Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 09:41 PM GMT

PDB ID	:	1Q23
Title	:	Crystal structure of Chloramphenicol acetyltransferase I complexed with Fusidic acid at 2.18 A resolution
Authors	:	Roidis, A.; Kokkinidis, M.
Deposited on	:	2003-07-23
Resolution	:	2.18 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

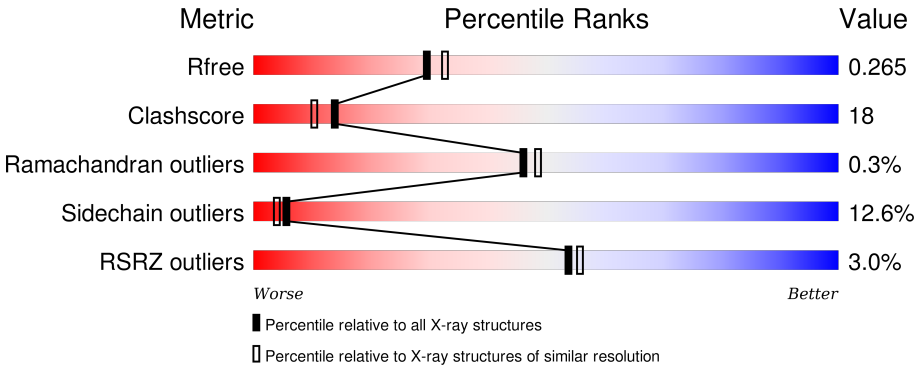
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.18 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}	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	219	% 57% 32% 8%
1	B	219	3% 68% 24% 6%
1	C	219	65% 22% 8%
1	D	219	% 56% 31% 10%
1	E	219	3% 61% 30% 7%

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Mol	Chain	Length	Quality of chain
1	F	219	61% 27% 7%
1	G	219	3% 63% 25% 7%
1	H	219	2% 58% 32% 6%
1	I	219	3% 55% 33% 8%
1	J	219	6% 60% 26% 9%
1	K	219	3% 62% 29% 5%
1	L	219	10% 53% 36% 6%

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
2	CA	A	801	-	-	-	X
3	FUA	A	702	X	-	-	-
3	FUA	B	703	X	-	-	-
3	FUA	C	701	X	-	-	-
3	FUA	D	705	X	-	-	-
3	FUA	E	706	X	-	-	-
3	FUA	F	704	X	-	-	-
3	FUA	G	708	X	-	-	-
3	FUA	H	709	X	-	-	-
3	FUA	I	707	X	-	-	-
3	FUA	J	711	X	-	-	-
3	FUA	K	712	X	-	-	-
3	FUA	L	710	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22280 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.

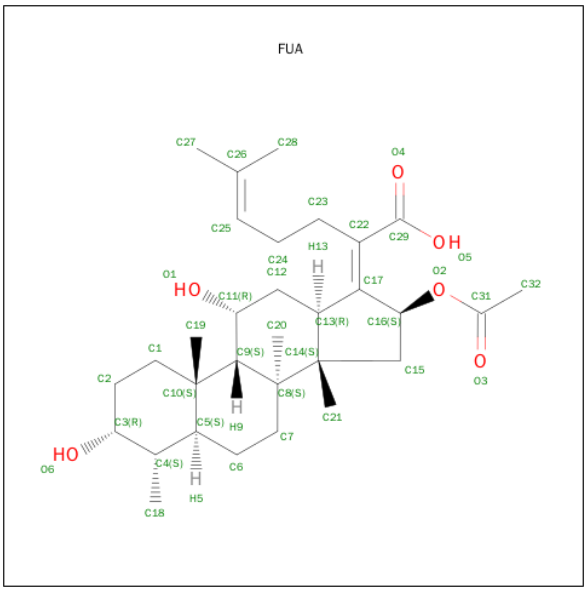
- Molecule 1 is a protein called Chloramphenicol acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1771	1150	291	317	13			
1	B	217	Total	C	N	O	S	0	0	0
			1798	1167	296	322	13			
1	C	213	Total	C	N	O	S	0	0	0
			1763	1144	290	316	13			
1	D	213	Total	C	N	O	S	0	0	0
			1763	1144	290	316	13			
1	E	215	Total	C	N	O	S	0	0	0
			1785	1160	294	318	13			
1	F	212	Total	C	N	O	S	0	0	0
			1759	1142	289	315	13			
1	G	213	Total	C	N	O	S	0	0	0
			1763	1144	290	316	13			
1	H	216	Total	C	N	O	S	0	0	0
			1785	1159	294	319	13			
1	I	215	Total	C	N	O	S	0	0	0
			1785	1160	294	318	13			
1	J	212	Total	C	N	O	S	0	0	0
			1763	1146	289	315	13			
1	K	213	Total	C	N	O	S	0	0	0
			1772	1153	291	315	13			
1	L	210	Total	C	N	O	S	0	0	0
			1746	1135	286	312	13			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 37 31 6	0	0
3	A	1	Total C O 37 31 6	0	0
3	B	1	Total C O 37 31 6	0	0
3	F	1	Total C O 37 31 6	0	0
3	D	1	Total C O 37 31 6	0	0
3	E	1	Total C O 37 31 6	0	0
3	I	1	Total C O 37 31 6	0	0
3	G	1	Total C O 37 31 6	0	0
3	H	1	Total C O 37 31 6	0	0
3	L	1	Total C O 37 31 6	0	0
3	J	1	Total C O 37 31 6	0	0
3	K	1	Total C O 37 31 6	0	0

- Molecule 4 is water.

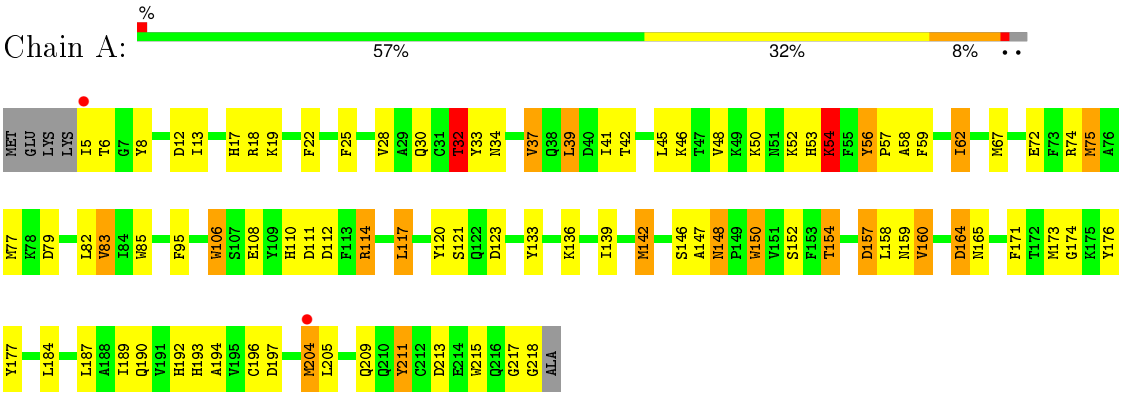
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	78	Total O 78 78	0	0
4	B	51	Total O 51 51	0	0
4	C	68	Total O 68 68	0	0
4	D	58	Total O 58 58	0	0
4	E	44	Total O 44 44	0	0
4	F	43	Total O 43 43	0	0
4	G	43	Total O 43 43	0	0
4	H	74	Total O 74 74	0	0
4	I	42	Total O 42 42	0	0
4	J	34	Total O 34 34	0	0
4	K	26	Total O 26 26	0	0
4	L	21	Total O 21 21	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

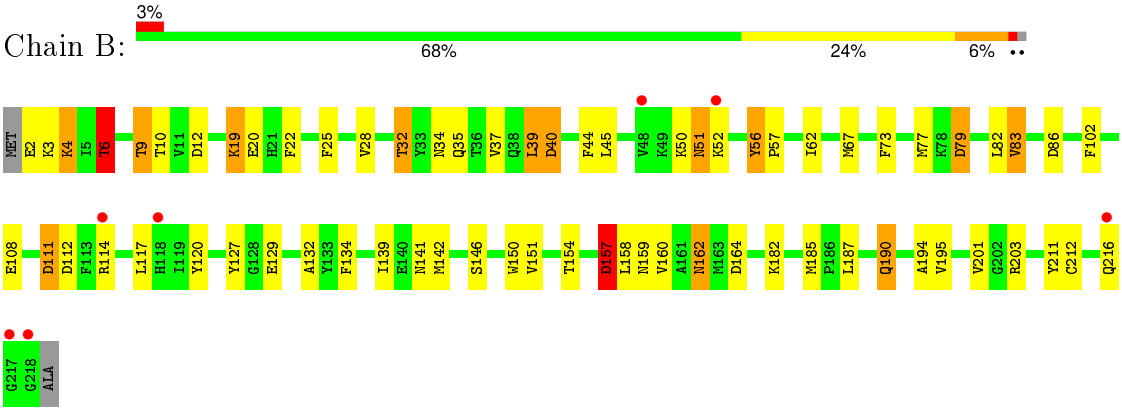
- Molecule 1: Chloramphenicol acetyltransferase

Chain A:



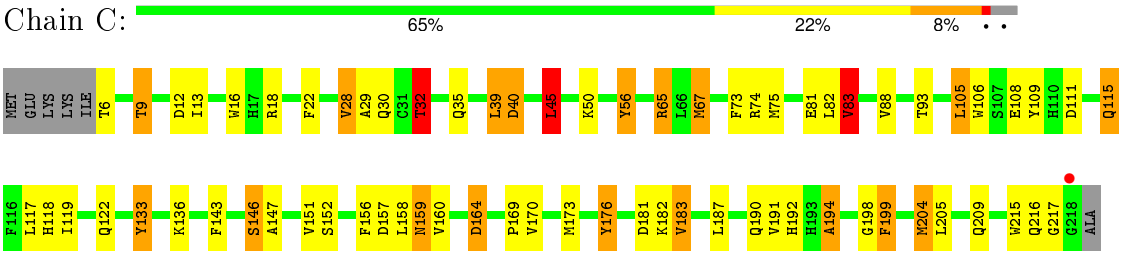
- Molecule 1: Chloramphenicol acetyltransferase

Chain B:

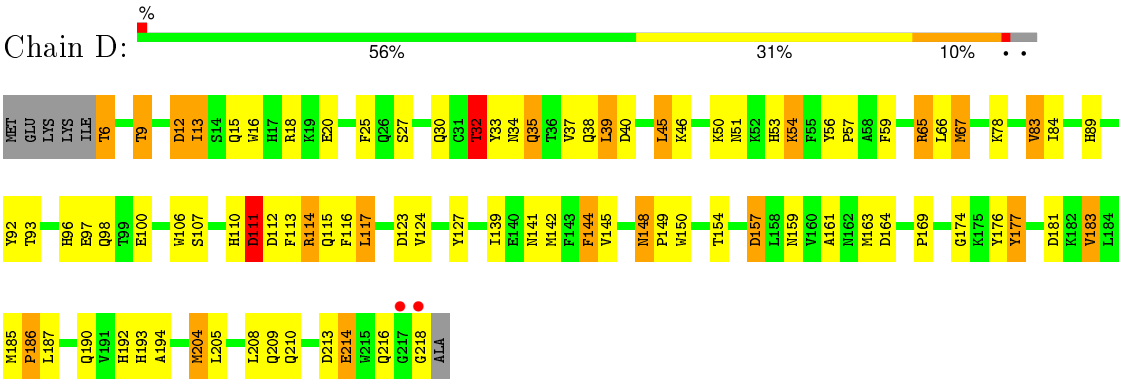


- Molecule 1: Chloramphenicol acetyltransferase

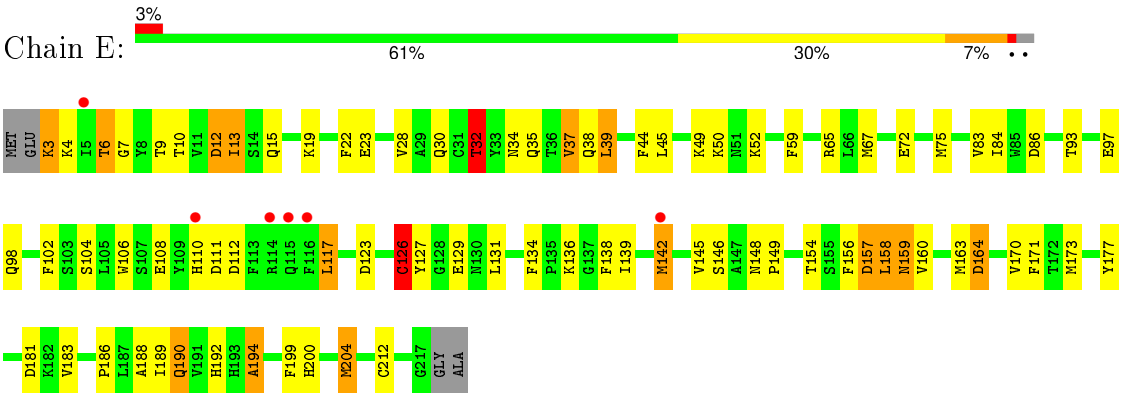
Chain C:



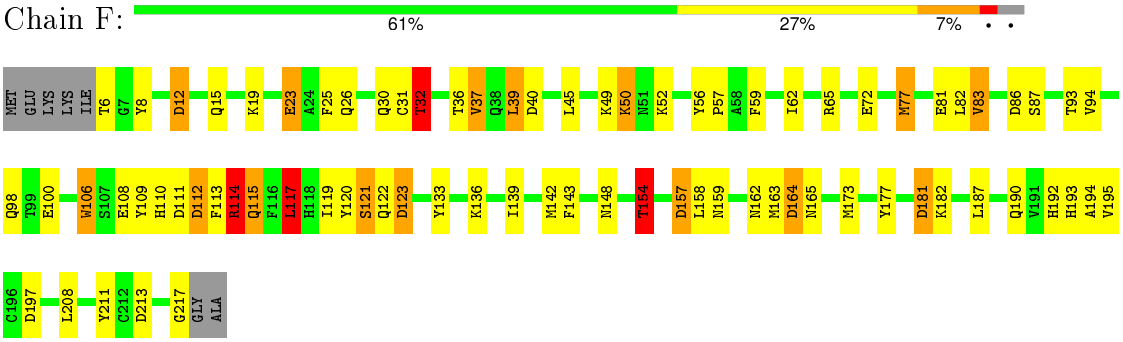
- Molecule 1: Chloramphenicol acetyltransferase



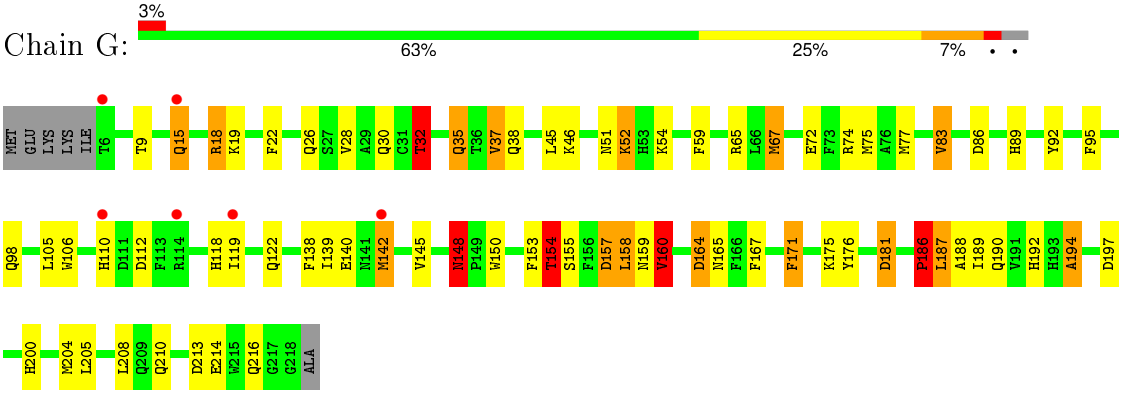
• Molecule 1: Chloramphenicol acetyltransferase



• Molecule 1: Chloramphenicol acetyltransferase

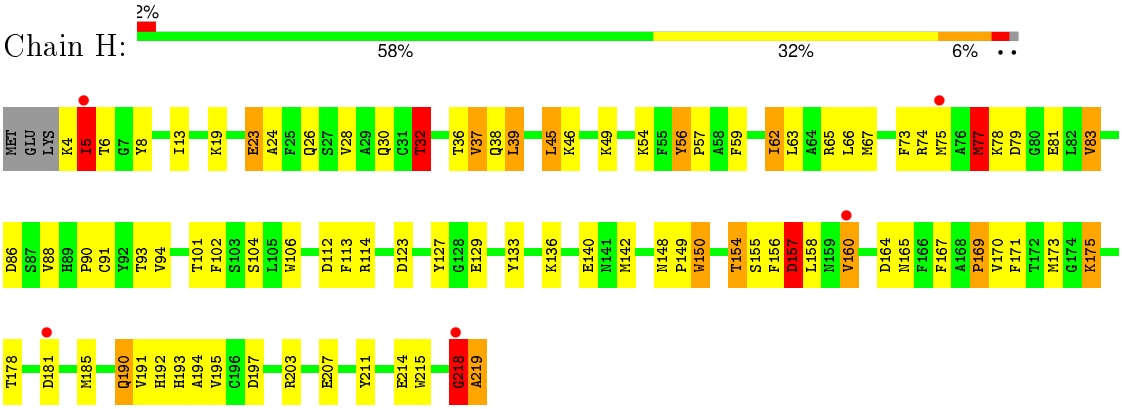


• Molecule 1: Chloramphenicol acetyltransferase



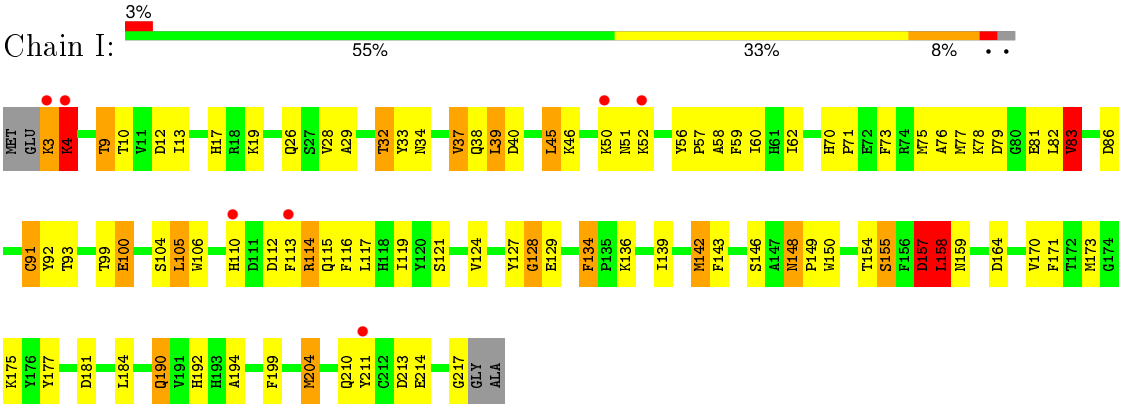
• Molecule 1: Chloramphenicol acetyltransferase

Chain H:



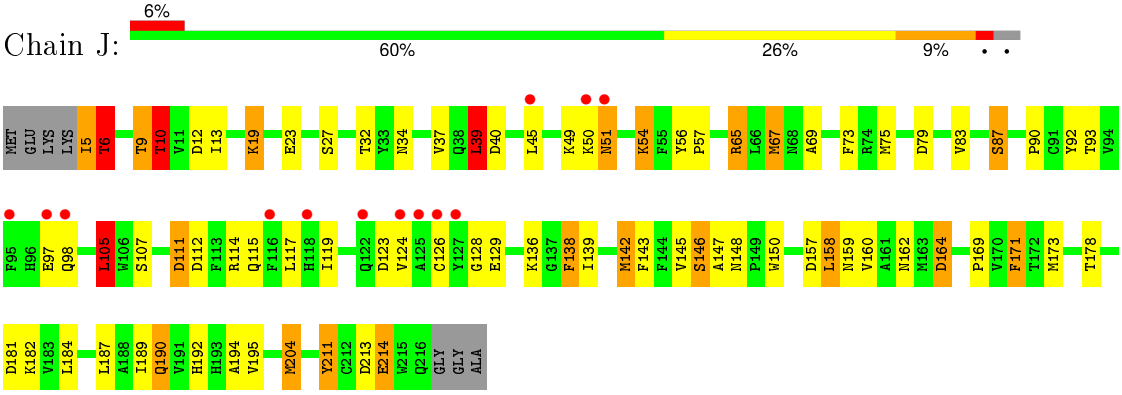
• Molecule 1: Chloramphenicol acetyltransferase

Chain I:



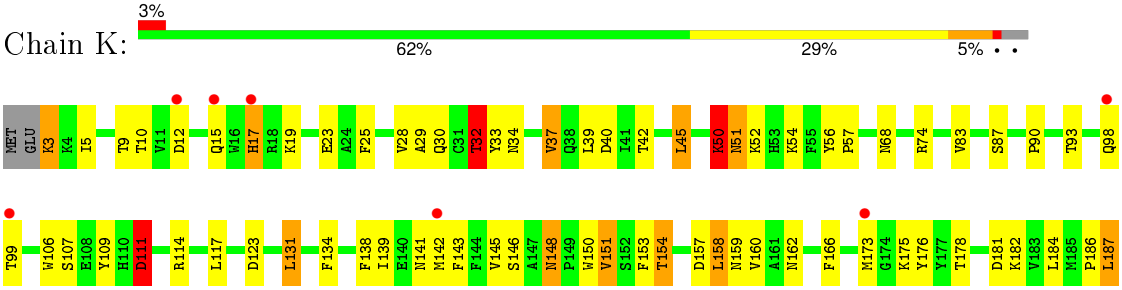
• Molecule 1: Chloramphenicol acetyltransferase

