN:OE1	2.11	0.51
1:E:325:ALA:O	1:G:80:HIS:HE1	1.94	0.51
2:F:11:ALA:HA	2:F:24:VAL:O	2.11	0.51
2:D:31:LYS:NZ	4:D:201:HOH:O	2.44	0.50
2:H:72:LEU:HD11	2:H:93:LEU:HD12	1.93	0.50
1:E:86:VAL:HG22	1:E:291:MET:HA	1.91	0.50
1:E:185:GLU:HG3	1:E:191:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:MET:HE3	1:C:71:LEU:HD21	1.92	0.50
1:E:144:ALA:HB2	1:E:209:PRO:HB2	1.93	0.50
1:G:39:GLU:HA	1:G:94:GLN:NE2	2.27	0.50
1:G:123:ASP:C	1:G:125:TYR:H	2.19	0.50
1:A:169:LEU:HD23	1:A:170:ARG:N	2.26	0.50
1:E:291:MET:HE3	1:E:294:CYS:SG	2.51	0.50
2:B:44:ARG:CD	2:B:51:ARG:HH12	2.24	0.50
1:C:245:LEU:HD11	1:C:307:LEU:HD11	1.94	0.50
1:G:243:ILE:HD12	1:G:243:ILE:N	2.27	0.50
2:D:81:PHE:HB3	2:D:94:SER:HB3	1.92	0.50
2:H:86:ASN:CG	2:H:89:THR:HB	2.37	0.50
1:C:41:PRO:HG2	1:C:80:HIS:CE1	2.47	0.50
2:H:77:ASN:ND2	2:H:79:GLY:H	2.09	0.50
1:C:133:ASP:O	1:C:137:GLN:HB2	2.12	0.50
1:A:57:GLU:HG2	1:A:72:TRP:CE3	2.46	0.50
1:A:299:LEU:C	1:A:299:LEU:HD23	2.36	0.49
1:G:166:LYS:CG	1:G:170:ARG:HH22	2.24	0.49
1:E:13:ILE:HB	1:E:14:PRO:HD3	1.93	0.49
1:E:323:ASP:OD2	1:E:323:ASP:N	2.42	0.49
1:A:78:GLU:OE2	3:A:990:KAA:NZ	2.45	0.49
1:A:254:ASP:OD2	1:A:254:ASP:C	2.55	0.49
1:E:94:GLN:NE2	1:E:96:CYS:HB3	2.27	0.49
1:E:107:TYR:CD1	1:E:306:MET:HE1	2.47	0.49
1:G:50:ASP:O	1:G:269:ARG:NH2	2.43	0.49
1:E:188:ARG:HH21	1:E:188:ARG:HG3	1.78	0.49
1:C:112:PHE:HE1	1:C:114:MET:CG	2.26	0.49
1:C:154:LEU:HD13	1:C:159:ILE:O	2.12	0.49
1:C:163:SER:O	1:C:164:ALA:C	2.56	0.49
2:B:5:TYR:HB2	2:B:8:ASP:OD2	2.12	0.49
1:E:67:GLN:NE2	1:E:67:GLN:N	2.61	0.49
1:E:166:LYS:HB2	1:E:170:ARG:HH11	1.76	0.49
1:G:144:ALA:CB	1:G:209:PRO:HB2	2.36	0.49
1:A:302:ASP:HB2	1:A:314:LEU:HD11	1.95	0.49
1:C:166:LYS:HG2	1:C:170:ARG:NH2	2.26	0.49
1:E:18:LYS:O	1:E:21:ALA:HB3	2.13	0.49
1:G:120:PRO:HA	1:G:294:CYS:CB	2.39	0.49
1:A:223:ALA:HB2	1:A:249:PHE:CB	2.42	0.49
2:D:4:TYR:CE2	2:D:13:LEU:HD11	2.48	0.49
2:D:167:PHE:HE1	2:D:186:ARG:NH2	2.11	0.49
1:G:234:GLU:O	1:G:249:PHE:HB2	2.13	0.49
1:A:23:MET:HE2	1:C:39:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:PRO:HG2	1:E:208:LYS:HB3	1.94	0.48
2:B:4:TYR:CE2	2:B:13:LEU:HD11	2.48	0.48
1:C:109:ASN:O	1:C:110:PRO:C	2.56	0.48
2:D:114:ILE:HB	2:D:126:THR:HB	1.96	0.48
1:G:135:LEU:HD11	1:G:238:VAL:HG11	1.95	0.48
2:B:4:TYR:CZ	2:B:13:LEU:HD11	2.48	0.48
1:C:112:PHE:CE1	1:C:114:MET:HG3	2.48	0.48
1:G:153:PHE:CE1	1:G:157:LEU:HD12	2.48	0.48
2:H:6:SER:HA	2:H:9:PHE:CE2	2.49	0.48
1:A:45:GLN:HG3	4:A:329:HOH:O	2.13	0.48
2:B:96:ASP:O	2:B:100:ILE:HG13	2.14	0.48
2:B:118:TRP:HB2	2:B:123:ILE:HD13	1.95	0.48
2:D:100:ILE:HD12	2:D:107:LEU:HD11	1.95	0.48
1:A:94:GLN:NE2	1:A:96:CYS:HB3	2.28	0.48
1:G:13:ILE:N	1:G:14:PRO:CD	2.76	0.48
1:G:179:SER:O	1:G:183:ASP:HB2	2.14	0.48
2:H:108:LEU:O	2:H:109:ASP:C	2.55	0.48
1:A:119:ARG:HB3	1:A:122:TYR:HB2	1.95	0.48
2:H:100:ILE:HD12	2:H:100:ILE:C	2.39	0.48
2:H:177:ASP:OD2	2:H:179:ARG:HD3	2.14	0.48
1:A:99:PHE:HD2	1:C:43:MET:HE2	1.79	0.48
2:B:66:ASP:OD1	2:B:119:ASN:HA	2.14	0.48
1:C:197:THR:HA	1:C:201:GLU:HG3	1.96	0.48
1:G:12:SER:CB	1:G:14:PRO:HD2	2.43	0.48
2:B:44:ARG:HG3	2:B:51:ARG:HH12	1.72	0.47
2:H:152:LYS:NZ	2:H:168:VAL:O	2.44	0.47
1:A:17:LEU:HD12	1:C:36:LEU:HD13	1.95	0.47
2:H:89:THR:O	2:H:90:PHE:HB2	2.14	0.47
2:B:14:LYS:HA	2:B:22:TYR:O	2.14	0.47
2:B:23:ALA:HB3	2:B:44:ARG:HB3	1.95	0.47
1:G:86:VAL:HG22	1:G:291:MET:HB2	1.96	0.47
1:A:18:LYS:CE	1:A:309:LEU:HD22	2.40	0.47
1:E:94:GLN:HE21	1:E:96:CYS:HB3	1.79	0.47
1:A:74:MET:HE2	1:A:74:MET:HA	1.96	0.47
2:F:6:SER:HB3	2:F:39:ALA:HB2	1.97	0.47
1:A:47:THR:CG2	1:A:277:HIS:HB3	2.45	0.47
2:B:71:ASN:ND2	2:B:71:ASN:N	2.49	0.47
1:C:243:ILE:O	1:C:245:LEU:HD13	2.15	0.47
1:E:79:TYR:CD2	1:E:283:LEU:HD22	2.49	0.47
1:G:43:MET:HG2	1:G:73:LEU:HD23	1.96	0.47
1:G:159:ILE:HG13	1:G:172:VAL:CG2	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LYS:O	1:A:272:ARG:HG3	2.14	0.47
1:C:36:LEU:HB3	1:C:92:VAL:HG12	1.96	0.47
1:G:147:LEU:O	1:G:212:VAL:HA	2.15	0.47
1:A:94:GLN:HE21	1:A:96:CYS:HB3	1.80	0.47
1:G:116:GLU:HG3	1:G:298:ALA:HA	1.97	0.47
2:B:28:GLU:HG3	4:B:189:HOH:O	2.14	0.46
1:E:285:GLU:HA	1:E:285:GLU:OE2	2.15	0.46
1:G:223:ALA:HB2	1:G:249:PHE:CG	2.50	0.46
1:E:153:PHE:CB	1:E:161:PRO:HD3	2.45	0.46
1:E:299:LEU:HD12	1:E:299:LEU:O	2.16	0.46
1:G:166:LYS:HD3	1:G:186:GLU:OE2	2.14	0.46
1:G:175:LYS:C	1:G:177:ASP:H	2.22	0.46
2:H:105:LYS:HE3	2:H:106:TRP:CZ2	2.50	0.46
1:G:257:GLU:HA	1:G:260:GLN:HG2	1.98	0.46
2:H:137:ASP:HA	2:H:170:ILE:CD1	2.46	0.46
1:E:188:ARG:HG3	1:E:188:ARG:NH2	2.31	0.46
1:E:264:GLN:OE1	1:E:264:GLN:HA	2.16	0.46
1:G:153:PHE:HB3	1:G:161:PRO:HD3	1.98	0.46
2:H:111:ALA:HB2	4:H:199:HOH:O	2.16	0.46
2:D:6:SER:HB3	2:D:39:ALA:CB	2.45	0.46
1:E:120:PRO:HA	1:E:294:CYS:HB3	1.97	0.46
1:E:278:PRO:HG2	4:E:350:HOH:O	2.16	0.46
1:G:29:PHE:CD1	1:G:29:PHE:C	2.94	0.46
1:A:102:GLU:HG3	1:C:61:VAL:CG1	2.37	0.46
1:E:13:ILE:N	1:E:14:PRO:CD	2.77	0.46
