Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 09:16 AM EST

PDB ID	:	3KP0
Title	:	Crystal Structure of ORNITHINE 4,5 AMINOMUTASE in complex with 2,4-diaminobutyrate (DAB) (Aerobic)
Authors	:	Wolthers, K.R.; Levy, C.W.; Scrutton, N.S.; Leys, D.
Deposited on	:	2009-11-14
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

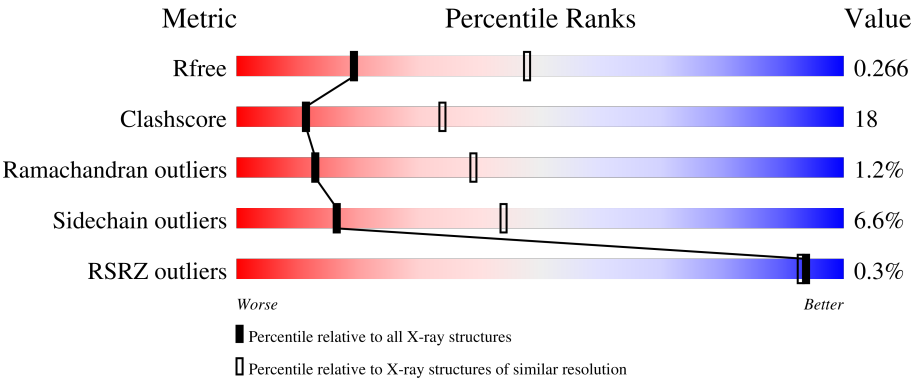
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	763	50% 24% • 24%
1	B	763	59% 33% • 5%
1	C	763	% 60% 32% • 5%
1	D	763	50% 23% •• 24%
2	E	121	60% 26% • 10%

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Mol	Chain	Length	Quality of chain
2	F	121	70% 18% 10%
2	G	121	% 63% 27% 10%
2	H	121	69% 19% 10%

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
5	B12	B	1801	X	-	X	-
5	B12	C	1801	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 24133 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 D-ornithine aminomutase E component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4537	2861	782	864	30			
1	B	728	Total	C	N	O	S	0	0	0
			5669	3576	984	1075	34			
1	C	728	Total	C	N	O	S	0	0	0
			5654	3570	981	1069	34			
1	D	578	Total	C	N	O	S	0	0	0
			4540	2864	782	864	30			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
A	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
A	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
A	744	SER	-	expression tag	UNP Q8VPJ5
A	745	GLU	-	expression tag	UNP Q8VPJ5
A	746	ASP	-	expression tag	UNP Q8VPJ5
A	747	PRO	-	expression tag	UNP Q8VPJ5
A	748	ASN	-	expression tag	UNP Q8VPJ5
A	749	SER	-	expression tag	UNP Q8VPJ5
A	750	SER	-	expression tag	UNP Q8VPJ5
A	751	SER	-	expression tag	UNP Q8VPJ5
A	752	VAL	-	expression tag	UNP Q8VPJ5
A	753	ASP	-	expression tag	UNP Q8VPJ5
A	754	LYS	-	expression tag	UNP Q8VPJ5
A	755	LEU	-	expression tag	UNP Q8VPJ5
A	756	ALA	-	expression tag	UNP Q8VPJ5
A	757	ALA	-	expression tag	UNP Q8VPJ5
A	758	ALA	-	expression tag	UNP Q8VPJ5
A	759	LEU	-	expression tag	UNP Q8VPJ5
A	760	GLU	-	expression tag	UNP Q8VPJ5
A	761	HIS	-	expression tag	UNP Q8VPJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	762	HIS	-	expression tag	UNP Q8VPJ5
A	763	HIS	-	expression tag	UNP Q8VPJ5
A	764	HIS	-	expression tag	UNP Q8VPJ5
A	765	HIS	-	expression tag	UNP Q8VPJ5
A	766	HIS	-	expression tag	UNP Q8VPJ5
B	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
B	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
B	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
B	744	SER	-	expression tag	UNP Q8VPJ5
B	745	GLU	-	expression tag	UNP Q8VPJ5
B	746	ASP	-	expression tag	UNP Q8VPJ5
B	747	PRO	-	expression tag	UNP Q8VPJ5
B	748	ASN	-	expression tag	UNP Q8VPJ5
B	749	SER	-	expression tag	UNP Q8VPJ5
B	750	SER	-	expression tag	UNP Q8VPJ5
B	751	SER	-	expression tag	UNP Q8VPJ5
B	752	VAL	-	expression tag	UNP Q8VPJ5
B	753	ASP	-	expression tag	UNP Q8VPJ5
B	754	LYS	-	expression tag	UNP Q8VPJ5
B	755	LEU	-	expression tag	UNP Q8VPJ5
B	756	ALA	-	expression tag	UNP Q8VPJ5
B	757	ALA	-	expression tag	UNP Q8VPJ5
B	758	ALA	-	expression tag	UNP Q8VPJ5
B	759	LEU	-	expression tag	UNP Q8VPJ5
B	760	GLU	-	expression tag	UNP Q8VPJ5
B	761	HIS	-	expression tag	UNP Q8VPJ5
B	762	HIS	-	expression tag	UNP Q8VPJ5
B	763	HIS	-	expression tag	UNP Q8VPJ5
B	764	HIS	-	expression tag	UNP Q8VPJ5
B	765	HIS	-	expression tag	UNP Q8VPJ5
B	766	HIS	-	expression tag	UNP Q8VPJ5
C	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
C	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
C	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
C	744	SER	-	expression tag	UNP Q8VPJ5
C	745	GLU	-	expression tag	UNP Q8VPJ5
C	746	ASP	-	expression tag	UNP Q8VPJ5
C	747	PRO	-	expression tag	UNP Q8VPJ5
C	748	ASN	-	expression tag	UNP Q8VPJ5
C	749	SER	-	expression tag	UNP Q8VPJ5
C	750	SER	-	expression tag	UNP Q8VPJ5
C	751	SER	-	expression tag	UNP Q8VPJ5

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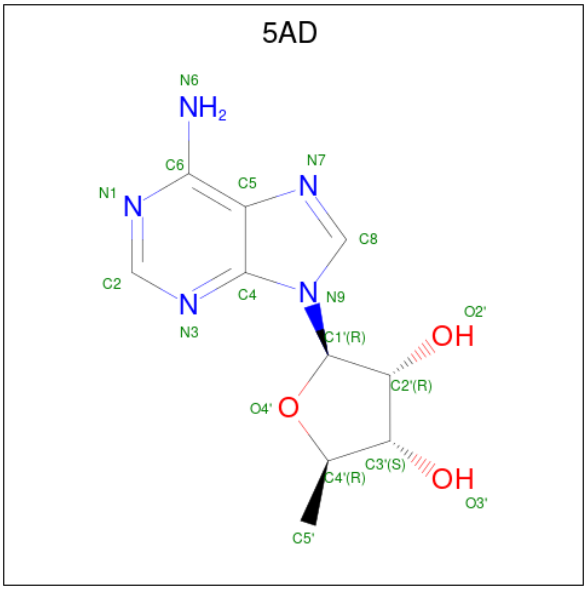
Chain	Residue	Modelled	Actual	Comment	Reference
C	752	VAL	-	expression tag	UNP Q8VPJ5
C	753	ASP	-	expression tag	UNP Q8VPJ5
C	754	LYS	-	expression tag	UNP Q8VPJ5
C	755	LEU	-	expression tag	UNP Q8VPJ5
C	756	ALA	-	expression tag	UNP Q8VPJ5
C	757	ALA	-	expression tag	UNP Q8VPJ5
C	758	ALA	-	expression tag	UNP Q8VPJ5
C	759	LEU	-	expression tag	UNP Q8VPJ5
C	760	GLU	-	expression tag	UNP Q8VPJ5
C	761	HIS	-	expression tag	UNP Q8VPJ5
C	762	HIS	-	expression tag	UNP Q8VPJ5
C	763	HIS	-	expression tag	UNP Q8VPJ5
C	764	HIS	-	expression tag	UNP Q8VPJ5
C	765	HIS	-	expression tag	UNP Q8VPJ5
C	766	HIS	-	expression tag	UNP Q8VPJ5
D	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
D	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
D	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
D	744	SER	-	expression tag	UNP Q8VPJ5
D	745	GLU	-	expression tag	UNP Q8VPJ5
D	746	ASP	-	expression tag	UNP Q8VPJ5
D	747	PRO	-	expression tag	UNP Q8VPJ5
D	748	ASN	-	expression tag	UNP Q8VPJ5
D	749	SER	-	expression tag	UNP Q8VPJ5
D	750	SER	-	expression tag	UNP Q8VPJ5
D	751	SER	-	expression tag	UNP Q8VPJ5
D	752	VAL	-	expression tag	UNP Q8VPJ5
D	753	ASP	-	expression tag	UNP Q8VPJ5
D	754	LYS	-	expression tag	UNP Q8VPJ5
D	755	LEU	-	expression tag	UNP Q8VPJ5
D	756	ALA	-	expression tag	UNP Q8VPJ5
D	757	ALA	-	expression tag	UNP Q8VPJ5
D	758	ALA	-	expression tag	UNP Q8VPJ5
D	759	LEU	-	expression tag	UNP Q8VPJ5
D	760	GLU	-	expression tag	UNP Q8VPJ5
D	761	HIS	-	expression tag	UNP Q8VPJ5
D	762	HIS	-	expression tag	UNP Q8VPJ5
D	763	HIS	-	expression tag	UNP Q8VPJ5
D	764	HIS	-	expression tag	UNP Q8VPJ5
D	765	HIS	-	expression tag	UNP Q8VPJ5
D	766	HIS	-	expression tag	UNP Q8VPJ5

- Molecule 2 is a protein called D-ornithine aminomutase S component.

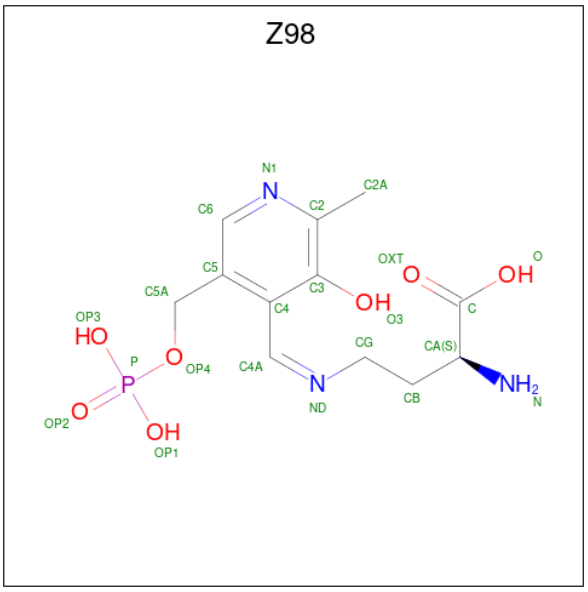
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			
2	F	109	Total	C	N	O	S	0	0	0
			858	539	152	163	4			
2	G	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			
2	H	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			

- Molecule 3 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



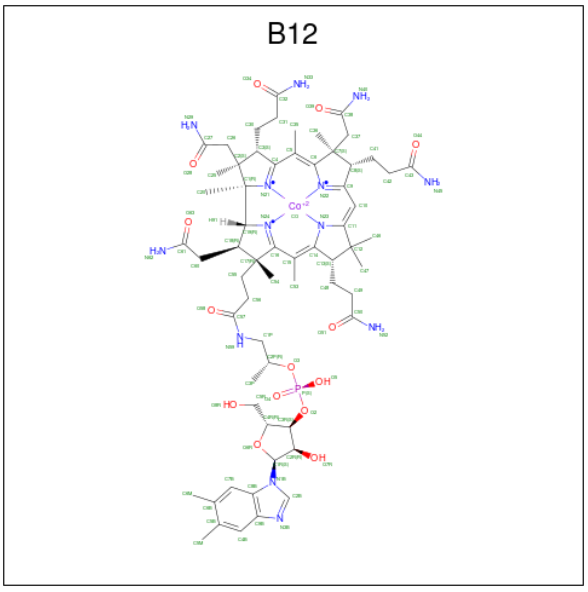
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	10	5	3		
3	D	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 4 is (2S)-2-amino-4-{[(1Z)-{3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene]amino}butanoic acid (three-letter code: Z98) (formula: $C_{12}H_{18}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	12	3	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	12	3	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	12	3	7	1		
4	D	1	Total	C	N	O	P	0	0
			23	12	3	7	1		

- Molecule 5 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



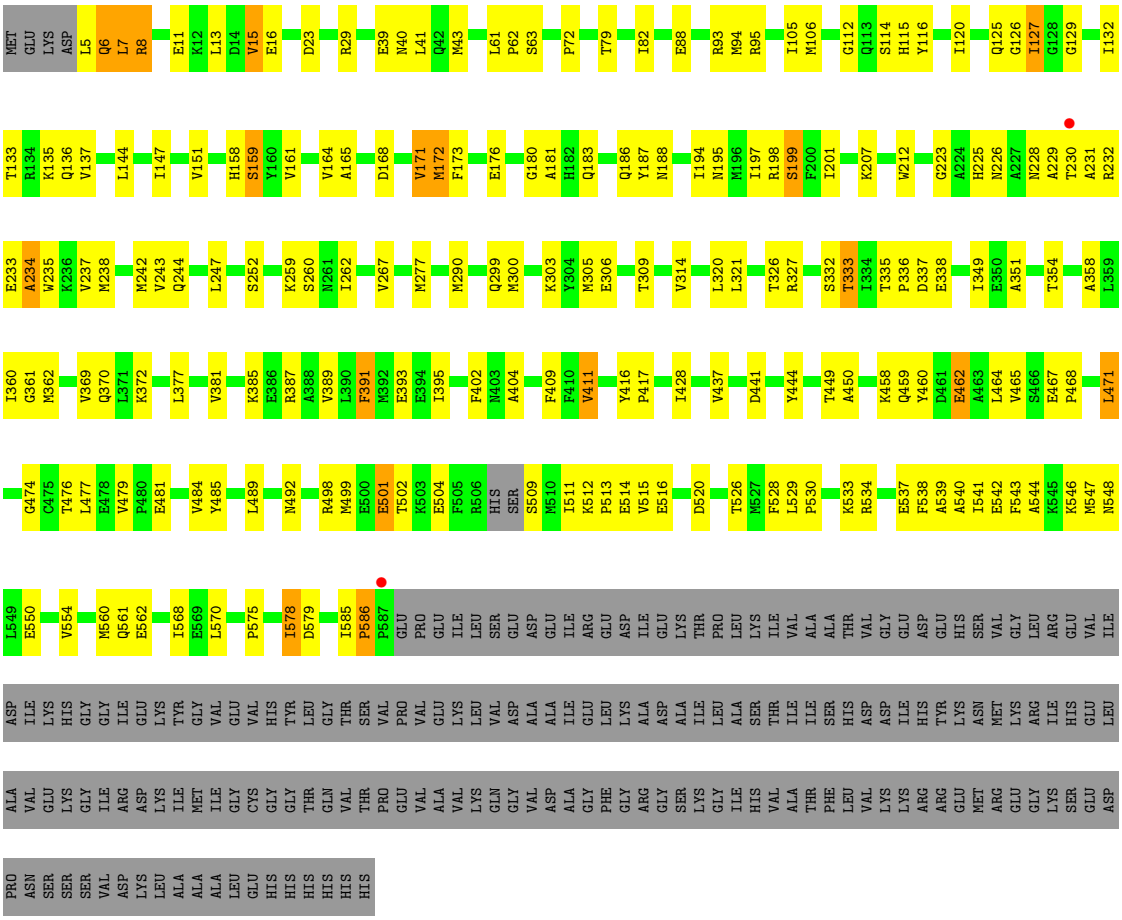
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
5	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

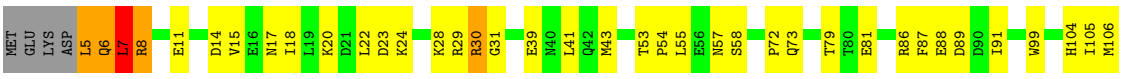
• Molecule 1: D-ornithine aminomutase E component