Chain J:

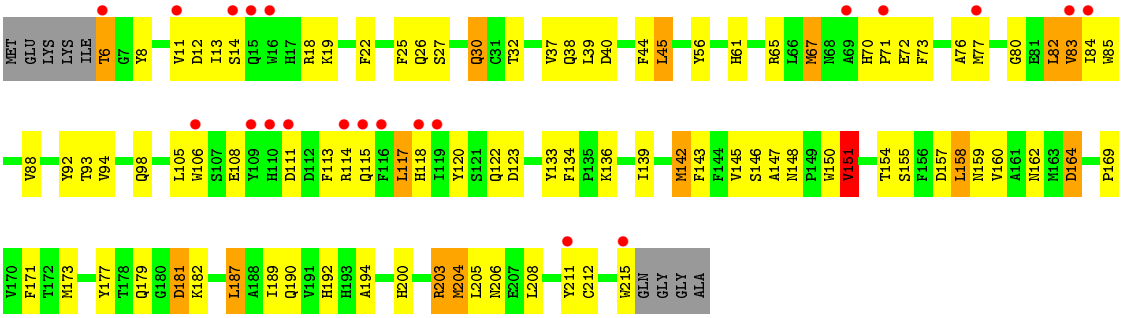


• Molecule 1: Chloramphenicol acetyltransferase

Chain K:



• Molecule 1: Chloramphenicol acetyltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	115.35Å 129.20Å 118.07Å 90.00° 108.30° 90.00°	Depositor
Resolution (Å)	111.80 – 2.18 53.34 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.7 (111.80-2.18) 98.0 (53.34-2.12)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.192 , 0.263 0.200 , 0.265	Depositor DCC
R_{free} test set	8605 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.0	EDS
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	2 of 182074 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22280	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, FUA

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	1.69	21/1830 (1.1%)	1.40	24/2484 (1.0%)
1	B	1.60	19/1857 (1.0%)	1.38	17/2518 (0.7%)
1	C	1.62	20/1822 (1.1%)	1.34	15/2473 (0.6%)
1	D	1.65	19/1822 (1.0%)	1.45	22/2473 (0.9%)
1	E	1.54	13/1844 (0.7%)	1.31	17/2501 (0.7%)
1	F	1.57	15/1818 (0.8%)	1.38	20/2468 (0.8%)
1	G	1.59	18/1822 (1.0%)	1.39	22/2473 (0.9%)
1	H	1.67	19/1844 (1.0%)	1.39	24/2502 (1.0%)
1	I	1.58	16/1844 (0.9%)	1.39	18/2501 (0.7%)
1	J	1.37	7/1822 (0.4%)	1.32	14/2474 (0.6%)
1	K	1.36	11/1831 (0.6%)	1.24	13/2484 (0.5%)
1	L	1.37	6/1805 (0.3%)	1.25	10/2451 (0.4%)
All	All	1.55	184/21961 (0.8%)	1.35	216/29802 (0.7%)

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	H	0	2
1	I	0	2
1	J	0	1
All	All	0	5

All (184) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	PHE	CE2-CZ	9.96	1.56	1.37
1	G	37	VAL	CB-CG2	-9.18	1.33	1.52
1	D	183	VAL	CB-CG2	9.01	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	59	PHE	CE1-CZ	8.92	1.54	1.37
1	D	157	ASP	CB-CG	8.88	1.70	1.51
1	B	28	VAL	CB-CG1	8.69	1.71	1.52
1	C	106	TRP	CE3-CZ3	8.35	1.52	1.38
1	K	145	VAL	CB-CG1	8.21	1.70	1.52
1	H	171	PHE	CE2-CZ	8.21	1.52	1.37
1	H	150	TRP	CE3-CZ3	8.05	1.52	1.38
1	B	162	ASN	CG-OD1	8.05	1.41	1.24
1	C	81	GLU	CD-OE2	7.92	1.34	1.25
1	B	20	GLU	CD-OE2	-7.90	1.17	1.25
1	B	102	PHE	CE2-CZ	7.62	1.51	1.37
1	D	111	ASP	CB-CG	-7.49	1.36	1.51
1	I	116	PHE	CE1-CZ	7.49	1.51	1.37
1	D	145	VAL	CB-CG1	7.33	1.68	1.52
1	A	28	VAL	CB-CG1	7.28	1.68	1.52
1	A	177	TYR	CG-CD2	7.23	1.48	1.39
1	C	160	VAL	CB-CG1	-7.17	1.37	1.52
1	E	106	TRP	CB-CG	7.16	1.63	1.50
1	A	33	TYR	CD1-CE1	7.15	1.50	1.39
1	I	33	TYR	CE1-CZ	7.02	1.47	1.38
1	D	27	SER	CA-CB	7.01	1.63	1.52
1	D	33	TYR	CD1-CE1	7.00	1.49	1.39
1	F	100	GLU	CD-OE1	7.00	1.33	1.25
1	H	215	TRP	CB-CG	6.91	1.62	1.50
1	E	159	ASN	CB-CG	6.90	1.67	1.51
1	A	177	TYR	CE1-CZ	6.89	1.47	1.38
1	F	8	TYR	CD2-CE2	6.83	1.49	1.39
1	C	16	TRP	CG-CD1	6.82	1.46	1.36
1	D	127	TYR	CD1-CE1	6.80	1.49	1.39
1	B	22	PHE	CD2-CE2	6.79	1.52	1.39
1	J	211	TYR	CD2-CE2	6.76	1.49	1.39
1	H	102	PHE	CD2-CE2	6.76	1.52	1.39
1	E	170	VAL	CB-CG2	6.74	1.67	1.52
1	E	126	CYS	CB-SG	-6.73	1.70	1.82
1	E	199	PHE	CE1-CZ	6.69	1.50	1.37
1	F	211	TYR	CD1-CE1	6.67	1.49	1.39
1	D	177	TYR	CD2-CE2	6.65	1.49	1.39
1	K	211	TYR	CD1-CE1	6.60	1.49	1.39
1	I	78	LYS	CE-NZ	6.59	1.65	1.49
1	K	29	ALA	CA-CB	6.59	1.66	1.52
1	G	83	VAL	CB-CG2	6.55	1.66	1.52
1	J	211	TYR	CD1-CE1	6.54	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	219	ALA	C-O	6.54	1.35	1.23
1	F	195	VAL	CB-CG1	6.53	1.66	1.52
1	G	22	PHE	CE1-CZ	6.50	1.49	1.37
1	A	211	TYR	CD2-CE2	6.49	1.49	1.39
1	A	56	TYR	CD1-CE1	6.43	1.49	1.39
1	J	87	SER	CB-OG	-6.43	1.33	1.42
1	C	159	ASN	CB-CG	6.42	1.65	1.51
1	E	183	VAL	CB-CG2	6.39	1.66	1.52
1	D	92	TYR	CD2-CE2	-6.39	1.29	1.39
1	I	37	VAL	CB-CG1	-6.33	1.39	1.52
1	K	37	VAL	CB-CG2	-6.32	1.39	1.52
1	I	177	TYR	CE1-CZ	6.32	1.46	1.38
1	B	77	MET	CG-SD	6.28	1.97	1.81
1	A	196	CYS	CB-SG	-6.27	1.71	1.82
1	A	211	TYR	CE2-CZ	6.20	1.46	1.38
1	H	112	ASP	N-CA	6.19	1.58	1.46
1	E	170	VAL	CB-CG1	6.18	1.65	1.52
1	G	194	ALA	CA-CB	6.16	1.65	1.52
1	I	143	PHE	CE2-CZ	6.15	1.49	1.37
1	I	76	ALA	CA-CB	6.13	1.65	1.52
1	E	188	ALA	CA-CB	6.11	1.65	1.52
1	H	77	MET	CB-CG	6.11	1.71	1.51
1	B	151	VAL	CB-CG2	6.10	1.65	1.52
1	D	124	VAL	CB-CG2	6.10	1.65	1.52
1	L	120	TYR	CE1-CZ	6.09	1.46	1.38
1	F	177	TYR	CE2-CZ	-6.08	1.30	1.38
1	B	195	VAL	CB-CG1	6.06	1.65	1.52
1	L	143	PHE	CE1-CZ	6.06	1.48	1.37
1	C	22	PHE	CE2-CZ	6.04	1.48	1.37
1	A	177	TYR	CD1-CE1	6.01	1.48	1.39
1	K	33	TYR	CD1-CE1	6.00	1.48	1.39
1	H	88	VAL	CB-CG1	6.00	1.65	1.52
1	F	211	TYR	CD2-CE2	5.93	1.48	1.39
1	H	83	VAL	CB-CG1	-5.92	1.40	1.52
1	C	199	PHE	CE1-CZ	5.89	1.48	1.37
1	A	176	TYR	CB-CG	5.88	1.60	1.51
1	C	191	VAL	CB-CG1	5.85	1.65	1.52
1	C	156	PHE	CG-CD2	5.84	1.47	1.38
1	G	77	MET	CG-SD	5.83	1.96	1.81
1	G	153	PHE	CD2-CE2	5.83	1.50	1.39
1	A	150	TRP	CE3-CZ3	5.82	1.48	1.38
1	E	194	ALA	CA-CB	5.81	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	134	PHE	CE1-CZ	5.80	1.48	1.37
1	G	75	MET	CG-SD	-5.78	1.66	1.81
1	C	194	ALA	CA-CB	5.78	1.64	1.52
1	E	22	PHE	CE2-CZ	5.77	1.48	1.37
1	D	127	TYR	CE2-CZ	5.75	1.46	1.38
1	F	122	GLN	CG-CD	5.72	1.64	1.51
1	A	85	TRP	CE3-CZ3	5.72	1.48	1.38
1	G	140	GLU	CD-OE2	5.71	1.31	1.25
1	C	109	TYR	CD2-CE2	5.71	1.48	1.39
1	J	143	PHE	CB-CG	-5.71	1.41	1.51
1	H	170	VAL	CB-CG1	5.70	1.64	1.52
1	D	116	PHE	CG-CD1	5.69	1.47	1.38
1	I	100	GLU	CD-OE1	5.66	1.31	1.25
1	B	102	PHE	CE1-CZ	5.65	1.48	1.37
1	C	183	VAL	CB-CG2	5.65	1.64	1.52
1	L	151	VAL	CB-CG1	5.62	1.64	1.52
1	K	54	LYS	CD-CE	5.62	1.65	1.51
1	B	56	TYR	CD2-CE2	5.59	1.47	1.39
1	C	88	VAL	CB-CG2	5.58	1.64	1.52
1	C	56	TYR	CG-CD2	5.57	1.46	1.39
1	I	170	VAL	CB-CG1	5.56	1.64	1.52
1	B	6	THR	CB-CG2	5.56	1.70	1.52
1	B	120	TYR	CE2-CZ	5.56	1.45	1.38
1	H	28	VAL	CB-CG1	5.55	1.64	1.52
1	J	6	THR	CB-CG2	5.55	1.70	1.52
1	B	150	TRP	CB-CG	-5.55	1.40	1.50
1	G	22	PHE	CE2-CZ	5.54	1.47	1.37
1	H	214	GLU	CD-OE2	-5.54	1.19	1.25
1	C	170	VAL	CB-CG1	5.53	1.64	1.52
1	H	171	PHE	CD2-CE2	5.53	1.50	1.39
1	G	35	GLN	CG-CD	5.52	1.63	1.51
1	D	35	GLN	CB-CG	-5.51	1.37	1.52
1	A	152	SER	CA-CB	5.49	1.61	1.52
1	D	92	TYR	CD1-CE1	-5.48	1.31	1.39
1	B	35	GLN	CB-CG	-5.46	1.37	1.52
1	L	151	VAL	CB-CG2	-5.46	1.41	1.52
1	B	194	ALA	CA-CB	-5.44	1.41	1.52
1	L	30	GLN	CG-CD	5.42	1.63	1.51
1	B	201	VAL	CB-CG1	5.42	1.64	1.52
1	C	181	ASP	CB-CG	5.41	1.63	1.51
1	C	133	TYR	C-O	5.41	1.33	1.23
1	F	114	ARG	CG-CD	5.40	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	VAL	CB-CG2	-5.39	1.41	1.52
1	A	83	VAL	CB-CG2	5.36	1.64	1.52
1	D	144	PHE	CE1-CZ	5.36	1.47	1.37
1	G	154	THR	CB-CG2	-5.35	1.34	1.52
1	A	58	ALA	CA-CB	5.35	1.63	1.52
1	C	152	SER	CA-CB	5.34	1.60	1.52
1	C	143	PHE	CG-CD1	-5.34	1.30	1.38
1	L	155	SER	CB-OG	-5.34	1.35	1.42
1	G	171	PHE	CD1-CE1	5.31	1.49	1.39
1	F	106	TRP	CB-CG	5.30	1.59	1.50
1	G	74	ARG	CB-CG	5.29	1.66	1.52
1	B	22	PHE	CE2-CZ	5.26	1.47	1.37
1	B	25	PHE	CE1-CZ	5.26	1.47	1.37
1	H	156	PHE	CD2-CE2	5.26	1.49	1.39
1	H	56	TYR	CD2-CE2	5.26	1.47	1.39
1	D	59	PHE	CE1-CZ	5.26	1.47	1.37
1	I	59	PHE	CE1-CZ	5.25	1.47	1.37
1	G	92	TYR	CD2-CE2	5.25	1.47	1.39
1	K	211	TYR	CD2-CE2	5.25	1.47	1.39
1	A	106	TRP	CE3-CZ3	5.24	1.47	1.38
1	A	95	PHE	CD2-CE2	5.23	1.49	1.39
1	I	78	LYS	CB-CG	5.22	1.66	1.52
1	D	209	GLN	CB-CG	5.22	1.66	1.52
1	I	28	VAL	CB-CG1	-5.21	1.42	1.52
1	G	95	PHE	CE1-CZ	5.21	1.47	1.37
1	K	134	PHE	CB-CG	-5.21	1.42	1.51
1	F	143	PHE	CE1-CZ	5.20	1.47	1.37
1	F	23	GLU	CD-OE2	5.19	1.31	1.25
1	J	171	PHE	CE1-CZ	5.19	1.47	1.37
1	D	15	GLN	CB-CG	5.18	1.66	1.52
1	J	69	ALA	CA-CB	5.17	1.63	1.52
1	K	211	TYR	CE1-CZ	5.17	1.45	1.38
1	E	102	PHE	CE2-CZ	5.15	1.47	1.37
1	K	109	TYR	CD1-CE1	5.15	1.47	1.39
1	A	174	GLY	CA-C	5.15	1.60	1.51
1	F	65	ARG	NE-CZ	5.14	1.39	1.33
1	C	136	LYS	CD-CE	5.14	1.64	1.51
1	F	133	TYR	CB-CG	5.14	1.59	1.51
1	G	148	ASN	CB-CG	5.13	1.62	1.51
1	D	106	TRP	CB-CG	5.12	1.59	1.50
1	I	199	PHE	CE1-CZ	5.12	1.47	1.37
1	F	72	GLU	CG-CD	5.11	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	143	PHE	CE1-CZ	5.09	1.47	1.37
1	A	54	LYS	CG-CD	5.08	1.69	1.52
1	E	28	VAL	CB-CG2	5.08	1.63	1.52
1	I	91	CYS	C-O	5.07	1.32	1.23
1	H	81	GLU	CG-CD	5.06	1.59	1.51
1	H	5	ILE	N-CA	5.06	1.56	1.46
1	H	211	TYR	CE2-CZ	5.06	1.45	1.38
1	B	127	TYR	CE2-CZ	5.04	1.45	1.38
1	H	165	ASN	CB-CG	5.04	1.62	1.51
1	G	46	LYS	CD-CE	5.04	1.63	1.51
1	I	157	ASP	CB-CG	5.04	1.62	1.51
1	F	109	TYR	CD1-CE1	-5.03	1.31	1.39
1	E	108	GLU	CD-OE2	5.03	1.31	1.25