2:H:109:ASP:O	2:H:110:GLN:CB	2.64	0.46
1:E:10:SER:HB3	1:E:324:ARG:HD3	1.97	0.46
1:A:4:THR:O	1:A:5:ALA:C	2.59	0.46
2:B:70:MET:HE3	2:B:86:ASN:HD21	1.80	0.46
1:G:33:ARG:NH2	1:G:33:ARG:CG	2.75	0.46
1:C:115:LEU:HD13	1:C:117:TRP:CZ3	2.51	0.46
1:G:37:GLU:HA	1:G:93:PHE:O	2.16	0.46
1:G:236:PHE:CD1	1:G:236:PHE:C	2.93	0.46
1:E:181:VAL:HG23	1:E:182:ALA:H	1.81	0.45
1:C:49:THR:O	1:C:50:ASP:C	2.59	0.45
1:C:206:LYS:N	1:C:206:LYS:CD	2.62	0.45
2:B:44:ARG:CG	2:B:51:ARG:NH1	2.71	0.45
2:D:100:ILE:HG21	2:D:104:ALA:HB2	1.98	0.45
1:C:112:PHE:HE1	1:C:114:MET:HG3	1.81	0.45
1:C:266:ASN:HB3	1:C:276:GLN:OE1	2.17	0.45
2:D:50:THR:CG2	2:D:51:ARG:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:CYS:O	1:G:73:LEU:HA	2.17	0.45
1:A:305:VAL:O	1:A:309:LEU:HG	2.17	0.45
1:C:78:GLU:OE2	1:C:222:LEU:HD22	2.16	0.45
1:C:148:SER:OG	1:C:151:GLN:HG2	2.17	0.45
1:C:165:ASP:CG	1:C:168:GLN:HE21	2.25	0.45
2:D:86:ASN:HB2	2:D:91:GLU:O	2.16	0.45
1:E:25:GLU:HG3	4:E:387:HOH:O	2.16	0.45
2:H:118:TRP:CE2	2:H:119:ASN:ND2	2.84	0.45
1:A:195:LEU:O	1:A:199:GLY:N	2.49	0.45
1:C:322:VAL:HG23	1:C:323:ASP:N	2.30	0.45
1:G:45:GLN:HE21	1:G:45:GLN:HB3	1.56	0.45
1:G:77:PRO:O	1:G:81:MET:HG3	2.17	0.45
2:H:56:PHE:N	2:H:56:PHE:CD1	2.85	0.45
2:H:139:ASP:O	2:H:152:LYS:CD	2.64	0.45
1:A:44:SER:C	1:A:71:LEU:HD12	2.41	0.45
1:A:258:GLN:NE2	1:A:262:PHE:CZ	2.85	0.45
1:E:99:PHE:CD1	1:E:99:PHE:N	2.84	0.45
1:G:74:MET:HE2	1:G:80:HIS:HD2	1.81	0.45
1:G:166:LYS:CA	1:G:166:LYS:HE3	2.46	0.45
2:H:12:GLY:O	2:H:14:LYS:HE3	2.16	0.45
1:E:168:GLN:O	1:E:172:VAL:HG23	2.17	0.45
1:E:182:ALA:O	1:E:185:GLU:HB3	2.17	0.45
1:G:79:TYR:CG	1:G:283:LEU:HD22	2.51	0.45
1:C:153:PHE:HB3	1:C:161:PRO:HD3	1.98	0.45
1:E:83:ARG:CZ	1:E:282:ASN:HB3	2.47	0.45
1:A:54:VAL:HG22	1:A:101:ASN:HB3	1.99	0.44
2:B:5:TYR:O	2:B:6:SER:C	2.61	0.44
1:A:169:LEU:HD23	1:A:169:LEU:C	2.43	0.44
1:E:155:ARG:HD2	1:E:156:TYR:CE1	2.53	0.44
1:G:170:ARG:HD3	1:G:183:ASP:HA	1.98	0.44
1:C:157:LEU:O	1:C:159:ILE:HG12	2.17	0.44
1:G:17:LEU:O	1:G:17:LEU:HD23	2.17	0.44
2:H:96:ASP:OD1	2:H:96:ASP:C	2.60	0.44
1:G:17:LEU:HD23	1:G:17:LEU:C	2.43	0.44
1:A:165:ASP:HB3	1:A:168:GLN:HE22	1.83	0.44
1:G:48:VAL:HG12	1:G:79:TYR:CZ	2.51	0.44
2:B:66:ASP:O	2:B:118:TRP:HD1	2.00	0.44
1:E:297:VAL:HG22	1:E:298:ALA:N	2.32	0.44
1:E:302:ASP:HB2	4:E:360:HOH:O	2.17	0.44
1:A:104:MET:HG2	1:A:105:GLY:N	2.32	0.44
1:E:79:TYR:CG	1:E:283:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:ARG:HG2	1:E:236:PHE:N	2.32	0.44
2:H:52:VAL:CG2	2:H:53:GLU:H	2.30	0.44
1:A:204:ILE:CG2	1:A:210:THR:HB	2.48	0.44
2:B:44:ARG:CG	2:B:51:ARG:HH12	2.30	0.44
1:A:36:LEU:HB3	1:A:92:VAL:HG12	2.00	0.44
1:A:43:MET:HE2	1:C:111:GLU:HB3	1.99	0.44
1:A:154:LEU:HD23	1:A:159:ILE:O	2.18	0.44
2:B:5:TYR:O	2:B:7:ASN:N	2.51	0.44
1:C:223:ALA:HB2	1:C:249:PHE:CB	2.47	0.44
2:D:44:ARG:HH12	2:D:51:ARG:HD3	1.83	0.44
1:E:49:THR:O	1:E:50:ASP:C	2.60	0.44
2:H:52:VAL:HG22	2:H:53:GLU:H	1.83	0.44
1:A:119:ARG:HG3	1:A:119:ARG:HH11	1.83	0.43
1:A:181:VAL:O	1:A:181:VAL:CG2	2.66	0.43
1:A:281:GLN:CD	1:A:281:GLN:N	2.68	0.43
2:B:73:THR:CG2	2:B:87:ASN:HD21	2.31	0.43
2:D:54:LYS:HE2	2:D:54:LYS:HB3	1.86	0.43
2:H:167:PHE:CE1	2:H:186:ARG:NH2	2.86	0.43
1:C:107:TYR:CE1	1:C:306:MET:HE1	2.53	0.43
1:C:181:VAL:HG21	1:C:194:LEU:HD11	1.98	0.43
1:G:105:GLY:HA3	2:H:29:PHE:HB3	1.99	0.43
1:C:149:TYR:CD2	1:C:216:PRO:HD3	2.54	0.43
2:D:10:ARG:O	2:D:11:ALA:C	2.61	0.43
1:E:256:ARG:HG2	1:E:260:GLN:NE2	2.33	0.43
1:A:204:ILE:CG2	1:A:205:GLY:N	2.81	0.43
1:C:221:SER:H	2:D:34:LYS:HZ3	1.66	0.43
1:E:116:GLU:HG3	1:E:298:ALA:CB	2.49	0.43
1:G:74:MET:HE3	1:G:76:SER:O	2.19	0.43
1:G:258:GLN:HG3	1:G:262:PHE:CE2	2.54	0.43
2:H:118:TRP:HB2	2:H:123:ILE:HD13	2.01	0.43
1:A:33:ARG:HH21	1:A:33:ARG:HG3	1.84	0.43
1:A:170:ARG:HD3	1:A:183:ASP:HA	2.00	0.43
1:C:189:ASP:OD2	1:C:218:SER:CB	2.64	0.43
2:F:27:SER:OG	2:F:41:VAL:HG22	2.19	0.43
2:D:170:ILE:HG22	2:D:171:GLY:N	2.33	0.43
1:E:165:ASP:CG	1:E:167:THR:HG1	2.25	0.43
2:F:46:LEU:O	2:F:47:LEU:C	2.62	0.43
1:G:143:ALA:O	1:G:208:LYS:HD2	2.18	0.43
1:C:200:VAL:O	1:C:204:ILE:HG23	2.18	0.43
1:E:256:ARG:HD3	1:E:260:GLN:HE22	1.83	0.43
1:G:123:ASP:OD2	1:G:123:ASP:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:GLU:OE2	2:H:63:GLU:HA	2.18	0.43
1:C:120:PRO:HA	1:C:294:CYS:CB	2.49	0.43
1:C:195:LEU:O	1:C:199:GLY:N	2.50	0.43
1:E:115:LEU:HD13	1:E:117:TRP:CZ3	2.54	0.43
1:A:7:TRP:CE2	1:A:8:GLN:HG3	2.53	0.42
1:A:163:SER:O	1:A:164:ALA:C	2.62	0.42
2:B:87:ASN:N	2:B:87:ASN:ND2	2.66	0.42
2:D:42:LYS:C	2:D:43:LEU:HD12	2.44	0.42
1:G:248:GLY:HA2	1:G:297:VAL:HA	2.01	0.42
1:A:115:LEU:HB2	1:A:301:VAL:CG2	2.49	0.42
1:C:51:ILE:H	1:C:51:ILE:HG13	1.59	0.42
2:D:109:ASP:O	2:D:110:GLN:CB	2.62	0.42
1:G:109:ASN:HB2	1:G:314:LEU:HD23	2.01	0.42
1:G:154:LEU:HD23	1:G:159:ILE:O	2.18	0.42
1:G:240:TYR:HD2	1:G:307:LEU:HD13	1.84	0.42