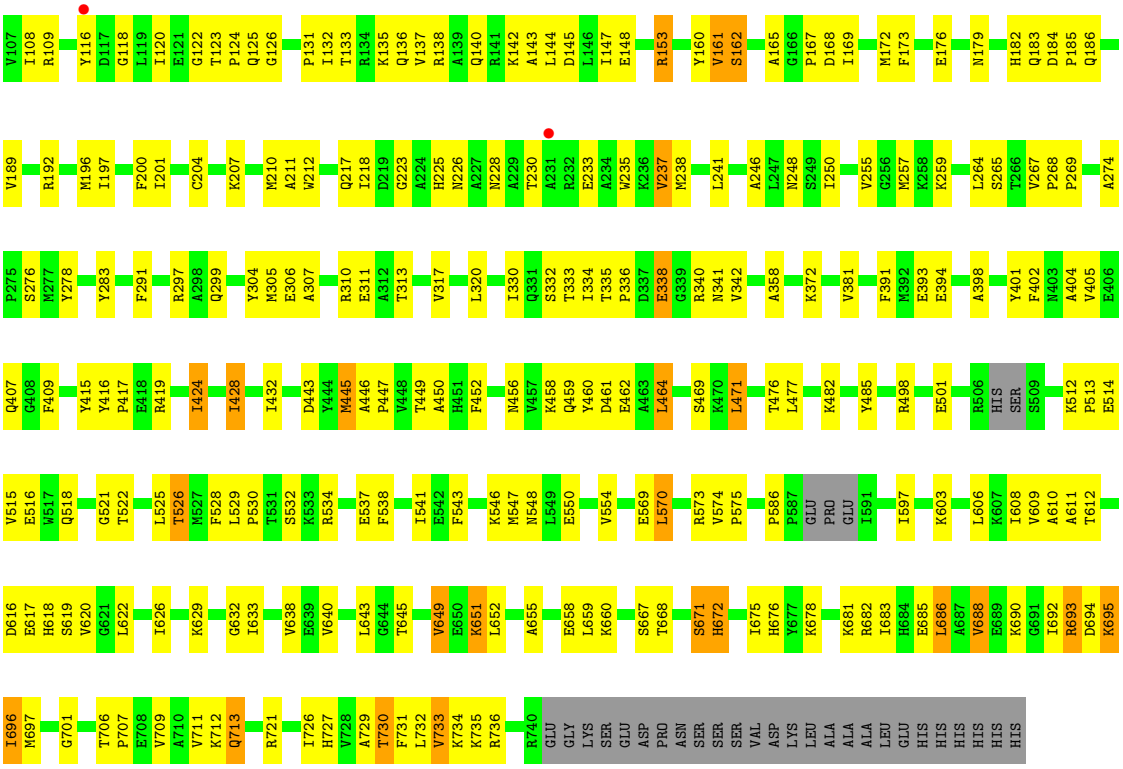
Chain A:



• Molecule 1: D-ornithine aminomutase E component

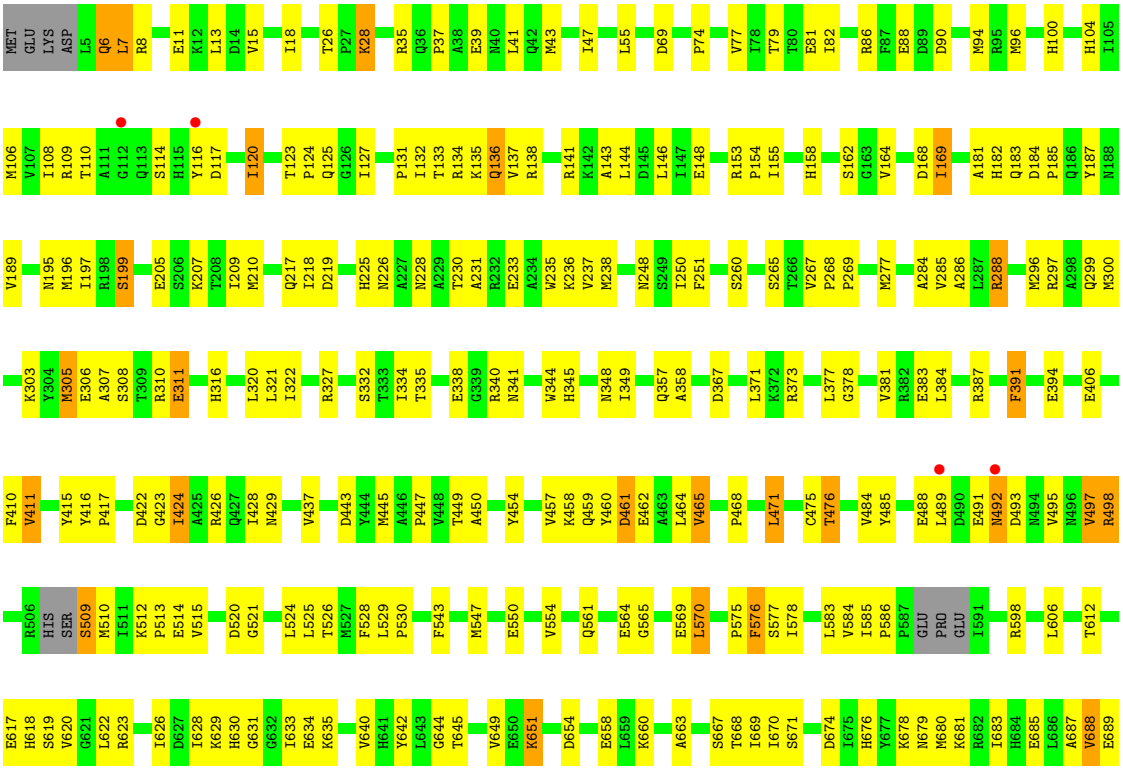
Chain B:

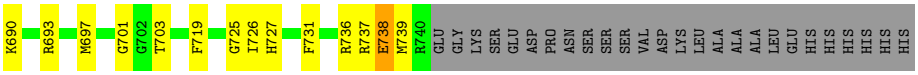




• Molecule 1: D-ornithine aminomutase E component

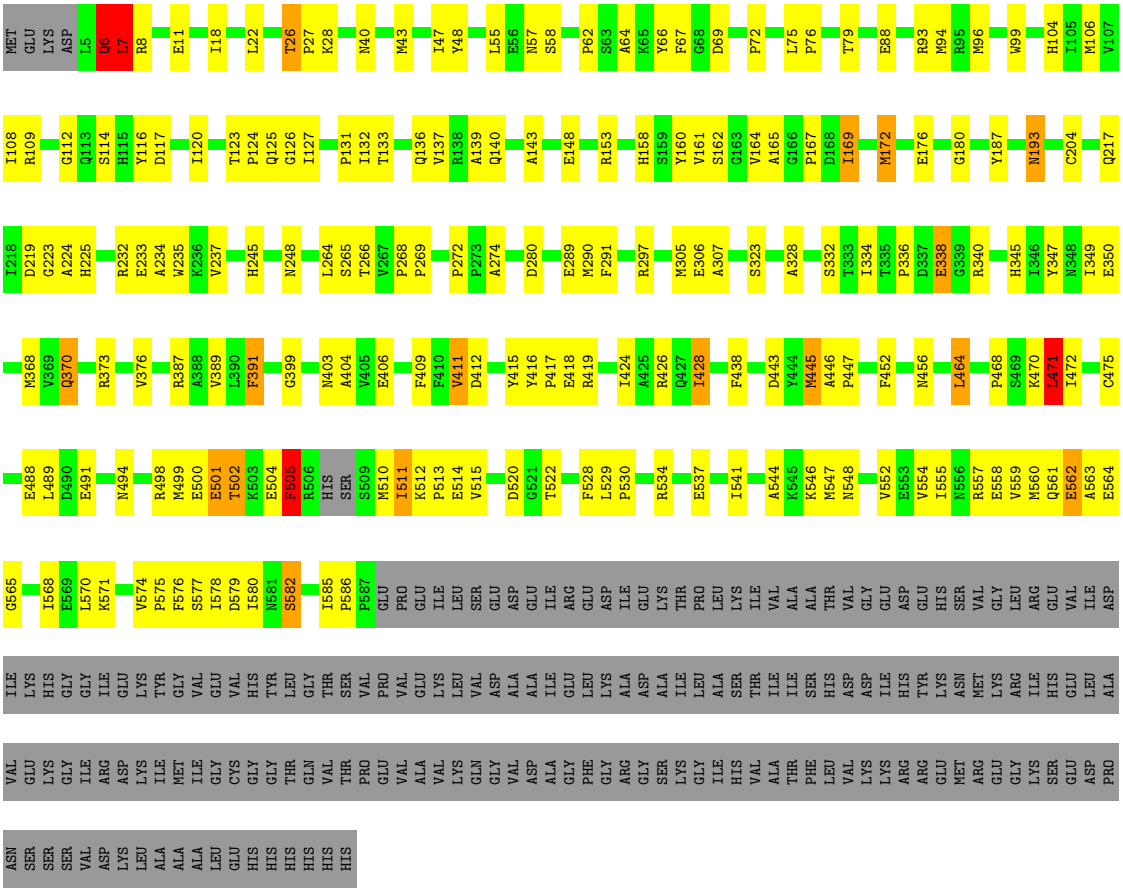
Chain C:





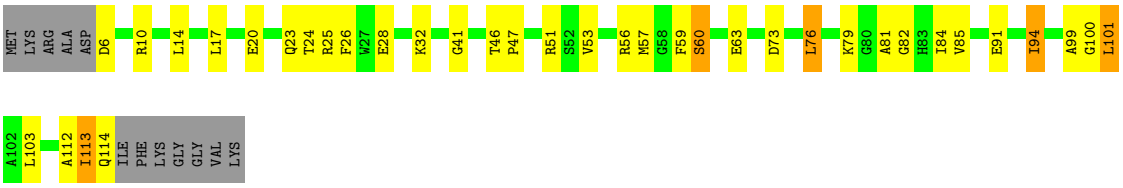
• Molecule 1: D-ornithine aminomutase E component

Chain D:



• Molecule 2: D-ornithine aminomutase S component

Chain E:

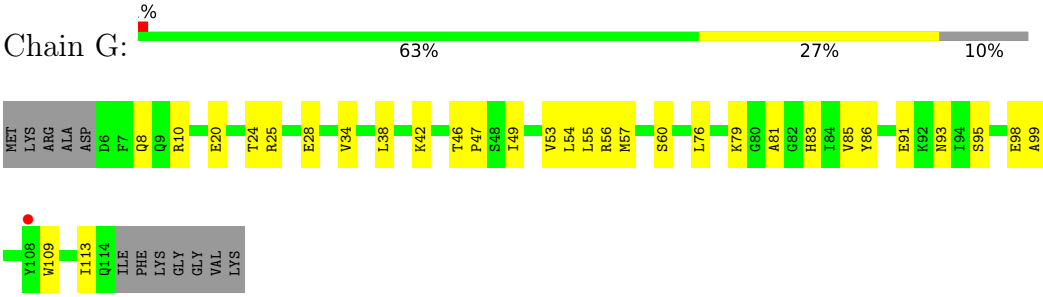


• Molecule 2: D-ornithine aminomutase S component

Chain F:

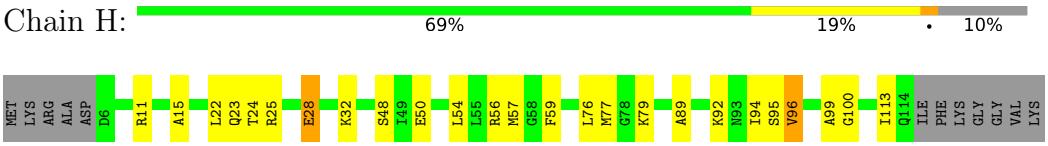
• Molecule 2: D-ornithine aminomutase S component

Chain G:



• Molecule 2: D-ornithine aminomutase S component

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.09Å 231.95Å 124.32Å 90.00° 103.24° 90.00°	Depositor
Resolution (Å)	63.11 – 2.80 64.33 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (63.11-2.80) 92.4 (64.33-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.5_2, REFMAC 5.5.0102	Depositor
R, R_{free}	0.191 , 0.270 0.186 , 0.266	Depositor DCC
R_{free} test set	4129 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.9	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24133	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5AD, Z98, B12

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.45	0/4628	0.63	0/6272
1	B	0.45	0/5774	0.61	0/7814
1	C	0.42	0/5759	0.59	0/7796
1	D	0.47	0/4631	0.63	0/6276
2	E	0.45	0/867	0.55	0/1163
2	F	0.43	0/870	0.59	0/1167
2	G	0.40	0/867	0.56	0/1163
2	H	0.45	0/867	0.58	0/1163
All	All	0.45	0/24263	0.61	0/32814