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	4	LYS	O-C-N	-17.03	95.45	122.70
1	D	157	ASP	CB-CG-OD2	13.29	130.26	118.30
1	D	65	ARG	NE-CZ-NH2	-13.11	113.75	120.30
1	G	213	ASP	CB-CG-OD2	12.42	129.48	118.30
1	B	164	ASP	CB-CG-OD2	11.94	129.05	118.30
1	I	12	ASP	CB-CG-OD2	10.74	127.97	118.30
1	F	86	ASP	CB-CG-OD2	10.54	127.78	118.30
1	E	157	ASP	CB-CG-OD2	10.37	127.63	118.30
1	F	213	ASP	CB-CG-OD2	10.35	127.61	118.30
1	B	157	ASP	CB-CG-OD1	-10.34	109.00	118.30
1	D	164	ASP	CB-CG-OD2	10.08	127.37	118.30
1	J	12	ASP	CB-CG-OD2	9.77	127.10	118.30
1	J	65	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	F	12	ASP	CB-CG-OD2	9.35	126.72	118.30
1	A	74	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	J	111	ASP	CB-CG-OD1	9.27	126.64	118.30
1	C	12	ASP	CB-CG-OD2	9.12	126.51	118.30
1	L	164	ASP	CB-CG-OD2	9.04	126.44	118.30
1	C	74	ARG	NE-CZ-NH2	-9.03	115.79	120.30
1	A	82	LEU	CB-CG-CD2	-9.01	95.68	111.00
1	I	181	ASP	CB-CG-OD2	8.72	126.15	118.30
1	H	157	ASP	CB-CG-OD2	8.64	126.08	118.30
1	A	75	MET	CG-SD-CE	8.63	114.01	100.20
1	I	4	LYS	CA-C-N	8.62	136.16	117.20
1	J	79	ASP	CB-CG-OD2	8.62	126.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	123	ASP	CB-CG-OD2	8.50	125.95	118.30
1	K	40	ASP	CB-CG-OD2	8.29	125.76	118.30
1	D	65	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	H	160	VAL	CG1-CB-CG2	8.07	123.81	110.90
1	A	79	ASP	CB-CG-OD2	7.97	125.47	118.30
1	J	105	LEU	CB-CG-CD2	-7.90	97.58	111.00
1	D	213	ASP	CB-CG-OD2	7.86	125.38	118.30
1	D	181	ASP	CB-CG-OD2	7.83	125.34	118.30
1	J	65	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	I	4	LYS	N-CA-C	7.78	132.02	111.00
1	C	65	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	B	111	ASP	CB-CG-OD2	7.67	125.20	118.30
1	G	181	ASP	CB-CG-OD2	7.65	125.18	118.30
1	A	12	ASP	CB-CG-OD2	7.61	125.15	118.30
1	G	112	ASP	CB-CG-OD2	7.61	125.15	118.30
1	E	65	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	D	111	ASP	CB-CG-OD1	-7.58	111.48	118.30
1	J	164	ASP	CB-CG-OD2	7.56	125.10	118.30
1	F	123	ASP	CB-CG-OD2	7.55	125.10	118.30
1	B	12	ASP	CB-CG-OD2	7.54	125.09	118.30
1	C	67	MET	CG-SD-CE	-7.52	88.17	100.20
1	G	18	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	E	65	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	B	112	ASP	CB-CG-OD1	7.45	125.01	118.30
1	K	111	ASP	CB-CG-OD2	7.40	124.96	118.30
1	I	157	ASP	CB-CG-OD1	7.38	124.94	118.30
1	F	40	ASP	CB-CG-OD2	7.36	124.92	118.30
1	I	51	ASN	O-C-N	-7.33	110.98	122.70
1	D	40	ASP	CB-CG-OD2	7.29	124.86	118.30
1	A	32	THR	N-CA-CB	-7.27	96.49	110.30
1	A	37	VAL	CG1-CB-CG2	7.21	122.43	110.90
1	I	40	ASP	CB-CG-OD2	7.19	124.77	118.30
1	L	12	ASP	CB-CG-OD2	7.17	124.76	118.30
1	G	186	PRO	CA-N-CD	-7.16	101.48	111.50
1	A	164	ASP	CB-CG-OD2	7.11	124.70	118.30
1	F	181	ASP	CB-CG-OD2	7.11	124.70	118.30
1	H	79	ASP	CB-CG-OD2	7.10	124.69	118.30
1	F	32	THR	N-CA-CB	-7.07	96.86	110.30
1	J	39	LEU	CB-CG-CD2	7.04	122.96	111.00
1	G	187	LEU	CB-CG-CD2	7.03	122.94	111.00
1	H	203	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	E	37	VAL	CA-CB-CG1	6.94	121.31	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	157	ASP	OD1-CG-OD2	-6.86	110.27	123.30
1	F	111	ASP	CB-CG-OD2	6.84	124.46	118.30
1	H	39	LEU	CA-CB-CG	6.82	130.99	115.30
1	C	164	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	197	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	77	MET	CG-SD-CE	-6.78	89.35	100.20
1	G	205	LEU	CB-CG-CD2	6.77	122.51	111.00
1	K	45	LEU	CA-CB-CG	6.74	130.80	115.30
1	F	197	ASP	CB-CG-OD2	6.70	124.33	118.30
1	D	32	THR	N-CA-CB	-6.63	97.71	110.30
1	G	158	LEU	CB-CG-CD2	-6.62	99.75	111.00
1	I	164	ASP	CB-CG-OD2	6.61	124.25	118.30
1	K	74	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	H	39	LEU	CB-CG-CD2	6.60	122.22	111.00
1	G	67	MET	CG-SD-CE	6.57	110.70	100.20
1	G	213	ASP	CB-CG-OD1	-6.57	112.39	118.30
1	G	32	THR	N-CA-CB	-6.56	97.84	110.30
1	D	37	VAL	CG1-CB-CG2	6.54	121.37	110.90
1	B	39	LEU	CB-CG-CD2	6.53	122.11	111.00
1	I	112	ASP	CB-CG-OD2	6.51	124.16	118.30
1	F	39	LEU	CB-CG-CD2	6.49	122.02	111.00
1	G	105	LEU	CA-CB-CG	6.41	130.04	115.30
1	J	213	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	74	ARG	CD-NE-CZ	6.41	132.57	123.60
1	E	12	ASP	CB-CG-OD2	6.39	124.05	118.30
1	D	12	ASP	CB-CG-OD2	6.36	124.02	118.30
1	H	123	ASP	CB-CG-OD2	6.36	124.02	118.30
1	L	111	ASP	CB-CG-OD2	6.35	124.02	118.30
1	C	32	THR	N-CA-CB	-6.32	98.28	110.30
1	D	111	ASP	CB-CA-C	-6.30	97.80	110.40
1	H	218	GLY	CA-C-O	-6.29	109.29	120.60
1	H	181	ASP	CB-CG-OD2	6.25	123.93	118.30
1	F	164	ASP	CB-CG-OD2	6.25	123.92	118.30
1	L	40	ASP	CB-CG-OD2	6.24	123.92	118.30
1	G	158	LEU	CB-CA-C	-6.22	98.39	110.20
1	A	112	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	74	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	L	158	LEU	CA-CB-CG	6.19	129.54	115.30
1	A	157	ASP	CB-CG-OD2	6.17	123.85	118.30
1	G	86	ASP	CB-CG-OD2	6.17	123.85	118.30
1	C	105	LEU	CB-CA-C	-6.17	98.49	110.20
1	B	203	ARG	NE-CZ-NH1	-6.16	117.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	83	VAL	CG1-CB-CG2	6.14	120.72	110.90
1	F	114	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	E	117	LEU	CB-CG-CD2	6.13	121.42	111.00
1	D	214	GLU	CB-CA-C	6.09	122.58	110.40
1	G	164	ASP	CB-CG-OD1	6.01	123.71	118.30
1	F	154	THR	N-CA-CB	-6.00	98.89	110.30
1	I	45	LEU	CB-CG-CD2	6.00	121.20	111.00
1	G	154	THR	CA-CB-CG2	5.99	120.79	112.40
1	L	123	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	83	VAL	CA-CB-CG1	5.96	119.83	110.90
1	F	117	LEU	CA-CB-CG	5.96	129.00	115.30
1	I	51	ASN	C-N-CA	-5.95	106.82	121.70
1	H	86	ASP	CB-CG-OD2	5.95	123.66	118.30
1	B	185	MET	CG-SD-CE	-5.94	90.70	100.20
1	F	112	ASP	CB-CG-OD1	5.92	123.63	118.30
1	E	181	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	213	ASP	CB-CG-OD2	5.88	123.59	118.30
1	C	39	LEU	CB-CG-CD2	5.88	120.99	111.00
1	J	112	ASP	CB-CG-OD1	5.87	123.59	118.30
1	E	32	THR	CA-CB-CG2	5.82	120.55	112.40
1	E	131	LEU	CB-CG-CD1	5.82	120.89	111.00
1	G	65	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	D	163	MET	CG-SD-CE	5.81	109.50	100.20
1	H	164	ASP	CB-CG-OD2	5.81	123.53	118.30
1	J	10	THR	N-CA-CB	-5.80	99.28	110.30
1	B	40	ASP	CB-CG-OD2	5.80	123.52	118.30
1	F	83	VAL	CG1-CB-CG2	5.74	120.08	110.90
1	C	40	ASP	CB-CG-OD2	5.73	123.45	118.30
1	I	51	ASN	CA-C-N	5.73	129.80	117.20
1	K	12	ASP	CB-CG-OD2	5.73	123.45	118.30
1	K	175	LYS	CD-CE-NZ	-5.72	98.54	111.70
1	A	205	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	H	214	GLU	CG-CD-OE1	5.67	129.64	118.30
1	D	18	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	B	86	ASP	CB-CG-OD1	5.66	123.39	118.30
1	H	207	GLU	OE1-CD-OE2	-5.63	116.55	123.30
1	F	72	GLU	OE1-CD-OE2	-5.61	116.56	123.30
1	C	83	VAL	CG1-CB-CG2	5.59	119.84	110.90
1	J	187	LEU	CA-CB-CG	-5.59	102.45	115.30
1	H	74	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	E	158	LEU	CA-CB-CG	5.58	128.13	115.30
1	F	154	THR	CA-CB-CG2	5.57	120.19	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	123	ASP	CB-CG-OD2	5.55	123.30	118.30
1	H	114	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	E	86	ASP	CB-CG-OD2	5.53	123.27	118.30
1	J	87	SER	N-CA-CB	-5.51	102.24	110.50
1	A	83	VAL	CG1-CB-CG2	5.49	119.69	110.90
1	I	79	ASP	CB-CG-OD2	5.49	123.24	118.30
1	G	157	ASP	CB-CG-OD2	5.48	123.23	118.30
1	E	39	LEU	CB-CA-C	-5.47	99.80	110.20
1	H	178	THR	OG1-CB-CG2	-5.47	97.42	110.00
1	B	157	ASP	CB-CG-OD2	5.46	123.22	118.30
1	H	83	VAL	N-CA-CB	-5.46	99.50	111.50
1	K	74	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	K	32	THR	N-CA-CB	-5.43	99.99	110.30
1	H	197	ASP	CB-CG-OD1	5.42	123.18	118.30
1	C	18	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	83	VAL	CG1-CB-CG2	5.41	119.55	110.90
1	D	214	GLU	CA-CB-CG	5.41	125.29	113.40
1	A	111	ASP	CB-CG-OD1	5.40	123.16	118.30
1	I	86	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	39	LEU	CB-CG-CD2	5.38	120.15	111.00
1	E	164	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	83	VAL	CA-CB-CG2	5.34	118.91	110.90
1	H	32	THR	N-CA-CB	-5.34	100.16	110.30
1	C	45	LEU	CB-CG-CD2	5.33	120.07	111.00
1	E	136	LYS	CD-CE-NZ	-5.33	99.45	111.70
1	B	79	ASP	CB-CG-OD2	5.32	123.09	118.30
1	I	158	LEU	CA-CB-CG	5.30	127.48	115.30
1	E	39	LEU	CB-CG-CD2	5.29	120.00	111.00
1	A	37	VAL	CA-CB-CG2	5.29	118.83	110.90
1	F	121	SER	N-CA-CB	5.28	118.42	110.50
1	H	171	PHE	CB-CA-C	-5.28	99.84	110.40
1	G	145	VAL	CG1-CB-CG2	-5.26	102.49	110.90
1	H	77	MET	CG-SD-CE	-5.25	91.79	100.20
1	F	39	LEU	CB-CA-C	-5.25	100.22	110.20
1	L	203	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	181	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	187	LEU	CA-CB-CG	-5.22	103.30	115.30
1	A	160	VAL	N-CA-C	-5.21	96.93	111.00
1	I	83	VAL	CG1-CB-CG2	5.20	119.23	110.90
1	D	123	ASP	CB-CG-OD2	5.19	122.97	118.30
1	K	181	ASP	CB-CG-OD2	5.19	122.97	118.30
1	K	54	LYS	CD-CE-NZ	5.17	123.59	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	213	ASP	CB-CG-OD2	5.15	122.94	118.30
1	K	197	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	184	LEU	CB-CG-CD1	5.15	119.76	111.00
1	H	63	LEU	CB-CG-CD1	-5.14	102.25	111.00
1	E	111	ASP	CB-CG-OD2	5.14	122.92	118.30
1	C	28	VAL	N-CA-CB	-5.13	100.20	111.50
1	H	83	VAL	CG1-CB-CG2	5.13	119.11	110.90
1	H	219	ALA	CB-CA-C	5.13	117.79	110.10
1	L	45	LEU	CA-CB-CG	5.12	127.06	115.30
1	L	187	LEU	CA-CB-CG	-5.11	103.54	115.30
1	B	151	VAL	CB-CA-C	-5.10	101.71	111.40
1	G	160	VAL	CG1-CB-CG2	5.10	119.06	110.90
1	D	9	THR	OG1-CB-CG2	-5.08	98.31	110.00
1	G	197	ASP	CB-CG-OD2	5.07	122.86	118.30
1	L	181	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	18	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	214	GLU	N-CA-CB	-5.06	101.49	110.60
1	C	12	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	G	51	ASN	C-N-CA	-5.05	109.08	121.70
1	B	82	LEU	CB-CG-CD1	-5.04	102.42	111.00
1	K	45	LEU	CB-CG-CD2	5.02	119.54	111.00
1	J	40	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	121	SER	CA-CB-OG	-5.00	97.69	111.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	218	GLY	Peptide
1	H	5	ILE	Peptide
1	I	3	LYS	Peptide
1	I	4	LYS	Mainchain
1	J	6	THR	Peptide

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	1771	0	1658	59	0
1	B	1798	0	1690	46	0
1	C	1763	0	1647	45	0
1	D	1763	0	1647	71	0
1	E	1785	0	1681	70	0
1	F	1759	0	1644	55	0
1	G	1763	0	1647	61	0
1	H	1785	0	1676	78	0
1	I	1785	0	1681	79	0
1	J	1763	0	1652	88	0
1	K	1772	0	1670	62	0
1	L	1746	0	1633	75	0
2	A	1	0	0	0	0
3	A	37	0	44	8	0
3	B	37	0	44	9	0
3	C	37	0	44	5	0
3	D	37	0	44	10	0
3	E	37	0	44	3	0
3	F	37	0	44	8	0
3	G	37	0	43	6	0
3	H	37	0	43	5	0
3	I	37	0	44	16	0
3	J	37	0	44	10	0
3	K	37	0	44	10	0
3	L	37	0	44	4	0
4	A	78	0	0	6	0
4	B	51	0	0	7	0
4	C	68	0	0	10	0
4	D	58	0	0	7	0
4	E	44	0	0	8	0
4	F	43	0	0	5	0
4	G	43	0	0	6	0
4	H	74	0	0	10	0
4	I	42	0	0	8	0
4	J	34	0	0	9	0
4	K	26	0	0	7	0
4	L	21	0	0	7	0
All	All	22280	0	20452	774	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 18.