2:H:46:LEU:HD13	2:H:67:VAL:HG11	2.00	0.42
1:A:57:GLU:CG	1:A:72:TRP:CZ3	3.02	0.42
1:C:13:ILE:N	1:C:14:PRO:CD	2.82	0.42
2:D:44:ARG:HH12	2:D:51:ARG:CD	2.32	0.42
1:G:85:LEU:HD12	1:G:85:LEU:HA	1.87	0.42
1:C:185:GLU:HG3	1:C:191:LEU:HG	2.01	0.42
1:E:245:LEU:HD21	1:E:307:LEU:HD12	2.01	0.42
2:F:20:GLU:HB2	2:F:22:TYR:CE1	2.54	0.42
2:H:77:ASN:ND2	2:H:78:ASP:N	2.67	0.42
1:A:236:PHE:CD1	1:A:236:PHE:C	2.97	0.42
2:B:40:ARG:NH1	2:B:55:THR:OG1	2.48	0.42
2:B:117:LEU:HD13	2:B:120:GLY:O	2.20	0.42
2:D:48:THR:C	2:D:50:THR:N	2.78	0.42
1:E:112:PHE:N	1:E:112:PHE:CD1	2.87	0.42
1:E:189:ASP:OD1	1:E:218:SER:CB	2.66	0.42
1:E:200:VAL:O	1:E:201:GLU:C	2.62	0.42
2:H:57:LYS:HB2	2:H:60:ASP:CG	2.45	0.42
2:H:71:ASN:O	2:H:72:LEU:HD23	2.20	0.42
1:C:8:GLN:HE21	1:C:8:GLN:HB3	1.60	0.42
2:D:6:SER:HB3	2:D:39:ALA:HB3	2.00	0.42
2:D:72:LEU:HD11	2:D:93:LEU:HD12	2.02	0.42
2:D:138:THR:OG1	2:D:152:LYS:HE2	2.19	0.42
1:G:40:THR:N	1:G:94:GLN:HE22	2.08	0.42
1:G:253:THR:O	1:G:253:THR:HG22	2.19	0.42
1:E:122:TYR:CD2	1:E:126:ARG:HB3	2.55	0.42
1:G:30:PHE:HE2	1:G:115:LEU:HD11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LEU:HD23	1:C:147:LEU:N	2.35	0.42
1:C:170:ARG:HD3	1:C:183:ASP:HA	2.01	0.42
1:C:201:GLU:HB2	1:C:202:PRO:HD3	2.02	0.42
1:E:47:THR:HB	1:E:72:TRP:CG	2.55	0.42
2:F:44:ARG:NE	2:F:51:ARG:NH1	2.50	0.42
2:H:177:ASP:O	2:H:181:GLY:N	2.49	0.42
1:A:281:GLN:O	1:A:285:GLU:HB2	2.20	0.42
2:B:77:ASN:HA	2:B:81:PHE:O	2.18	0.42
1:E:235:ARG:HG3	1:E:249:PHE:HD2	1.85	0.42
1:G:83:ARG:CZ	1:G:282:ASN:HB3	2.50	0.42
1:G:166:LYS:HB3	1:G:167:THR:H	1.65	0.42
1:G:201:GLU:CB	1:G:202:PRO:HD3	2.50	0.42
1:G:166:LYS:HG2	1:G:170:ARG:HH22	1.85	0.41
1:A:311:ALA:HB1	1:A:316:GLU:OE2	2.19	0.41
1:C:116:GLU:OE2	1:C:118:TYR:OH	2.34	0.41
1:E:153:PHE:HB3	1:E:161:PRO:HD3	2.03	0.41
1:A:166:LYS:CB	1:A:170:ARG:HH22	2.22	0.41
1:C:119:ARG:HB3	1:C:122:TYR:CG	2.56	0.41
2:D:44:ARG:HG3	2:D:44:ARG:NH2	2.35	0.41
1:E:181:VAL:HG23	1:E:194:LEU:CD2	2.50	0.41
1:G:122:TYR:CE2	1:G:126:ARG:HD2	2.55	0.41
1:A:48:VAL:HG12	1:A:79:TYR:CZ	2.55	0.41
1:A:165:ASP:N	1:A:168:GLN:OE1	2.48	0.41
1:C:79:TYR:N	1:C:79:TYR:CD2	2.88	0.41
1:C:223:ALA:CB	1:C:249:PHE:HB2	2.50	0.41
1:E:79:TYR:CD2	1:E:79:TYR:N	2.87	0.41
1:G:229:ASP:OD1	1:G:231:ARG:HB2	2.20	0.41
2:H:44:ARG:HH12	2:H:51:ARG:HD3	1.83	0.41
2:H:132:GLU:HG2	2:H:187:VAL:HG21	2.03	0.41
2:H:46:LEU:CD1	2:H:67:VAL:HG11	2.50	0.41
1:C:124:MET:HE1	1:C:214:HIS:CD2	2.56	0.41
2:D:183:TYR:OH	2:D:186:ARG:HG3	2.19	0.41
1:E:223:ALA:HB2	1:E:249:PHE:CB	2.50	0.41
2:B:76:TYR:CD1	2:B:76:TYR:C	2.98	0.41
1:E:154:LEU:HD12	1:E:154:LEU:HA	1.91	0.41
1:G:162:LEU:HD12	1:G:162:LEU:N	2.36	0.41
1:G:247:ASN:HB3	3:G:993:KAA:HN8	1.86	0.41
1:A:150:GLN:CG	1:A:162:LEU:HD22	2.50	0.41
1:A:154:LEU:HD23	1:A:159:ILE:C	2.45	0.41
1:C:223:ALA:HB2	1:C:249:PHE:HB2	2.02	0.41
1:E:201:GLU:N	1:E:202:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:LEU:HG	2:F:15:ILE:HG23	2.02	0.41
1:G:124:MET:HE1	1:G:213:TYR:CB	2.42	0.41
1:C:239:TYR:CD1	1:C:239:TYR:N	2.88	0.41
2:F:8:ASP:O	2:F:10:ARG:N	2.54	0.41
2:F:26:ALA:O	2:F:41:VAL:HG13	2.21	0.41
1:G:129:ASN:O	1:G:132:ASP:HB3	2.21	0.41
1:G:249:PHE:CZ	3:G:993:KAA:HE2	2.56	0.41
1:G:299:LEU:HD23	1:G:299:LEU:C	2.45	0.41
2:D:116:THR:HB	2:D:124:SER:OG	2.21	0.41
1:A:220:ALA:O	1:A:221:SER:HB3	2.21	0.40
1:C:99:PHE:CD1	1:C:99:PHE:N	2.89	0.40
1:C:221:SER:H	2:D:34:LYS:NZ	2.18	0.40
1:E:115:LEU:HD13	1:E:117:TRP:HZ3	1.85	0.40
2:B:86:ASN:HB3	2:B:89:THR:HB	2.03	0.40
2:B:114:ILE:HB	2:B:126:THR:HB	2.02	0.40
1:C:161:PRO:HG2	1:C:162:LEU:HD13	2.02	0.40
2:D:135:ILE:HD12	2:D:168:VAL:HG12	2.02	0.40
1:E:81:MET:O	1:E:85:LEU:HD22	2.22	0.40
1:G:130:GLU:O	1:G:133:ASP:OD1	2.39	0.40
1:A:204:ILE:HD13	1:A:204:ILE:HA	1.86	0.40
1:A:258:GLN:HG3	1:A:262:PHE:CE2	2.56	0.40
1:C:118:TYR:CE2	1:C:296:GLY:HA3	2.57	0.40
1:C:178:LEU:CD2	2:D:55:THR:HB	2.52	0.40
1:C:178:LEU:HD22	2:D:55:THR:HB	2.03	0.40
2:D:82:TRP:CG	2:D:100:ILE:HG13	2.57	0.40
1:G:79:TYR:CD2	1:G:283:LEU:HD22	2.57	0.40
2:D:152:LYS:NZ	2:D:166:LEU:O	2.53	0.40
2:H:39:ALA:O	2:H:41:VAL:HG12	2.20	0.40
2:H:57:LYS:O	2:H:58:SER:C	2.62	0.40
1:A:8:GLN:HA	1:A:9:PRO:HD3	1.87	0.40
1:A:119:ARG:HG2	1:A:122:TYR:CE2	2.57	0.40
1:A:165:ASP:HA	1:A:188:ARG:HH22	1.86	0.40
1:C:118:TYR:CD2	1:C:296:GLY:HA3	2.56	0.40
2:F:17:LEU:HB2	2:F:22:TYR:CD1	2.57	0.40
1:G:162:LEU:CD1	1:G:162:LEU:N	2.85	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	321/328 (98%)	303 (94%)	18 (6%)	0	100	100
1	C	322/328 (98%)	299 (93%)	21 (6%)	2 (1%)	21	38
1	E	321/328 (98%)	304 (95%)	16 (5%)	1 (0%)	36	55
1	G	319/328 (97%)	283 (89%)	31 (10%)	5 (2%)	7	14
2	B	132/191 (69%)	113 (86%)	14 (11%)	5 (4%)	2	3
2	D	171/191 (90%)	154 (90%)	17 (10%)	0	100	100
2	F	57/191 (30%)	49 (86%)	5 (9%)	3 (5%)	1	1
2	H	171/191 (90%)	151 (88%)	18 (10%)	2 (1%)	10	20
All	All	1814/2076 (87%)	1656 (91%)	140 (8%)	18 (1%)	12	24