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
2	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	113	ILE	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	4537	0	4469	154	0
1	B	5669	0	5635	238	0
1	C	5654	0	5621	229	0
1	D	4540	0	4478	160	0
2	E	855	0	863	34	0
2	F	858	0	865	23	0
2	G	855	0	863	24	0
2	H	855	0	863	29	0
3	A	18	0	11	3	0
3	D	18	0	10	1	0
4	A	23	0	15	4	0
4	B	23	0	15	4	0
4	C	23	0	15	4	0
4	D	23	0	15	3	0
5	B	91	0	87	24	0
5	C	91	0	87	17	0
All	All	24133	0	23912	849	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 (849) 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:C:158:HIS:HE1	1:C:218:ILE:HD12	1.16	1.11
1:B:398:ALA:HB1	1:B:407:GLN:HE22	1.25	0.98
1:A:225:HIS:O	1:A:228:ASN:HB2	1.64	0.97
1:B:172:MET:HE2	1:B:173:PHE:HD1	1.30	0.95
1:B:526:THR:HG23	1:B:569:GLU:HG2	1.47	0.95
1:B:393:GLU:HG3	2:F:29:MET:HE1	1.48	0.95
1:C:225:HIS:O	1:C:228:ASN:HB2	1.67	0.94
2:F:54:LEU:HA	2:F:57:MET:HE2	1.49	0.93
1:B:464:LEU:HD23	1:B:471:LEU:HD13	1.52	0.92
1:B:79:THR:HB	1:B:332:SER:HA	1.53	0.91
5:B:1801:B12:H8	5:B:1801:B12:H401	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ILE:HG12	1:C:133:THR:HG22	1.53	0.89
1:C:158:HIS:CE1	1:C:218:ILE:HD12	2.06	0.88
5:C:1801:B12:N40	5:C:1801:B12:H8	1.89	0.88
1:C:183:GLN:HB3	1:C:217:GLN:HE21	1.38	0.87
1:A:231:ALA:O	1:A:303:LYS:HE2	1.76	0.86
1:B:393:GLU:HG3	2:F:29:MET:CE	2.05	0.85
1:B:17:ASN:HA	1:B:20:LYS:HE2	1.58	0.84
1:D:120:ILE:HG13	1:D:133:THR:HG22	1.59	0.84
1:C:6:GLN:CD	1:C:7:LEU:H	1.80	0.84
1:D:406:GLU:OE2	1:D:428:ILE:HG22	1.78	0.84
1:B:18:ILE:HG23	1:B:142:LYS:HD3	1.60	0.83
5:C:1801:B12:H8	5:C:1801:B12:H401	1.43	0.83
1:B:688:VAL:HG23	1:B:693:ARG:HG2	1.59	0.83
5:B:1801:B12:H362	5:B:1801:B12:H351	1.60	0.83
1:D:234:ALA:O	1:D:237:VAL:HG12	1.80	0.82
5:B:1801:B12:H531	5:B:1801:B12:H552	1.61	0.81
1:B:649:VAL:HG22	1:B:683:ILE:HG13	1.62	0.81
1:C:525:LEU:HB3	1:C:570:LEU:HD12	1.61	0.81
1:B:372:LYS:HG2	1:D:370:GLN:HG2	1.63	0.80
1:A:112:GLY:HA3	1:C:620:VAL:HG13	1.64	0.80
5:C:1801:B12:O28	5:C:1801:B12:H3	1.79	0.80
1:B:30:ARG:HG2	1:B:30:ARG:HH11	1.47	0.80
2:F:54:LEU:HD23	2:F:57:MET:HE1	1.64	0.79
5:C:1801:B12:H362	5:C:1801:B12:H351	1.63	0.79
1:B:678:LYS:HB3	1:B:682:ARG:NH1	1.97	0.78
1:C:134:ARG:HD3	1:C:138:ARG:HH21	1.48	0.78
1:C:612:THR:HB	1:C:645:THR:HG22	1.66	0.77
1:D:537:GLU:HG3	1:D:554:VAL:HG21	1.65	0.77
2:H:24:THR:O	2:H:28:GLU:HG2	1.83	0.77
1:B:622:LEU:HB2	1:B:667:SER:HB2	1.67	0.77
1:C:484:VAL:HG11	2:G:60:SER:HB3	1.67	0.77
1:C:286:ALA:HB2	1:C:381:VAL:HG13	1.67	0.77
2:H:54:LEU:HD23	2:H:57:MET:CE	2.15	0.76
1:C:681:LYS:O	1:C:685:GLU:HG3	1.86	0.76
1:B:398:ALA:HB1	1:B:407:GLN:NE2	2.00	0.75
1:B:612:THR:HG22	1:B:616:ASP:HB3	1.69	0.74
1:B:138:ARG:NH1	1:B:485:TYR:CD1	2.55	0.74
1:B:5:LEU:O	1:B:6:GLN:HB2	1.87	0.74
1:B:464:LEU:HD23	1:B:471:LEU:CD1	2.16	0.74
5:B:1801:B12:H8	5:B:1801:B12:N40	2.02	0.74
1:A:172:MET:HE2	1:A:176:GLU:HG3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LYS:HB2	1:A:513:PRO:HD2	1.70	0.74
5:C:1801:B12:O7R	5:C:1801:B12:H2B	1.88	0.73
1:B:172:MET:HE2	1:B:173:PHE:CD1	2.21	0.73
1:B:161:VAL:HG12	1:B:161:VAL:O	1.88	0.73
1:C:6:GLN:CG	1:C:7:LEU:N	2.52	0.72
1:B:372:LYS:CG	1:D:370:GLN:HG2	2.19	0.72
1:A:550:GLU:HG3	1:A:575:PRO:HG3	1.70	0.72
1:C:123:THR:HG23	1:C:135:LYS:HD3	1.71	0.72
2:E:20:GLU:HB3	1:D:47:ILE:HD11	1.70	0.72
1:C:411:VAL:HG12	1:C:411:VAL:O	1.87	0.72
1:C:411:VAL:HG11	1:C:424:ILE:HD11	1.72	0.71
1:B:109:ARG:HG2	1:B:132:ILE:HG13	1.72	0.70
1:B:443:ASP:OD1	2:F:79:LYS:HE2	1.92	0.70
1:C:187:TYR:CZ	4:C:767:Z98:H5AA	2.27	0.70
1:C:577:SER:O	1:C:578:ILE:HD12	1.92	0.70
1:A:43:MET:CE	1:A:72:PRO:HA	2.21	0.69
1:C:308:SER:HB3	1:C:311:GLU:HB2	1.74	0.69
1:C:525:LEU:HB3	1:C:570:LEU:CD1	2.22	0.69
1:C:134:ARG:O	1:C:138:ARG:HG3	1.93	0.69
2:G:54:LEU:HD23	2:G:57:MET:HE1	1.74	0.69
1:B:116:TYR:CE2	1:B:120:ILE:HD13	2.27	0.69
1:D:416:TYR:CD1	1:D:417:PRO:HA	2.27	0.69
1:D:290:MET:SD	2:H:23:GLN:HG3	2.33	0.68
1:A:233:GLU:HB3	1:A:235:TRP:CH2	2.29	0.68
1:B:610:ALA:HB1	1:B:622:LEU:HD21	1.75	0.68
2:H:54:LEU:HA	2:H:57:MET:HE3	1.76	0.68
2:E:57:MET:HE1	2:E:82:GLY:HA3	1.76	0.67
1:A:43:MET:HE1	1:A:72:PRO:HA	1.76	0.67
1:A:161:VAL:HG23	1:A:181:ALA:HB1	1.74	0.67
1:D:510:MET:CE	1:D:577:SER:HB2	2.25	0.67
1:C:460:TYR:O	1:C:461:ASP:HB2	1.94	0.67
1:B:311:GLU:OE1	1:D:62:PRO:HB2	1.95	0.67
1:C:619:SER:HB3	1:C:645:THR:HG21	1.77	0.67
1:C:288:ARG:HG3	1:C:296:MET:CE	2.25	0.67
1:B:543:PHE:CZ	1:D:578:ILE:HD13	2.31	0.66
1:C:689:GLU:O	1:C:689:GLU:HG2	1.95	0.66
1:C:631:GLY:O	1:C:725:GLY:HA3	1.94	0.66
1:B:8:ARG:CZ	1:B:8:ARG:HB3	2.25	0.66
5:C:1801:B12:O7R	5:C:1801:B12:C2B	2.42	0.66
1:B:238:MET:SD	1:B:283:TYR:HB2	2.35	0.65
1:C:528:PHE:CZ	1:C:565:GLY:HA3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:510:MET:HE2	1:D:577:SER:HB2	1.78	0.65
1:D:389:VAL:HG21	2:H:22:LEU:CD1	2.26	0.65
1:B:686:LEU:O	1:B:690:LYS:HG2	1.96	0.65
1:B:697:MET:HE1	1:B:736:ARG:HA	1.76	0.65
1:C:525:LEU:HD23	1:C:570:LEU:HD11	1.79	0.65
1:C:183:GLN:HB3	1:C:217:GLN:NE2	2.10	0.65
1:C:205:GLU:O	1:C:209:ILE:HD12	1.96	0.65
2:G:95:SER:O	2:G:98:GLU:HB2	1.96	0.65
1:B:668:THR:O	1:B:668:THR:HG23	1.95	0.65
1:C:668:THR:HG23	1:C:668:THR:O	1.97	0.64
1:C:416:TYR:CG	1:C:417:PRO:HA	2.31	0.64
1:B:226:ASN:O	1:B:230:THR:HG23	1.97	0.64
1:C:79:THR:HB	1:C:332:SER:HA	1.78	0.64
1:D:428:ILE:HG12	1:D:428:ILE:O	1.96	0.64
1:C:207:LYS:NZ	1:C:217:GLN:HE22	1.96	0.63
1:C:231:ALA:O	1:C:303:LYS:HE2	1.98	0.63
1:C:526:THR:HG23	1:C:569:GLU:HG3	1.79	0.63
1:D:93:ARG:HD3	1:D:345:HIS:HA	1.80	0.63
1:C:6:GLN:HG2	1:C:7:LEU:N	2.12	0.63
1:B:678:LYS:HB3	1:B:682:ARG:HH12	1.61	0.63
1:C:226:ASN:O	1:C:230:THR:HG23	1.99	0.63
1:A:267:VAL:CG2	1:A:299:GLN:HB3	2.29	0.63
1:A:515:VAL:HG23	1:A:516:GLU:HG2	1.80	0.63
5:C:1801:B12:H531	5:C:1801:B12:H543	1.79	0.63
1:B:537:GLU:HG3	1:B:554:VAL:HG21	1.80	0.63
1:C:492:ASN:N	1:C:492:ASN:HD22	1.97	0.63
1:A:387:ARG:NH1	1:A:417:PRO:HD2	2.14	0.62
1:B:459:GLN:HG3	1:B:460:TYR:CD2	2.34	0.62
1:C:41:LEU:CD2	1:C:43:MET:HE2	2.29	0.62
1:D:416:TYR:CG	1:D:417:PRO:HA	2.34	0.62
1:C:476:THR:OG1	2:G:56:ARG:HA	2.00	0.62
1:D:472:ILE:HG22	2:H:96:VAL:HG21	1.80	0.62
1:B:196:MET:SD	1:B:402:PHE:HD1	2.23	0.62
1:C:132:ILE:HA	1:C:136:GLN:OE1	2.00	0.62
1:C:654:ASP:OD1	1:C:690:LYS:NZ	2.32	0.62
5:C:1801:B12:H262	5:C:1801:B12:H601	1.82	0.62
1:A:578:ILE:HG23	1:A:579:ASP:N	2.15	0.61
2:F:54:LEU:HD23	2:F:57:MET:CE	2.29	0.61
1:C:135:LYS:NZ	1:C:488:GLU:OE2	2.32	0.61
1:C:233:GLU:HG2	1:C:235:TRP:CH2	2.35	0.61
1:D:443:ASP:OD1	2:H:79:LYS:HE3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ARG:NH1	1:C:11:GLU:OE2	2.33	0.61
3:A:1500:5AD:H5'3	5:C:1801:B12:C16	2.30	0.61
1:D:124:PRO:O	1:D:131:PRO:HG2	2.00	0.61
1:D:187:TYR:CZ	4:D:767:Z98:H5AA	2.36	0.61
1:B:28:LYS:HD2	1:B:145:ASP:CG	2.21	0.61
1:D:411:VAL:HB	1:D:424:ILE:HG13	1.81	0.61
1:C:688:VAL:HG23	1:C:693:ARG:HG2	1.81	0.61
1:C:626:ILE:HD13	1:C:640:VAL:HG11	1.83	0.61
1:D:245:HIS:CG	1:D:264:LEU:HD23	2.35	0.61
1:D:475:CYS:HB2	2:H:56:ARG:O	2.01	0.61
1:D:132:ILE:HA	1:D:136:GLN:OE1	2.00	0.61
1:A:112:GLY:HA3	1:C:620:VAL:CG1	2.30	0.61
1:B:81:GLU:HG3	1:B:106:MET:O	2.01	0.61
5:B:1801:B12:H552	5:B:1801:B12:C53	2.31	0.61
1:A:391:PHE:HA	1:A:416:TYR:CZ	2.36	0.60
1:B:212:TRP:CH2	1:B:477:LEU:HB3	2.36	0.60
5:B:1801:B12:H601	5:B:1801:B12:H262	1.82	0.60
1:C:492:ASN:N	1:C:492:ASN:ND2	2.48	0.60
1:D:307:ALA:HB1	1:D:340:ARG:HG3	1.83	0.60
1:A:501:GLU:OE1	1:A:502:THR:HG23	2.01	0.60
1:C:153:ARG:HG2	1:C:154:PRO:HD2	1.83	0.60
1:A:88:GLU:OE2	1:A:498:ARG:HD2	2.01	0.60
1:B:447:PRO:O	1:B:469:SER:HA	2.01	0.60
1:D:116:TYR:CE2	1:D:120:ILE:HD13	2.36	0.60
1:A:116:TYR:CE1	1:C:620:VAL:HG21	2.36	0.60
5:B:1801:B12:H492	5:B:1801:B12:C47	2.32	0.60
1:C:288:ARG:HG3	1:C:296:MET:HE3	1.84	0.60
1:C:327:ARG:NH1	1:C:327:ARG:HB3	2.16	0.60
1:C:543:PHE:O	1:C:547:MET:HG3	2.02	0.60
1:C:514:GLU:HA	1:C:520:ASP:OD1	2.02	0.59
1:C:618:HIS:CE1	5:C:1801:B12:N22	2.70	0.59
2:E:81:ALA:O	2:E:85:VAL:HG23	2.02	0.59
1:A:132:ILE:HA	1:A:136:GLN:OE1	2.02	0.59
1:D:193:ASN:OD1	1:D:426:ARG:HD2	2.02	0.59
1:C:462:GLU:O	1:C:465:VAL:HG23	2.01	0.59
1:B:160:TYR:CD1	1:B:182:HIS:HB2	2.38	0.59
1:B:534:ARG:HG3	1:B:534:ARG:HH11	1.67	0.59
1:A:459:GLN:HG3	1:A:460:TYR:CD2	2.37	0.59
1:B:416:TYR:CG	1:B:417:PRO:HA	2.38	0.58
1:D:515:VAL:HG13	1:D:522:THR:HB	1.85	0.58
5:B:1801:B12:H203	5:B:1801:B12:H301	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:579:ASP:HB3	1:D:582:SER:OG	2.03	0.58
1:A:464:LEU:CD2	1:A:471:LEU:HD13	2.34	0.58
1:B:688:VAL:HA	1:B:693:ARG:HB2	1.86	0.58
1:D:399:GLY:HA3	1:D:403:ASN:HD22	1.68	0.58
1:D:541:ILE:HD11	1:D:554:VAL:HG23	1.84	0.58
1:B:14:ASP:HB3	1:B:17:ASN:HB3	1.85	0.58
1:D:415:TYR:O	1:D:418:GLU:HB3	2.04	0.58
1:D:6:GLN:CG	1:D:7:LEU:H	2.15	0.58
1:B:118:GLY:H	1:B:165:ALA:HB2	1.67	0.58
1:B:693:ARG:HG3	1:B:693:ARG:O	2.03	0.58
1:C:327:ARG:HB3	1:C:327:ARG:HH11	1.69	0.58
1:C:575:PRO:HD2	1:C:576:PHE:CE2	2.38	0.58
1:A:161:VAL:O	1:A:161:VAL:HG12	2.04	0.57
1:A:267:VAL:HG22	1:A:299:GLN:HB3	1.86	0.57
1:A:541:ILE:HD11	1:A:554:VAL:HG23	1.85	0.57
4:A:767:Z98:HG	4:A:767:Z98:O3	2.04	0.57
1:B:619:SER:HB3	1:B:645:THR:HG21	1.85	0.57
1:C:554:VAL:HA	1:C:570:LEU:HB3	1.86	0.57
1:A:385:LYS:O	1:A:389:VAL:HG23	2.04	0.57
1:C:701:GLY:HA2	1:C:719:PHE:O	2.03	0.57
1:D:106:MET:HG3	1:D:158:HIS:CD2	2.39	0.57
1:C:327:ARG:HH11	1:C:327:ARG:CB	2.17	0.57
1:C:488:GLU:O	1:C:489:LEU:HD23	2.04	0.57
2:G:38:LEU:O	2:G:42:LYS:HG3	2.04	0.57
2:E:60:SER:OG	2:E:63:GLU:HG3	2.03	0.57
1:C:495:VAL:HA	1:C:498:ARG:NH1	2.19	0.57
1:B:697:MET:HE1	1:B:736:ARG:CA	2.33	0.57
1:A:116:TYR:HE1	1:C:620:VAL:HG21	1.68	0.57
1:A:464:LEU:HD23	1:A:471:LEU:HD13	1.87	0.57
1:C:117:ASP:HA	1:C:164:VAL:HG23	1.86	0.57
1:C:284:ALA:O	1:C:288:ARG:HD2	2.05	0.57
2:G:53:VAL:HG12	2:G:57:MET:HE2	1.85	0.57
1:A:114:SER:OG	4:A:767:Z98:OP1	2.23	0.57
1:B:57:ASN:HB3	1:B:99:TRP:CH2	2.40	0.57
1:D:187:TYR:OH	4:D:767:Z98:H5AA	2.05	0.57
1:C:158:HIS:CD2	1:C:181:ALA:HA	2.40	0.56
1:C:235:TRP:O	1:C:238:MET:HG3	2.05	0.56
1:A:514:GLU:HA	1:A:520:ASP:OD1	2.05	0.56
3:A:1500:5AD:C4'	5:C:1801:B12:N23	2.68	0.56
1:B:116:TYR:HE2	1:B:120:ILE:HD13	1.70	0.56
1:C:459:GLN:HG3	1:C:460:TYR:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:LEU:HD11	1:D:139:ALA:HB2	1.86	0.56
2:H:54:LEU:HD23	2:H:57:MET:HE2	1.87	0.56
1:D:43:MET:HB2	1:D:48:TYR:HE2	1.70	0.56
1:B:30:ARG:HH11	1:B:30:ARG:CG	2.16	0.56
1:B:512:LYS:HB2	1:B:513:PRO:CD	2.36	0.56
2:F:92:LYS:HE3	2:F:108:TYR:CE1	2.41	0.56
1:B:622:LEU:HD12	1:B:622:LEU:O	2.06	0.56
1:C:79:THR:HG21	1:C:106:MET:HE3	1.87	0.56
5:B:1801:B12:H362	5:B:1801:B12:C35	2.33	0.56
2:H:25:ARG:HA	2:H:28:GLU:HG3	1.87	0.56
1:D:389:VAL:HG21	2:H:22:LEU:HD11	1.88	0.56
1:A:416:TYR:CG	1:A:417:PRO:HA	2.41	0.55
1:B:196:MET:SD	1:B:402:PHE:CD1	2.99	0.55
1:A:43:MET:HE3	1:A:72:PRO:CB	2.36	0.55
1:C:584:VAL:HG12	1:C:584:VAL:O	2.05	0.55
1:C:622:LEU:HB2	1:C:667:SER:HB2	1.87	0.55
1:A:8:ARG:HD3	1:A:11:GLU:CD	2.27	0.55
1:C:250:ILE:HG23	2:G:34:VAL:HG21	1.87	0.55
1:D:219:ASP:HB3	1:D:248:ASN:HD22	1.71	0.55
1:B:160:TYR:CE1	1:B:182:HIS:CG	2.94	0.55
1:B:735:LYS:O	1:B:735:LYS:HG3	2.06	0.55
1:C:79:THR:CG2	1:C:106:MET:HE3	2.37	0.55
1:A:578:ILE:CG2	1:A:579:ASP:N	2.69	0.55
1:C:6:GLN:CG	1:C:7:LEU:H	2.16	0.55
1:A:6:GLN:O	1:A:7:LEU:HB2	2.06	0.55
1:A:232:ARG:HH21	1:C:598:ARG:NH2	2.05	0.55
1:B:8:ARG:CZ	1:B:8:ARG:CB	2.84	0.55
1:B:274:ALA:O	1:B:276:SER:N	2.40	0.55
1:B:393:GLU:OE2	2:F:25:ARG:NH1	2.36	0.55
1:B:87:PHE:HB2	1:B:140:GLN:NE2	2.22	0.55
1:B:246:ALA:O	1:B:250:ILE:HG22	2.07	0.55
1:B:394:GLU:CD	1:B:419:ARG:HH22	2.10	0.55
1:A:333:THR:OG1	1:A:351:ALA:HB1	2.06	0.55
1:A:560:MET:HB3	1:C:96:MET:HE3	1.89	0.55
1:A:79:THR:HB	1:A:332:SER:HA	1.87	0.55
1:D:412:ASP:OD1	1:D:419:ARG:HG3	2.06	0.55
1:A:243:VAL:O	1:A:247:LEU:HG	2.06	0.55
1:A:534:ARG:NH1	1:A:538:PHE:HE2	2.05	0.54
1:B:81:GLU:OE2	1:B:108:ILE:HG13	2.07	0.54
1:A:229:ALA:C	1:A:231:ALA:H	2.09	0.54
1:B:212:TRP:CZ2	1:B:477:LEU:HB3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:ASP:O	2:F:10:ARG:HG3	2.08	0.54
1:B:445:MET:HB3	2:F:83:HIS:CD2	2.43	0.54
1:D:514:GLU:HA	1:D:520:ASP:OD1	2.07	0.54
1:C:110:THR:HG22	1:C:131:PRO:HA	1.89	0.54
1:A:393:GLU:OE2	2:E:25:ARG:NH1	2.41	0.54
1:B:55:LEU:HD12	1:B:58:SER:HB3	1.89	0.54
1:B:217:GLN:NE2	1:B:257:MET:CE	2.70	0.54
1:A:381:VAL:O	1:A:385:LYS:HG3	2.07	0.54
1:B:223:GLY:O	1:B:226:ASN:HB2	2.08	0.54
1:D:577:SER:C	1:D:578:ILE:HD12	2.28	0.54
1:A:5:LEU:C	1:A:5:LEU:HD23	2.28	0.54
1:D:445:MET:HE2	1:D:447:PRO:N	2.23	0.54
1:A:441:ASP:OD2	2:E:79:LYS:HE3	2.08	0.54
2:E:53:VAL:HG12	2:E:57:MET:CE	2.38	0.54
1:B:109:ARG:NH1	1:B:169:ILE:HD13	2.22	0.54
1:C:81:GLU:HG2	1:C:108:ILE:HD11	1.90	0.54
1:C:377:LEU:O	1:C:381:VAL:HG23	2.08	0.54
1:D:404:ALA:HB1	1:D:409:PHE:CD2	2.43	0.54
1:B:428:ILE:O	1:B:428:ILE:HG13	2.08	0.53