All (774) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:ILE:H	1:E:142:MET:CE	1.31	1.37
1:E:139:ILE:N	1:E:142:MET:HE3	1.39	1.36
1:H:218:GLY:HA2	1:H:219:ALA:O	1.36	1.24
1:E:67:MET:CE	1:E:171:PHE:HE1	1.49	1.24
1:J:67:MET:CE	1:J:67:MET:HA	1.71	1.20
1:G:139:ILE:N	1:G:142:MET:HE3	1.56	1.20
1:G:139:ILE:H	1:G:142:MET:CE	1.58	1.16
1:E:67:MET:HE2	1:E:171:PHE:HE1	1.02	1.15
1:D:154:THR:O	1:F:154:THR:HG23	1.46	1.12
1:C:67:MET:HE1	1:C:169:PRO:HG2	1.17	1.12
1:D:67:MET:HE3	1:D:169:PRO:HG2	1.23	1.12
1:A:154:THR:HG23	1:B:154:THR:O	1.50	1.11
1:K:139:ILE:N	1:K:142:MET:HE3	1.64	1.09
1:J:67:MET:HA	1:J:67:MET:HE2	1.27	1.08
1:D:67:MET:CE	1:D:169:PRO:HG2	1.82	1.08
1:A:6:THR:HG21	4:A:837:HOH:O	1.52	1.08
1:K:154:THR:HG23	1:L:154:THR:O	1.53	1.07
1:H:154:THR:CG2	1:I:154:THR:O	2.02	1.07
1:C:67:MET:CE	1:C:73:PHE:HB3	1.85	1.06
1:E:67:MET:HE2	1:E:171:PHE:CE1	1.90	1.06
1:C:146:SER:HB3	4:C:709:HOH:O	1.53	1.06
1:K:139:ILE:H	1:K:142:MET:CE	1.69	1.05
1:H:154:THR:HG23	1:I:154:THR:O	1.54	1.05
1:E:67:MET:CE	1:E:171:PHE:CE1	2.39	1.05
1:G:154:THR:HG23	1:H:154:THR:O	1.54	1.05
1:L:67:MET:HE3	1:L:169:PRO:HG2	1.34	1.04
1:J:171:PHE:HZ	1:J:204:MET:CE	1.71	1.03
1:F:114:ARG:HD3	4:F:729:HOH:O	1.58	1.02
1:C:67:MET:CE	1:C:169:PRO:HG2	1.89	1.01
1:K:139:ILE:H	1:K:142:MET:HE3	0.87	1.01
1:G:139:ILE:H	1:G:142:MET:HE3	0.84	1.00
1:D:154:THR:HG23	1:E:154:THR:O	1.60	1.00
1:C:40:ASP:OD1	1:C:182:LYS:HD2	1.60	1.00
1:H:67:MET:HE3	1:H:73:PHE:HB3	1.44	0.99
1:H:8:TYR:CE2	1:H:78:LYS:HE2	1.97	0.99
1:J:171:PHE:CZ	1:J:204:MET:CE	2.47	0.97
1:C:115:GLN:O	1:C:119:ILE:CD1	2.13	0.96
1:E:139:ILE:O	1:E:142:MET:SD	2.22	0.96
1:C:115:GLN:O	1:C:119:ILE:HD12	1.65	0.95
1:I:139:ILE:HG13	1:I:142:MET:SD	2.07	0.95
1:J:115:GLN:O	1:J:119:ILE:HD12	1.67	0.94
1:F:123:ASP:OD1	1:F:136:LYS:HE2	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:ASN:HB3	1:H:32:THR:HG22	1.49	0.94
1:E:154:THR:HG23	1:F:154:THR:O	1.68	0.93
1:F:192:HIS:HD1	1:F:194:ALA:H	1.13	0.93
1:G:32:THR:HG22	1:I:159:ASN:HB3	1.49	0.93
1:A:159:ASN:HB3	1:B:32:THR:HG22	1.51	0.92
1:L:106:TRP:CD1	1:L:142:MET:CE	2.53	0.92
1:H:75:MET:SD	1:H:195:VAL:HB	2.09	0.92
1:I:171:PHE:CZ	1:I:204:MET:CE	2.53	0.91
1:L:11:VAL:CG1	1:L:82:LEU:HB3	2.00	0.91
1:H:218:GLY:HA2	1:H:219:ALA:C	1.90	0.91
1:L:67:MET:CE	1:L:169:PRO:HG2	1.99	0.91
1:C:67:MET:HE1	1:C:73:PHE:HB3	1.52	0.91
1:B:67:MET:HE3	1:B:73:PHE:CG	2.05	0.91
1:I:134:PHE:CE1	3:I:707:FUA:H282	2.06	0.90
1:C:67:MET:HE3	1:C:73:PHE:HB3	1.54	0.89
1:E:34:ASN:ND2	1:E:190:GLN:HB3	1.88	0.89
1:D:157:ASP:OD2	1:F:157:ASP:HB2	1.74	0.88
1:G:154:THR:O	1:I:154:THR:HG23	1.72	0.88
1:J:93:THR:HG21	3:J:711:FUA:H22	1.54	0.88
1:H:106:TRP:HB3	1:H:142:MET:CE	2.03	0.88
1:G:38:GLN:HE22	1:G:186:PRO:HG3	1.38	0.88
1:E:192:HIS:HD1	1:E:194:ALA:H	1.21	0.87
1:I:171:PHE:CZ	1:I:204:MET:HE3	2.07	0.87
1:L:8:TYR:HB2	1:L:83:VAL:HG13	1.57	0.85
1:K:99:THR:HG21	1:K:131:LEU:HD11	1.57	0.85
1:D:111:ASP:OD2	1:J:65:ARG:HD2	1.75	0.85
1:L:162:ASN:CG	4:L:723:HOH:O	2.14	0.85
1:E:67:MET:HE1	1:E:171:PHE:CE1	2.11	0.84
1:C:65:ARG:HD2	4:C:765:HOH:O	1.77	0.84
1:D:159:ASN:HB3	1:E:32:THR:HG22	1.60	0.84
1:E:67:MET:HE1	1:E:171:PHE:HE1	1.43	0.83
1:J:5:ILE:HA	4:J:740:HOH:O	1.78	0.83
1:J:67:MET:CA	1:J:67:MET:CE	2.55	0.83
1:H:192:HIS:HD1	1:H:194:ALA:H	1.27	0.83
1:D:210:GLN:O	1:D:214:GLU:HB3	1.78	0.82
1:I:171:PHE:HZ	1:I:204:MET:CE	1.90	0.82
1:H:155:SER:CB	1:I:155:SER:HB2	2.09	0.82
1:D:32:THR:HG21	4:D:709:HOH:O	1.78	0.82
1:F:59:PHE:CD2	1:F:173:MET:SD	2.73	0.82
1:I:3:LYS:N	4:I:748:HOH:O	2.12	0.82
1:G:192:HIS:HD1	1:G:194:ALA:H	1.25	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TRP:CD1	1:A:142:MET:CE	2.62	0.82
1:A:154:THR:CG2	1:B:154:THR:O	2.28	0.81
1:A:123:ASP:OD1	1:A:136:LYS:NZ	2.13	0.81
1:A:192:HIS:HD1	1:A:194:ALA:H	1.28	0.81
1:K:192:HIS:HD1	1:K:194:ALA:H	1.29	0.81
1:H:113:PHE:H	1:H:219:ALA:HB1	1.44	0.80
1:H:155:SER:HB2	1:I:155:SER:HB2	1.62	0.80
1:D:157:ASP:OD2	1:F:157:ASP:CB	2.29	0.80
1:G:15:GLN:HA	1:G:15:GLN:HE21	1.46	0.80
1:J:146:SER:HB3	3:J:711:FUA:H3	1.63	0.80
1:D:56:TYR:HB3	1:D:57:PRO:CD	2.12	0.80
1:L:11:VAL:HG12	1:L:82:LEU:HB3	1.65	0.79
1:A:56:TYR:HD1	1:A:173:MET:HE1	1.47	0.79
1:C:40:ASP:OD1	1:C:182:LYS:CD	2.30	0.79
1:F:77:MET:HE1	1:F:82:LEU:N	1.98	0.78
1:D:6:THR:HG23	4:D:733:HOH:O	1.83	0.78
1:E:139:ILE:H	1:E:142:MET:HE3	0.62	0.78
1:J:171:PHE:CZ	1:J:204:MET:HE3	2.18	0.78
1:J:192:HIS:HD1	1:J:194:ALA:H	1.29	0.78
1:I:192:HIS:HD1	1:I:194:ALA:H	1.31	0.78
1:L:204:MET:HE1	1:L:205:LEU:HD23	1.66	0.78
1:J:171:PHE:HZ	1:J:204:MET:HE3	1.49	0.77
1:H:32:THR:HG21	4:H:731:HOH:O	1.83	0.77
1:B:50:LYS:HG3	1:B:51:ASN:ND2	2.00	0.77
1:E:38:GLN:HE22	1:E:186:PRO:HG3	1.48	0.77
1:A:123:ASP:CG	1:A:136:LYS:HZ1	1.87	0.77
1:D:110:HIS:HD2	1:D:112:ASP:H	1.33	0.77
1:L:22:PHE:CZ	1:L:82:LEU:HD12	2.19	0.77
1:A:67:MET:HA	1:A:67:MET:HE2	1.66	0.76
1:F:114:ARG:NH2	1:F:217:GLY:O	2.19	0.76
1:B:2:GLU:N	4:B:714:HOH:O	2.17	0.76
1:B:56:TYR:HB3	1:B:57:PRO:CD	2.13	0.76
1:H:149:PRO:O	1:H:175:LYS:HG2	1.86	0.76
1:J:171:PHE:CZ	1:J:204:MET:HE1	2.20	0.75
1:I:171:PHE:HZ	1:I:204:MET:HE3	1.47	0.75
1:H:106:TRP:HB3	1:H:142:MET:HE2	1.68	0.75
1:G:158:LEU:HD11	3:G:708:FUA:H72	1.67	0.75
1:C:192:HIS:HD1	1:C:194:ALA:H	1.34	0.75
1:I:139:ILE:CG1	1:I:142:MET:SD	2.75	0.75
1:D:114:ARG:HH21	1:D:218:GLY:HA3	1.51	0.75
1:G:139:ILE:O	1:G:142:MET:SD	2.46	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:MET:HE3	1:F:77:MET:HA	1.69	0.74
1:E:139:ILE:N	1:E:142:MET:CE	2.16	0.74
1:J:93:THR:CG2	3:J:711:FUA:H22	2.17	0.74
1:F:77:MET:CE	1:F:81:GLU:C	2.56	0.74
1:K:3:LYS:CB	4:K:720:HOH:O	2.36	0.73
1:B:32:THR:HG21	4:B:707:HOH:O	1.87	0.73
1:J:65:ARG:HD3	4:J:727:HOH:O	1.89	0.73
1:E:157:ASP:OD1	4:E:744:HOH:O	2.07	0.73
1:A:171:PHE:HZ	1:A:204:MET:CE	2.02	0.73
1:L:204:MET:CE	1:L:205:LEU:HD23	2.20	0.72
1:F:110:HIS:HD2	1:F:119:ILE:HD13	1.54	0.72
1:D:13:ILE:HD12	1:D:16:TRP:CE3	2.24	0.72
1:C:119:ILE:H	1:C:119:ILE:HD12	1.53	0.72
1:I:171:PHE:CE2	1:I:204:MET:HE1	2.25	0.72
1:E:129:GLU:CB	4:E:729:HOH:O	2.37	0.72
3:B:703:FUA:C28	1:C:29:ALA:HB2	2.20	0.72
1:D:65:ARG:HD2	1:J:111:ASP:OD2	1.89	0.72
1:I:26:GLN:NE2	4:I:749:HOH:O	2.23	0.71
3:B:703:FUA:H282	1:C:29:ALA:HB2	1.72	0.71
1:E:171:PHE:CZ	1:E:204:MET:CE	2.73	0.71
1:K:138:PHE:HA	1:K:142:MET:HE1	1.72	0.71
1:F:77:MET:HA	1:F:77:MET:CE	2.20	0.71
1:A:106:TRP:CD1	1:A:142:MET:HE3	2.25	0.71
3:F:704:FUA:C12	3:F:704:FUA:H232	2.20	0.71
1:H:167:PHE:O	1:H:169:PRO:HD3	1.91	0.71
1:I:9:THR:HG23	4:I:721:HOH:O	1.90	0.71
1:K:3:LYS:HB3	4:K:720:HOH:O	1.89	0.71
1:L:106:TRP:CD1	1:L:142:MET:HE3	2.25	0.70
1:D:148:ASN:ND2	1:D:150:TRP:HE3	1.89	0.70
1:D:114:ARG:NH2	1:D:218:GLY:HA3	2.05	0.70
1:L:11:VAL:HG11	1:L:82:LEU:HB3	1.71	0.70
1:J:9:THR:HG23	4:J:712:HOH:O	1.92	0.70
1:H:56:TYR:HE1	1:H:173:MET:CE	2.05	0.70
1:J:13:ILE:HG22	1:J:19:LYS:HE3	1.74	0.70
1:E:145:VAL:HG11	1:E:173:MET:HE3	1.73	0.70
1:H:218:GLY:CA	1:H:219:ALA:O	2.30	0.70
1:E:159:ASN:HB3	1:F:32:THR:HG22	1.72	0.70
1:L:67:MET:HE3	1:L:169:PRO:CG	2.19	0.70
1:J:90:PRO:HD2	1:J:107:SER:O	1.92	0.69
1:F:114:ARG:CD	4:F:729:HOH:O	2.27	0.69
1:L:106:TRP:CG	1:L:142:MET:HE3	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:138:PHE:HA	1:K:142:MET:CE	2.22	0.69
3:I:707:FUA:H283	3:I:707:FUA:H122	1.72	0.69
1:J:67:MET:HA	1:J:67:MET:HE3	1.71	0.69
1:B:56:TYR:HB3	1:B:57:PRO:HD3	1.72	0.69
1:D:13:ILE:HD12	1:D:16:TRP:HE3	1.57	0.68
1:I:139:ILE:O	1:I:142:MET:SD	2.51	0.68
1:A:32:THR:HG22	1:C:159:ASN:HB3	1.76	0.68
1:B:67:MET:HE2	1:B:73:PHE:HB3	1.74	0.68
1:E:129:GLU:HB2	4:E:729:HOH:O	1.92	0.68
1:F:110:HIS:HD2	1:F:119:ILE:CD1	2.06	0.68
1:E:139:ILE:HG12	1:E:142:MET:CE	2.24	0.67
1:E:171:PHE:HZ	1:E:204:MET:CE	2.07	0.67
1:I:134:PHE:HE1	3:I:707:FUA:H282	1.57	0.67
1:E:9:THR:HG22	4:E:725:HOH:O	1.93	0.67
1:F:77:MET:CE	1:F:82:LEU:N	2.56	0.67
1:H:23:GLU:HG2	4:H:727:HOH:O	1.94	0.67
1:E:171:PHE:CZ	1:E:204:MET:HE3	2.28	0.67
1:J:67:MET:CE	1:J:73:PHE:CG	2.78	0.67
1:E:6:THR:HB	1:E:7:GLY:O	1.94	0.67
3:D:705:FUA:C12	3:D:705:FUA:H232	2.25	0.67
1:I:56:TYR:HB3	1:I:57:PRO:HD3	1.77	0.67
1:J:67:MET:HE1	1:J:73:PHE:CD1	2.29	0.67
1:C:32:THR:HG21	4:C:726:HOH:O	1.92	0.67
1:G:38:GLN:HE22	1:G:186:PRO:CG	2.08	0.67
1:D:148:ASN:HD22	1:D:150:TRP:HE3	1.43	0.67
1:J:139:ILE:H	1:J:142:MET:HE3	1.60	0.67
3:B:703:FUA:C12	3:B:703:FUA:H232	2.25	0.67
1:J:157:ASP:OD1	1:L:157:ASP:OD2	2.12	0.66
1:A:171:PHE:CZ	1:A:204:MET:CE	2.77	0.66
1:B:50:LYS:CG	1:B:51:ASN:ND2	2.58	0.66
1:J:56:TYR:CE1	1:J:173:MET:CE	2.78	0.66
1:D:13:ILE:CD1	1:D:16:TRP:CE3	2.78	0.66
3:I:707:FUA:H283	3:I:707:FUA:H232	1.76	0.66
1:B:114:ARG:HG3	1:B:114:ARG:HH11	1.59	0.66
1:J:67:MET:CE	1:J:73:PHE:CD1	2.79	0.66
1:B:162:ASN:HB3	4:B:712:HOH:O	1.96	0.66
1:K:3:LYS:N	4:K:733:HOH:O	2.29	0.66
1:D:67:MET:CE	1:D:169:PRO:CG	2.68	0.65
1:G:110:HIS:HD2	1:G:119:ILE:CD1	2.09	0.65
1:H:67:MET:HE2	1:H:169:PRO:HB2	1.77	0.65
3:I:707:FUA:C28	3:I:707:FUA:H232	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ASN:OD1	1:D:157:ASP:OD1	2.12	0.65
1:J:19:LYS:HE2	1:J:23:GLU:OE2	1.95	0.65
1:I:32:THR:HG21	4:I:708:HOH:O	1.97	0.65
1:D:204:MET:HE3	1:D:205:LEU:N	2.12	0.65
1:H:65:ARG:HH22	1:H:219:ALA:HB2	1.62	0.64
1:K:111:ASP:N	1:K:111:ASP:OD1	2.30	0.64
1:J:67:MET:CA	1:J:67:MET:HE3	2.27	0.64
1:H:218:GLY:CA	1:H:219:ALA:C	2.65	0.64
1:J:67:MET:SD	1:J:73:PHE:HB3	2.38	0.64
1:H:56:TYR:HE1	1:H:173:MET:HE3	1.60	0.64
1:E:138:PHE:HA	1:E:142:MET:HE1	1.80	0.64
1:D:32:THR:HG22	1:F:159:ASN:HB3	1.79	0.64
1:A:106:TRP:CG	1:A:142:MET:HE3	2.32	0.64
1:L:106:TRP:CD1	1:L:142:MET:HE1	2.33	0.63
1:H:113:PHE:H	1:H:219:ALA:CB	2.11	0.63
1:E:171:PHE:HZ	1:E:204:MET:HE3	1.64	0.63
1:I:56:TYR:HB3	1:I:57:PRO:CD	2.29	0.63
1:C:119:ILE:HD12	1:C:119:ILE:N	2.13	0.63
1:B:67:MET:CE	1:B:73:PHE:HB3	2.28	0.63
1:E:34:ASN:ND2	1:E:190:GLN:CB	2.62	0.63
1:J:105:LEU:HD23	1:J:105:LEU:H	1.63	0.63
1:A:67:MET:HE1	1:A:204:MET:SD	2.38	0.63
1:G:67:MET:HE1	1:G:204:MET:SD	2.39	0.62
1:H:75:MET:SD	1:H:195:VAL:CB	2.87	0.62
1:K:139:ILE:HD12	1:K:141:ASN:OD1	1.99	0.62
1:E:148:ASN:N	1:E:149:PRO:CD	2.63	0.62
1:L:44:PHE:HB2	1:L:212:CYS:O	1.99	0.62
1:I:134:PHE:HE1	3:I:707:FUA:C28	2.12	0.62
1:L:146:SER:OG	3:L:710:FUA:H3	1.99	0.62
1:A:56:TYR:HD1	1:A:173:MET:CE	2.13	0.62
1:G:38:GLN:NE2	1:G:186:PRO:HD3	2.15	0.62
1:L:67:MET:HB3	1:L:88:VAL:HG21	1.81	0.62
1:L:22:PHE:CZ	1:L:82:LEU:CD1	2.83	0.62
1:I:134:PHE:CE1	3:I:707:FUA:C28	2.82	0.61
1:F:57:PRO:HG3	1:F:120:TYR:CE2	2.35	0.61
1:F:56:TYR:HB3	1:F:57:PRO:HD3	1.82	0.61
1:I:149:PRO:O	1:I:175:LYS:HG3	2.00	0.61
1:H:113:PHE:N	1:H:219:ALA:HB1	2.14	0.61
1:E:145:VAL:HG11	1:E:173:MET:CE	2.30	0.61
1:H:23:GLU:HG3	1:H:24:ALA:N	2.15	0.61
1:E:148:ASN:N	1:E:149:PRO:HD3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:SER:HB2	1:H:155:SER:HB2	1.82	0.61
1:E:110:HIS:HD2	1:E:112:ASP:H	1.47	0.61
1:H:56:TYR:HB3	1:H:57:PRO:HD3	1.81	0.61
1:J:105:LEU:N	1:J:105:LEU:HD23	2.14	0.61
1:H:8:TYR:CD2	1:H:78:LYS:HE2	2.35	0.61
1:L:98:GLN:HG2	4:L:725:HOH:O	2.00	0.61
1:B:159:ASN:HB3	1:C:32:THR:HG22	1.83	0.61
1:H:91:CYS:HB2	1:H:142:MET:HE2	1.83	0.61
1:G:158:LEU:HD13	1:G:160:VAL:HG23	1.81	0.61
1:G:15:GLN:HA	1:G:15:GLN:NE2	2.16	0.60
1:A:133:TYR:CE2	3:A:702:FUA:H272	2.35	0.60
1:L:179:GLN:HG3	1:L:179:GLN:O	2.00	0.60
1:A:215:TRP:CZ2	1:A:217:GLY:HA2	2.37	0.60
1:G:210:GLN:O	1:G:214:GLU:HG3	2.00	0.60
1:H:30:GLN:NE2	4:H:761:HOH:O	2.35	0.60
1:B:114:ARG:CG	1:B:114:ARG:HH11	2.14	0.60
1:A:56:TYR:CD1	1:A:173:MET:HE1	2.34	0.60
1:K:106:TRP:CD1	1:K:142:MET:CE	2.85	0.59
1:H:101:THR:HG21	1:I:17:HIS:HB3	1.83	0.59
1:E:139:ILE:N	1:E:142:MET:SD	2.74	0.59
1:L:67:MET:CE	1:L:169:PRO:CG	2.79	0.59
1:J:157:ASP:OD2	1:K:157:ASP:OD2	2.20	0.59
1:B:51:ASN:N	1:B:51:ASN:HD22	2.00	0.59
1:J:159:ASN:HB3	1:K:32:THR:HG22	1.83	0.59
1:I:62:ILE:HG23	1:I:211:TYR:HD1	1.66	0.59
1:C:9:THR:HG22	4:C:712:HOH:O	2.00	0.59
1:F:115:GLN:O	1:F:119:ILE:HD12	2.03	0.59
3:D:705:FUA:C22	3:D:705:FUA:H283	2.32	0.59
1:B:4:LYS:HE2	1:B:108:GLU:OE1	2.02	0.59
1:C:159:ASN:ND2	4:C:768:HOH:O	2.07	0.59
1:L:139:ILE:HG12	1:L:142:MET:SD	2.41	0.59
1:E:13:ILE:HG22	1:E:19:LYS:HG3	1.85	0.59
1:I:106:TRP:CD1	1:I:142:MET:HE1	2.37	0.59
1:G:110:HIS:CD2	1:G:119:ILE:CD1	2.86	0.58
1:G:187:LEU:HD22	1:G:208:LEU:HD21	1.82	0.58
1:J:67:MET:HE1	1:J:73:PHE:CG	2.38	0.58
1:J:56:TYR:HE1	1:J:173:MET:CE	2.15	0.58
1:H:67:MET:CE	1:H:169:PRO:HG2	2.34	0.58
1:H:106:TRP:CB	1:H:142:MET:CE	2.81	0.58
1:I:26:GLN:HE21	1:I:26:GLN:HA	1.69	0.58
1:D:154:THR:CG2	1:E:154:THR:O	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:162:ASN:ND2	4:L:723:HOH:O	2.36	0.58
1:G:30:GLN:HE22	1:G:164:ASP:HA	1.69	0.58
1:H:23:GLU:CG	4:H:727:HOH:O	2.52	0.58
1:I:4:LYS:HE2	1:I:4:LYS:HA	1.86	0.57
1:D:12:ASP:O	1:J:10:THR:HG23	2.04	0.57
1:A:123:ASP:CG	1:A:136:LYS:NZ	2.56	0.57
1:D:56:TYR:HB3	1:D:57:PRO:HD2	1.86	0.57
1:G:32:THR:HG21	4:G:725:HOH:O	2.03	0.57
1:J:148:ASN:ND2	1:J:150:TRP:HE3	2.01	0.57
1:G:171:PHE:HZ	1:G:204:MET:SD	2.27	0.57
1:L:26:GLN:HA	1:L:26:GLN:OE1	2.02	0.57
1:J:93:THR:HG21	3:J:711:FUA:C2	2.32	0.57
1:A:171:PHE:CZ	1:A:204:MET:HE3	2.39	0.57
1:A:67:MET:CA	1:A:67:MET:HE2	2.35	0.57
1:F:110:HIS:CD2	1:F:119:ILE:HD13	2.38	0.57
1:G:154:THR:CG2	1:H:154:THR:O	2.44	0.56
1:K:3:LYS:CG	4:K:720:HOH:O	2.52	0.56
1:L:145:VAL:HG11	1:L:173:MET:CE	2.34	0.56
1:A:117:LEU:HD22	1:A:117:LEU:O	2.06	0.56
1:A:114:ARG:NH2	1:L:80:GLY:O	2.38	0.56
1:L:11:VAL:O	1:L:11:VAL:HG13	2.06	0.56
1:H:106:TRP:CG	1:H:142:MET:HE3	2.40	0.56
1:G:118:HIS:O	1:G:122:GLN:HG3	2.05	0.56
1:F:110:HIS:CD2	1:F:119:ILE:CD1	2.88	0.56
1:G:154:THR:HG21	1:H:38:GLN:OE1	2.06	0.56
1:F:56:TYR:HB3	1:F:57:PRO:CD	2.36	0.56
1:K:139:ILE:HG13	1:K:142:MET:HG3	1.88	0.56
1:I:146:SER:CB	3:I:707:FUA:H3	2.35	0.56
1:E:93:THR:HG21	3:E:706:FUA:H22	1.88	0.56
1:K:90:PRO:HD2	1:K:107:SER:O	2.06	0.56
1:D:56:TYR:HB3	1:D:57:PRO:HD3	1.88	0.55
1:A:30:GLN:NE2	4:A:802:HOH:O	2.38	0.55
1:L:76:ALA:HA	4:L:729:HOH:O	2.05	0.55
1:C:30:GLN:HE22	1:C:164:ASP:HA	1.70	0.55
1:B:3:LYS:H	1:I:10:THR:HB	1.69	0.55
1:J:56:TYR:CD1	1:J:173:MET:CE	2.89	0.55
1:I:105:LEU:HD11	1:I:127:TYR:HB2	1.86	0.55
1:D:157:ASP:OD2	1:F:157:ASP:HB3	2.05	0.55
1:I:93:THR:CG2	3:I:707:FUA:H22	2.37	0.55
1:K:148:ASN:HD21	1:K:151:VAL:HG13	1.71	0.55
1:K:139:ILE:HG13	1:K:142:MET:CG	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:707:FUA:C28	3:I:707:FUA:H122	2.37	0.55
1:A:114:ARG:HH11	1:A:218:GLY:HA2	1.72	0.55
1:K:148:ASN:HD22	1:K:148:ASN:C	2.10	0.55
1:K:187:LEU:HG	1:K:188:ALA:N	2.18	0.55
1:D:12:ASP:O	1:J:10:THR:CG2	2.55	0.55
1:B:114:ARG:NH1	1:B:114:ARG:CG	2.68	0.55
1:H:148:ASN:OD1	1:H:150:TRP:HE3	1.90	0.54
1:H:8:TYR:CE2	1:H:78:LYS:CE	2.83	0.54
1:J:49:LYS:O	1:J:51:ASN:O	2.25	0.54
1:E:171:PHE:CE2	1:E:204:MET:HE1	2.41	0.54
1:I:190:GLN:C	1:I:190:GLN:HE21	2.10	0.54
1:D:46:LYS:HE2	4:D:749:HOH:O	2.07	0.54
1:H:155:SER:HB3	1:I:155:SER:HB2	1.89	0.54
1:E:154:THR:CG2	1:F:154:THR:O	2.51	0.54
1:J:171:PHE:CE2	1:J:204:MET:HE1	2.42	0.54
1:K:148:ASN:HD21	1:K:151:VAL:CG1	2.19	0.54
1:L:71:PRO:HD3	4:L:714:HOH:O	2.08	0.54
1:E:104:SER:HB2	1:E:134:PHE:CE2	2.42	0.54
1:G:139:ILE:HG12	1:G:142:MET:CE	2.39	0.53
1:G:67:MET:CE	1:G:204:MET:SD	2.96	0.53
1:H:77:MET:CA	1:H:77:MET:HE2	2.38	0.53
1:E:34:ASN:HD22	1:E:190:GLN:HB3	1.67	0.53
1:A:139:ILE:HG13	1:A:142:MET:HG3	1.89	0.53
1:K:25:PHE:O	1:K:30:GLN:HG3	2.08	0.53
1:K:150:TRP:HB3	1:L:206:ASN:HD21	1.74	0.53
1:H:56:TYR:CE1	1:H:173:MET:HE3	2.41	0.53
1:A:106:TRP:CD1	1:A:142:MET:HE1	2.42	0.53
1:L:22:PHE:CE2	1:L:82:LEU:HD11	2.43	0.53
1:A:56:TYR:CD1	1:A:173:MET:CE	2.91	0.53
1:H:133:TYR:HH	3:H:709:FUA:HO1	1.56	0.53
1:K:34:ASN:ND2	1:K:158:LEU:H	2.06	0.53
1:K:148:ASN:ND2	1:K:151:VAL:HG13	2.23	0.53
1:L:145:VAL:CG1	1:L:173:MET:CE	2.87	0.53
1:C:115:GLN:O	1:C:119:ILE:HD13	2.05	0.52
1:G:158:LEU:HD11	3:G:708:FUA:C7	2.38	0.52
3:F:704:FUA:H121	3:F:704:FUA:H232	1.92	0.52
1:L:204:MET:HE2	1:L:205:LEU:N	2.24	0.52
1:J:67:MET:HE2	1:J:73:PHE:CD1	2.44	0.52
1:J:123:ASP:OD1	1:J:136:LYS:HE3	2.10	0.52
1:H:54:LYS:HG3	4:H:768:HOH:O	2.08	0.52
1:I:124:VAL:O	1:I:128:GLY:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:TRP:CB	1:H:142:MET:HE3	2.39	0.52
1:A:59:PHE:CD2	1:A:173:MET:SD	3.03	0.52
1:K:3:LYS:CA	4:K:733:HOH:O	2.58	0.52
1:I:34:ASN:ND2	1:I:158:LEU:H	2.07	0.52
1:I:34:ASN:ND2	1:I:190:GLN:HB2	2.24	0.52
1:H:106:TRP:HB3	1:H:142:MET:HE3	1.91	0.52
3:A:702:FUA:H122	3:A:702:FUA:H25	1.91	0.52
1:G:106:TRP:CD1	1:G:142:MET:CE	2.92	0.52
1:F:77:MET:HE1	1:F:81:GLU:C	2.26	0.52
1:D:144:PHE:CZ	3:D:705:FUA:H231	2.44	0.52
1:J:148:ASN:HD22	1:J:150:TRP:HE3	1.57	0.52
3:E:706:FUA:H232	3:E:706:FUA:C12	2.40	0.52
1:J:157:ASP:OD2	1:K:157:ASP:CG	2.47	0.52
1:E:44:PHE:HB2	1:E:212:CYS:HB3	1.91	0.52
1:B:67:MET:CE	1:B:73:PHE:CG	2.86	0.51
1:L:30:GLN:HE22	1:L:164:ASP:HA	1.75	0.51
1:J:56:TYR:CD1	1:J:173:MET:HE3	2.44	0.51
1:H:93:THR:HG21	3:H:709:FUA:H22	1.93	0.51
3:K:712:FUA:H282	3:K:712:FUA:H232	1.91	0.51
1:J:171:PHE:CE2	1:J:204:MET:CE	2.93	0.51
1:I:91:CYS:SG	1:I:104:SER:HB3	2.50	0.51
1:H:56:TYR:CE1	1:H:173:MET:CE	2.91	0.51
1:J:56:TYR:CE1	1:J:173:MET:HE3	2.45	0.51
1:G:26:GLN:NE2	4:G:740:HOH:O	2.43	0.51
1:B:51:ASN:H	1:B:51:ASN:HD22	1.56	0.51
1:J:56:TYR:CE1	1:J:147:ALA:HB2	2.46	0.51
1:B:146:SER:HB3	3:B:703:FUA:H22	1.91	0.51
1:I:92:TYR:OH	1:I:105:LEU:HD23	2.11	0.51
1:D:154:THR:O	1:F:154:THR:CG2	2.39	0.51
1:L:8:TYR:HB2	1:L:83:VAL:CG1	2.36	0.51
1:E:19:LYS:O	1:E:23:GLU:HG3	2.11	0.51
1:L:145:VAL:HG11	1:L:173:MET:HE2	1.92	0.51
1:J:92:TYR:CE1	1:J:105:LEU:HD21	2.45	0.51