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	66	SER
1	G	166	LYS
2	B	6	SER
2	F	9	PHE
1	G	228	GLU
1	C	228	GLU
2	F	6	SER
1	G	124	MET
2	B	8	ASP
2	B	9	PHE
2	B	47	LEU
1	C	164	ALA
2	F	45	ARG
2	B	129	ASN
1	G	170	ARG
2	H	109	ASP
2	H	49	GLY

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Mol	Chain	Res	Type
1	G	51	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	277/281 (99%)	255 (92%)	22 (8%)	11	24
1	C	278/281 (99%)	260 (94%)	18 (6%)	15	32
1	E	277/281 (99%)	256 (92%)	21 (8%)	12	26
1	G	277/281 (99%)	254 (92%)	23 (8%)	10	22
2	B	113/157 (72%)	105 (93%)	8 (7%)	13	29
2	D	148/157 (94%)	138 (93%)	10 (7%)	14	31
2	F	49/157 (31%)	47 (96%)	2 (4%)	27	53
2	H	148/157 (94%)	140 (95%)	8 (5%)	20	41
All	All	1567/1752 (89%)	1455 (93%)	112 (7%)	13	29

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	61	VAL
1	A	65	HIS
1	A	67	GLN
1	A	71	LEU
1	A	85	LEU
1	A	115	LEU
1	A	119	ARG
1	A	126	ARG
1	A	147	LEU
1	A	155	ARG
1	A	159	ILE
1	A	162	LEU
1	A	169	LEU