1:B:443:ASP:CG	2:F:79:LYS:HE2	2.29	0.53
1:B:586:PRO:O	1:D:534:ARG:NH2	2.40	0.53
1:B:651:LYS:HE3	1:B:651:LYS:N	2.24	0.53
1:B:237:VAL:HG13	1:B:241:LEU:HG	1.90	0.53
1:C:668:THR:HG22	1:C:701:GLY:O	2.08	0.53
2:H:92:LYS:HB2	2:H:94:ILE:HG12	1.91	0.53
1:A:528:PHE:HB3	1:C:514:GLU:O	2.08	0.53
1:B:335:THR:O	1:B:338:GLU:HB2	2.09	0.53
1:B:649:VAL:HG22	1:B:683:ILE:CG1	2.35	0.53
5:B:1801:B12:H492	5:B:1801:B12:H471	1.90	0.53
1:A:29:ARG:HG3	1:A:29:ARG:HH11	1.73	0.53
1:A:568:ILE:HG22	1:A:570:LEU:CD1	2.39	0.53
1:C:144:LEU:O	1:C:148:GLU:HG2	2.09	0.53
1:C:153:ARG:HG2	1:C:154:PRO:CD	2.39	0.53
2:H:32:LYS:NZ	2:H:32:LYS:HB3	2.24	0.53
1:A:238:MET:O	1:A:242:MET:HG3	2.09	0.53
1:A:361:GLY:O	1:C:277:MET:HG2	2.09	0.53
1:B:534:ARG:HG3	1:B:534:ARG:NH1	2.24	0.53
1:C:288:ARG:HG3	1:C:296:MET:HE2	1.90	0.53
1:D:26:THR:HG22	1:D:27:PRO:HD2	1.91	0.53
1:B:73:GLN:HE21	1:B:153:ARG:HH22	1.56	0.53
1:B:79:THR:HA	1:B:104:HIS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:99:ALA:O	2:E:103:LEU:HD12	2.09	0.52
1:B:608:ILE:HD13	1:B:638:VAL:CG1	2.39	0.52
1:B:612:THR:CG2	1:B:616:ASP:HB3	2.37	0.52
1:C:141:ARG:NH2	1:C:148:GLU:OE2	2.41	0.52
1:C:550:GLU:HG2	1:C:575:PRO:HG3	1.91	0.52
1:B:445:MET:HE2	1:B:446:ALA:C	2.28	0.52
2:G:46:THR:HB	2:G:47:PRO:HD2	1.92	0.52
1:D:389:VAL:HG21	2:H:22:LEU:HD12	1.90	0.52
1:B:168:ASP:OD2	2:F:48:SER:HB2	2.10	0.52
1:B:449:THR:HG22	1:B:450:ALA:N	2.24	0.52
1:A:389:VAL:HG22	2:E:26:PHE:HB2	1.92	0.52
1:B:649:VAL:CG2	1:B:683:ILE:HG13	2.37	0.52
1:C:445:MET:HE1	1:C:447:PRO:HB3	1.91	0.52
1:B:618:HIS:CE1	5:B:1801:B12:N22	2.78	0.52
1:D:504:GLU:O	1:D:505:PHE:CD1	2.62	0.52
4:B:767:Z98:HGA	4:B:767:Z98:O3	2.10	0.52
1:C:187:TYR:OH	4:C:767:Z98:H5AA	2.10	0.52
1:C:226:ASN:N	1:C:226:ASN:HD22	2.07	0.52
1:D:28:LYS:HE3	1:D:148:GLU:OE1	2.09	0.52
1:B:138:ARG:NH1	1:B:485:TYR:HD1	2.05	0.52
1:B:416:TYR:CD1	1:B:417:PRO:HA	2.44	0.52
1:B:28:LYS:HD2	1:B:145:ASP:HB3	1.92	0.52
1:B:668:THR:O	1:B:668:THR:CG2	2.57	0.52
1:C:35:ARG:HH12	1:C:74:PRO:HD2	1.75	0.52
1:B:124:PRO:O	1:B:131:PRO:HG2	2.10	0.52
1:B:445:MET:HE1	1:B:447:PRO:CA	2.40	0.51
1:D:472:ILE:CG2	2:H:96:VAL:HG21	2.40	0.51
2:H:11:ARG:HH22	2:H:15:ALA:HA	1.75	0.51
1:B:458:LYS:NZ	1:B:462:GLU:CB	2.73	0.51
1:B:537:GLU:O	1:B:541:ILE:HG12	2.10	0.51
1:C:120:ILE:CG1	1:C:133:THR:HG22	2.33	0.51
1:C:288:ARG:HA	1:C:296:MET:CE	2.40	0.51
1:C:41:LEU:HD21	1:C:43:MET:HE2	1.91	0.51
1:D:464:LEU:HD23	1:D:471:LEU:HD13	1.92	0.51
2:E:94:ILE:HD12	2:E:99:ALA:HB2	1.92	0.51
1:B:608:ILE:HD13	1:B:638:VAL:HG13	1.93	0.51
1:B:707:PRO:O	1:B:711:VAL:HG23	2.10	0.51
1:C:86:ARG:HB3	1:C:88:GLU:OE2	2.10	0.51
1:C:443:ASP:OD1	2:G:79:LYS:HE2	2.11	0.51
2:G:113:ILE:HG22	2:G:113:ILE:O	2.10	0.51
1:D:438:PHE:CE2	2:H:77:MET:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ALA:O	1:A:362:MET:HG3	2.10	0.51
1:C:406:GLU:HG2	1:C:426:ARG:O	2.10	0.51
1:A:229:ALA:O	1:A:231:ALA:N	2.39	0.51
1:B:692:ILE:O	1:B:694:ASP:N	2.44	0.51
1:C:663:ALA:HB2	1:C:697:MET:HB2	1.93	0.51
1:D:126:GLY:HA3	1:D:131:PRO:HD3	1.92	0.51
1:A:165:ALA:HB1	1:A:168:ASP:OD2	2.11	0.51
1:B:730:THR:O	1:B:734:LYS:HB2	2.10	0.51
1:D:64:ALA:O	1:D:67:PHE:N	2.43	0.51
1:D:237:VAL:HG22	1:D:237:VAL:O	2.09	0.51
1:C:678:LYS:O	1:C:681:LYS:HB3	2.09	0.51
5:C:1801:B12:H362	5:C:1801:B12:C35	2.37	0.51
1:A:300:MET:CE	1:A:320:LEU:HD21	2.41	0.51
1:C:457:VAL:HG13	1:C:471:LEU:HD21	1.93	0.51
1:B:729:ALA:O	1:B:733:VAL:HG13	2.11	0.50
1:A:537:GLU:HG3	1:A:554:VAL:HG21	1.93	0.50
2:E:113:ILE:O	2:E:113:ILE:HG22	2.11	0.50
2:E:59:PHE:CE1	2:E:100:GLY:HA3	2.46	0.50
1:B:692:ILE:HD12	1:B:696:ILE:HD13	1.93	0.50
1:D:161:VAL:HG12	1:D:161:VAL:O	2.11	0.50
1:B:609:VAL:HG23	1:B:652:LEU:HD11	1.93	0.50
1:C:642:TYR:CE2	1:C:644:GLY:HA2	2.46	0.50
1:D:43:MET:HE3	1:D:72:PRO:HB3	1.92	0.50
1:D:534:ARG:HG3	1:D:534:ARG:HH11	1.76	0.50
1:A:449:THR:HG22	1:A:450:ALA:N	2.26	0.50
1:C:86:ARG:HD3	1:C:498:ARG:HD2	1.93	0.50
1:D:245:HIS:HB3	1:D:264:LEU:HD23	1.93	0.50
1:A:82:ILE:HG12	1:A:93:ARG:HD2	1.94	0.50
1:D:18:ILE:HD13	1:D:143:ALA:HB2	1.93	0.50
1:D:43:MET:HE1	1:D:72:PRO:HA	1.94	0.50
1:D:57:ASN:HB3	1:D:99:TRP:CH2	2.46	0.50
2:H:54:LEU:HA	2:H:57:MET:CE	2.40	0.50
2:E:6:ASP:O	2:E:10:ARG:HG2	2.12	0.50
1:B:143:ALA:O	1:B:147:ILE:HG13	2.12	0.50
1:B:200:PHE:CZ	1:B:401:TYR:CE2	3.00	0.50
1:C:6:GLN:CD	1:C:7:LEU:N	2.55	0.50
1:C:138:ARG:CZ	1:C:485:TYR:HD1	2.25	0.50
1:B:393:GLU:CG	2:F:29:MET:HE1	2.33	0.49
1:A:61:LEU:O	1:A:62:PRO:C	2.50	0.49
1:A:207:LYS:HE3	1:A:252:SER:OG	2.12	0.49
1:B:514:GLU:OE2	1:B:518:GLN:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:113:ILE:C	2:E:114:GLN:HG2	2.32	0.49
1:B:498:ARG:O	1:B:501:GLU:HB2	2.11	0.49
1:B:651:LYS:HE3	1:B:651:LYS:CA	2.42	0.49
1:C:619:SER:HB3	1:C:645:THR:CG2	2.40	0.49
2:G:53:VAL:HG12	2:G:57:MET:CE	2.43	0.49
1:A:94:MET:HG2	1:A:105:ILE:HG21	1.95	0.49
1:A:137:VAL:HG11	1:A:172:MET:HE1	1.94	0.49
1:A:172:MET:CE	1:A:176:GLU:HG3	2.39	0.49
1:A:197:ILE:CG2	1:A:437:VAL:HG21	2.43	0.49
1:A:197:ILE:HG22	1:A:437:VAL:HG21	1.94	0.49
1:C:79:THR:CB	1:C:332:SER:HA	2.42	0.49
1:C:182:HIS:HB3	4:C:767:Z98:H2AA	1.94	0.49
1:C:411:VAL:HB	1:C:424:ILE:HG12	1.92	0.49
1:B:28:LYS:HD2	1:B:145:ASP:CB	2.43	0.49
1:B:445:MET:HE1	1:B:447:PRO:HA	1.95	0.49
1:D:43:MET:CE	1:D:72:PRO:HA	2.43	0.49
1:D:272:PRO:HA	1:D:274:ALA:N	2.28	0.49
1:D:578:ILE:HD12	1:D:578:ILE:N	2.27	0.49
1:A:43:MET:HE3	1:A:72:PRO:CA	2.43	0.49
1:B:122:GLY:O	1:B:133:THR:HG21	2.11	0.49
1:A:159:SER:HB3	1:A:173:PHE:CZ	2.48	0.49
1:C:207:LYS:HZ2	1:C:217:GLN:HE22	1.61	0.49
1:D:445:MET:HE2	1:D:446:ALA:C	2.33	0.49
2:E:57:MET:CE	2:E:82:GLY:HA3	2.41	0.49
2:F:107:LYS:O	2:F:108:TYR:HB2	2.13	0.49
1:C:510:MET:CE	1:C:577:SER:HB2	2.43	0.49
1:D:79:THR:HB	1:D:332:SER:HA	1.95	0.49
1:C:187:TYR:CE2	4:C:767:Z98:H5AA	2.48	0.48
1:D:411:VAL:HG12	1:D:411:VAL:O	2.12	0.48
1:D:488:GLU:O	1:D:489:LEU:HD23	2.12	0.48
1:B:547:MET:O	1:B:548:ASN:HB2	2.13	0.48
1:D:307:ALA:CB	1:D:340:ARG:HG3	2.41	0.48
2:H:54:LEU:HD23	2:H:57:MET:HE1	1.95	0.48
1:A:126:GLY:HA3	1:A:129:GLY:O	2.13	0.48
1:A:309:THR:HG22	1:A:336:PRO:HB2	1.95	0.48
1:B:597:ILE:HG23	1:B:733:VAL:HG11	1.95	0.48
1:C:228:ASN:HD21	1:C:269:PRO:HA	1.78	0.48
1:C:320:LEU:HD13	1:C:358:ALA:HB3	1.94	0.48
1:C:679:ASN:O	1:C:683:ILE:HG13	2.14	0.48
1:D:219:ASP:HB3	1:D:248:ASN:ND2	2.26	0.48
1:A:484:VAL:HG11	2:E:60:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:GLU:HG3	2:F:29:MET:HE3	1.94	0.48
1:B:443:ASP:HA	1:B:456:ASN:HD22	1.78	0.48
1:C:305:MET:HE2	1:C:305:MET:HA	1.94	0.48
1:A:147:ILE:O	1:A:151:VAL:HG22	2.13	0.48
2:E:24:THR:HG21	1:D:47:ILE:HD13	1.95	0.48
1:C:82:ILE:HG22	1:C:90:ASP:HB3	1.95	0.48
1:C:207:LYS:HE3	1:C:251:PHE:HD2	1.78	0.48
1:D:568:ILE:HG22	1:D:570:LEU:HD12	1.95	0.48
1:B:137:VAL:HG11	1:B:172:MET:HE1	1.95	0.48
1:B:334:ILE:HG23	1:B:338:GLU:HG3	1.94	0.48
1:B:515:VAL:HG23	1:B:516:GLU:HG2	1.94	0.48
1:B:697:MET:HE3	1:B:736:ARG:HB2	1.96	0.48
5:B:1801:B12:N23	3:D:1500:5AD:C4'	2.76	0.48
1:C:236:LYS:HB3	1:C:415:TYR:HB2	1.95	0.48
1:C:300:MET:HB2	1:C:334:ILE:HG12	1.96	0.48
1:D:264:LEU:HD21	1:D:291:PHE:CD1	2.48	0.48
1:A:188:ASN:HB3	1:A:194:ILE:HB	1.95	0.48
1:A:223:GLY:HA3	4:A:767:Z98:H2A	1.96	0.48
1:A:411:VAL:HG12	1:A:411:VAL:O	2.14	0.48
4:A:767:Z98:O3	4:A:767:Z98:CG	2.62	0.48
1:B:126:GLY:HA3	1:B:131:PRO:HD3	1.94	0.48
1:D:438:PHE:CD2	2:H:77:MET:HG3	2.48	0.48
1:D:561:GLN:HB3	1:D:564:GLU:HB2	1.95	0.48
2:E:112:ALA:C	2:E:114:GLN:H	2.16	0.48
1:C:158:HIS:NE2	1:C:181:ALA:HA	2.29	0.48
1:C:210:MET:HE2	1:C:217:GLN:HB2	1.96	0.48
1:C:668:THR:O	1:C:668:THR:CG2	2.61	0.48
1:D:268:PRO:HA	1:D:269:PRO:HD3	1.68	0.48
1:D:510:MET:HE3	1:D:577:SER:HB2	1.95	0.48
2:E:28:GLU:HG2	1:D:40:ASN:ND2	2.29	0.48
1:B:184:ASP:OD1	1:B:186:GLN:HG3	2.14	0.48
1:B:701:GLY:HA3	5:B:1801:B12:C9B	2.44	0.48
1:C:195:ASN:O	1:C:199:SER:HB2	2.14	0.48
2:H:89:ALA:HB2	2:H:99:ALA:CB	2.43	0.48
1:C:41:LEU:HD23	1:C:43:MET:HE2	1.94	0.48
1:C:629:LYS:HE3	1:C:630:HIS:NE2	2.29	0.48
5:C:1801:B12:H301	5:C:1801:B12:H203	1.96	0.48
2:E:46:THR:HB	2:E:47:PRO:HD2	1.96	0.47
1:B:109:ARG:HH12	1:B:169:ILE:HD13	1.79	0.47
1:D:123:THR:O	1:D:498:ARG:NH2	2.47	0.47
1:A:171:VAL:HG12	1:A:172:MET:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:GLU:CG	2:F:29:MET:CE	2.86	0.47
2:F:71:THR:HG23	2:F:76:LEU:HB3	1.96	0.47
1:C:416:TYR:CD2	1:C:417:PRO:HA	2.48	0.47
1:C:475:CYS:HB2	2:G:56:ARG:O	2.15	0.47
1:A:116:TYR:CE2	1:A:120:ILE:HD13	2.50	0.47
1:B:267:VAL:HG22	1:B:299:GLN:O	2.14	0.47
1:B:432:ILE:N	1:B:432:ILE:HD13	2.29	0.47
1:C:658:GLU:O	1:C:658:GLU:HG2	2.15	0.47
1:D:55:LEU:HD12	1:D:58:SER:HB3	1.96	0.47
1:D:269:PRO:HD2	1:D:280:ASP:CG	2.35	0.47
1:A:259:LYS:HA	1:A:262:ILE:HD12	1.96	0.47
1:A:474:GLY:HA3	1:A:479:VAL:CG2	2.44	0.47
1:C:344:TRP:CG	1:C:515:VAL:HB	2.49	0.47
1:C:411:VAL:O	1:C:423:GLY:HA2	2.14	0.47
1:D:109:ARG:NH1	1:D:169:ILE:HD12	2.30	0.47
1:D:334:ILE:HG23	1:D:338:GLU:HG3	1.96	0.47
2:H:11:ARG:HH12	2:H:15:ALA:HB2	1.80	0.47
1:A:402:PHE:HB3	1:A:428:ILE:HG12	1.96	0.47
1:A:542:GLU:O	1:A:546:LYS:HG2	2.15	0.47
2:F:27:TRP:O	2:F:28:GLU:C	2.53	0.47
1:C:307:ALA:O	1:C:340:ARG:HD3	2.15	0.47
1:D:470:LYS:O	1:D:472:ILE:N	2.48	0.47
1:D:547:MET:O	1:D:548:ASN:HB2	2.14	0.47
1:B:204:CYS:HB3	1:B:452:PHE:CD2	2.50	0.47
1:B:217:GLN:NE2	1:B:257:MET:HE1	2.30	0.47
1:C:82:ILE:HD12	1:C:94:MET:HG2	1.96	0.47
1:C:406:GLU:OE1	1:C:428:ILE:HG13	2.15	0.47
1:C:577:SER:C	1:C:578:ILE:HD12	2.35	0.47
1:D:336:PRO:HD2	1:D:347:TYR:HB3	1.97	0.47
1:D:529:LEU:HA	1:D:530:PRO:HD3	1.74	0.47
2:H:50:GLU:HG3	2:H:77:MET:HE3	1.95	0.47
1:A:5:LEU:HD23	1:A:6:GLN:HB2	1.97	0.47
1:A:354:THR:OG1	1:C:310:ARG:HD2	2.14	0.47
1:C:228:ASN:ND2	1:C:269:PRO:HA	2.30	0.47
1:C:529:LEU:HA	1:C:530:PRO:HD3	1.74	0.47
2:G:81:ALA:O	2:G:85:VAL:HG23	2.15	0.47
1:A:484:VAL:HG11	2:E:60:SER:CB	2.45	0.47
1:B:197:ILE:HG22	1:B:201:ILE:HD12	1.97	0.47
1:C:267:VAL:HG22	1:C:299:GLN:HB3	1.97	0.47
1:D:224:ALA:HB3	1:D:245:HIS:CE1	2.50	0.47
1:B:132:ILE:HA	1:B:136:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLU:HG2	1:C:108:ILE:CD1	2.45	0.46
1:C:305:MET:HA	1:C:305:MET:CE	2.45	0.46
1:A:300:MET:HE1	1:A:320:LEU:HD21	1.97	0.46
1:C:738:GLU:O	1:C:738:GLU:HG2	2.14	0.46
1:D:109:ARG:HG2	1:D:132:ILE:HG13	1.98	0.46
1:A:7:LEU:HA	1:A:7:LEU:HD23	1.56	0.46
1:B:228:ASN:OD1	1:B:241:LEU:HD11	2.15	0.46
1:B:515:VAL:HG13	1:B:522:THR:HB	1.98	0.46
1:B:659:LEU:O	1:B:660:LYS:HB3	2.15	0.46
1:B:726:ILE:HG23	1:B:727:HIS:H	1.80	0.46
1:C:554:VAL:HG22	1:C:570:LEU:HD23	1.98	0.46
1:A:526:THR:HB	1:C:524:LEU:HB3	1.97	0.46
1:B:546:LYS:HD3	1:D:576:PHE:CE1	2.51	0.46
1:C:416:TYR:CD1	1:C:417:PRO:HA	2.51	0.46
1:D:104:HIS:CE1	1:D:106:MET:CE	2.98	0.46
1:B:30:ARG:CG	1:B:30:ARG:NH1	2.78	0.46
1:D:541:ILE:CD1	1:D:554:VAL:HG23	2.45	0.46
1:B:264:LEU:HD21	1:B:291:PHE:CD1	2.51	0.46
1:B:307:ALA:O	1:B:340:ARG:HD3	2.16	0.46
1:C:491:GLU:C	1:C:492:ASN:HD22	2.19	0.46
1:A:561:GLN:O	1:A:562:GLU:C	2.54	0.46
5:B:1801:B12:H473	5:B:1801:B12:C49	2.24	0.46
1:C:219:ASP:HB3	1:C:248:ASN:ND2	2.30	0.46
1:C:373:ARG:NH1	1:C:378:GLY:HA2	2.31	0.46
1:A:314:VAL:HB	1:C:357:GLN:NE2	2.30	0.46
1:A:543:PHE:CZ	1:C:578:ILE:HD13	2.51	0.46
1:B:116:TYR:CD2	1:B:120:ILE:HD13	2.51	0.46
1:B:313:THR:O	1:B:317:VAL:HG23	2.16	0.46
1:B:697:MET:CE	1:B:736:ARG:HB2	2.45	0.46
1:C:35:ARG:O	1:C:37:PRO:HD3	2.16	0.46
1:C:77:VAL:CG1	1:C:104:HIS:HB2	2.46	0.46
1:A:43:MET:CE	1:A:72:PRO:CA	2.93	0.46
1:B:79:THR:HB	1:B:332:SER:CA	2.35	0.46
1:B:333:THR:O	1:B:334:ILE:HD13	2.16	0.46
1:C:561:GLN:OE1	1:C:564:GLU:HG2	2.16	0.46
1:D:94:MET:HE3	1:D:140:GLN:NE2	2.31	0.46
1:D:233:GLU:HB3	1:D:235:TRP:CH2	2.51	0.46
2:H:50:GLU:HG3	2:H:77:MET:CE	2.46	0.46
1:A:63:SER:HB2	1:C:311:GLU:OE2	2.15	0.46
1:B:660:LYS:O	1:B:660:LYS:HG2	2.16	0.46
1:C:411:VAL:O	1:C:411:VAL:CG1	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:633:ILE:O	1:C:634:GLU:C	2.53	0.46
1:D:552:VAL:CG1	1:D:570:LEU:HD23	2.46	0.46
1:A:95:ARG:HG3	1:A:147:ILE:HG12	1.99	0.45
1:A:481:GLU:CD	1:A:481:GLU:H	2.20	0.45
1:D:297:ARG:O	1:D:297:ARG:HD3	2.16	0.45
1:D:334:ILE:HD13	1:D:334:ILE:HA	1.83	0.45
1:A:212:TRP:CH2	1:A:477:LEU:HD22	2.52	0.45
5:C:1801:B12:H301	5:C:1801:B12:H253	1.62	0.45
1:D:158:HIS:HA	1:D:180:GLY:O	2.16	0.45
1:A:537:GLU:O	1:A:540:ALA:HB3	2.16	0.45
1:B:200:PHE:CE1	1:B:401:TYR:HE2	2.33	0.45
1:B:464:LEU:HD12	1:B:464:LEU:HA	1.76	0.45
1:D:6:GLN:CG	1:D:7:LEU:N	2.79	0.45
1:D:94:MET:CE	1:D:140:GLN:NE2	2.80	0.45
1:B:446:ALA:HA	1:B:447:PRO:HD3	1.80	0.45
1:A:195:ASN:O	1:A:199:SER:HB2	2.16	0.45
1:B:88:GLU:HG2	1:B:89:ASP:N	2.32	0.45
1:B:197:ILE:HG22	1:B:201:ILE:CD1	2.46	0.45
1:B:255:VAL:HG23	2:F:38:LEU:HD21	1.99	0.45
1:C:197:ILE:HG22	1:C:437:VAL:HG21	1.98	0.45
1:A:13:LEU:HG	1:A:95:ARG:HD2	1.98	0.45
1:A:277:MET:HE1	1:A:321:LEU:HG	1.99	0.45
1:C:513:PRO:O	1:C:521:GLY:HA2	2.16	0.45
1:D:137:VAL:HG21	1:D:172:MET:HE1	1.98	0.45
1:A:290:MET:CE	1:A:385:LYS:HD3	2.47	0.45