1:I:159:ASN:ND2	4:I:726:HOH:O	2.16	0.51
1:C:9:THR:CG2	4:C:712:HOH:O	2.57	0.51
1:A:37:VAL:CG2	1:C:151:VAL:HG13	2.41	0.51
3:I:707:FUA:H283	3:I:707:FUA:C23	2.40	0.51
1:H:46:LYS:NZ	4:H:734:HOH:O	2.44	0.51
4:J:724:HOH:O	1:K:159:ASN:ND2	2.25	0.50
1:I:171:PHE:CZ	1:I:204:MET:HE1	2.34	0.50
1:J:50:LYS:C	1:J:51:ASN:O	2.48	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:84:ILE:HG22	1:L:85:TRP:O	2.12	0.50
3:I:707:FUA:C28	3:I:707:FUA:C23	2.89	0.50
1:I:13:ILE:CG2	1:I:13:ILE:O	2.59	0.50
1:F:19:LYS:O	1:F:23:GLU:HG3	2.11	0.50
1:H:154:THR:HG21	1:I:154:THR:O	2.05	0.50
1:E:97:GLU:HG3	4:E:750:HOH:O	2.10	0.50
1:L:67:MET:HE3	1:L:73:PHE:HB3	1.92	0.50
1:G:28:VAL:HG12	4:G:742:HOH:O	2.11	0.50
1:K:106:TRP:CG	1:K:142:MET:HE2	2.47	0.50
1:J:158:LEU:HD11	3:J:711:FUA:H72	1.93	0.50
1:A:171:PHE:CZ	1:A:204:MET:HE1	2.46	0.50
1:I:58:ALA:HA	1:I:113:PHE:CE1	2.46	0.50
1:H:190:GLN:HE21	1:H:190:GLN:C	2.15	0.50
1:D:25:PHE:O	1:D:30:GLN:HG3	2.12	0.49
1:G:139:ILE:HG13	1:G:142:MET:CG	2.41	0.49
1:J:146:SER:CB	3:J:711:FUA:H3	2.40	0.49
1:E:139:ILE:HG12	1:E:142:MET:HE3	1.93	0.49
1:H:167:PHE:O	1:H:169:PRO:CD	2.58	0.49
1:E:177:TYR:HE2	1:E:186:PRO:HD3	1.76	0.49
1:D:110:HIS:CD2	1:D:112:ASP:H	2.22	0.49
3:B:703:FUA:H232	3:B:703:FUA:H121	1.94	0.49
1:F:113:PHE:CZ	1:F:117:LEU:HG	2.47	0.49
1:C:215:TRP:CZ2	1:C:217:GLY:HA2	2.48	0.49
1:C:93:THR:HG21	3:C:701:FUA:H22	1.95	0.49
1:A:72:GLU:OE2	4:A:868:HOH:O	2.18	0.49
1:K:139:ILE:O	1:K:142:MET:SD	2.71	0.49
1:J:32:THR:HG22	1:L:159:ASN:HB3	1.94	0.49
1:I:56:TYR:O	1:I:60:ILE:HG13	2.13	0.49
1:I:99:THR:O	1:I:100:GLU:HB2	2.13	0.49
1:G:52:LYS:HE2	4:G:735:HOH:O	2.12	0.49
1:H:75:MET:SD	1:H:195:VAL:CG1	3.01	0.48
3:G:708:FUA:H232	3:G:708:FUA:H121	1.94	0.48
1:D:13:ILE:HD11	1:D:16:TRP:CE3	2.48	0.48
1:K:159:ASN:HB3	1:L:32:THR:CG2	2.43	0.48
1:B:9:THR:HG23	4:B:721:HOH:O	2.12	0.48
1:C:204:MET:HE2	1:C:205:LEU:HA	1.93	0.48
1:B:67:MET:CE	1:B:73:PHE:CB	2.91	0.48
1:E:32:THR:HG21	4:E:707:HOH:O	2.13	0.48
1:B:162:ASN:CA	4:B:712:HOH:O	2.60	0.48
1:I:136:LYS:NZ	4:I:717:HOH:O	2.42	0.48
1:A:34:ASN:ND2	1:A:158:LEU:H	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:ILE:HG13	1:D:142:MET:HG3	1.94	0.48
1:D:115:GLN:HE21	1:J:214:GLU:HG3	1.79	0.48
1:A:48:VAL:HG13	1:A:53:HIS:O	2.14	0.48
1:I:13:ILE:HG22	1:I:13:ILE:O	2.12	0.48
1:A:39:LEU:HD22	1:A:209:GLN:OE1	2.14	0.48
1:B:51:ASN:ND2	1:B:51:ASN:N	2.60	0.48
1:B:6:THR:HG21	1:B:141:ASN:HD21	1.78	0.48
1:D:20:GLU:OE2	4:D:727:HOH:O	2.20	0.48
1:A:32:THR:HG21	4:A:812:HOH:O	2.14	0.48
1:K:68:ASN:OD1	1:K:87:SER:HA	2.13	0.48
1:J:39:LEU:O	1:J:184:LEU:HA	2.14	0.48
1:E:138:PHE:HA	1:E:142:MET:CE	2.44	0.48
1:J:67:MET:N	1:J:67:MET:HE3	2.29	0.48
1:F:93:THR:CG2	3:F:704:FUA:H22	2.44	0.48
1:L:18:ARG:O	1:L:19:LYS:C	2.52	0.48
1:K:32:THR:HG21	4:K:714:HOH:O	2.13	0.47
1:E:30:GLN:HE22	1:E:164:ASP:HA	1.78	0.47
1:K:176:TYR:HA	1:K:184:LEU:O	2.14	0.47
1:C:67:MET:CE	1:C:73:PHE:CB	2.76	0.47
1:J:5:ILE:N	4:J:740:HOH:O	2.47	0.47
1:F:162:ASN:O	3:F:704:FUA:H321	2.14	0.47
1:A:62:ILE:HD13	1:A:211:TYR:HD2	1.80	0.47
1:L:38:GLN:NE2	1:L:177:TYR:OH	2.46	0.47
1:G:139:ILE:CG1	1:G:142:MET:CE	2.92	0.47
1:L:65:ARG:NH2	1:L:211:TYR:CD2	2.81	0.47
1:F:93:THR:HG21	3:F:704:FUA:H22	1.95	0.47
1:L:148:ASN:OD1	1:L:151:VAL:HG13	2.15	0.47
1:F:187:LEU:CD2	1:F:208:LEU:HD21	2.44	0.47
1:G:139:ILE:HG13	1:G:142:MET:SD	2.55	0.47
1:A:30:GLN:HE22	1:A:164:ASP:HA	1.80	0.47
1:G:139:ILE:HG13	1:G:142:MET:HG3	1.95	0.47
1:K:138:PHE:CA	1:K:142:MET:CE	2.92	0.47
1:L:11:VAL:CG1	1:L:11:VAL:O	2.63	0.47
1:J:139:ILE:N	1:J:142:MET:HE3	2.28	0.47
1:L:150:TRP:HB2	1:L:151:VAL:HG12	1.97	0.47
1:K:51:ASN:N	1:K:51:ASN:OD1	2.46	0.47
1:D:174:GLY:HA3	1:D:186:PRO:HB2	1.96	0.47
1:G:157:ASP:OD1	1:H:157:ASP:HB2	2.15	0.47
1:I:110:HIS:CD2	1:I:119:ILE:HD13	2.49	0.47
1:F:26:GLN:NE2	4:F:717:HOH:O	2.48	0.47
1:K:106:TRP:CD1	1:K:142:MET:HE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ASN:ND2	4:C:768:HOH:O	2.33	0.47
1:C:30:GLN:NE2	4:C:708:HOH:O	2.47	0.47
3:K:712:FUA:C28	3:K:712:FUA:H232	2.45	0.47
1:L:61:HIS:O	1:L:65:ARG:HG3	2.14	0.47
1:K:56:TYR:HB3	1:K:57:PRO:CD	2.45	0.47
1:L:113:PHE:O	1:L:114:ARG:C	2.52	0.47
1:E:12:ASP:OD2	1:E:15:GLN:HG2	2.15	0.47
1:D:45:LEU:HD12	1:D:183:VAL:HG11	1.97	0.47
1:F:123:ASP:OD1	1:F:136:LYS:CE	2.53	0.46
3:D:705:FUA:H151	3:D:705:FUA:H203	1.50	0.46
1:G:38:GLN:HE22	1:G:186:PRO:CD	2.29	0.46
1:J:56:TYR:HB3	1:J:57:PRO:CD	2.45	0.46
1:B:34:ASN:CB	1:B:157:ASP:HB3	2.45	0.46
1:H:90:PRO:O	1:H:106:TRP:HA	2.15	0.46
1:K:99:THR:HG21	1:K:131:LEU:CD1	2.39	0.46
1:K:146:SER:HB3	3:K:712:FUA:H3	1.97	0.46
1:G:176:TYR:N	4:G:736:HOH:O	2.25	0.46
1:K:17:HIS:N	1:K:17:HIS:ND1	2.62	0.46
1:D:110:HIS:HD2	1:D:112:ASP:N	2.09	0.46
1:B:67:MET:HE3	1:B:73:PHE:CB	2.44	0.46
1:I:92:TYR:CZ	1:I:105:LEU:HD23	2.50	0.46
1:L:187:LEU:HD22	1:L:208:LEU:HD21	1.96	0.46
1:A:54:LYS:HD3	4:A:818:HOH:O	2.16	0.46
1:I:77:MET:HE1	1:I:82:LEU:HB2	1.98	0.46
1:G:171:PHE:CZ	1:G:204:MET:CE	2.98	0.46
1:H:67:MET:HE1	1:H:73:PHE:CD2	2.51	0.46
1:A:159:ASN:OD1	1:B:159:ASN:ND2	2.48	0.46
1:E:156:PHE:O	1:E:157:ASP:OD1	2.34	0.46
1:D:6:THR:CG2	4:D:733:HOH:O	2.54	0.46
1:A:133:TYR:HE2	3:A:702:FUA:H272	1.77	0.46
1:D:9:THR:HG23	4:D:730:HOH:O	2.16	0.46
1:I:93:THR:HG21	3:I:707:FUA:H22	1.97	0.46
1:L:164:ASP:HB2	4:L:723:HOH:O	2.15	0.46
1:F:77:MET:HG3	1:F:165:ASN:CG	2.36	0.46
1:H:26:GLN:NE2	4:H:761:HOH:O	2.47	0.46
1:F:187:LEU:HD22	1:F:208:LEU:HD21	1.98	0.46
1:B:67:MET:HE3	1:B:73:PHE:CD1	2.49	0.46
1:B:146:SER:CB	3:B:703:FUA:H3	2.46	0.46
1:D:89:HIS:O	1:D:142:MET:HA	2.15	0.46
1:J:124:VAL:O	1:J:128:GLY:N	2.47	0.46
1:I:148:ASN:HB3	1:I:173:MET:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:HIS:O	1:D:100:GLU:N	2.49	0.46
1:E:126:CYS:HB3	1:E:127:TYR:CD2	2.51	0.46
1:G:138:PHE:HA	1:G:142:MET:CE	2.45	0.46
3:J:711:FUA:H72	3:J:711:FUA:H212	1.57	0.46
1:E:59:PHE:HD2	1:E:173:MET:HE1	1.81	0.46
1:L:187:LEU:HD22	1:L:208:LEU:CD2	2.45	0.46
1:A:67:MET:HA	1:A:67:MET:CE	2.43	0.45
1:C:192:HIS:HD1	1:C:194:ALA:N	2.08	0.45
3:A:702:FUA:H151	3:A:702:FUA:H203	1.71	0.45
1:H:59:PHE:O	1:H:62:ILE:HG22	2.15	0.45
1:E:35:GLN:HG3	4:E:731:HOH:O	2.15	0.45
1:H:106:TRP:CD1	1:H:142:MET:HE3	2.51	0.45
1:D:159:ASN:OD1	4:D:761:HOH:O	2.21	0.45
3:L:710:FUA:H232	3:L:710:FUA:C12	2.47	0.45
1:E:75:MET:HA	1:E:83:VAL:O	2.16	0.45
3:B:703:FUA:H203	3:B:703:FUA:H151	1.42	0.45
1:C:204:MET:HE3	1:C:204:MET:O	2.17	0.45
1:J:92:TYR:HA	1:J:145:VAL:O	2.17	0.45
1:B:34:ASN:ND2	1:B:190:GLN:HB2	2.32	0.45
1:G:175:LYS:HA	4:G:736:HOH:O	2.16	0.45
1:A:13:ILE:HG22	1:A:19:LYS:HG3	1.99	0.45
1:K:106:TRP:CD1	1:K:142:MET:HE1	2.52	0.45
1:J:138:PHE:CE2	3:J:711:FUA:H283	2.52	0.45
3:H:709:FUA:C29	3:H:709:FUA:O2	2.64	0.45
1:F:49:LYS:O	1:F:50:LYS:C	2.55	0.45
1:J:204:MET:SD	1:J:204:MET:C	2.95	0.45
1:E:156:PHE:C	1:E:157:ASP:OD1	2.55	0.45
1:J:34:ASN:HD21	1:J:158:LEU:H	1.64	0.45
1:J:65:ARG:NH1	1:J:211:TYR:CE2	2.85	0.45
3:F:704:FUA:H122	3:F:704:FUA:H232	1.96	0.45
1:J:37:VAL:HG23	4:J:726:HOH:O	2.15	0.45
1:J:105:LEU:N	1:J:105:LEU:CD2	2.80	0.45
3:C:701:FUA:H151	3:C:701:FUA:H203	1.14	0.45
1:A:34:ASN:OD1	1:A:157:ASP:OD2	2.35	0.45
1:I:37:VAL:HG12	1:I:38:GLN:N	2.32	0.45
1:K:146:SER:HB3	3:K:712:FUA:H22	1.99	0.45
1:F:25:PHE:O	1:F:30:GLN:HA	2.17	0.45
1:H:45:LEU:HD22	1:H:49:LYS:HD2	1.99	0.45
1:J:162:ASN:ND2	1:J:164:ASP:H	2.15	0.45
1:C:75:MET:HA	1:C:83:VAL:O	2.17	0.45
1:F:106:TRP:O	1:F:136:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:166:PHE:CZ	3:K:712:FUA:H211	2.52	0.45
1:L:72:GLU:HG3	1:L:200:HIS:HB3	1.99	0.45
1:C:45:LEU:HD12	1:C:183:VAL:HG11	1.99	0.45
1:I:75:MET:HA	1:I:83:VAL:O	2.16	0.45
3:G:708:FUA:H203	3:G:708:FUA:H151	1.83	0.44
1:I:56:TYR:N	1:I:57:PRO:HD2	2.32	0.44
1:C:133:TYR:HH	3:C:701:FUA:HO1	1.65	0.44
1:B:139:ILE:HG13	1:B:142:MET:HG2	1.97	0.44
1:C:198:GLY:O	1:C:199:PHE:C	2.56	0.44
1:J:67:MET:HE2	1:J:73:PHE:CG	2.52	0.44
1:I:91:CYS:HB2	1:I:142:MET:HE2	1.99	0.44
1:E:9:THR:CG2	1:E:84:ILE:HB	2.46	0.44
1:B:162:ASN:CB	4:B:712:HOH:O	2.62	0.44
1:D:214:GLU:HG3	1:J:115:GLN:NE2	2.32	0.44
1:A:159:ASN:ND2	4:C:768:HOH:O	2.09	0.44
1:H:56:TYR:HE1	1:H:173:MET:HE1	1.80	0.44
3:D:705:FUA:H72	3:D:705:FUA:H212	1.65	0.44
1:L:145:VAL:CG1	1:L:173:MET:HE2	2.46	0.44
1:J:75:MET:HE3	1:J:195:VAL:HB	1.98	0.44
1:I:70:HIS:HB2	1:I:73:PHE:CD1	2.52	0.44
1:H:65:ARG:HH22	1:H:219:ALA:CB	2.28	0.44
3:D:705:FUA:C12	3:D:705:FUA:C23	2.95	0.44
1:L:117:LEU:HD12	1:L:117:LEU:O	2.17	0.44
1:C:176:TYR:CD1	1:C:176:TYR:C	2.91	0.44
1:F:12:ASP:OD1	1:F:15:GLN:HG2	2.18	0.44
1:H:67:MET:HE3	1:H:73:PHE:CB	2.32	0.44
1:G:110:HIS:HD2	1:G:119:ILE:HD12	1.81	0.44
1:F:36:THR:HG22	1:F:37:VAL:N	2.32	0.44
1:C:56:TYR:CE1	1:C:147:ALA:HB2	2.53	0.44
1:C:118:HIS:O	1:C:122:GLN:HG3	2.17	0.44
1:J:159:ASN:HD22	1:L:159:ASN:ND2	2.15	0.44
1:D:30:GLN:HE21	1:D:192:HIS:HE2	1.66	0.44
1:A:57:PRO:HB3	1:A:120:TYR:CD2	2.52	0.44
1:L:92:TYR:HA	1:L:145:VAL:O	2.16	0.44
1:L:72:GLU:OE1	1:L:203:ARG:NH2	2.51	0.44
1:G:35:GLN:O	1:G:188:ALA:HA	2.17	0.44
1:D:111:ASP:OD2	1:J:65:ARG:CD	2.58	0.44
1:E:9:THR:HG23	1:E:84:ILE:HB	2.00	0.44
3:D:705:FUA:H121	3:D:705:FUA:H232	1.97	0.44
1:J:67:MET:SD	1:J:169:PRO:HG2	2.58	0.44
1:J:34:ASN:ND2	1:J:158:LEU:H	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:701:FUA:H212	3:C:701:FUA:H72	1.72	0.44
1:I:77:MET:CE	1:I:82:LEU:HD13	2.48	0.44
3:K:712:FUA:H151	3:K:712:FUA:H203	1.43	0.43
1:G:38:GLN:HE22	1:G:186:PRO:HD3	1.81	0.43
1:E:145:VAL:CG1	1:E:173:MET:CE	2.97	0.43
1:E:104:SER:CB	1:E:134:PHE:CE2	3.01	0.43
1:K:93:THR:HG23	1:K:146:SER:HA	1.99	0.43
1:C:40:ASP:HB3	1:C:209:GLN:HE22	1.81	0.43
1:I:134:PHE:CZ	3:I:707:FUA:H282	2.52	0.43
1:J:138:PHE:CD1	1:J:138:PHE:O	2.72	0.43
1:A:56:TYR:CE1	1:A:147:ALA:HB2	2.53	0.43
1:G:158:LEU:HD23	1:G:158:LEU:HA	1.68	0.43
1:D:149:PRO:HD2	1:D:150:TRP:CZ3	2.53	0.43
1:G:187:LEU:HD22	1:G:208:LEU:CD2	2.46	0.43
3:K:712:FUA:H72	3:K:712:FUA:H212	1.62	0.43
1:A:41:ILE:O	1:A:42:THR:C	2.56	0.43
1:I:26:GLN:HA	1:I:26:GLN:NE2	2.33	0.43
1:K:162:ASN:O	3:K:712:FUA:H321	2.17	0.43
1:H:127:TYR:CD2	1:H:136:LYS:HG2	2.53	0.43
1:I:34:ASN:HD21	1:I:158:LEU:H	1.67	0.43
1:J:67:MET:HE2	1:J:73:PHE:CB	2.49	0.43
1:G:106:TRP:CD1	1:G:142:MET:HE2	2.53	0.43
1:I:171:PHE:HE2	1:I:204:MET:HE1	1.81	0.43
1:J:54:LYS:HG3	1:J:57:PRO:HG3	2.01	0.43
1:K:50:LYS:C	1:K:51:ASN:O	2.54	0.43
1:D:177:TYR:HE2	1:D:186:PRO:HD3	1.83	0.43
1:I:19:LYS:HD2	4:I:727:HOH:O	2.18	0.43
1:G:139:ILE:HG12	1:G:142:MET:HE3	2.01	0.43
1:F:77:MET:HE3	1:F:82:LEU:HA	2.00	0.43
1:K:159:ASN:HB3	1:L:32:THR:HG22	2.01	0.43
1:K:158:LEU:HD11	3:K:712:FUA:H72	2.01	0.43
1:B:50:LYS:HG2	1:B:51:ASN:ND2	2.32	0.43
1:F:30:GLN:NE2	4:F:717:HOH:O	2.52	0.43
1:B:6:THR:CG2	1:B:141:ASN:HD21	2.32	0.43
1:L:30:GLN:HG3	1:L:192:HIS:CE1	2.54	0.43
1:E:49:LYS:O	1:E:50:LYS:C	2.56	0.43
1:G:72:GLU:HG3	1:G:200:HIS:HB3	2.01	0.43
1:D:176:TYR:HA	1:D:185:MET:HA	2.00	0.43
1:I:139:ILE:HG12	1:I:142:MET:SD	2.59	0.42
3:H:709:FUA:H72	3:H:709:FUA:H212	1.66	0.42
1:B:19:LYS:HB2	1:B:19:LYS:HE2	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:HB3	3:A:702:FUA:H22	2.01	0.42
3:H:709:FUA:H283	1:I:29:ALA:HB2	2.00	0.42
1:F:163:MET:O	1:F:164:ASP:C	2.56	0.42
1:A:148:ASN:ND2	1:A:150:TRP:HE3	2.17	0.42
1:K:138:PHE:HA	1:K:142:MET:HE3	1.99	0.42
1:K:93:THR:HG21	3:K:712:FUA:H22	2.01	0.42
1:D:113:PHE:O	1:D:117:LEU:HB2	2.20	0.42
1:G:89:HIS:O	1:G:142:MET:HA	2.19	0.42
1:I:171:PHE:HZ	1:I:204:MET:SD	2.42	0.42
1:G:138:PHE:HA	1:G:142:MET:HE1	2.02	0.42
1:L:8:TYR:N	1:L:8:TYR:CD2	2.86	0.42
1:H:36:THR:HG22	1:H:37:VAL:N	2.34	0.42
1:L:133:TYR:CZ	1:L:134:PHE:HE1	2.37	0.42
1:K:139:ILE:N	1:K:142:MET:CE	2.49	0.42
1:L:162:ASN:OD1	4:L:723:HOH:O	2.22	0.42
1:B:50:LYS:CG	1:B:51:ASN:HD22	2.30	0.42
3:F:704:FUA:H72	3:F:704:FUA:H212	1.76	0.42
1:H:56:TYR:HB3	1:H:57:PRO:CD	2.49	0.42
3:D:705:FUA:C23	3:D:705:FUA:C28	2.98	0.42
1:B:9:THR:CG2	4:B:721:HOH:O	2.68	0.42
1:I:70:HIS:HA	1:I:71:PRO:HD2	1.87	0.42
1:D:176:TYR:HB3	1:D:185:MET:HB2	2.01	0.42
1:L:56:TYR:CE1	1:L:147:ALA:HB2	2.55	0.42
1:K:153:PHE:O	1:K:186:PRO:HB3	2.20	0.42
1:G:106:TRP:CG	1:G:142:MET:HE2	2.54	0.42
3:J:711:FUA:H151	3:J:711:FUA:H203	1.47	0.42
1:F:77:MET:HG3	1:F:165:ASN:OD1	2.20	0.42
1:F:110:HIS:CD2	1:F:119:ILE:HD11	2.55	0.42
1:H:157:ASP:OD1	1:I:157:ASP:OD2	2.38	0.42
1:D:25:PHE:HB2	1:D:194:ALA:HA	2.01	0.42
1:F:30:GLN:HE22	1:F:164:ASP:HA	1.85	0.42
1:C:13:ILE:HD11	1:C:82:LEU:HD23	2.00	0.42
1:D:65:ARG:CD	1:J:111:ASP:OD2	2.64	0.42
1:J:56:TYR:CD1	1:J:173:MET:HE1	2.54	0.42
1:E:160:VAL:HA	1:F:31:CYS:HB3	2.02	0.42
1:I:39:LEU:O	1:I:184:LEU:HA	2.20	0.42
3:F:704:FUA:H151	3:F:704:FUA:H203	1.53	0.42
1:D:204:MET:HE1	1:D:205:LEU:HG	2.02	0.42
1:H:140:GLU:HG2	4:H:778:HOH:O	2.20	0.42
1:E:3:LYS:N	4:E:748:HOH:O	2.53	0.42
1:A:108:GLU:OE1	1:A:110:HIS:NE2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:ILE:HG23	1:H:13:ILE:HD12	1.74	0.42
3:D:705:FUA:H232	3:D:705:FUA:H122	2.01	0.41
1:E:104:SER:O	1:E:134:PHE:HD2	2.03	0.41
1:K:56:TYR:HB3	1:K:57:PRO:HD3	2.02	0.41
1:I:148:ASN:ND2	1:I:150:TRP:HE3	2.18	0.41
1:A:133:TYR:HE2	3:A:702:FUA:C27	2.32	0.41
1:K:148:ASN:ND2	1:K:150:TRP:HE3	2.18	0.41
1:D:54:LYS:HZ3	1:D:54:LYS:HG2	1.59	0.41
1:L:6:THR:O	1:L:6:THR:HG23	2.20	0.41
1:D:38:GLN:OE1	1:F:154:THR:HG21	2.20	0.41
1:J:158:LEU:HD11	3:J:711:FUA:C7	2.50	0.41
3:G:708:FUA:C12	3:G:708:FUA:H232	2.51	0.41
1:H:56:TYR:CE1	1:H:173:MET:HE1	2.56	0.41
1:F:32:THR:HG21	4:F:705:HOH:O	2.18	0.41
1:D:185:MET:HB3	1:D:185:MET:HE2	1.88	0.41
1:L:171:PHE:CE2	1:L:189:ILE:HD13	2.54	0.41
1:E:72:GLU:HG3	1:E:200:HIS:HB3	2.02	0.41
1:C:119:ILE:H	1:C:119:ILE:CD1	2.26	0.41
1:B:134:PHE:CE1	3:B:703:FUA:H273	2.55	0.41
1:G:187:LEU:HA	1:G:187:LEU:HD12	1.89	0.41
1:I:115:GLN:O	1:I:119:ILE:HD12	2.20	0.41
1:D:66:LEU:HD11	1:D:208:LEU:HA	2.01	0.41
1:A:6:THR:CG2	4:A:837:HOH:O	2.34	0.41
3:I:707:FUA:H203	3:I:707:FUA:H151	1.72	0.41
3:G:708:FUA:H202	3:G:708:FUA:C5	2.50	0.41
1:D:84:ILE:HD13	1:J:9:THR:HG21	2.02	0.41
1:D:93:THR:HG21	3:D:705:FUA:H22	2.01	0.41
1:E:93:THR:CG2	3:E:706:FUA:H22	2.49	0.41
1:K:34:ASN:HD21	1:K:158:LEU:H	1.68	0.41
1:G:165:ASN:HA	1:G:167:PHE:CE1	2.56	0.41
1:A:17:HIS:HD2	4:C:750:HOH:O	2.03	0.41
1:H:66:LEU:HD23	4:H:715:HOH:O	2.20	0.41
1:D:110:HIS:HE1	4:J:725:HOH:O	2.02	0.41
3:A:702:FUA:H72	3:A:702:FUA:H212	1.71	0.41
1:J:123:ASP:OD1	1:J:136:LYS:CE	2.68	0.41
1:C:93:THR:CG2	3:C:701:FUA:H22	2.51	0.41
1:H:104:SER:OG	4:H:783:HOH:O	2.22	0.41
1:C:67:MET:HE2	1:C:169:PRO:HG2	1.95	0.41
1:K:150:TRP:HB3	1:L:206:ASN:ND2	2.34	0.41
1:J:189:ILE:HD12	1:J:190:GLN:N	2.36	0.41
1:D:157:ASP:HB2	1:E:157:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PHE:HB2	1:A:194:ALA:HA	2.03	0.41
1:L:204:MET:HE2	1:L:205:LEU:CA	2.51	0.41
1:F:112:ASP:HB3	1:F:115:GLN:HB2	2.01	0.41
1:A:8:TYR:HB2	1:A:83:VAL:HG13	2.02	0.41
1:B:40:ASP:OD1	1:B:182:LYS:HG2	2.20	0.41
1:F:139:ILE:HG13	1:F:142:MET:HG2	2.03	0.41
1:L:204:MET:CE	1:L:205:LEU:HA	2.51	0.41
1:J:9:THR:CG2	4:J:712:HOH:O	2.62	0.41
1:L:93:THR:HG21	3:L:710:FUA:H22	2.02	0.41
1:A:75:MET:HA	1:A:83:VAL:O	2.21	0.41
1:G:18:ARG:O	1:G:19:LYS:C	2.59	0.41
1:H:67:MET:CE	1:H:169:PRO:CB	3.00	0.40
3:A:702:FUA:H121	3:A:702:FUA:H232	2.03	0.40
1:I:4:LYS:HE2	1:I:4:LYS:CA	2.51	0.40
1:L:70:HIS:HA	1:L:71:PRO:HD2	1.70	0.40
1:C:204:MET:HE2	1:C:205:LEU:CA	2.51	0.40
1:I:70:HIS:HB2	1:I:73:PHE:CE1	2.56	0.40
1:B:62:ILE:HG23	1:B:211:TYR:HD1	1.85	0.40
1:D:141:ASN:N	1:D:141:ASN:OD1	2.52	0.40
3:L:710:FUA:H212	3:L:710:FUA:H72	1.63	0.40
3:B:703:FUA:H72	3:B:703:FUA:H212	1.79	0.40
1:H:23:GLU:CG	1:H:24:ALA:N	2.83	0.40
4:J:724:HOH:O	1:L:159:ASN:OD1	2.22	0.40
1:D:51:ASN:HB3	1:D:53:HIS:CD2	2.57	0.40
3:I:707:FUA:H232	3:I:707:FUA:C12	2.52	0.40
1:K:25:PHE:HB2	1:K:194:ALA:HA	2.03	0.40
1:D:204:MET:HB3	1:D:204:MET:HE2	1.72	0.40
1:D:161:ALA:HB2	1:E:163:MET:SD	2.61	0.40
1:I:114:ARG:HH22	1:I:217:GLY:C	2.25	0.40
1:L:25:PHE:HB2	1:L:194:ALA:HA	2.03	0.40
1:G:38:GLN:NE2	1:G:186:PRO:HG3	2.20	0.40
1:K:3:LYS:HG2	4:K:720:HOH:O	2.21	0.40
1:I:81:GLU:HB2	4:I:739:HOH:O	2.20	0.40
1:B:44:PHE:HB2	1:B:212:CYS:O	2.21	0.40
1:G:148:ASN:HD22	1:G:150:TRP:HE3	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/219 (97%)	205 (97%)	6 (3%)	1 (0%)	34	33
1	B	215/219 (98%)	206 (96%)	8 (4%)	1 (0%)	34	33
1	C	211/219 (96%)	202 (96%)	9 (4%)	0	100	100
1	D	211/219 (96%)	207 (98%)	4 (2%)	0	100	100
1	E	213/219 (97%)	202 (95%)	11 (5%)	0	100	100
1	F	210/219 (96%)	201 (96%)	8 (4%)	1 (0%)	34	33
1	G	211/219 (96%)	206 (98%)	5 (2%)	0	100	100
1	H	214/219 (98%)	208 (97%)	6 (3%)	0	100	100
1	I	213/219 (97%)	206 (97%)	6 (3%)	1 (0%)	34	33
1	J	210/219 (96%)	202 (96%)	6 (3%)	2 (1%)	19	15
1	K	211/219 (96%)	202 (96%)	8 (4%)	1 (0%)	34	33
1	L	208/219 (95%)	200 (96%)	8 (4%)	0	100	100
All	All	2539/2628 (97%)	2447 (96%)	85 (3%)	7 (0%)	46	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	50	LYS
1	I	128	GLY
1	J	51	ASN
1	F	52	LYS
1	A	165	ASN
1	B	132	ALA
1	J	27	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/194 (98%)	171 (90%)	19 (10%)	9	7
1	B	193/194 (100%)	171 (89%)	22 (11%)	7	5
1	C	189/194 (97%)	166 (88%)	23 (12%)	6	4
1	D	189/194 (97%)	165 (87%)	24 (13%)	5	4
1	E	192/194 (99%)	173 (90%)	19 (10%)	10	8
1	F	189/194 (97%)	164 (87%)	25 (13%)	5	3
1	G	189/194 (97%)	171 (90%)	18 (10%)	11	9
1	H	191/194 (98%)	167 (87%)	24 (13%)	5	4
1	I	192/194 (99%)	170 (88%)	22 (12%)	7	5
1	J	190/194 (98%)	161 (85%)	29 (15%)	3	2
1	K	191/194 (98%)	157 (82%)	34 (18%)	2	1
1	L	188/194 (97%)	160 (85%)	28 (15%)	4	2
All	All	2283/2328 (98%)	1996 (87%)	287 (13%)	5	4