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Mol	Chain	Res	Type
1	A	170	ARG
1	A	175	LYS
1	A	189	ASP
1	A	192	LEU
1	A	194	LEU
1	A	228	GLU
1	A	281	GLN
1	A	323	ASP
2	B	51	ARG
2	B	71	ASN
2	B	87	ASN
2	B	91	GLU
2	B	108	LEU
2	B	109	ASP
2	B	117	LEU
2	B	134	GLU
1	C	3	GLU
1	C	23	MET
1	C	45	GLN
1	C	54	VAL
1	C	85	LEU
1	C	114	MET
1	C	115	LEU
1	C	137	GLN
1	C	147	LEU
1	C	153	PHE
1	C	154	LEU
1	C	157	LEU
1	C	169	LEU
1	C	176	LEU
1	C	192	LEU
1	C	206	LYS
1	C	218	SER
1	C	253	THR
2	D	28	GLU
2	D	41	VAL
2	D	43	LEU
2	D	63	GLU
2	D	92	GLN
2	D	139	ASP
2	D	152	LYS
2	D	156	LEU

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Mol	Chain	Res	Type
2	D	176	VAL
2	D	179	ARG
1	E	3	GLU
1	E	38	VAL
1	E	45	GLN
1	E	53	LEU
1	E	54	VAL
1	E	61	VAL
1	E	65	HIS
1	E	67	GLN
1	E	85	LEU
1	E	115	LEU
1	E	126	ARG
1	E	129	ASN
1	E	154	LEU
1	E	191	LEU
1	E	206	LYS
1	E	222	LEU
1	E	256	ARG
1	E	299	LEU
1	E	322	VAL
1	E	323	ASP
1	E	324	ARG
2	F	51	ARG
2	F	57	LYS
1	G	16	LEU
1	G	28	ARG
1	G	45	GLN
1	G	47	THR
1	G	49	THR
1	G	54	VAL
1	G	61	VAL
1	G	69	MET
1	G	71	LEU
1	G	85	LEU
1	G	115	LEU
1	G	126	ARG
1	G	130	GLU
1	G	133	ASP
1	G	147	LEU
1	G	153	PHE
1	G	166	LYS

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Mol	Chain	Res	Type
1	G	168	GLN
1	G	169	LEU
1	G	230	HIS
1	G	259	GLN
1	G	285	GLU
1	G	312	GLU
2	H	41	VAL
2	H	43	LEU
2	H	56	PHE
2	H	92	GLN
2	H	126	THR
2	H	139	ASP
2	H	156	LEU
2	H	176	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	15	ASN
1	A	65	HIS
1	A	94	GLN
1	A	108	HIS
1	A	121	HIS
1	A	129	ASN
1	A	136	GLN
1	A	137	GLN
1	A	150	GLN
1	A	219	GLN
1	A	276	GLN
1	A	282	ASN
2	B	71	ASN
2	B	77	ASN
2	B	86	ASN
2	B	87	ASN
2	B	92	GLN
2	B	110	GLN
2	B	129	ASN
1	C	8	GLN
1	C	15	ASN
1	C	67	GLN
1	C	94	GLN

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Mol	Chain	Res	Type
1	C	129	ASN
1	C	136	GLN
1	C	150	GLN
1	C	168	GLN
1	C	214	HIS
1	C	219	GLN
1	C	224	GLN
1	C	247	ASN
1	C	259	GLN
2	D	7	ASN
2	D	77	ASN
2	D	129	ASN
2	D	169	GLN
1	E	8	GLN
1	E	15	ASN
1	E	45	GLN
1	E	67	GLN
1	E	94	GLN
1	E	136	GLN
1	E	137	GLN
1	E	203	ASN
1	E	219	GLN
1	E	247	ASN
1	E	250	HIS
1	E	258	GLN
1	E	260	GLN
1	E	281	GLN
1	G	8	GLN
1	G	15	ASN
1	G	45	GLN
1	G	52	HIS
1	G	67	GLN
1	G	80	HIS
1	G	94	GLN
1	G	150	GLN
1	G	168	GLN
1	G	203	ASN
1	G	214	HIS
1	G	219	GLN
1	G	224	GLN
1	G	258	GLN
1	G	259	GLN

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Mol	Chain	Res	Type
1	G	260	GLN
1	G	276	GLN
2	H	36	GLN
2	H	77	ASN
2	H	83	HIS
2	H	87	ASN
2	H	110	GLN
2	H	119	ASN
2	H	129	ASN
2	H	169	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	KAA	A	990	-	34,34,34	2.79	8 (23%)	46,49,49	2.14	13 (28%)
3	KAA	C	991	-	34,34,34	2.80	8 (23%)	46,49,49	2.13	12 (26%)
3	KAA	E	992	-	34,34,34	2.80	8 (23%)	46,49,49	2.18	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	KAA	G	993	-	34,34,34	2.82	8 (23%)	46,49,49	2.16	12 (26%)