5:B:1801:B12:H531	5:B:1801:B12:C55	2.36	0.45
1:C:110:THR:CG2	1:C:131:PRO:HA	2.46	0.45
1:C:231:ALA:O	1:C:303:LYS:CE	2.63	0.45
1:C:334:ILE:HG23	1:C:338:GLU:HG3	1.98	0.45
1:D:162:SER:CB	4:D:767:Z98:H6	2.47	0.45
1:A:234:ALA:O	1:A:237:VAL:HG12	2.17	0.45
1:B:701:GLY:HA3	5:B:1801:B12:C8B	2.47	0.45
1:C:383:GLU:HG2	1:C:387:ARG:HE	1.81	0.45
1:D:546:LYS:HE3	1:D:546:LYS:HB3	1.72	0.45
1:B:461:ASP:HB3	1:B:464:LEU:HB2	1.99	0.45
1:C:612:THR:HG21	1:C:618:HIS:O	2.16	0.45
1:A:115:HIS:ND1	1:C:623:ARG:NH1	2.54	0.44
1:A:391:PHE:CE2	1:A:395:ILE:HD11	2.52	0.44
1:B:167:PRO:HD2	2:F:48:SER:OG	2.17	0.44
1:B:207:LYS:HG2	1:B:217:GLN:NE2	2.32	0.44
1:D:104:HIS:CE1	1:D:106:MET:HE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:GLU:OE1	1:D:176:GLU:HA	2.16	0.44
1:A:229:ALA:C	1:A:231:ALA:N	2.71	0.44
1:B:456:ASN:O	1:B:459:GLN:HG2	2.17	0.44
1:C:391:PHE:HA	1:C:416:TYR:CZ	2.53	0.44
1:C:651:LYS:CA	1:C:651:LYS:HE3	2.47	0.44
1:D:43:MET:HB2	1:D:48:TYR:CE2	2.51	0.44
1:D:117:ASP:HA	1:D:164:VAL:HG23	2.00	0.44
1:B:692:ILE:C	1:B:694:ASP:H	2.21	0.44
1:C:189:VAL:HG22	1:C:196:MET:HA	2.00	0.44
2:E:76:LEU:HD23	2:E:84:ILE:HD12	1.98	0.44
1:C:116:TYR:HD2	1:C:120:ILE:HG22	1.82	0.44
2:G:24:THR:O	2:G:28:GLU:HG2	2.17	0.44
1:A:15:VAL:HG22	1:A:499:MET:CE	2.47	0.44
1:B:161:VAL:O	1:B:161:VAL:CG1	2.59	0.44
1:B:695:LYS:HB2	1:B:695:LYS:HE3	1.61	0.44
1:C:462:GLU:CD	1:C:462:GLU:H	2.20	0.44
1:D:233:GLU:HB3	1:D:235:TRP:CZ3	2.53	0.44
1:D:445:MET:HG3	1:D:456:ASN:O	2.18	0.44
1:A:201:ILE:HG12	2:E:41:GLY:HA2	2.00	0.44
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.74	0.44
1:B:88:GLU:OE1	1:B:498:ARG:NH1	2.50	0.44
1:D:446:ALA:HA	1:D:447:PRO:HD3	1.70	0.44
1:A:39:GLU:O	1:A:41:LEU:N	2.51	0.44
1:A:233:GLU:HB3	1:A:235:TRP:CZ3	2.52	0.44
1:A:544:ALA:HB2	1:A:570:LEU:HD23	2.00	0.44
1:C:238:MET:CE	1:C:384:LEU:HD21	2.48	0.44
1:C:373:ARG:HA	1:C:377:LEU:HD23	2.00	0.44
1:C:628:ILE:HD12	1:C:635:LYS:HA	1.99	0.44
2:G:20:GLU:CD	2:G:20:GLU:H	2.21	0.44
1:D:6:GLN:HG2	1:D:7:LEU:N	2.33	0.44
1:D:500:GLU:C	1:D:502:THR:H	2.21	0.44
1:A:372:LYS:HD2	1:C:367:ASP:O	2.17	0.44
1:B:162:SER:HB2	4:B:767:Z98:H6	2.00	0.44
1:B:228:ASN:HD22	1:B:267:VAL:HB	1.83	0.44
1:C:123:THR:CG2	1:C:135:LYS:HD3	2.44	0.44
1:C:676:HIS:O	1:C:680:MET:HG3	2.17	0.44
1:A:232:ARG:NH2	1:C:598:ARG:NH2	2.66	0.44
1:D:116:TYR:CD2	1:D:120:ILE:HD13	2.53	0.44
1:A:29:ARG:HG3	1:A:29:ARG:NH1	2.32	0.43
1:A:127:ILE:HG13	5:C:1801:B12:H1P1	2.00	0.43
1:A:335:THR:HB	1:A:337:ASP:OD1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:LYS:HZ3	1:B:462:GLU:CB	2.31	0.43
1:C:207:LYS:NZ	1:C:217:GLN:NE2	2.63	0.43
1:D:511:ILE:O	1:D:511:ILE:CG2	2.66	0.43
1:D:555:ILE:HG21	1:D:571:LYS:HD3	2.00	0.43
1:A:137:VAL:HG11	1:A:172:MET:CE	2.48	0.43
1:A:186:GLN:OE1	1:A:244:GLN:HG2	2.18	0.43
1:A:233:GLU:HB3	1:A:235:TRP:CZ2	2.54	0.43
1:A:369:VAL:HG12	1:A:370:GLN:N	2.33	0.43
1:B:525:LEU:HD23	1:B:570:LEU:CD1	2.49	0.43
1:B:606:LEU:HD21	1:B:732:LEU:HB3	2.00	0.43
1:C:55:LEU:HD21	1:C:153:ARG:CZ	2.48	0.43
2:G:99:ALA:O	2:G:103:LEU:HD12	2.18	0.43
1:D:289:GLU:CD	1:D:373:ARG:HH21	2.22	0.43
1:D:559:VAL:O	1:D:559:VAL:HG12	2.17	0.43
1:B:160:TYR:HD1	1:B:182:HIS:HB2	1.81	0.43
1:B:162:SER:CB	4:B:767:Z98:H6	2.48	0.43
1:B:185:PRO:O	1:B:189:VAL:HG23	2.18	0.43
1:B:278:TYR:CE1	1:D:368:MET:HE2	2.53	0.43
1:B:459:GLN:HG3	1:B:460:TYR:CE2	2.53	0.43
1:B:671:SER:O	1:B:672:HIS:C	2.57	0.43
1:D:167:PRO:HG2	2:H:48:SER:OG	2.18	0.43
1:D:323:SER:HB3	1:D:328:ALA:HB2	1.99	0.43
1:B:391:PHE:HA	1:B:416:TYR:CZ	2.54	0.43
1:C:116:TYR:HD2	1:C:120:ILE:CG2	2.31	0.43
1:D:391:PHE:HA	1:D:416:TYR:CZ	2.52	0.43
1:A:377:LEU:O	1:A:381:VAL:HG23	2.19	0.43
2:E:32:LYS:HE2	2:E:32:LYS:HB3	1.70	0.43
1:B:123:THR:HG23	1:B:135:LYS:HD3	1.99	0.43
1:B:626:ILE:HD13	1:B:640:VAL:HG11	1.99	0.43
1:C:148:GLU:HB3	1:C:155:ILE:HG13	2.00	0.43
1:C:205:GLU:HG2	2:G:49:ILE:HG23	2.00	0.43
1:A:161:VAL:HG23	1:A:181:ALA:CB	2.44	0.43
1:B:144:LEU:O	1:B:148:GLU:HG2	2.18	0.43
1:B:529:LEU:HA	1:B:530:PRO:HD3	1.75	0.43
1:B:655:ALA:O	1:B:659:LEU:HG	2.17	0.43
1:C:100:HIS:ND1	1:C:349:ILE:HG23	2.34	0.43
2:G:54:LEU:HD23	2:G:57:MET:CE	2.45	0.43
1:A:172:MET:HE2	1:A:176:GLU:CG	2.44	0.43
2:E:47:PRO:O	2:E:51:ARG:HG3	2.19	0.43
1:B:81:GLU:OE2	1:B:108:ILE:CG1	2.66	0.43
1:B:574:VAL:HA	1:B:575:PRO:HD3	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:THR:HB	1:B:709:VAL:HB	1.99	0.43
5:B:1801:B12:C47	5:B:1801:B12:C49	2.82	0.43
1:A:116:TYR:HE2	1:A:120:ILE:HD13	1.81	0.43
1:A:546:LYS:HB2	1:C:576:PHE:CE1	2.54	0.43
1:B:611:ALA:HB2	1:B:643:LEU:HB2	2.00	0.43
1:B:726:ILE:HG23	1:B:727:HIS:N	2.34	0.43
2:G:10:ARG:HE	2:G:10:ARG:HB3	1.65	0.43
1:A:158:HIS:HA	1:A:180:GLY:O	2.18	0.43
1:B:225:HIS:CG	1:B:265:SER:HG	2.37	0.43
5:B:1801:B12:H262	5:B:1801:B12:C60	2.48	0.43
5:B:1801:B12:H562	5:B:1801:B12:H18	1.88	0.43
1:C:133:THR:O	1:C:137:VAL:HG23	2.18	0.43
1:D:64:ALA:HB1	1:D:69:ASP:HA	2.00	0.43
1:A:126:GLY:C	1:A:127:ILE:HD13	2.39	0.43
1:B:185:PRO:HD2	1:B:248:ASN:OD1	2.19	0.43
1:B:449:THR:CG2	1:B:450:ALA:N	2.82	0.43
5:B:1801:B12:H301	5:B:1801:B12:H253	1.74	0.43
5:B:1801:B12:H412	5:B:1801:B12:H363	1.66	0.43
1:C:35:ARG:NH1	1:C:74:PRO:HD2	2.34	0.43
2:H:59:PHE:CZ	2:H:100:GLY:HA3	2.54	0.43
1:A:411:VAL:O	1:A:411:VAL:CG1	2.67	0.42
2:E:17:LEU:HD23	2:E:17:LEU:HA	1.76	0.42
1:B:401:TYR:O	1:B:405:VAL:HG23	2.19	0.42
1:C:124:PRO:HA	1:C:493:ASP:OD2	2.19	0.42
1:C:445:MET:O	2:G:83:HIS:HB2	2.18	0.42
1:D:399:GLY:CA	1:D:403:ASN:HD22	2.31	0.42
1:A:528:PHE:O	1:C:513:PRO:HA	2.19	0.42
1:B:43:MET:CE	1:B:72:PRO:HA	2.49	0.42
1:B:268:PRO:HA	1:B:269:PRO:HD3	1.81	0.42
1:B:617:GLU:HB2	5:B:1801:B12:C43	2.49	0.42
5:B:1801:B12:H473	5:B:1801:B12:H481	1.31	0.42
1:C:268:PRO:HA	1:C:269:PRO:HD3	1.84	0.42
1:C:667:SER:HA	5:C:1801:B12:H4B	2.01	0.42
1:A:106:MET:HE2	1:A:158:HIS:CE1	2.55	0.42
1:B:304:TYR:HD1	1:D:66:TYR:CD2	2.38	0.42
5:C:1801:B12:H531	5:C:1801:B12:H551	2.01	0.42
1:A:539:ALA:HB2	1:C:583:LEU:HD11	2.02	0.42
1:B:7:LEU:HD23	1:B:7:LEU:HA	1.60	0.42
1:B:297:ARG:HA	1:B:330:ILE:HB	2.01	0.42
1:B:320:LEU:HD13	1:B:358:ALA:HB3	2.01	0.42
1:B:335:THR:HA	1:B:336:PRO:HD3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ILE:HA	1:B:424:ILE:HD13	1.61	0.42
1:C:468:PRO:O	1:C:471:LEU:HB2	2.19	0.42
1:D:8:ARG:HD2	1:D:11:GLU:OE1	2.18	0.42
2:H:94:ILE:HD12	2:H:99:ALA:HA	2.01	0.42
1:B:200:PHE:CE1	1:B:401:TYR:CE2	3.07	0.42
1:B:233:GLU:HG2	1:B:235:TRP:CH2	2.53	0.42
1:B:620:VAL:HG13	1:D:112:GLY:HA3	2.01	0.42
2:H:57:MET:HE3	2:H:57:MET:HB2	1.79	0.42
1:A:467:GLU:N	1:A:468:PRO:HD3	2.34	0.42
1:B:8:ARG:NH1	1:B:11:GLU:HG3	2.34	0.42
1:B:176:GLU:OE1	1:B:176:GLU:HA	2.19	0.42
1:B:550:GLU:CG	1:B:575:PRO:HG3	2.50	0.42
1:C:286:ALA:CB	1:C:381:VAL:HG13	2.42	0.42
1:C:492:ASN:O	1:C:497:VAL:HG11	2.18	0.42
1:D:204:CYS:HB3	1:D:452:PHE:CD2	2.54	0.42
1:A:299:GLN:OE1	1:A:299:GLN:HA	2.20	0.42
1:A:360:ILE:HD13	1:A:360:ILE:HA	1.66	0.42
1:A:444:TYR:CD2	1:A:444:TYR:C	2.93	0.42
1:B:86:ARG:HB3	1:B:88:GLU:CD	2.40	0.42
1:B:218:ILE:CG2	1:B:265:SER:HB2	2.49	0.42
1:D:574:VAL:HA	1:D:575:PRO:HD3	1.70	0.42
1:B:538:PHE:CE2	1:D:585:ILE:HG23	2.54	0.42
1:B:543:PHE:CE2	1:D:578:ILE:HD13	2.54	0.42
1:B:693:ARG:O	1:B:693:ARG:NH1	2.52	0.42
1:C:509:SER:O	1:C:509:SER:OG	2.36	0.42
1:D:528:PHE:CZ	1:D:565:GLY:HA3	2.55	0.42
1:A:158:HIS:CD2	1:A:159:SER:N	2.88	0.42
1:A:476:THR:OG1	2:E:56:ARG:HA	2.20	0.42
1:B:225:HIS:HB3	1:B:265:SER:O	2.20	0.42
1:B:546:LYS:HB3	1:D:576:PHE:CZ	2.55	0.42
2:F:23:GLN:O	2:F:26:PHE:HB3	2.19	0.42
1:C:622:LEU:HD23	1:C:642:TYR:HE1	1.85	0.42
1:D:512:LYS:HB2	1:D:513:PRO:CD	2.49	0.42
1:B:8:ARG:HH12	1:B:11:GLU:HG3	1.84	0.42
1:B:53:THR:HA	1:B:54:PRO:HD3	1.69	0.42
1:B:225:HIS:CE1	1:B:265:SER:OG	2.73	0.42
1:D:137:VAL:HG21	1:D:172:MET:CE	2.50	0.42
1:D:585:ILE:HA	1:D:586:PRO:HD2	1.93	0.42
1:A:444:TYR:HA	2:E:79:LYS:O	2.19	0.41
1:D:558:GLU:O	1:D:560:MET:HE3	2.20	0.41
1:A:458:LYS:HE3	1:A:462:GLU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:GLN:HE21	1:B:713:GLN:N	2.18	0.41
1:C:96:MET:CE	1:C:345:HIS:HB3	2.49	0.41
1:C:267:VAL:CG2	1:C:299:GLN:HB3	2.50	0.41
1:A:120:ILE:HG13	1:A:133:THR:HG22	2.01	0.41
1:A:233:GLU:O	1:A:235:TRP:N	2.53	0.41
1:A:547:MET:O	1:A:548:ASN:HB2	2.19	0.41
1:B:310:ARG:HD3	1:D:350:GLU:HG2	2.02	0.41
1:B:528:PHE:CZ	1:D:96:MET:HE1	2.55	0.41
1:C:410:PHE:O	1:C:411:VAL:HB	2.20	0.41
1:C:471:LEU:HD12	2:G:86:TYR:OH	2.20	0.41
1:D:123:THR:O	1:D:494:ASN:HA	2.21	0.41
1:A:511:ILE:HG22	1:A:578:ILE:HG22	2.01	0.41
2:G:25:ARG:HA	2:G:28:GLU:HG2	2.02	0.41
2:E:28:GLU:CG	1:D:40:ASN:HD21	2.33	0.41
1:B:192:ARG:NH2	4:B:767:Z98:OP3	2.53	0.41
1:D:387:ARG:NH1	1:D:416:TYR:O	2.52	0.41
1:D:445:MET:CE	1:D:471:LEU:HD23	2.50	0.41
1:D:561:GLN:O	1:D:563:ALA:N	2.53	0.41
1:A:135:LYS:HG3	1:A:485:TYR:OH	2.20	0.41
1:A:585:ILE:HA	1:A:586:PRO:HD2	1.93	0.41
2:E:101:LEU:HD13	2:E:101:LEU:HA	1.68	0.41
1:B:31:GLY:O	1:B:179:ASN:ND2	2.53	0.41
1:B:675:ILE:HA	1:B:678:LYS:HB2	2.03	0.41
1:D:165:ALA:O	1:D:169:ILE:HG13	2.20	0.41
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.84	0.41
1:A:489:LEU:O	3:A:1500:5AD:C2	2.69	0.41
2:E:94:ILE:CD1	2:E:99:ALA:HB2	2.51	0.41
1:B:404:ALA:HB1	1:B:409:PHE:CD2	2.56	0.41
1:C:344:TRP:O	1:C:345:HIS:C	2.59	0.41
1:C:617:GLU:HA	1:C:617:GLU:OE2	2.21	0.41
1:C:668:THR:HG21	1:C:680:MET:HE2	2.03	0.41
1:D:534:ARG:HG3	1:D:534:ARG:NH1	2.35	0.41
2:H:95:SER:O	2:H:96:VAL:C	2.59	0.41
1:B:41:LEU:HD23	1:B:43:MET:HE2	2.01	0.41
1:B:118:GLY:N	1:B:165:ALA:HB2	2.35	0.41
1:B:237:VAL:HG13	1:B:237:VAL:O	2.20	0.41
1:B:712:LYS:HA	1:B:712:LYS:HD3	1.95	0.41
5:B:1801:B12:H601	5:B:1801:B12:H252	2.03	0.41
2:F:25:ARG:O	2:F:29:MET:HG3	2.20	0.41
1:D:468:PRO:O	1:D:471:LEU:HB2	2.21	0.41
1:D:579:ASP:O	1:D:580:ILE:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:TYR:HD1	1:A:226:ASN:ND2	2.19	0.41
1:A:212:TRP:CZ3	1:A:477:LEU:HD22	2.55	0.41
1:A:290:MET:HG3	1:A:290:MET:O	2.21	0.41
1:A:404:ALA:O	1:A:409:PHE:HB2	2.21	0.41
1:A:547:MET:O	1:C:547:MET:HB3	2.21	0.41
1:B:476:THR:HG22	1:B:482:LYS:HB2	2.03	0.41
1:B:521:GLY:HA3	1:B:573:ARG:HG3	2.02	0.41
1:B:550:GLU:HB2	1:B:573:ARG:HB3	2.03	0.41
1:B:620:VAL:CG1	1:D:112:GLY:HA3	2.51	0.41
1:C:106:MET:HE3	1:C:106:MET:HB2	1.89	0.41
1:C:109:ARG:NH1	1:C:169:ILE:CD1	2.84	0.41
1:C:143:ALA:O	1:C:146:LEU:HB2	2.21	0.41
1:C:316:HIS:CE1	1:C:334:ILE:HB	2.55	0.41
1:C:449:THR:HG22	1:C:450:ALA:N	2.36	0.41
1:C:726:ILE:HG23	1:C:727:HIS:N	2.36	0.41
1:C:737:ARG:C	1:C:739:MET:H	2.24	0.41
1:D:399:GLY:HA3	1:D:403:ASN:ND2	2.34	0.41
1:D:561:GLN:O	1:D:562:GLU:C	2.59	0.41
2:E:59:PHE:CZ	2:E:100:GLY:HA3	2.55	0.41
1:C:79:THR:HG21	1:C:106:MET:CE	2.51	0.41
1:D:500:GLU:O	1:D:502:THR:N	2.54	0.41
1:A:233:GLU:HG2	1:A:235:TRP:CH2	2.56	0.40
1:B:681:LYS:O	1:B:685:GLU:HG3	2.21	0.40
1:D:88:GLU:OE1	1:D:498:ARG:NH1	2.54	0.40
1:D:544:ALA:HB3	1:D:552:VAL:HG11	2.03	0.40
1:B:22:LEU:HD23	1:B:22:LEU:HA	1.93	0.40
1:B:23:ASP:OD2	1:B:24:LYS:HG2	2.20	0.40
1:B:210:MET:HE2	1:B:210:MET:HB3	1.88	0.40
1:B:415:TYR:O	1:B:416:TYR:C	2.59	0.40
1:C:109:ARG:HG2	1:C:132:ILE:HG13	2.03	0.40
1:C:394:GLU:HG2	1:C:394:GLU:O	2.21	0.40
1:D:75:LEU:N	1:D:76:PRO:CD	2.84	0.40
1:D:266:THR:O	1:D:266:THR:HG23	2.22	0.40
2:E:112:ALA:O	2:E:114:GLN:N	2.51	0.40
1:B:6:GLN:HG2	1:B:8:ARG:HG3	2.03	0.40
1:B:211:ALA:HB2	1:B:257:MET:HG2	2.03	0.40
1:B:449:THR:O	2:F:56:ARG:NH1	2.52	0.40
1:C:285:VAL:HG21	1:C:371:LEU:HD13	2.04	0.40
1:C:651:LYS:HE3	1:C:651:LYS:HA	2.03	0.40
1:C:651:LYS:HA	1:C:651:LYS:CE	2.51	0.40
2:G:103:LEU:HD23	2:G:109:TRP:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:THR:OG1	1:A:327:ARG:N	2.52	0.40
1:A:416:TYR:CD1	1:A:417:PRO:HA	2.57	0.40
1:B:87:PHE:O	1:B:91:ILE:HG12	2.21	0.40
1:B:632:GLY:O	1:B:633:ILE:C	2.60	0.40
1:C:184:ASP:HA	1:C:185:PRO:HD2	1.82	0.40
1:C:277:MET:HE2	1:C:321:LEU:HD23	2.03	0.40
1:C:335:THR:HG22	1:C:348:ASN:HA	2.03	0.40
1:C:422:ASP:N	1:C:422:ASP:OD1	2.55	0.40
1:C:585:ILE:HA	1:C:586:PRO:HD3	1.94	0.40
1:C:649:VAL:HG22	1:C:683:ILE:HG12	2.03	0.40
1:C:687:ALA:HB3	1:C:693:ARG:HD3	2.03	0.40
2:G:91:GLU:C	2:G:93:ASN:H	2.25	0.40
1:D:223:GLY:HA2	1:D:225:HIS:CE1	2.57	0.40
1:D:471:LEU:HD12	1:D:471:LEU:HA	1.67	0.40
2:E:14:LEU:O	2:E:17:LEU:HB2	2.22	0.40
1:C:28:LYS:HB3	1:C:28:LYS:HE2	1.90	0.40
1:C:458:LYS:C	1:C:460:TYR:H	2.25	0.40
1:D:108:ILE:HA	1:D:160:TYR:CE2	2.56	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	574/763 (75%)	525 (92%)	41 (7%)	8 (1%)	11 34
1	B	722/763 (95%)	662 (92%)	54 (8%)	6 (1%)	19 49
1	C	722/763 (95%)	666 (92%)	47 (6%)	9 (1%)	13 39
1	D	574/763 (75%)	534 (93%)	31 (5%)	9 (2%)	9 31
2	E	107/121 (88%)	104 (97%)	2 (2%)	1 (1%)	17 46
2	F	107/121 (88%)	98 (92%)	8 (8%)	1 (1%)	17 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	107/121 (88%)	99 (92%)	8 (8%)	0	100	100
2	H	107/121 (88%)	102 (95%)	4 (4%)	1 (1%)	17	46
All	All	3020/3536 (85%)	2790 (92%)	195 (6%)	35 (1%)	13	39