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	32	THR
1	A	39	LEU
1	A	45	LEU
1	A	46	LYS
1	A	50	LYS
1	A	52	LYS
1	A	54	LYS
1	A	62	ILE
1	A	114	ARG
1	A	117	LEU
1	A	142	MET
1	A	148	ASN
1	A	154	THR

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Mol	Chain	Res	Type
1	A	160	VAL
1	A	189	ILE
1	A	190	GLN
1	A	193	HIS
1	A	204	MET
1	B	4	LYS
1	B	6	THR
1	B	9	THR
1	B	10	THR
1	B	19	LYS
1	B	32	THR
1	B	37	VAL
1	B	39	LEU
1	B	45	LEU
1	B	51	ASN
1	B	52	LYS
1	B	79	ASP
1	B	83	VAL
1	B	111	ASP
1	B	117	LEU
1	B	129	GLU
1	B	157	ASP
1	B	158	LEU
1	B	160	VAL
1	B	187	LEU
1	B	190	GLN
1	B	216	GLN
1	C	6	THR
1	C	9	THR
1	C	28	VAL
1	C	32	THR
1	C	35	GLN
1	C	39	LEU
1	C	45	LEU
1	C	50	LYS
1	C	83	VAL
1	C	105	LEU
1	C	108	GLU
1	C	111	ASP
1	C	115	GLN
1	C	117	LEU
1	C	146	SER

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Mol	Chain	Res	Type
1	C	157	ASP
1	C	158	LEU
1	C	173	MET
1	C	176	TYR
1	C	187	LEU
1	C	190	GLN
1	C	204	MET
1	C	216	GLN
1	D	6	THR
1	D	13	ILE
1	D	32	THR
1	D	35	GLN
1	D	39	LEU
1	D	45	LEU
1	D	50	LYS
1	D	54	LYS
1	D	67	MET
1	D	78	LYS
1	D	83	VAL
1	D	97	GLU
1	D	98	GLN
1	D	107	SER
1	D	111	ASP
1	D	114	ARG
1	D	117	LEU
1	D	148	ASN
1	D	186	PRO
1	D	187	LEU
1	D	190	GLN
1	D	193	HIS
1	D	204	MET
1	D	216	GLN
1	E	3	LYS
1	E	4	LYS
1	E	6	THR
1	E	10	THR
1	E	13	ILE
1	E	32	THR
1	E	37	VAL
1	E	39	LEU
1	E	45	LEU
1	E	52	LYS

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Mol	Chain	Res	Type
1	E	98	GLN
1	E	117	LEU
1	E	126	CYS
1	E	142	MET
1	E	146	SER
1	E	158	LEU
1	E	189	ILE
1	E	190	GLN
1	E	204	MET
1	F	6	THR
1	F	32	THR
1	F	37	VAL
1	F	39	LEU
1	F	45	LEU
1	F	50	LYS
1	F	62	ILE
1	F	77	MET
1	F	83	VAL
1	F	87	SER
1	F	94	VAL
1	F	98	GLN
1	F	108	GLU
1	F	114	ARG
1	F	115	GLN
1	F	117	LEU
1	F	121	SER
1	F	148	ASN
1	F	154	THR
1	F	157	ASP
1	F	158	LEU
1	F	181	ASP
1	F	182	LYS
1	F	190	GLN
1	F	193	HIS
1	G	9	THR
1	G	15	GLN
1	G	32	THR
1	G	37	VAL
1	G	45	LEU
1	G	52	LYS
1	G	54	LYS
1	G	83	VAL

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Mol	Chain	Res	Type
1	G	98	GLN
1	G	142	MET
1	G	148	ASN
1	G	154	THR
1	G	160	VAL
1	G	181	ASP
1	G	186	PRO
1	G	189	ILE
1	G	190	GLN
1	G	216	GLN
1	H	4	LYS
1	H	5	ILE
1	H	6	THR
1	H	19	LYS
1	H	23	GLU
1	H	32	THR
1	H	37	VAL
1	H	39	LEU
1	H	45	LEU
1	H	62	ILE
1	H	77	MET
1	H	83	VAL
1	H	94	VAL
1	H	129	GLU
1	H	154	THR
1	H	157	ASP
1	H	158	LEU
1	H	160	VAL
1	H	169	PRO
1	H	175	LYS
1	H	185	MET
1	H	190	GLN
1	H	191	VAL
1	H	193	HIS
1	I	9	THR
1	I	32	THR
1	I	39	LEU
1	I	45	LEU
1	I	46	LYS
1	I	50	LYS
1	I	52	LYS
1	I	83	VAL

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Mol	Chain	Res	Type
1	I	105	LEU
1	I	114	ARG
1	I	117	LEU
1	I	121	SER
1	I	129	GLU
1	I	142	MET
1	I	148	ASN
1	I	155	SER
1	I	157	ASP
1	I	158	LEU
1	I	190	GLN
1	I	204	MET
1	I	210	GLN
1	I	214	GLU
1	J	5	ILE
1	J	6	THR
1	J	9	THR
1	J	10	THR
1	J	19	LYS
1	J	39	LEU
1	J	45	LEU
1	J	54	LYS
1	J	67	MET
1	J	83	VAL
1	J	87	SER
1	J	97	GLU
1	J	98	GLN
1	J	105	LEU
1	J	114	ARG
1	J	117	LEU
1	J	126	CYS
1	J	129	GLU
1	J	138	PHE
1	J	142	MET
1	J	146	SER
1	J	158	LEU
1	J	160	VAL
1	J	178	THR
1	J	181	ASP
1	J	182	LYS
1	J	190	GLN
1	J	204	MET

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Mol	Chain	Res	Type
1	J	214	GLU
1	K	3	LYS
1	K	5	ILE
1	K	9	THR
1	K	10	THR
1	K	15	GLN
1	K	17	HIS
1	K	19	LYS
1	K	23	GLU
1	K	28	VAL
1	K	32	THR
1	K	37	VAL
1	K	39	LEU
1	K	42	THR
1	K	45	LEU
1	K	50	LYS
1	K	51	ASN
1	K	52	LYS
1	K	83	VAL
1	K	98	GLN
1	K	111	ASP
1	K	114	ARG
1	K	117	LEU
1	K	131	LEU
1	K	148	ASN
1	K	151	VAL
1	K	154	THR
1	K	158	LEU
1	K	160	VAL
1	K	173	MET
1	K	178	THR
1	K	182	LYS
1	K	187	LEU
1	K	190	GLN
1	K	203	ARG
1	L	6	THR
1	L	13	ILE
1	L	14	SER
1	L	27	SER
1	L	37	VAL
1	L	39	LEU
1	L	45	LEU

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Mol	Chain	Res	Type
1	L	67	MET
1	L	77	MET
1	L	82	LEU
1	L	83	VAL
1	L	94	VAL
1	L	105	LEU
1	L	108	GLU
1	L	115	GLN
1	L	117	LEU
1	L	118	HIS
1	L	122	GLN
1	L	136	LYS
1	L	142	MET
1	L	151	VAL
1	L	158	LEU
1	L	160	VAL
1	L	181	ASP
1	L	182	LYS
1	L	190	GLN
1	L	204	MET
1	L	215	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	30	GLN
1	A	34	ASN
1	A	38	GLN
1	A	148	ASN
1	A	190	GLN
1	B	26	GLN
1	B	34	ASN
1	B	51	ASN
1	B	210	GLN
1	C	26	GLN
1	C	30	GLN
1	C	34	ASN
1	C	38	GLN
1	C	190	GLN
1	D	26	GLN
1	D	30	GLN

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Mol	Chain	Res	Type
1	D	110	HIS
1	D	115	GLN
1	D	190	GLN
1	E	15	GLN
1	E	26	GLN
1	E	30	GLN
1	E	34	ASN
1	E	38	GLN
1	E	98	GLN
1	E	110	HIS
1	F	17	HIS
1	F	26	GLN
1	F	30	GLN
1	F	34	ASN
1	F	110	HIS
1	F	148	ASN
1	F	190	GLN
1	G	15	GLN
1	G	26	GLN
1	G	30	GLN
1	G	38	GLN
1	G	110	HIS
1	G	148	ASN
1	G	159	ASN
1	G	190	GLN
1	G	210	GLN
1	H	17	HIS
1	H	26	GLN
1	H	30	GLN
1	H	34	ASN
1	H	35	GLN
1	H	159	ASN
1	H	190	GLN
1	I	26	GLN
1	I	30	GLN
1	I	34	ASN
1	I	38	GLN
1	I	98	GLN
1	I	148	ASN
1	I	190	GLN
1	J	15	GLN
1	J	30	GLN