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	KAA	A	990	-	-	3/23/40/40	0/3/3/3
3	KAA	C	991	-	-	0/23/40/40	0/3/3/3
3	KAA	E	992	-	-	0/23/40/40	0/3/3/3
3	KAA	G	993	-	-	2/23/40/40	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	991	KAA	O1S-S1	9.17	1.50	1.42
3	E	992	KAA	O2S-S1	9.16	1.50	1.42
3	G	993	KAA	O1S-S1	9.15	1.50	1.42
3	G	993	KAA	O2S-S1	9.14	1.50	1.42
3	A	990	KAA	O2S-S1	9.06	1.50	1.42
3	E	992	KAA	O1S-S1	9.01	1.50	1.42
3	C	991	KAA	O2S-S1	8.99	1.50	1.42
3	A	990	KAA	O1S-S1	8.96	1.50	1.42
3	G	993	KAA	O5'-S1	-8.16	1.43	1.60
3	C	991	KAA	O5'-S1	-8.12	1.43	1.60
3	A	990	KAA	O5'-S1	-8.11	1.43	1.60
3	E	992	KAA	O5'-S1	-8.09	1.43	1.60
3	G	993	KAA	C5-N7	-3.13	1.33	1.39
3	C	991	KAA	C5-N7	-3.13	1.33	1.39
3	A	990	KAA	C5-N7	-3.10	1.33	1.39
3	E	992	KAA	C5-N7	-3.05	1.33	1.39
3	A	990	KAA	C8-N9	-2.37	1.33	1.37
3	E	992	KAA	C8-N9	-2.37	1.33	1.37
3	G	993	KAA	C8-N9	-2.37	1.33	1.37
3	A	990	KAA	C-N8	-2.35	1.33	1.37
3	A	990	KAA	S1-N8	2.35	1.63	1.59
3	G	993	KAA	C-N8	-2.34	1.33	1.37
3	E	992	KAA	C-N8	-2.34	1.33	1.37
3	C	991	KAA	C8-N9	-2.29	1.33	1.37
3	G	993	KAA	S1-N8	2.28	1.63	1.59
3	C	991	KAA	S1-N8	2.23	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	991	KAA	C-N8	-2.23	1.33	1.37
3	E	992	KAA	S1-N8	2.20	1.63	1.59
3	G	993	KAA	C4-N9	-2.17	1.33	1.37
3	C	991	KAA	C4-N9	-2.07	1.33	1.37
3	A	990	KAA	C4-N9	-2.03	1.33	1.37
3	E	992	KAA	C4-N9	-2.00	1.33	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	991	KAA	O2S-S1-O1S	-7.75	109.24	120.85
3	E	992	KAA	O2S-S1-O1S	-7.70	109.31	120.85
3	A	990	KAA	O2S-S1-O1S	-7.63	109.42	120.85
3	G	993	KAA	O2S-S1-O1S	-7.57	109.51	120.85
3	E	992	KAA	C5-C4-N3	-5.35	119.35	126.72
3	A	990	KAA	C5-C4-N3	-5.26	119.47	126.72
3	G	993	KAA	C5-C4-N3	-5.16	119.61	126.72
3	C	991	KAA	C5-C4-N3	-5.10	119.70	126.72
3	G	993	KAA	N1-C2-N3	-4.66	121.53	128.58
3	C	991	KAA	N1-C2-N3	-4.65	121.55	128.58
3	E	992	KAA	N1-C2-N3	-4.60	121.62	128.58
3	A	990	KAA	N1-C2-N3	-4.53	121.73	128.58
3	E	992	KAA	N3-C4-N9	3.92	133.84	127.17
3	A	990	KAA	N3-C4-N9	3.80	133.63	127.17
3	G	993	KAA	C-N8-S1	-3.70	110.53	124.07
3	G	993	KAA	N3-C4-N9	3.67	133.42	127.17
3	E	992	KAA	C2-N3-C4	3.63	120.70	111.83
3	C	991	KAA	N3-C4-N9	3.62	133.32	127.17
3	E	992	KAA	C-N8-S1	-3.58	110.99	124.07
3	G	993	KAA	C2-N3-C4	3.55	120.51	111.83
3	A	990	KAA	C2-N3-C4	3.55	120.50	111.83
3	C	991	KAA	C-N8-S1	-3.53	111.14	124.07
3	C	991	KAA	C2-N3-C4	3.53	120.45	111.83
3	A	990	KAA	C-N8-S1	-3.41	111.61	124.07
3	G	993	KAA	N9-C8-N7	-3.20	109.39	113.94
3	C	991	KAA	N9-C8-N7	-3.08	109.56	113.94
3	E	992	KAA	N9-C8-N7	-3.03	109.64	113.94
3	A	990	KAA	N9-C8-N7	-2.92	109.79	113.94
3	G	993	KAA	C5-N7-C8	2.82	107.88	103.45
3	G	993	KAA	C2'-C3'-C4'	-2.82	97.16	102.61
3	C	991	KAA	C5-N7-C8	2.76	107.78	103.45
3	G	993	KAA	C4-C5-N7	-2.74	107.45	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	992	KAA	C5-N7-C8	2.71	107.71	103.45
3	C	991	KAA	C4-C5-N7	-2.64	107.56	110.58
3	A	990	KAA	C5-N7-C8	2.63	107.59	103.45
3	E	992	KAA	C4-C5-N7	-2.61	107.60	110.58
3	A	990	KAA	C4-C5-N7	-2.56	107.65	110.58
3	G	993	KAA	C4-N9-C8	2.44	108.30	105.74
3	E	992	KAA	C4-N9-C8	2.37	108.23	105.74
3	G	993	KAA	O5'-C5'-C4'	2.35	111.76	107.57
3	C	991	KAA	C4-N9-C8	2.29	108.14	105.74
3	C	991	KAA	O5'-C5'-C4'	2.25	111.58	107.57
3	A	990	KAA	O5'-S1-N8	2.25	111.50	105.69
3	A	990	KAA	C4-N9-C8	2.22	108.06	105.74
3	E	992	KAA	C5'-O5'-S1	2.21	121.62	116.97
3	C	991	KAA	C2'-C3'-C4'	-2.17	98.42	102.61
3	E	992	KAA	O5'-C5'-C4'	2.16	111.42	107.57
3	A	990	KAA	C2'-C3'-C4'	-2.10	98.54	102.61
3	A	990	KAA	O5'-C5'-C4'	2.09	111.29	107.57
3	E	992	KAA	O5'-S1-N8	2.07	111.05	105.69

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	990	KAA	O-C-CA-CB
3	A	990	KAA	N8-C-CA-CB
3	G	993	KAA	O-C-CA-CB
3	G	993	KAA	N8-C-CA-CB
3	A	990	KAA	N-CA-CB-CG

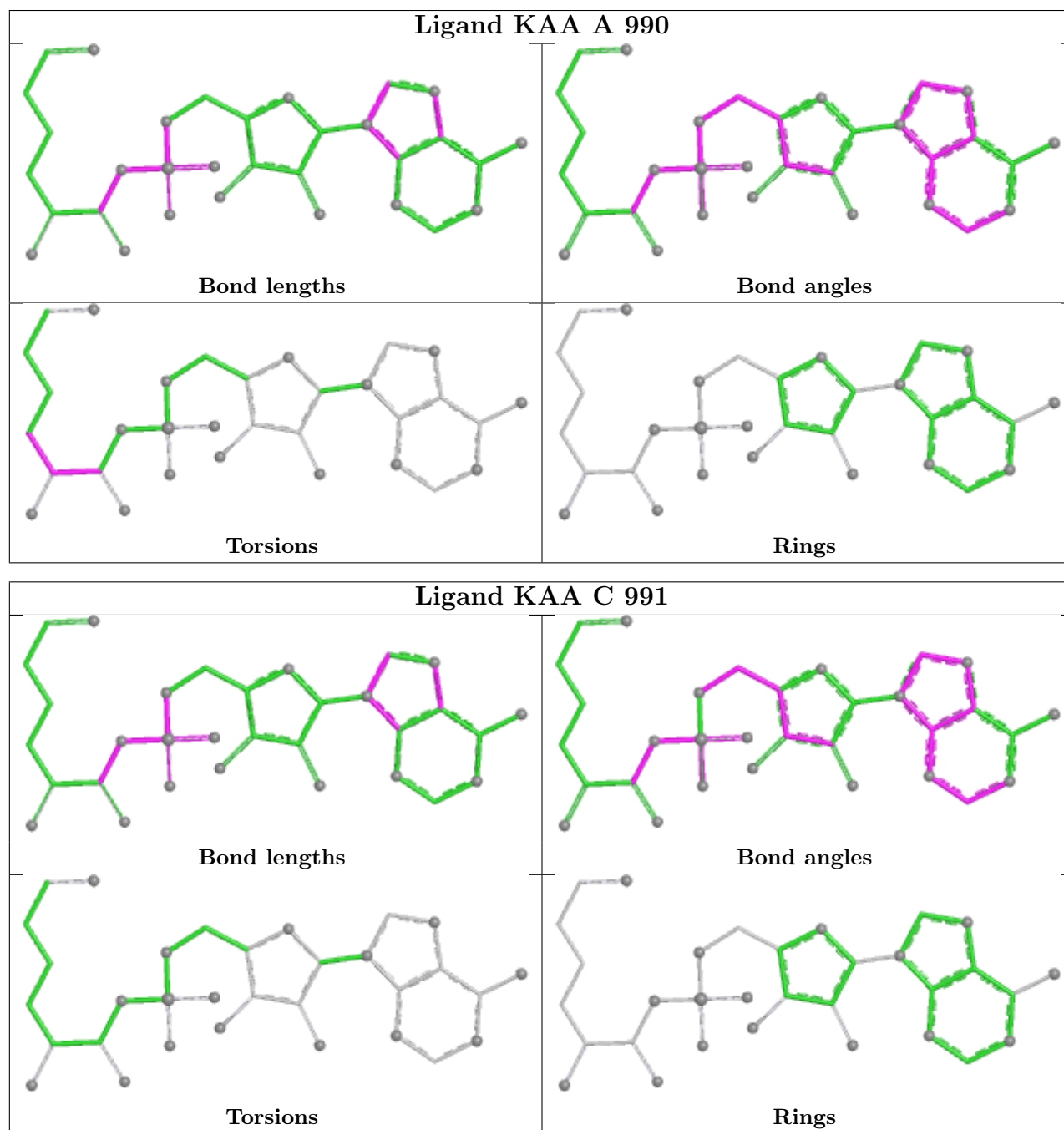
There are no ring outliers.