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	230	THR
1	A	234	ALA
1	A	504	GLU
1	B	6	GLN
1	B	7	LEU
1	C	461	ASP
1	D	6	GLN
1	D	471	LEU
1	D	505	PHE
1	A	7	LEU
2	E	113	ILE
1	B	658	GLU
1	B	672	HIS
1	B	693	ARG
2	F	75	GLY
1	C	738	GLU
1	D	7	LEU
1	A	411	VAL
1	C	454	TYR
1	D	411	VAL
1	D	501	GLU
1	D	562	GLU
1	C	69	ASP
1	D	232	ARG
2	H	96	VAL
1	C	670	ILE
1	C	674	ASP
1	D	193	ASN
1	A	586	PRO
1	C	669	ILE
1	C	411	VAL
1	C	465	VAL
1	B	161	VAL

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Mol	Chain	Res	Type
1	A	171	VAL

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	484/644 (75%)	456 (94%)	28 (6%)	20	50
1	B	603/644 (94%)	560 (93%)	43 (7%)	14	39
1	C	600/644 (93%)	551 (92%)	49 (8%)	11	33
1	D	485/644 (75%)	455 (94%)	30 (6%)	18	47
2	E	89/100 (89%)	82 (92%)	7 (8%)	12	34
2	F	90/100 (90%)	85 (94%)	5 (6%)	21	51
2	G	89/100 (89%)	85 (96%)	4 (4%)	27	60
2	H	89/100 (89%)	87 (98%)	2 (2%)	52	83
All	All	2529/2976 (85%)	2361 (93%)	168 (7%)	16	44