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Mol	Chain	Res	Type
1	J	34	ASN
1	J	38	GLN
1	J	162	ASN
1	K	30	GLN
1	K	34	ASN
1	K	38	GLN
1	K	98	GLN
1	K	148	ASN
1	K	190	GLN
1	L	30	GLN
1	L	35	GLN
1	L	159	ASN
1	L	179	GLN
1	L	206	ASN
1	L	210	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 1 is 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	FUA	A	702	-	37,40,40	2.21	13 (35%)	45,64,64	5.14	32 (71%)
3	FUA	B	703	-	37,40,40	2.10	12 (32%)	45,64,64	5.43	29 (64%)
3	FUA	C	701	-	37,40,40	2.11	12 (32%)	45,64,64	5.54	30 (66%)
3	FUA	D	705	-	37,40,40	1.97	9 (24%)	45,64,64	5.38	28 (62%)
3	FUA	E	706	-	37,40,40	1.76	7 (18%)	45,64,64	5.12	30 (66%)
3	FUA	F	704	-	37,40,40	1.95	8 (21%)	45,64,64	4.87	26 (57%)
3	FUA	G	708	-	37,40,40	1.65	7 (18%)	45,64,64	5.22	32 (71%)
3	FUA	H	709	-	37,40,40	1.99	10 (27%)	45,64,64	5.62	31 (68%)
3	FUA	I	707	-	37,40,40	1.65	8 (21%)	45,64,64	4.90	28 (62%)
3	FUA	J	711	-	37,40,40	1.69	7 (18%)	45,64,64	5.50	31 (68%)
3	FUA	K	712	-	37,40,40	1.73	5 (13%)	45,64,64	5.14	22 (48%)
3	FUA	L	710	-	37,40,40	1.83	7 (18%)	45,64,64	4.96	29 (64%)

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	FUA	A	702	-	3/3/15/16	0/10/92/92	0/4/4/4
3	FUA	B	703	-	4/4/15/16	0/10/92/92	0/4/4/4
3	FUA	C	701	-	3/3/15/16	0/10/92/92	0/4/4/4
3	FUA	D	705	-	2/2/15/16	0/10/92/92	0/4/4/4
3	FUA	E	706	-	4/4/15/16	0/10/92/92	0/4/4/4
3	FUA	F	704	-	3/3/15/16	0/10/92/92	0/4/4/4
3	FUA	G	708	-	4/4/15/16	0/10/92/92	0/4/4/4
3	FUA	H	709	-	3/3/15/16	0/10/92/92	0/4/4/4
3	FUA	I	707	-	2/2/15/16	0/10/92/92	0/4/4/4
3	FUA	J	711	-	2/2/15/16	0/10/92/92	0/4/4/4
3	FUA	K	712	-	3/3/15/16	0/10/92/92	0/4/4/4
3	FUA	L	710	-	3/3/15/16	0/10/92/92	0/4/4/4

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	705	FUA	C14-C8	-6.70	1.46	1.58
3	A	702	FUA	C14-C8	-6.05	1.47	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	FUA	C14-C8	-5.94	1.47	1.58
3	A	702	FUA	C8-C9	-5.66	1.47	1.56
3	C	701	FUA	C14-C8	-5.49	1.48	1.58
3	F	704	FUA	C14-C8	-5.33	1.48	1.58
3	J	711	FUA	C14-C8	-5.12	1.49	1.58
3	K	712	FUA	C14-C8	-5.09	1.49	1.58
3	F	704	FUA	C8-C9	-5.07	1.48	1.56
3	L	710	FUA	C14-C8	-4.87	1.49	1.58
3	I	707	FUA	C8-C9	-4.73	1.48	1.56
3	E	706	FUA	C14-C8	-4.63	1.50	1.58
3	H	709	FUA	C14-C8	-4.55	1.50	1.58
3	H	709	FUA	C4-C5	-4.53	1.46	1.54
3	E	706	FUA	O2-C16	-4.40	1.36	1.45
3	A	702	FUA	C14-C13	-4.23	1.43	1.57
3	J	711	FUA	C8-C9	-4.12	1.49	1.56
3	D	705	FUA	C8-C9	-4.11	1.49	1.56
3	L	710	FUA	C29-C22	-3.86	1.44	1.51
3	B	703	FUA	C1-C10	-3.79	1.46	1.54
3	C	701	FUA	C7-C6	-3.69	1.45	1.53
3	F	704	FUA	C29-C22	-3.69	1.44	1.51
3	C	701	FUA	C8-C9	-3.57	1.50	1.56
3	G	708	FUA	C14-C8	-3.51	1.52	1.58
3	B	703	FUA	O2-C16	-3.38	1.38	1.45
3	B	703	FUA	C6-C5	-3.30	1.47	1.53
3	H	709	FUA	C14-C13	-3.28	1.46	1.57
3	C	701	FUA	C6-C5	-3.22	1.48	1.53
3	I	707	FUA	C14-C8	-3.21	1.52	1.58
3	E	706	FUA	C8-C9	-3.15	1.51	1.56
3	H	709	FUA	C13-C17	-3.12	1.47	1.52
3	A	702	FUA	C15-C14	-3.05	1.48	1.54
3	D	705	FUA	C10-C9	-3.02	1.52	1.57
3	K	712	FUA	C10-C9	-3.02	1.52	1.57
3	E	706	FUA	C14-C13	-2.98	1.47	1.57
3	B	703	FUA	C8-C9	-2.87	1.51	1.56
3	H	709	FUA	C10-C9	-2.86	1.52	1.57
3	E	706	FUA	C1-C10	-2.81	1.48	1.54
3	A	702	FUA	C10-C5	-2.78	1.50	1.56
3	C	701	FUA	C14-C13	-2.75	1.48	1.57
3	K	712	FUA	C8-C9	-2.75	1.52	1.56
3	A	702	FUA	C7-C6	-2.67	1.47	1.53
3	H	709	FUA	C8-C9	-2.63	1.52	1.56
3	D	705	FUA	C14-C13	-2.62	1.48	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	711	FUA	O2-C16	-2.53	1.40	1.45
3	I	707	FUA	C10-C9	-2.53	1.52	1.57
3	F	704	FUA	C13-C17	-2.47	1.48	1.52
3	C	701	FUA	C4-C5	-2.45	1.50	1.54
3	K	712	FUA	O2-C16	-2.41	1.40	1.45
3	I	707	FUA	C29-C22	-2.39	1.47	1.51
3	B	703	FUA	C7-C8	-2.38	1.49	1.54
3	I	707	FUA	C1-C10	-2.36	1.49	1.54
3	A	702	FUA	C1-C10	-2.29	1.49	1.54
3	D	705	FUA	C29-C22	-2.26	1.47	1.51
3	C	701	FUA	C10-C5	-2.26	1.51	1.56
3	J	711	FUA	C29-C22	-2.24	1.47	1.51
3	H	709	FUA	O2-C16	-2.22	1.41	1.45
3	A	702	FUA	C29-C22	-2.22	1.47	1.51
3	A	702	FUA	C7-C8	-2.22	1.50	1.54
3	D	705	FUA	C1-C10	-2.21	1.49	1.54
3	B	703	FUA	C13-C17	-2.20	1.49	1.52
3	B	703	FUA	C7-C6	-2.16	1.48	1.53
3	D	705	FUA	C4-C5	-2.14	1.50	1.54
3	C	701	FUA	C29-C22	-2.12	1.47	1.51
3	J	711	FUA	C10-C5	-2.11	1.52	1.56
3	I	707	FUA	C14-C13	-2.09	1.50	1.57
3	J	711	FUA	C14-C13	-2.06	1.50	1.57
3	G	708	FUA	C8-C9	-2.03	1.53	1.56
3	A	702	FUA	C4-C5	-2.02	1.50	1.54
3	H	709	FUA	C10-C5	-2.01	1.52	1.56
3	L	710	FUA	C10-C9	-2.01	1.53	1.57
3	A	702	FUA	C9-C11	-2.00	1.51	1.54
3	L	710	FUA	C19-C10	2.10	1.58	1.54
3	C	701	FUA	C2-C3	2.22	1.55	1.52
3	E	706	FUA	C19-C10	2.25	1.58	1.54
3	G	708	FUA	C12-C11	2.28	1.56	1.52
3	B	703	FUA	C19-C10	2.29	1.58	1.54
3	F	704	FUA	O6-C3	2.36	1.48	1.43
3	F	704	FUA	C2-C3	2.41	1.55	1.52
3	I	707	FUA	C19-C10	2.43	1.58	1.54
3	L	710	FUA	C12-C13	2.44	1.58	1.54
3	H	709	FUA	C18-C4	2.50	1.59	1.53
3	L	710	FUA	C12-C11	2.53	1.56	1.52
3	B	703	FUA	C20-C8	2.56	1.59	1.54
3	A	702	FUA	C2-C3	2.56	1.55	1.52
3	G	708	FUA	C23-C22	2.57	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	704	FUA	C19-C10	2.80	1.59	1.54
3	D	705	FUA	C12-C11	2.81	1.57	1.52
3	G	708	FUA	C9-C11	2.87	1.59	1.54
3	G	708	FUA	C2-C3	2.94	1.56	1.52
3	C	701	FUA	C12-C13	3.12	1.60	1.54
3	B	703	FUA	C12-C11	3.16	1.57	1.52
3	C	701	FUA	C19-C10	3.41	1.60	1.54
3	I	707	FUA	O2-C31	3.93	1.44	1.35
3	E	706	FUA	O2-C31	4.04	1.44	1.35
3	B	703	FUA	O2-C31	4.24	1.45	1.35
3	D	705	FUA	O2-C31	4.27	1.45	1.35
3	F	704	FUA	O2-C31	4.63	1.46	1.35
3	A	702	FUA	O2-C31	4.65	1.46	1.35
3	J	711	FUA	O2-C31	4.74	1.46	1.35
3	G	708	FUA	O2-C31	4.83	1.46	1.35
3	C	701	FUA	O2-C31	5.05	1.46	1.35
3	H	709	FUA	O2-C31	5.06	1.47	1.35
3	K	712	FUA	O2-C31	5.34	1.47	1.35
3	L	710	FUA	O2-C31	6.05	1.49	1.35