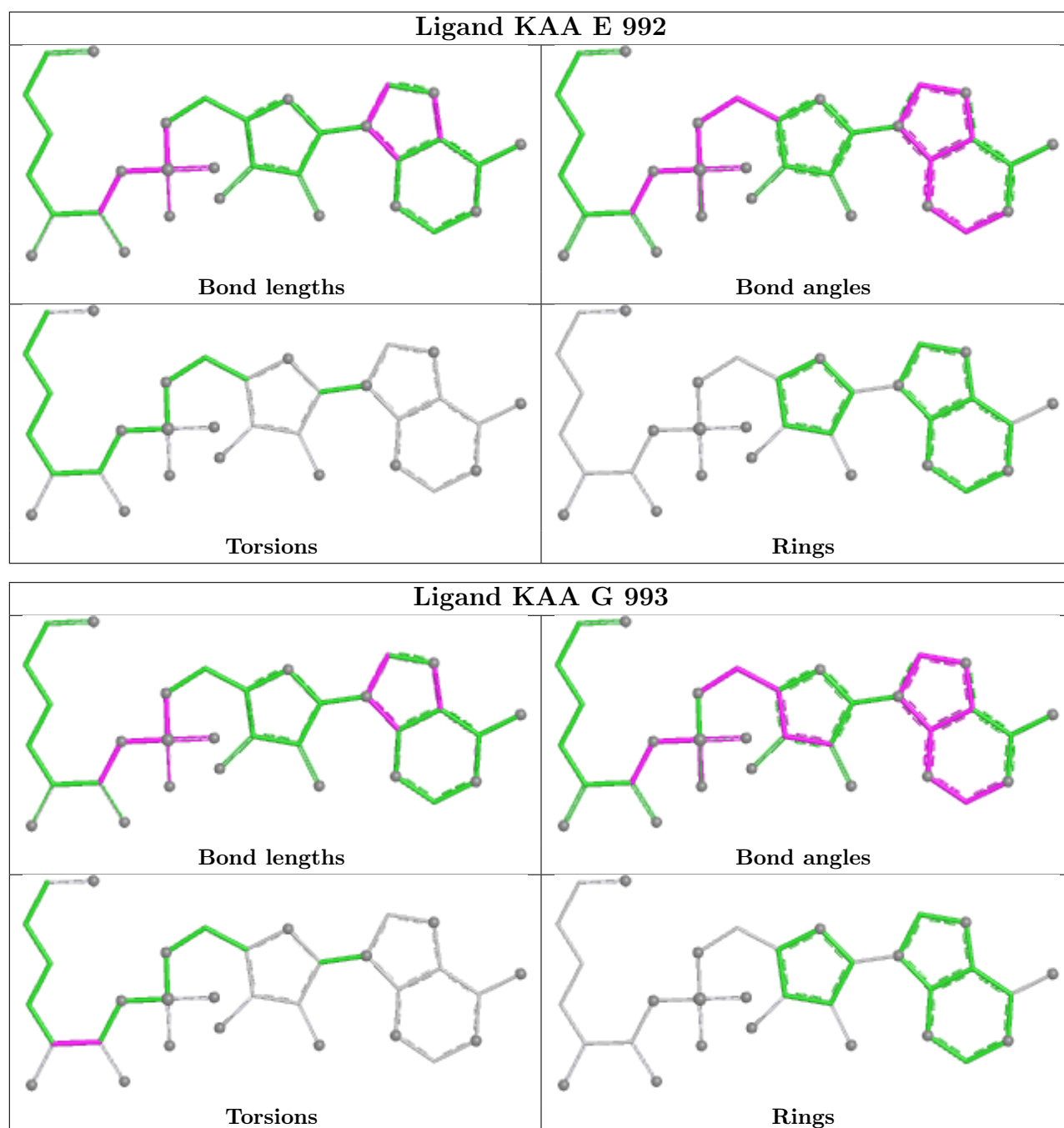
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	990	KAA	2	0
3	C	991	KAA	2	0
3	E	992	KAA	1	0
3	G	993	KAA	7	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 than 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.