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	8	ARG
1	A	15	VAL
1	A	16	GLU
1	A	23	ASP
1	A	125	GLN
1	A	127	ILE
1	A	159	SER
1	A	164	VAL
1	A	172	MET
1	A	183	GLN
1	A	198	ARG
1	A	199	SER
1	A	260	SER

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Mol	Chain	Res	Type
1	A	305	MET
1	A	306	GLU
1	A	333	THR
1	A	338	GLU
1	A	349	ILE
1	A	391	PHE
1	A	462	GLU
1	A	465	VAL
1	A	471	LEU
1	A	492	ASN
1	A	501	GLU
1	A	509	SER
1	A	533	LYS
1	A	578	ILE
2	E	23	GLN
2	E	60	SER
2	E	73	ASP
2	E	76	LEU
2	E	91	GLU
2	E	94	ILE
2	E	101	LEU
1	B	5	LEU
1	B	7	LEU
1	B	8	ARG
1	B	15	VAL
1	B	29	ARG
1	B	30	ARG
1	B	39	GLU
1	B	105	ILE
1	B	125	GLN
1	B	153	ARG
1	B	162	SER
1	B	183	GLN
1	B	237	VAL
1	B	259	LYS
1	B	305	MET
1	B	306	GLU
1	B	338	GLU
1	B	341	ASN
1	B	342	VAL
1	B	381	VAL
1	B	424	ILE

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Mol	Chain	Res	Type
1	B	428	ILE
1	B	445	MET
1	B	464	LEU
1	B	471	LEU
1	B	526	THR
1	B	532	SER
1	B	570	LEU
1	B	603	LYS
1	B	629	LYS
1	B	649	VAL
1	B	651	LYS
1	B	671	SER
1	B	676	HIS
1	B	686	LEU
1	B	688	VAL
1	B	695	LYS
1	B	696	ILE
1	B	713	GLN
1	B	721	ARG
1	B	730	THR
1	B	731	PHE
1	B	733	VAL
2	F	61	SER
2	F	76	LEU
2	F	79	LYS
2	F	97	ARG
2	F	111	ASP
1	C	6	GLN
1	C	7	LEU
1	C	13	LEU
1	C	15	VAL
1	C	18	ILE
1	C	26	THR
1	C	28	LYS
1	C	39	GLU
1	C	47	ILE
1	C	114	SER
1	C	120	ILE
1	C	125	GLN
1	C	127	ILE
1	C	136	GLN
1	C	162	SER

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Mol	Chain	Res	Type
1	C	168	ASP
1	C	169	ILE
1	C	199	SER
1	C	237	VAL
1	C	260	SER
1	C	265	SER
1	C	288	ARG
1	C	297	ARG
1	C	305	MET
1	C	306	GLU
1	C	311	GLU
1	C	322	ILE
1	C	341	ASN
1	C	391	PHE
1	C	424	ILE
1	C	429	ASN
1	C	464	LEU
1	C	471	LEU
1	C	476	THR
1	C	492	ASN
1	C	497	VAL
1	C	498	ARG
1	C	509	SER
1	C	512	LYS
1	C	570	LEU
1	C	576	PHE
1	C	606	LEU
1	C	651	LYS
1	C	660	LYS
1	C	671	SER
1	C	688	VAL
1	C	703	THR
1	C	731	PHE
1	C	736	ARG
2	G	8	GLN
2	G	55	LEU
2	G	76	LEU
2	G	101	LEU
1	D	6	GLN
1	D	7	LEU
1	D	26	THR
1	D	114	SER

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Mol	Chain	Res	Type
1	D	125	GLN
1	D	127	ILE
1	D	153	ARG
1	D	169	ILE
1	D	172	MET
1	D	217	GLN
1	D	265	SER
1	D	305	MET
1	D	306	GLU
1	D	338	GLU
1	D	349	ILE
1	D	370	GLN
1	D	376	VAL
1	D	391	PHE
1	D	428	ILE
1	D	445	MET
1	D	464	LEU
1	D	471	LEU
1	D	491	GLU
1	D	499	MET
1	D	501	GLU
1	D	502	THR
1	D	505	PHE
1	D	511	ILE
1	D	557	ARG
1	D	582	SER
2	H	28	GLU
2	H	76	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	226	ASN
1	A	301	ASN
1	A	331	GLN
1	B	73	GLN
1	B	217	GLN
1	B	301	ASN
1	B	331	GLN
1	B	407	GLN
1	B	492	ASN

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Mol	Chain	Res	Type
1	B	518	GLN
1	B	713	GLN
1	C	217	GLN
1	C	226	ASN
1	C	228	ASN
1	C	245	HIS
1	C	316	HIS
1	C	319	ASN
1	C	331	GLN
1	C	341	ASN
1	C	492	ASN
1	C	518	GLN
2	G	16	ASN
1	D	40	ASN
1	D	42	GLN
1	D	301	ASN
1	D	331	GLN
1	D	403	ASN
1	D	492	ASN
1	D	518	GLN
2	H	16	ASN
2	H	93	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	5AD	D	1500	5	17,20,20	2.94	7 (41%)	15,30,30	2.71	8 (53%)
5	B12	B	1801	3,1	90,101,101	1.43	10 (11%)	137,166,166	2.23	30 (21%)
4	Z98	D	767	-	22,23,23	3.87	9 (40%)	29,32,32	1.76	6 (20%)
4	Z98	A	767	-	22,23,23	4.02	8 (36%)	29,32,32	2.07	12 (41%)
5	B12	C	1801	3,1	90,101,101	1.39	8 (8%)	137,166,166	2.50	33 (24%)
4	Z98	B	767	-	22,23,23	4.13	10 (45%)	29,32,32	1.75	5 (17%)
4	Z98	C	767	-	22,23,23	4.16	10 (45%)	29,32,32	1.60	9 (31%)
3	5AD	A	1500	5	17,20,20	2.76	7 (41%)	15,30,30	3.46	8 (53%)

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	5AD	D	1500	5	-	0/0/20/20	0/3/3/3
5	B12	B	1801	3,1	1/1/36/38	5/52/223/223	0/3/11/11
4	Z98	D	767	-	-	8/17/17/17	0/1/1/1
5	B12	C	1801	3,1	1/1/36/38	14/52/223/223	0/3/11/11
4	Z98	A	767	-	-	5/17/17/17	0/1/1/1
4	Z98	B	767	-	-	7/17/17/17	0/1/1/1
4	Z98	C	767	-	-	7/17/17/17	0/1/1/1
3	5AD	A	1500	5	-	0/0/20/20	0/3/3/3

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	767	Z98	C4-C5	8.63	1.52	1.42
4	C	767	Z98	C4-C5	8.46	1.52	1.42
4	C	767	Z98	C2-N1	8.07	1.49	1.33
4	A	767	Z98	C6-N1	7.79	1.50	1.34
4	B	767	Z98	C2-N1	7.75	1.48	1.33
4	A	767	Z98	C2-N1	7.74	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	767	Z98	C6-N1	7.72	1.50	1.34
4	B	767	Z98	C6-N1	7.70	1.50	1.34
4	D	767	Z98	C4-C5	7.48	1.51	1.42
4	D	767	Z98	C6-N1	7.38	1.50	1.34
4	A	767	Z98	C4-C5	7.29	1.51	1.42
4	D	767	Z98	C2-N1	7.05	1.47	1.33
4	B	767	Z98	C3-C2	6.84	1.47	1.40
5	B	1801	B12	C14-N23	6.68	1.43	1.35
4	A	767	Z98	C3-C2	6.62	1.47	1.40
3	D	1500	5AD	C2-N3	6.57	1.42	1.32
4	A	767	Z98	C4-C3	6.51	1.50	1.40
4	C	767	Z98	C3-C2	6.50	1.47	1.40
3	D	1500	5AD	C4-N3	6.24	1.44	1.35
4	C	767	Z98	C4A-ND	6.19	1.48	1.27
4	D	767	Z98	C3-C2	6.18	1.47	1.40
3	A	1500	5AD	C2-N3	6.17	1.42	1.32
4	B	767	Z98	C4-C3	5.95	1.49	1.40
3	A	1500	5AD	C4-N3	5.83	1.43	1.35
4	D	767	Z98	C4-C3	5.74	1.49	1.40
4	D	767	Z98	C4A-ND	5.73	1.46	1.27
4	A	767	Z98	OXT-C	5.73	1.39	1.22
4	B	767	Z98	C4A-ND	5.73	1.46	1.27
5	C	1801	B12	C14-N23	5.67	1.42	1.35
4	A	767	Z98	C4A-ND	5.63	1.46	1.27
4	D	767	Z98	OXT-C	5.57	1.39	1.22
4	C	767	Z98	OXT-C	5.50	1.38	1.22
4	C	767	Z98	C4-C3	5.44	1.49	1.40
4	B	767	Z98	OXT-C	5.28	1.38	1.22
3	D	1500	5AD	O4'-C1'	4.92	1.47	1.41
3	A	1500	5AD	O4'-C1'	4.49	1.47	1.41
5	C	1801	B12	C19-N24	-4.39	1.40	1.48
5	C	1801	B12	C9-N22	4.39	1.42	1.30
5	B	1801	B12	C19-N24	-4.21	1.41	1.48
5	B	1801	B12	C9-N22	4.14	1.41	1.30
5	B	1801	B12	C8B-C9B	4.07	1.48	1.40
4	C	767	Z98	C6-C5	4.03	1.46	1.37
5	C	1801	B12	C8B-C9B	3.96	1.48	1.40
5	C	1801	B12	C16-C15	-3.90	1.33	1.44
4	B	767	Z98	C6-C5	3.84	1.45	1.37
4	D	767	Z98	C6-C5	3.53	1.45	1.37
4	A	767	Z98	C6-C5	3.46	1.44	1.37
3	D	1500	5AD	C6-N6	3.38	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1801	B12	C11-N23	3.37	1.43	1.37
5	B	1801	B12	C16-C15	-3.37	1.35	1.44
3	A	1500	5AD	C6-N6	3.26	1.45	1.34
5	B	1801	B12	C6B-C5B	3.16	1.48	1.40
5	B	1801	B12	C11-N23	3.10	1.43	1.37
3	A	1500	5AD	C8-N7	2.98	1.40	1.34
5	C	1801	B12	C6B-C5B	2.95	1.48	1.40
5	B	1801	B12	C10-C9	2.79	1.47	1.39
3	D	1500	5AD	C8-N7	2.74	1.39	1.34
4	C	767	Z98	O-C	-2.60	1.22	1.30
4	B	767	Z98	O-C	-2.56	1.22	1.30
3	D	1500	5AD	O3'-C3'	-2.53	1.37	1.43
3	D	1500	5AD	C6-N1	2.52	1.48	1.37
5	C	1801	B12	C10-C9	2.46	1.46	1.39
4	D	767	Z98	O-C	-2.38	1.22	1.30
3	A	1500	5AD	C6-N1	2.33	1.47	1.37
5	B	1801	B12	C14-C15	2.19	1.47	1.38
5	B	1801	B12	O6R-C1R	2.10	1.44	1.41
4	C	767	Z98	P-OP2	2.06	1.57	1.50
3	A	1500	5AD	O3'-C3'	-2.04	1.38	1.43
4	B	767	Z98	C4-C4A	2.02	1.50	1.46

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1801	B12	C20-C1-C19	-9.75	99.96	109.36
5	B	1801	B12	C1-C19-N24	8.82	116.16	106.24
5	B	1801	B12	C13-C12-C11	-7.95	91.97	100.97
5	C	1801	B12	C1-C19-N24	7.86	115.08	106.24
5	C	1801	B12	C47-C12-C46	7.81	122.55	109.35
3	A	1500	5AD	C5'-C4'-C3'	7.42	123.49	115.70
5	C	1801	B12	C13-C12-C11	-7.21	92.81	100.97
5	B	1801	B12	C46-C12-C13	-7.04	84.03	112.72
5	C	1801	B12	C46-C12-C13	-7.00	84.20	112.72
5	B	1801	B12	C1-C19-C18	6.87	133.16	121.88
5	C	1801	B12	C1-C19-C18	6.87	133.15	121.88
5	B	1801	B12	C20-C1-C19	-6.75	102.85	109.36
5	C	1801	B12	C55-C17-C16	-6.66	103.50	116.65
3	A	1500	5AD	N3-C2-N1	-6.30	118.83	128.68
3	D	1500	5AD	N3-C2-N1	-6.21	118.97	128.68
5	C	1801	B12	C26-C2-C1	6.21	119.67	110.01
5	C	1801	B12	C12-C11-C10	-6.18	115.32	123.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1801	B12	C12-C11-N23	6.10	120.33	111.83
5	B	1801	B12	C47-C12-C46	6.10	119.66	109.35
5	C	1801	B12	C47-C12-C13	-5.87	88.83	112.72
4	B	767	Z98	OP4-C5A-C5	5.66	120.13	109.35
5	C	1801	B12	C18-C19-N24	5.50	110.69	102.31
3	A	1500	5AD	O3'-C3'-C4'	5.37	123.63	110.47
4	D	767	Z98	OP4-C5A-C5	5.17	119.21	109.35
5	B	1801	B12	C12-C11-C10	-5.09	116.75	123.37
5	C	1801	B12	C2-C1-C19	4.93	126.38	118.60
5	B	1801	B12	C12-C11-N23	4.91	118.67	111.83
5	B	1801	B12	C47-C12-C13	-4.90	92.75	112.72
5	B	1801	B12	C18-C19-N24	4.76	109.55	102.31
5	B	1801	B12	C2-C1-N21	4.59	108.17	101.77
5	B	1801	B12	C15-C14-N23	-4.34	120.96	126.26
3	A	1500	5AD	O2'-C2'-C3'	4.13	125.17	111.82
5	B	1801	B12	C26-C2-C1	4.10	116.40	110.01
5	C	1801	B12	C19-C1-N21	4.08	106.35	102.16
5	C	1801	B12	C2-C1-N21	4.04	107.39	101.77
3	A	1500	5AD	C1'-N9-C4	-4.01	119.60	126.64
4	A	767	Z98	CB-CA-N	3.85	120.27	110.17
4	A	767	Z98	CG-ND-C4A	-3.77	107.34	118.90
4	A	767	Z98	OP4-C5A-C5	3.75	116.50	109.35
5	B	1801	B12	C2-C1-C19	3.74	124.51	118.60
5	C	1801	B12	C12-C13-C14	3.70	108.45	102.26
5	B	1801	B12	C20-C1-C2	-3.68	107.14	113.28
3	D	1500	5AD	O2'-C2'-C3'	3.68	123.71	111.82
3	D	1500	5AD	C5'-C4'-C3'	3.60	119.48	115.70
4	C	767	Z98	OP4-C5A-C5	3.58	116.18	109.35
5	B	1801	B12	C25-C2-C1	-3.58	108.38	113.78
3	D	1500	5AD	O3'-C3'-C4'	3.51	119.06	110.47
4	B	767	Z98	CB-CG-ND	3.42	119.29	110.92
5	B	1801	B12	C47-C12-C11	3.39	122.27	110.08
4	D	767	Z98	CG-CB-CA	3.36	121.16	112.72
5	C	1801	B12	C9-C10-C11	-3.31	121.19	125.97
4	A	767	Z98	CB-CG-ND	3.29	118.98	110.92
5	B	1801	B12	C19-C1-N21	3.29	105.54	102.16
5	C	1801	B12	C13-C14-N23	3.27	113.55	109.10
5	C	1801	B12	C18-C60-C61	-3.26	105.84	113.97
5	C	1801	B12	C2P-C1P-N59	-3.23	108.17	112.93
4	A	767	Z98	C5-C6-N1	-3.22	118.46	123.82
5	C	1801	B12	C30-C3-C2	-3.16	112.41	119.09
5	C	1801	B12	C25-C2-C1	-3.14	109.05	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1801	B12	C55-C17-C16	-3.02	110.69	116.65
5	C	1801	B12	C47-C12-C11	2.90	120.52	110.08
4	A	767	Z98	OXT-C-CA	-2.82	112.18	122.14
5	B	1801	B12	C12-C13-C14	2.79	106.93	102.26
4	C	767	Z98	CB-CA-N	2.76	117.41	110.17
4	B	767	Z98	C5-C6-N1	-2.71	119.31	123.82
5	B	1801	B12	C18-C17-C16	2.70	103.95	100.67
3	D	1500	5AD	O2'-C2'-C1'	2.69	120.79	110.85
5	B	1801	B12	O6R-C1R-C2R	-2.69	103.00	106.93
5	C	1801	B12	C18-C17-C16	2.68	103.93	100.67
4	D	767	Z98	CB-CA-N	2.60	116.98	110.17
4	A	767	Z98	C5-C4-C4A	-2.57	117.33	121.56
5	C	1801	B12	C20-C1-C2	-2.56	109.01	113.28
3	D	1500	5AD	O4'-C4'-C5'	2.55	122.78	110.29
4	C	767	Z98	C2A-C2-N1	2.53	122.62	117.67
4	D	767	Z98	C4-C4A-ND	-2.52	112.72	124.31
5	C	1801	B12	C20-C1-N21	-2.52	106.13	110.27
3	D	1500	5AD	C3'-C2'-C1'	2.52	104.77	100.98
5	B	1801	B12	C13-C14-N23	2.50	112.51	109.10
5	B	1801	B12	C30-C3-C2	-2.49	113.83	119.09
4	D	767	Z98	OP4-P-OP2	2.45	113.33	106.47
4	C	767	Z98	C3-C4-C4A	-2.43	115.89	120.41
5	B	1801	B12	C7-C6-N22	2.39	112.31	107.94
5	B	1801	B12	C3R-C2R-C1R	2.39	105.19	99.89
3	D	1500	5AD	O3'-C3'-C2'	2.37	119.49	111.82
4	B	767	Z98	CG-ND-C4A	-2.31	111.82	118.90
5	B	1801	B12	C54-C17-C18	-2.30	109.58	112.98
5	C	1801	B12	C7-C6-N22	2.29	112.12	107.94
5	C	1801	B12	C55-C56-C57	-2.27	106.28	111.23
3	A	1500	5AD	O4'-C4'-C5'	2.23	121.25	110.29
5	B	1801	B12	C46-C12-C11	2.22	118.07	110.08
5	C	1801	B12	C3R-C2R-C1R	2.22	104.80	99.89
4	C	767	Z98	C2A-C2-C3	-2.21	118.16	120.89
5	C	1801	B12	C2-C26-C27	-2.21	109.02	115.22
4	C	767	Z98	C5-C6-N1	-2.20	120.15	123.82
3	A	1500	5AD	O2'-C2'-C1'	2.20	118.97	110.85
4	A	767	Z98	CG-CB-CA	2.19	118.23	112.72
4	D	767	Z98	C3-C4-C5	2.17	119.93	118.26
4	A	767	Z98	OP3-P-OP4	2.17	112.51	106.73
4	B	767	Z98	O-C-OXT	-2.17	119.17	124.09
4	A	767	Z98	C2A-C2-C3	-2.16	118.22	120.89
5	C	1801	B12	C7-C6-C5	-2.15	124.68	128.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	767	Z98	CB-CG-ND	2.14	116.16	110.92
3	A	1500	5AD	C3'-C2'-C1'	2.12	104.17	100.98
5	B	1801	B12	C7-C6-C5	-2.12	124.74	128.07
4	C	767	Z98	OP4-P-OP2	2.11	112.39	106.47
5	B	1801	B12	C18-C60-C61	-2.09	108.76	113.97
5	C	1801	B12	C54-C17-C18	-2.08	109.91	112.98
4	A	767	Z98	C2A-C2-N1	2.04	121.65	117.67
5	C	1801	B12	C15-C14-N23	-2.02	123.79	126.26
4	C	767	Z98	CG-CB-CA	2.02	117.79	112.72
4	A	767	Z98	C6-C5-C4	2.01	121.84	118.15