All (348) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	709	FUA	C21-C14-C8	-16.80	94.81	112.33
3	J	711	FUA	C21-C14-C8	-15.30	96.38	112.33
3	B	703	FUA	C19-C10-C1	-14.39	83.99	108.20
3	K	712	FUA	C19-C10-C1	-13.12	86.13	108.20
3	D	705	FUA	C19-C10-C5	-12.81	91.97	111.18
3	K	712	FUA	C21-C14-C8	-12.76	99.03	112.33
3	C	701	FUA	C19-C10-C5	-12.34	92.68	111.18
3	B	703	FUA	O6-C3-C4	-11.87	86.81	110.69
3	J	711	FUA	C19-C10-C5	-11.76	93.55	111.18
3	L	710	FUA	C21-C14-C8	-11.65	100.17	112.33
3	F	704	FUA	C19-C10-C1	-11.45	88.94	108.20
3	E	706	FUA	C19-C10-C1	-11.23	89.31	108.20
3	C	701	FUA	O6-C3-C4	-11.16	88.24	110.69
3	J	711	FUA	C20-C8-C14	-11.06	90.96	110.84
3	I	707	FUA	C19-C10-C1	-10.70	90.20	108.20
3	G	708	FUA	C19-C10-C5	-10.60	95.28	111.18
3	G	708	FUA	C20-C8-C9	-10.52	91.51	112.26
3	E	706	FUA	C20-C8-C9	-10.37	91.81	112.26
3	D	705	FUA	C20-C8-C9	-10.25	92.03	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	FUA	C19-C10-C1	-10.23	91.00	108.20
3	A	702	FUA	O6-C3-C4	-10.01	90.56	110.69
3	A	702	FUA	C19-C10-C5	-9.96	96.25	111.18
3	H	709	FUA	C20-C8-C9	-9.90	92.74	112.26
3	F	704	FUA	C20-C8-C9	-9.84	92.84	112.26
3	A	702	FUA	C20-C8-C9	-9.84	92.85	112.26
3	C	701	FUA	C20-C8-C14	-9.81	93.21	110.84
3	G	708	FUA	C19-C10-C1	-9.80	91.72	108.20
3	I	707	FUA	C20-C8-C9	-9.75	93.01	112.26
3	E	706	FUA	O6-C3-C4	-9.66	91.26	110.69
3	C	701	FUA	C20-C8-C7	-9.53	90.96	107.99
3	L	710	FUA	C19-C10-C5	-9.45	97.01	111.18
3	F	704	FUA	C21-C14-C8	-9.12	102.82	112.33
3	H	709	FUA	C19-C10-C9	-9.10	89.62	113.04
3	D	705	FUA	O6-C3-C4	-9.07	92.46	110.69
3	C	701	FUA	C19-C10-C1	-9.05	92.98	108.20
3	H	709	FUA	C19-C10-C5	-8.97	97.73	111.18
3	K	712	FUA	C20-C8-C14	-8.82	94.99	110.84
3	L	710	FUA	C19-C10-C1	-8.70	93.57	108.20
3	L	710	FUA	C20-C8-C14	-8.64	95.31	110.84
3	D	705	FUA	C21-C14-C8	-8.55	103.41	112.33
3	B	703	FUA	C20-C8-C14	-8.50	95.56	110.84
3	L	710	FUA	C19-C10-C9	-8.44	91.32	113.04
3	A	702	FUA	C21-C14-C8	-8.41	103.56	112.33
3	H	709	FUA	O6-C3-C4	-8.36	93.88	110.69
3	D	705	FUA	C20-C8-C14	-8.34	95.85	110.84
3	B	703	FUA	C20-C8-C7	-8.34	93.09	107.99
3	F	704	FUA	O6-C3-C4	-8.25	94.09	110.69
3	I	707	FUA	C21-C14-C8	-8.18	103.79	112.33
3	D	705	FUA	C19-C10-C1	-8.07	94.63	108.20
3	K	712	FUA	C20-C8-C9	-8.06	96.36	112.26
3	L	710	FUA	C20-C8-C7	-8.00	93.69	107.99
3	J	711	FUA	C19-C10-C9	-7.97	92.52	113.04
3	F	704	FUA	C19-C10-C9	-7.84	92.86	113.04
3	B	703	FUA	C21-C14-C8	-7.61	104.39	112.33
3	E	706	FUA	C20-C8-C7	-7.50	94.58	107.99
3	L	710	FUA	O6-C3-C4	-7.49	95.63	110.69
3	I	707	FUA	C19-C10-C5	-7.45	100.01	111.18
3	J	711	FUA	O6-C3-C4	-7.42	95.77	110.69
3	I	707	FUA	C19-C10-C9	-7.40	93.98	113.04
3	K	712	FUA	C19-C10-C9	-7.40	93.99	113.04
3	G	708	FUA	C19-C10-C9	-7.40	93.99	113.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	707	FUA	O6-C3-C4	-7.37	95.88	110.69
3	E	706	FUA	C19-C10-C5	-7.24	100.33	111.18
3	I	707	FUA	C20-C8-C14	-7.21	97.88	110.84
3	I	707	FUA	O6-C3-C2	-7.19	93.63	109.93
3	E	706	FUA	C19-C10-C9	-7.13	94.69	113.04
3	G	708	FUA	O6-C3-C4	-7.08	96.44	110.69
3	G	708	FUA	C20-C8-C7	-7.08	95.33	107.99
3	G	708	FUA	C21-C14-C8	-7.02	105.01	112.33
3	F	704	FUA	C20-C8-C14	-6.81	98.59	110.84
3	B	703	FUA	C21-C14-C13	-6.73	95.88	113.10
3	A	702	FUA	C19-C10-C9	-6.69	95.82	113.04
3	H	709	FUA	C19-C10-C1	-6.56	97.16	108.20
3	E	706	FUA	C21-C14-C13	-6.55	96.34	113.10
3	H	709	FUA	C20-C8-C7	-6.43	96.49	107.99
3	A	702	FUA	C20-C8-C14	-6.42	99.31	110.84
3	B	703	FUA	C20-C8-C9	-6.38	99.68	112.26
3	L	710	FUA	C20-C8-C9	-6.33	99.76	112.26
3	J	711	FUA	C19-C10-C1	-6.33	97.55	108.20
3	B	703	FUA	C19-C10-C9	-6.30	96.83	113.04
3	J	711	FUA	C20-C8-C7	-6.24	96.83	107.99
3	J	711	FUA	C20-C8-C9	-6.24	99.95	112.26
3	K	712	FUA	C20-C8-C7	-6.22	96.86	107.99
3	A	702	FUA	C20-C8-C7	-6.21	96.89	107.99
3	K	712	FUA	O6-C3-C4	-6.20	98.22	110.69
3	I	707	FUA	C21-C14-C13	-6.15	97.36	113.10
3	H	709	FUA	O6-C3-C2	-6.05	96.22	109.93
3	J	711	FUA	C16-O2-C31	-6.01	107.44	117.14
3	G	708	FUA	C21-C14-C13	-5.96	97.84	113.10
3	A	702	FUA	C21-C14-C13	-5.94	97.89	113.10
3	H	709	FUA	C20-C8-C14	-5.93	100.19	110.84
3	D	705	FUA	C19-C10-C9	-5.83	98.02	113.04
3	E	706	FUA	C20-C8-C14	-5.82	100.38	110.84
3	K	712	FUA	O6-C3-C2	-5.80	96.79	109.93
3	C	701	FUA	C21-C14-C8	-5.79	106.29	112.33
3	F	704	FUA	C20-C8-C7	-5.79	97.65	107.99
3	K	712	FUA	C19-C10-C5	-5.67	102.68	111.18
3	F	704	FUA	C21-C14-C13	-5.64	98.66	113.10
3	H	709	FUA	C21-C14-C15	-5.43	91.77	109.15
3	I	707	FUA	C20-C8-C7	-5.36	98.40	107.99
3	F	704	FUA	C19-C10-C5	-5.20	103.39	111.18
3	J	711	FUA	O6-C3-C2	-5.15	98.25	109.93
3	D	705	FUA	C8-C9-C10	-5.14	111.03	116.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	701	FUA	C21-C14-C13	-5.09	100.06	113.10
3	D	705	FUA	C21-C14-C13	-5.08	100.10	113.10
3	C	701	FUA	C20-C8-C9	-5.03	102.33	112.26
3	B	703	FUA	C19-C10-C5	-4.97	103.72	111.18
3	G	708	FUA	C20-C8-C14	-4.89	102.05	110.84
3	E	706	FUA	C21-C14-C8	-4.87	107.25	112.33
3	K	712	FUA	C21-C14-C13	-4.74	100.97	113.10
3	C	701	FUA	C19-C10-C9	-4.72	100.87	113.04
3	D	705	FUA	C20-C8-C7	-4.58	99.80	107.99
3	H	709	FUA	C21-C14-C13	-4.38	101.88	113.10
3	D	705	FUA	C21-C14-C15	-4.25	95.55	109.15
3	F	704	FUA	O1-C11-C9	-4.24	99.04	110.71
3	J	711	FUA	O2-C31-O3	-4.22	114.49	122.92
3	A	702	FUA	C21-C14-C15	-4.05	96.19	109.15
3	L	710	FUA	C21-C14-C13	-4.03	102.79	113.10
3	G	708	FUA	C8-C9-C10	-3.88	112.36	116.45
3	B	703	FUA	O6-C3-C2	-3.85	101.20	109.93
3	J	711	FUA	C21-C14-C13	-3.82	103.33	113.10
3	G	708	FUA	C21-C14-C15	-3.76	97.14	109.15
3	B	703	FUA	C21-C14-C15	-3.73	97.21	109.15
3	A	702	FUA	O6-C3-C2	-3.73	101.48	109.93
3	F	704	FUA	C6-C5-C4	-3.70	108.05	114.18
3	B	703	FUA	O1-C11-C9	-3.45	101.19	110.71
3	J	711	FUA	C8-C9-C10	-3.41	112.85	116.45
3	I	707	FUA	C21-C14-C15	-3.38	98.33	109.15
3	D	705	FUA	O1-C11-C9	-3.34	101.51	110.71
3	E	706	FUA	O1-C11-C9	-3.33	101.53	110.71
3	J	711	FUA	C21-C14-C15	-3.29	98.62	109.15
3	E	706	FUA	C21-C14-C15	-3.27	98.69	109.15
3	B	703	FUA	C18-C4-C3	-3.21	107.05	111.37
3	A	702	FUA	O2-C31-O3	-3.17	116.59	122.92
3	E	706	FUA	O6-C3-C2	-3.07	102.97	109.93
3	A	702	FUA	C24-C25-C26	-3.05	116.00	127.73
3	C	701	FUA	C21-C14-C15	-3.02	99.50	109.15
3	F	704	FUA	O6-C3-C2	-2.95	103.25	109.93
3	H	709	FUA	O1-C11-C9	-2.93	102.63	110.71
3	C	701	FUA	O6-C3-C2	-2.81	103.56	109.93
3	B	703	FUA	C6-C5-C4	-2.79	109.55	114.18
3	K	712	FUA	C8-C9-C10	-2.73	113.58	116.45
3	D	705	FUA	O6-C3-C2	-2.56	104.13	109.93
3	A	702	FUA	O1-C11-C9	-2.52	103.78	110.71
3	F	704	FUA	C18-C4-C5	-2.47	109.21	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	704	FUA	C24-C25-C26	-2.38	118.56	127.73
3	A	702	FUA	C16-O2-C31	-2.34	113.37	117.14
3	E	706	FUA	C6-C5-C4	-2.31	110.36	114.18
3	L	710	FUA	O6-C3-C2	-2.24	104.85	109.93
3	C	701	FUA	C6-C5-C4	-2.23	110.49	114.18
3	G	708	FUA	O2-C31-O3	-2.18	118.56	122.92
3	J	711	FUA	C24-C25-C26	-2.16	119.42	127.73
3	D	705	FUA	C16-O2-C31	-2.13	113.71	117.14
3	A	702	FUA	C28-C26-C25	-2.09	115.90	122.61
3	L	710	FUA	C8-C9-C10	-2.07	114.27	116.45
3	I	707	FUA	O1-C11-C9	-2.03	105.11	110.71
3	E	706	FUA	C2-C3-C4	2.01	123.07	113.23
3	E	706	FUA	C5-C4-C3	2.01	114.28	110.53
3	C	701	FUA	O1-C11-C12	2.02	115.01	110.06
3	L	710	FUA	C7-C6-C5	2.03	116.53	113.10
3	I	707	FUA	O2-C31-C32	2.07	115.00	111.10
3	H	709	FUA	C2-C3-C4	2.07	123.37	113.23
3	I	707	FUA	C2-C3-C4	2.08	123.42	113.23
3	J	711	FUA	C13-C17-C16	2.12	110.59	107.19
3	A	702	FUA	C28-C26-C27	2.16	119.94	114.64
3	G	708	FUA	C7-C6-C5	2.17	116.75	113.10
3	F	704	FUA	C2-C3-C4	2.17	123.89	113.23
3	H	709	FUA	C1-C10-C9	2.18	114.68	109.21
3	G	708	FUA	C7-C8-C14	2.19	112.77	110.72
3	G	708	FUA	O6-C3-C2	2.20	114.92	109.93
3	H	709	FUA	C5-C4-C3	2.24	114.71	110.53
3	L	710	FUA	C2-C1-C10	2.25	116.86	112.84
3	A	702	FUA	C23-C24-C25	2.26	117.61	111.69
3	H	709	FUA	C16-O2-C31	2.28	120.83	117.14
3	D	705	FUA	C6-C7-C8	2.35	116.80	112.80
3	C	701	FUA	C6-C7-C8	2.38	116.86	112.80
3	B	703	FUA	C2-C3-C4	2.39	124.94	113.23
3	H	709	FUA	O2-C31-C32	2.41	115.64	111.10
3	H	709	FUA	C7-C6-C5	2.42	117.17	113.10
3	F	704	FUA	C7-C6-C5	2.42	117.18	113.10
3	E	706	FUA	C13-C17-C16	2.42	111.07	107.19
3	B	703	FUA	C13-C17-C16	2.43	111.08	107.19
3	A	702	FUA	C5-C4-C3	2.45	115.11	110.53
3	L	710	FUA	O1-C11-C12	2.49	116.17	110.06
3	J	711	FUA	C5-C4-C3	2.49	115.18	110.53
3	L	710	FUA	C28-C26-C27	2.50	120.78	114.64
3	G	708	FUA	O1-C11-C9	2.51	117.64	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	708	FUA	O2-C31-C32	2.52	115.86	111.10
3	G	708	FUA	C1-C10-C9	2.53	115.56	109.21
3	G	708	FUA	C16-O2-C31	2.53	121.23	117.14
3	F	704	FUA	C10-C9-C11	2.55	119.76	114.79
3	G	708	FUA	O1-C11-C12	2.61	116.45	110.06
3	H	709	FUA	C10-C9-C11	2.62	119.88	114.79
3	C	701	FUA	C23-C24-C25	2.63	118.57	111.69
3	G	708	FUA	C6-C7-C8	2.68	117.36	112.80
3	I	707	FUA	C7-C6-C5	2.68	117.62	113.10
3	C	701	FUA	C7-C6-C5	2.72	117.68	113.10
3	A	702	FUA	O2-C31-C32	2.72	116.23	111.10
3	E	706	FUA	C12-C11-C9	2.73	119.04	112.27
3	D	705	FUA	C5-C4-C3	2.79	115.73	110.53
3	H	709	FUA	C24-C25-C26	2.79	138.46	127.73
3	F	704	FUA	O2-C31-C32	2.79	116.36	111.10
3	K	712	FUA	C13-C17-C16	2.84	111.74	107.19
3	J	711	FUA	C1-C10-C9	2.84	116.35	109.21
3	B	703	FUA	C12-C11-C9	2.87	119.38	112.27
3	I	707	FUA	C1-C10-C9	2.92	116.55	109.21
3	L	710	FUA	C13-C17-C16	3.01	112.01	107.19
3	K	712	FUA	C7-C6-C5	3.02	118.19	113.10
3	I	707	FUA	C15-C14-C8	3.07	120.31	116.75
3	D	705	FUA	O2-C31-C32	3.09	116.92	111.10
3	E	706	FUA	C7-C6-C5	3.14	118.39	113.10
3	C	701	FUA	C5-C4-C3	3.24	116.58	110.53
3	I	707	FUA	C10-C9-C11	3.28	121.17	114.79
3	D	705	FUA	C13-C17-C16	3.32	112.52	107.19
3	H	709	FUA	C15-C14-C8	3.33	120.61	116.75
3	G	708	FUA	C24-C23-C22	3.38	120.43	112.02
3	I	707	FUA	C18-C4-C3	3.42	115.97	111.37
3	E	706	FUA	C28-C26-C27	3.44	123.09	114.64
3	J	711	FUA	C7-C8-C14	3.47	113.96	110.72
3	L	710	FUA	O2-C31-C32	3.57	117.83	111.10
3	I	707	FUA	C6-C7-C8	3.57	118.88	112.80
3	A	702	FUA	C7-C6-C5	3.64	119.23	113.10
3	D	705	FUA	C24-C23-C22	3.68	121.18	112.02
3	G	708	FUA	C15-C14-C8	3.73	121.07	116.75
3	A	702	FUA	C1-C10-C9	3.74	118.61	109.21
3	J	711	FUA	C18-C4-C5	3.76	118.42	112.86
3	K	712	FUA	C1-C10-C9	3.76	118.67	109.21
3	J	711	FUA	C15-C14-C8	3.77	121.11	116.75
3	K	712	FUA	C10-C9-C11	3.77	122.14	114.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	703	FUA	O1-C11-C12	3.78	119.32	110.06
3	E	706	FUA	C16-O2-C31	3.82	123.32	117.14
3	L	710	FUA	C10-C9-C11	3.86	122.30	114.79
3	A	702	FUA	C18-C4-C3	3.87	116.58	111.37
3	I	707	FUA	C7-C8-C14	3.87	114.34	110.72
3	C	701	FUA	C13-C17-C16	3.88	113.42	107.19
3	C	701	FUA	C10-C9-C11	3.92	122.41	114.79
3	B	703	FUA	C10-C9-C11	3.94	122.46	114.79
3	H	709	FUA	C13-C12-C11	3.97	117.33	111.95
3	C	701	FUA	C1-C10-C9	4.05	119.39	109.21
3	E	706	FUA	C18-C4-C5	4.11	118.94	112.86
3	J	711	FUA	C6-C7-C8	4.12	119.81	112.80
3	L	710	FUA	C6-C7-C8	4.17	119.90	112.80
3	A	702	FUA	C10-C9-C11	4.19	122.94	114.79
3	E	706	FUA	O1-C11-C12	4.22	120.39	110.06
3	A	702	FUA	C15-C14-C8	4.22	121.64	116.75
3	B	703	FUA	C13-C12-C11	4.23	117.69	111.95
3	L	710	FUA	C1-C10-C9	4.30	120.04	109.21
3	B	703	FUA	C23-C24-C25	4.38	123.16	111.69
3	L	710	FUA	C5-C4-C3	4.39	118.73	110.53
3	C	701	FUA	O2-C31-C32	4.42	119.43	111.10
3	J	711	FUA	C18-C4-C3	4.44	117.36	111.37
3	C	701	FUA	C16-O2-C31	4.46	124.36	117.14
3	L	710	FUA	C18-C4-C3	4.51	117.45	111.37
3	I	707	FUA	C18-C4-C5	4.54	119.57	112.86
3	F	704	FUA	C13-C12-C11	4.57	118.15	111.95
3	D	705	FUA	C18-C4-C3	4.61	117.58	111.37
3	J	711	FUA	C10-C9-C11	4.62	123.77	114.79
3	A	702	FUA	C1-C2-C3	4.65	121.00	111.48
3	F	704	FUA	C13-C17-C16	4.68	114.69	107.19
3	E	706	FUA	C1-C2-C3	4.68	121.06	111.48
3	D	705	FUA	C10-C9-C11	4.68	123.91	114.79
3	G	708	FUA	C10-C9-C11	4.69	123.92	114.79
3	H	709	FUA	C7-C8-C14	4.74	115.15	110.72
3	H	709	FUA	C1-C2-C3	4.86	121.42	111.48
3	B	703	FUA	C7-C6-C5	4.91	121.38	113.10
3	H	709	FUA	C23-C24-C25	4.96	124.68	111.69
3	B	703	FUA	C1-C10-C9	4.96	121.69	109.21
3	F	704	FUA	C1-C10-C9	5.02	121.84	109.21
3	B	703	FUA	C1-C2-C3	5.04	121.80	111.48
3	C	701	FUA	C1-C2-C3	5.07	121.85	111.48
3	J	711	FUA	C1-C2-C3	5.16	122.04	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	705	FUA	C13-C12-C11	5.16	118.95	111.95
3	L	710	FUA	C8-C14-C13	5.30	119.94	110.01
3	L	710	FUA	C1-C2-C3	5.31	122.34	111.48
3	E	706	FUA	C1-C10-C9	5.36	122.70	109.21
3	E	706	FUA	C10-C9-C11	5.40	125.29	114.79
3	F	704	FUA	C1-C2-C3	5.42	122.57	111.48
3	I	707	FUA	C1-C2-C3	5.47	122.67	111.48
3	D	705	FUA	C1-C2-C3	5.52	122.78	111.48
3	C	701	FUA	C18-C4-C5	5.53	121.04	112.86
3	J	711	FUA	C13-C12-C11	5.63	119.58	111.95
3	K	712	FUA	C1-C2-C3	5.77	123.30	111.48
3	D	705	FUA	C18-C4-C5	5.88	121.55	112.86
3	J	711	FUA	O2-C31-C32	5.89	122.20	111.10
3	F	704	FUA	C8-C14-C13	5.93	121.10	110.01
3	L	710	FUA	C18-C4-C5	5.97	121.69	112.86
3	A	702	FUA	C18-C4-C5	6.00	121.73	112.86
3	G	708	FUA	C5-C4-C3	6.06	121.85	110.53
3	A	702	FUA	C13-C12-C11	6.09	120.21	111.95
3	G	708	FUA	C1-C2-C3	6.28	124.33	111.48
3	G	708	FUA	C13-C12-C11	6.49	120.75	111.95
3	G	708	FUA	C8-C14-C13	6.52	122.22	110.01
3	I	707	FUA	C6-C5-C10	6.63	120.56	111.57
3	H	709	FUA	C8-C14-C13	6.72	122.58	110.01
3	K	712	FUA	C13-C12-C11	6.79	121.16	111.95
3	H	709	FUA	C18-C4-C5	6.80	122.91	112.86
3	K	712	FUA	C18-C4-C5	6.88	123.04	112.86
3	J	711	FUA	C8-C14-C13	6.89	122.90	110.01
3	E	706	FUA	C8-C14-C13	6.91	122.95	110.01
3	L	710	FUA	C7-C8-C9	6.93	123.67	108.88
3	C	701	FUA	C8-C14-C13	6.95	123.02	110.01
3	A	702	FUA	C8-C14-C13	7.08	123.25	110.01
3	D	705	FUA	C8-C14-C13	7.08	123.27	110.01
3	I	707	FUA	C8-C14-C13	7.09	123.28	110.01
3	K	712	FUA	C8-C14-C13	7.14	123.37	110.01
3	H	709	FUA	C18-C4-C3	7.19	121.05	111.37
3	I	707	FUA	C7-C8-C9	7.23	124.31	108.88
3	E	706	FUA	C13-C12-C11	7.33	121.89	111.95
3	I	707	FUA	C13-C12-C11	7.34	121.91	111.95
3	J	711	FUA	C7-C8-C9	7.51	124.89	108.88
3	C	701	FUA	C18-C4-C3	7.57	121.57	111.37
3	A	702	FUA	C6-C5-C10	7.66	121.96	111.57
3	B	703	FUA	C8-C14-C13	7.68	124.39	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	710	FUA	C1-C10-C5	7.76	118.50	107.90
3	L	710	FUA	C13-C12-C11	7.77	122.49	111.95
3	B	703	FUA	C7-C8-C9	7.83	125.58	108.88
3	K	712	FUA	C6-C5-C10	7.95	122.36	111.57
3	L	710	FUA	C6-C5-C10	8.08	122.53	111.57
3	A	702	FUA	C7-C8-C9	8.09	126.13	108.88
3	C	701	FUA	C7-C8-C9	8.10	126.15	108.88
3	G	708	FUA	C7-C8-C9	8.11	126.17	108.88
3	E	706	FUA	C7-C8-C9	8.23	126.43	108.88
3	H	709	FUA	C7-C8-C9	8.31	126.60	108.88
3	F	704	FUA	C7-C8-C9	8.40	126.81	108.88
3	B	703	FUA	C18-C4-C5	8.55	125.51	112.86
3	G	708	FUA	C6-C5-C10	8.63	123.27	111.57
3	H	709	FUA	C6-C5-C10	8.90	123.64	111.57
3	J	711	FUA	C6-C5-C10	8.92	123.67	111.57
3	K	712	FUA	C7-C8-C9	9.04	128.16	108.88
3	K	712	FUA	C1-C10-C5	9.06	120.29	107.90
3	D	705	FUA	C7-C8-C9	9.23	128.57	108.88
3	F	704	FUA	C1-C10-C5	9.35	120.68	107.90
3	G	708	FUA	C18-C4-C5	9.36	126.71	112.86
3	B	703	FUA	C6-C5-C10	9.44	124.38	111.57
3	E	706	FUA	C1-C10-C5	9.46	120.83	107.90
3	J	711	FUA	C1-C10-C5	9.70	121.16	107.90
3	I	707	FUA	C1-C10-C5	9.71	121.17	107.90
3	F	704	FUA	C6-C5-C10	9.81	124.88	111.57
3	D	705	FUA	C6-C5-C10	9.92	125.03	111.57
3	E	706	FUA	C6-C5-C10	10.16	125.35	111.57
3	A	702	FUA	C1-C10-C5	10.25	121.91	107.90
3	C	701	FUA	C13-C12-C11	10.51	126.20	111.95
3	B	703	FUA	C1-C10-C5	10.54	122.30	107.90
3	G	708	FUA	C1-C10-C5	10.54	122.31	107.90
3	C	701	FUA	C6-C5-C10	10.55	125.89	111.57
3	C	701	FUA	C1-C10-C5	10.78	122.64	107.90
3	H	709	FUA	C1-C10-C5	11.95	124.23	107.90
3	D	705	FUA	C1-C10-C5	12.47	124.94	107.90

All (36) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	J	711	FUA	C13
3	J	711	FUA	C9
3	D	705	FUA	C13

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Mol	Chain	Res	Type	Atom
3	D	705	FUA	C9
3	C	701	FUA	C4
3	C	701	FUA	C13
3	C	701	FUA	C9
3	E	706	FUA	C13
3	E	706	FUA	C5
3	E	706	FUA	C4
3	E	706	FUA	C9
3	F	704	FUA	C13
3	F	704	FUA	C4
3	F	704	FUA	C9
3	A	702	FUA	C13
3	A	702	FUA	C10
3	A	702	FUA	C9
3	G	708	FUA	C4
3	G	708	FUA	C13
3	G	708	FUA	C10
3	G	708	FUA	C9
3	H	709	FUA	C4
3	H	709	FUA	C13
3	H	709	FUA	C9
3	B	703	FUA	C13
3	B	703	FUA	C5
3	B	703	FUA	C4
3	B	703	FUA	C9
3	K	712	FUA	C13
3	K	712	FUA	C10
3	K	712	FUA	C9
3	I	707	FUA	C13
3	I	707	FUA	C9
3	L	710	FUA	C13
3	L	710	FUA	C10
3	L	710	FUA	C9

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	FUA	8	0
3	B	703	FUA	9	0
3	C	701	FUA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	705	FUA	10	0
3	E	706	FUA	3	0
3	F	704	FUA	8	0
3	G	708	FUA	6	0
3	H	709	FUA	5	0
3	I	707	FUA	16	0
3	J	711	FUA	10	0
3	K	712	FUA	10	0
3	L	710	FUA	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	214/219 (97%)	0.17	2 (0%) 85 86	14, 24, 41, 64	0
1	B	217/219 (99%)	0.25	7 (3%) 51 53	17, 28, 50, 71	0
1	C	213/219 (97%)	0.12	1 (0%) 91 92	16, 27, 48, 63	0
1	D	213/219 (97%)	0.31	2 (0%) 85 86	18, 26, 44, 70	0
1	E	215/219 (98%)	0.23	6 (2%) 56 58	19, 30, 47, 66	0
1	F	212/219 (96%)	0.07	0 100 100	19, 29, 49, 56	0
1	G	213/219 (97%)	0.20	6 (2%) 56 58	21, 30, 47, 57	0
1	H	216/219 (98%)	0.33	5 (2%) 64 65	14, 26, 40, 63	0
1	I	215/219 (98%)	0.28	7 (3%) 50 52	19, 32, 51, 68	0
1	J	212/219 (96%)	0.49	13 (6%) 25 26	25, 36, 55, 60	0
1	K	213/219 (97%)	0.30	7 (3%) 50 52	28, 39, 57, 64	0
1	L	210/219 (95%)	0.63	21 (10%) 9 10	26, 42, 63, 75	0
All	All	2563/2628 (97%)	0.28	77 (3%) 54 56	14, 31, 52, 75	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	217	GLY	7.6
1	D	218	GLY	6.3
1	H	5	ILE	4.9
1	L	11	VAL	4.6
1	H	218	GLY	4.4
1	L	114	ARG	4.4
1	J	124	VAL	4.3
1	L	15	GLN	4.2
1	B	218	GLY	3.8
1	L	77	MET	3.6
1	B	217	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	118	HIS	3.6
1	C	218	GLY	3.5
1	G	6	THR	3.4
1	E	5	ILE	3.3
1	E	114	ARG	3.3
1	K	12	ASP	3.3
1	A	5	ILE	3.2
1	J	98	GLN	3.2
1	L	84	ILE	3.1
1	J	118	HIS	3.1
1	J	95	PHE	3.1
1	K	15	GLN	3.1
1	L	211	TYR	3.0
1	E	116	PHE	3.0
1	J	50	LYS	2.9
1	J	127	TYR	2.9
1	B	48	VAL	2.9
1	K	142	MET	2.8
1	I	4	LYS	2.8
1	I	211	TYR	2.8
1	L	83	VAL	2.7
1	L	106	TRP	2.7
1	H	181	ASP	2.7
1	E	142	MET	2.6
1	A	204	MET	2.6
1	L	109	TYR	2.6
1	B	114	ARG	2.6
1	L	119	ILE	2.6
1	B	52	LYS	2.6
1	L	71	PRO	2.5
1	G	110	HIS	2.5
1	G	119	ILE	2.5
1	L	16	TRP	2.5
1	B	118	HIS	2.5
1	L	215	TRP	2.5
1	I	50	LYS	2.4
1	J	126	CYS	2.4
1	J	97	GLU	2.4
1	L	14	SER	2.4
1	L	69	ALA	2.4
1	I	110	HIS	2.4
1	E	110	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	17	HIS	2.3
1	L	111	ASP	2.3
1	H	160	VAL	2.2
1	J	51	ASN	2.2
1	B	216	GLN	2.2
1	E	115	GLN	2.2
1	K	99	THR	2.2
1	L	6	THR	2.2
1	J	122	GLN	2.2
1	L	110	HIS	2.2
1	I	52	LYS	2.2
1	G	142	MET	2.1
1	K	98	GLN	2.1
1	J	45	LEU	2.1
1	I	113	PHE	2.1
1	L	115	GLN	2.1
1	J	125	ALA	2.1
1	I	3	LYS	2.1
1	K	173	MET	2.1
1	H	75	MET	2.1
1	G	15	GLN	2.1
1	J	116	PHE	2.1
1	L	116	PHE	2.0
1	G	114	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	A	801	1/1	0.99	0.29	34.61	5,5,5,5	1
3	FUA	D	705	37/37	0.89	0.19	2.00	31,37,58,62	0
3	FUA	H	709	37/37	0.88	0.20	1.87	28,38,60,60	0
3	FUA	J	711	37/37	0.89	0.16	1.45	43,50,60,64	0
3	FUA	L	710	37/37	0.84	0.18	1.44	33,59,71,72	0
3	FUA	K	712	37/37	0.86	0.16	1.35	42,55,72,74	0
3	FUA	G	708	37/37	0.85	0.17	1.33	43,55,68,70	0
3	FUA	A	702	37/37	0.92	0.16	1.15	19,34,40,44	0
3	FUA	F	704	37/37	0.89	0.14	1.08	27,40,55,55	0
3	FUA	I	707	37/37	0.88	0.15	0.87	36,42,51,55	0
3	FUA	C	701	37/37	0.90	0.15	0.78	31,41,52,55	0
3	FUA	E	706	37/37	0.90	0.14	0.67	33,42,51,57	0
3	FUA	B	703	37/37	0.93	0.13	0.48	25,35,57,59	0

6.5 Other polymers

There are no such residues in this entry.