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	323/328 (98%)	-0.05	0 100 100	33, 51, 73, 103	0
1	C	324/328 (98%)	0.05	3 (0%) 81 78	34, 54, 81, 96	0
1	E	323/328 (98%)	-0.13	1 (0%) 90 87	31, 48, 75, 108	0
1	G	323/328 (98%)	0.58	11 (3%) 48 43	34, 73, 102, 110	0
2	B	134/191 (70%)	0.86	19 (14%) 6 5	39, 86, 123, 134	0
2	D	175/191 (91%)	0.40	7 (4%) 42 38	47, 65, 91, 107	0
2	F	59/191 (30%)	0.94	11 (18%) 3 2	48, 97, 130, 139	0
2	H	175/191 (91%)	0.69	8 (4%) 37 33	49, 73, 100, 114	0
All	All	1836/2076 (88%)	0.28	60 (3%) 49 45	31, 60, 101, 139	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	64	GLY	4.2
2	B	135	ILE	3.8
2	B	130	PHE	3.5
2	B	5	TYR	3.4
2	H	140	PRO	3.3
2	F	15	ILE	3.3
2	B	106	TRP	3.2
2	B	136	VAL	3.1
2	F	16	MET	3.1
2	H	151	GLY	3.0
2	F	5	TYR	3.0
2	F	6	SER	3.0
1	G	147	LEU	2.9
2	H	5	TYR	2.8
2	F	47	LEU	2.8
1	G	230	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	3	THR	2.8
2	D	5	TYR	2.7
2	B	129	ASN	2.6
2	B	107	LEU	2.6
2	D	86	ASN	2.5
2	D	90	PHE	2.5
2	B	7	ASN	2.5
2	H	6	SER	2.5
2	D	88	GLU	2.4
2	B	70	MET	2.4
2	F	23	ALA	2.4
2	F	9	PHE	2.4
2	B	134	GLU	2.4
1	E	89	CYS	2.3
2	F	3	THR	2.3
2	B	9	PHE	2.3
1	C	2	SER	2.2
2	D	140	PRO	2.2
2	B	72	LEU	2.2
2	F	21	PRO	2.2
2	H	7	ASN	2.2
2	B	90	PHE	2.2
1	C	64	GLY	2.2
2	B	133	LEU	2.2
2	F	43	LEU	2.2
1	G	154	LEU	2.1
2	H	34	LYS	2.1
1	C	162	LEU	2.1
2	F	14	LYS	2.1
1	G	181	VAL	2.1
1	G	176	LEU	2.1
2	H	120	GLY	2.1
2	B	93	LEU	2.1
1	G	190	THR	2.1
2	B	6	SER	2.1
1	G	141	CYS	2.1
2	D	187	VAL	2.0
2	B	108	LEU	2.0
1	G	243	ILE	2.0
1	G	1	MET	2.0
1	G	179	SER	2.0
2	H	24	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	19	GLY	2.0
2	D	7	ASN	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](#)

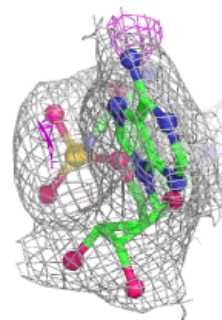
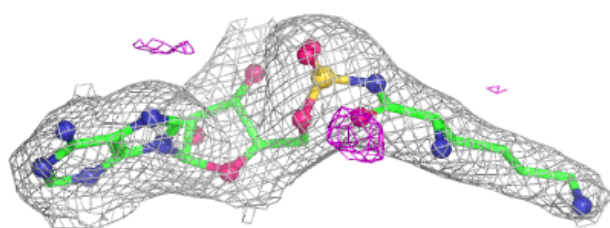
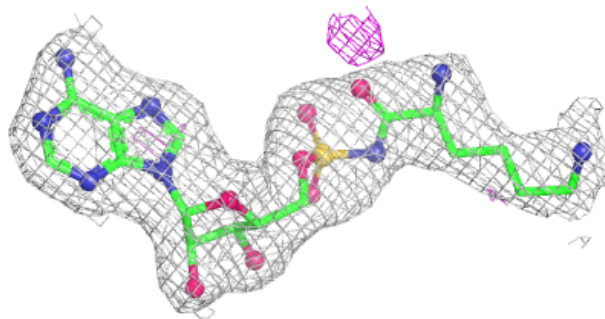
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	KAA	G	993	32/32	0.95	0.07	47,56,61,62	0
3	KAA	E	992	32/32	0.96	0.07	36,39,43,45	0
3	KAA	C	991	32/32	0.96	0.07	41,45,47,49	0
3	KAA	A	990	32/32	0.97	0.06	30,39,44,44	0

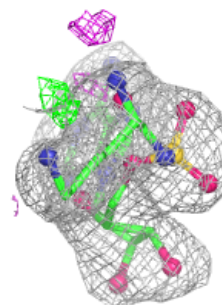
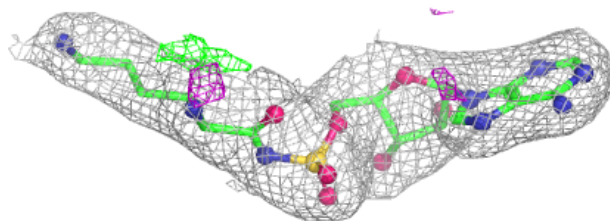
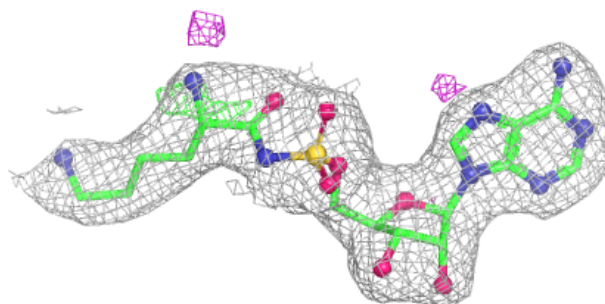
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KAA G 993:

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

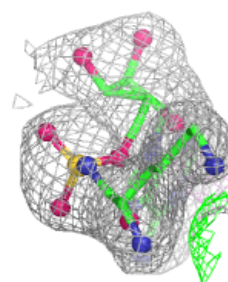
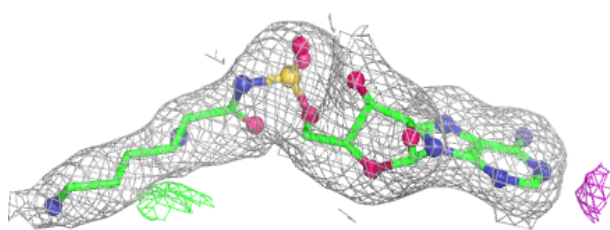
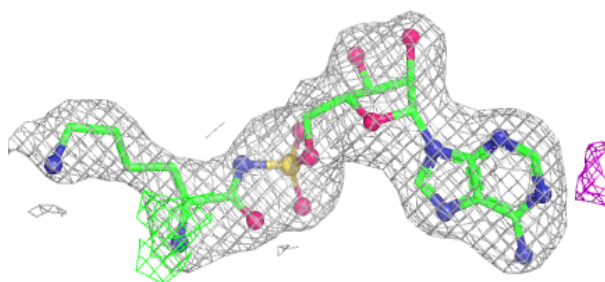
**Electron density around KAA E 992:**

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

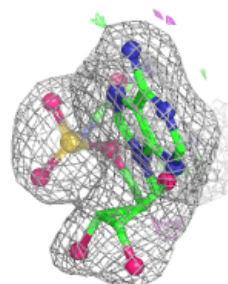
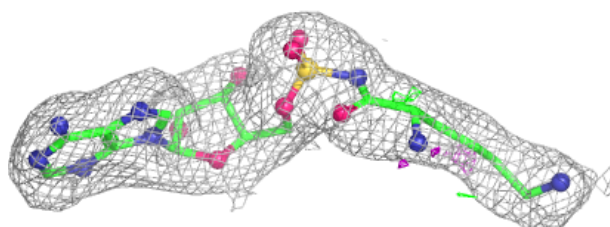
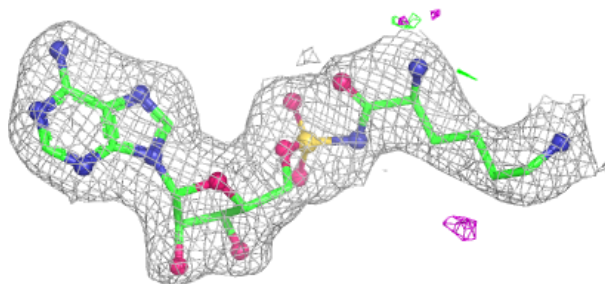


Electron density around KAA C 991:

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

**Electron density around KAA A 990:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.