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1801	B12	C19
5	C	1801	B12	C19

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	767	Z98	C5A-OP4-P-OP1
4	A	767	Z98	C5A-OP4-P-OP3
4	A	767	Z98	C4-C4A-ND-CG
4	B	767	Z98	C5A-OP4-P-OP1
4	B	767	Z98	C5A-OP4-P-OP2
4	B	767	Z98	C5A-OP4-P-OP3
4	B	767	Z98	N-CA-CB-CG
4	B	767	Z98	C4-C4A-ND-CG
4	C	767	Z98	C5A-OP4-P-OP1
4	C	767	Z98	C5A-OP4-P-OP3
4	C	767	Z98	C4-C4A-ND-CG
4	D	767	Z98	C-CA-CB-CG
4	D	767	Z98	N-CA-CB-CG
4	D	767	Z98	CA-CB-CG-ND
5	B	1801	B12	C7-C37-C38-O39
5	B	1801	B12	C16-C17-C55-C56
5	C	1801	B12	C16-C17-C55-C56
5	C	1801	B12	C54-C17-C55-C56
5	C	1801	B12	C18-C17-C55-C56
5	C	1801	B12	C56-C57-N59-C1P
5	C	1801	B12	O58-C57-N59-C1P
4	B	767	Z98	CB-CG-ND-C4A

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Mol	Chain	Res	Type	Atoms
5	C	1801	B12	C42-C41-C8-C9
4	D	767	Z98	C4-C4A-ND-CG
5	B	1801	B12	C7-C37-C38-N40
5	C	1801	B12	C14-C13-C48-C49
4	C	767	Z98	O-C-CA-N
4	C	767	Z98	C3-C4-C4A-ND
5	B	1801	B12	C18-C17-C55-C56
5	C	1801	B12	C2-C3-C30-C31
4	A	767	Z98	O-C-CA-CB
4	A	767	Z98	C5A-OP4-P-OP2
4	D	767	Z98	C3-C4-C4A-ND
4	C	767	Z98	OXT-C-CA-N
5	C	1801	B12	C12-C13-C48-C49
5	C	1801	B12	C7-C37-C38-N40
5	C	1801	B12	C4-C3-C30-C31
4	D	767	Z98	OXT-C-CA-CB
4	B	767	Z98	O-C-CA-CB
4	C	767	Z98	CB-CG-ND-C4A
5	C	1801	B12	C7-C37-C38-O39
4	D	767	Z98	O-C-CA-CB
5	B	1801	B12	C19-C18-C60-C61
4	D	767	Z98	C5-C4-C4A-ND
5	C	1801	B12	C17-C18-C60-C61
5	C	1801	B12	C19-C18-C60-C61

There are no ring outliers.

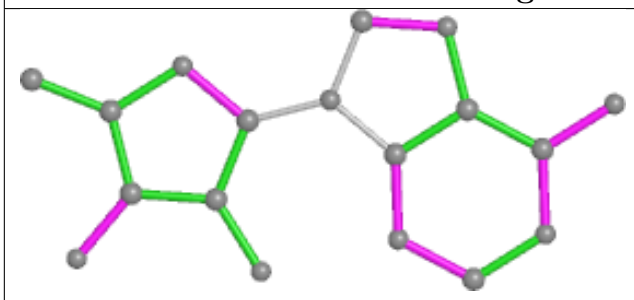
8 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1500	5AD	1	0
5	B	1801	B12	24	0
4	D	767	Z98	3	0
4	A	767	Z98	4	0
5	C	1801	B12	17	0
4	B	767	Z98	4	0
4	C	767	Z98	4	0
3	A	1500	5AD	3	0

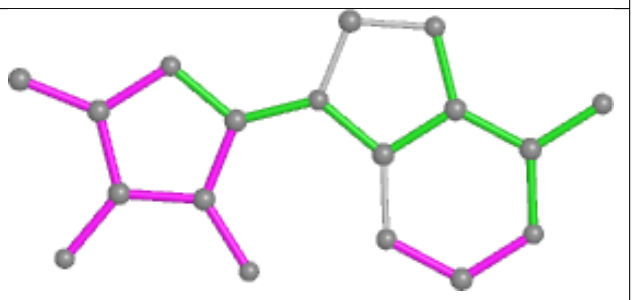
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

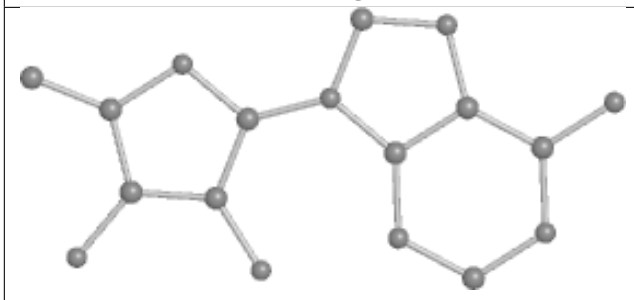
Ligand 5AD D 1500



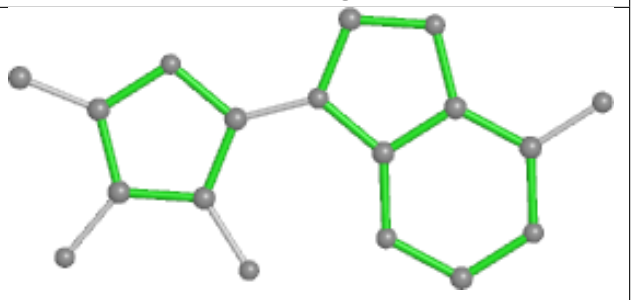
Bond lengths



Bond angles

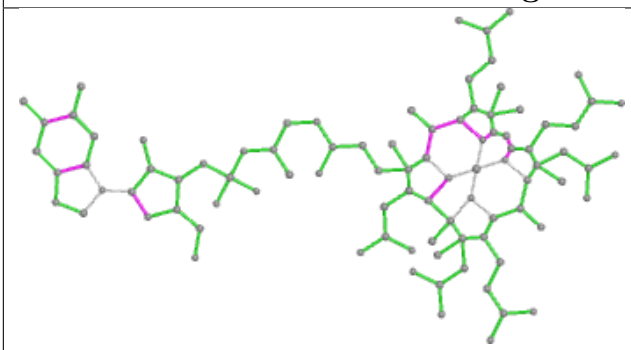


Torsions

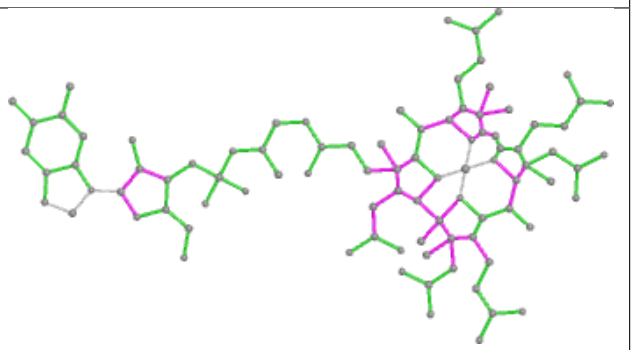


Rings

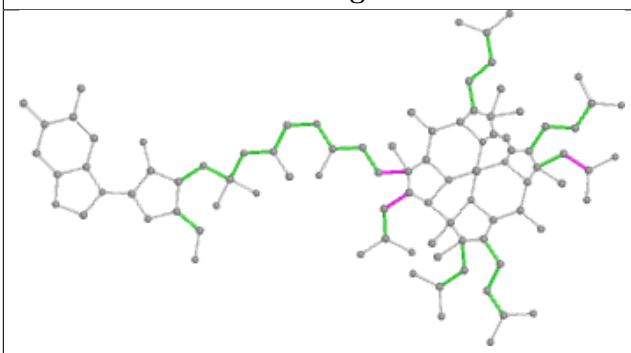
Ligand B12 B 1801



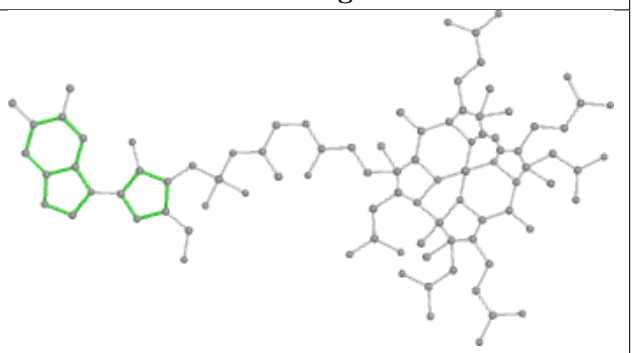
Bond lengths



Bond angles

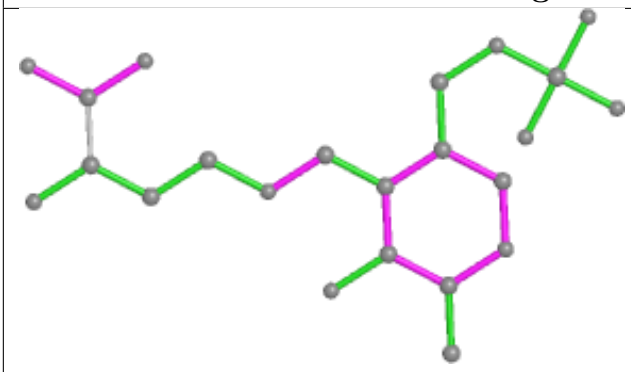


Torsions

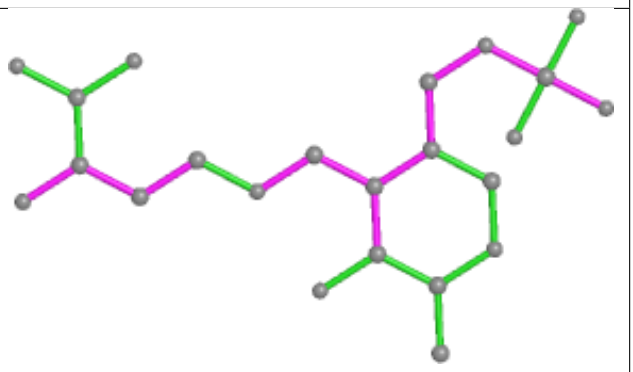


Rings

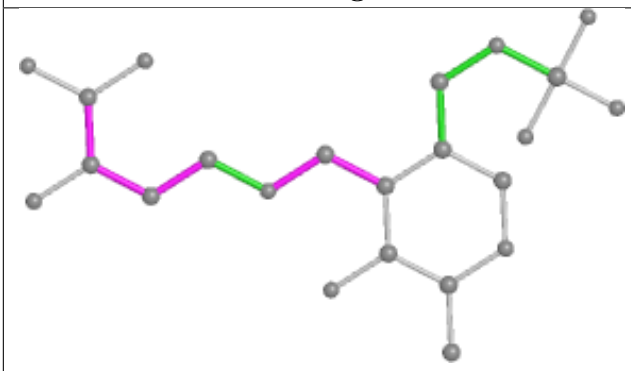
Ligand Z98 D 767



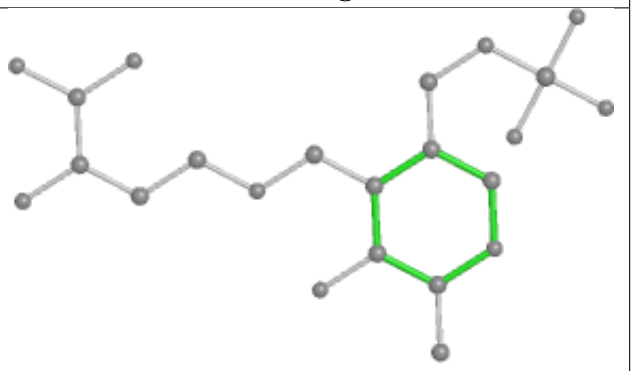
Bond lengths



Bond angles

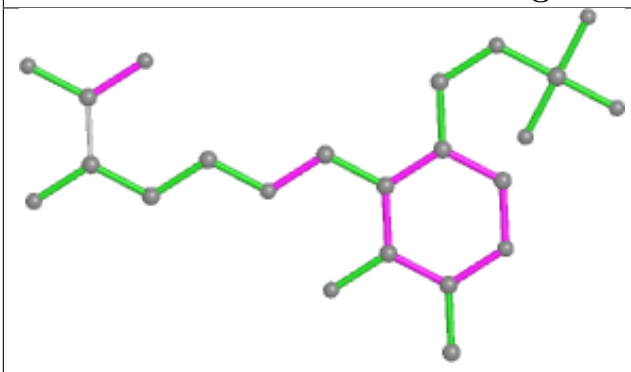


Torsions



Rings

Ligand Z98 A 767



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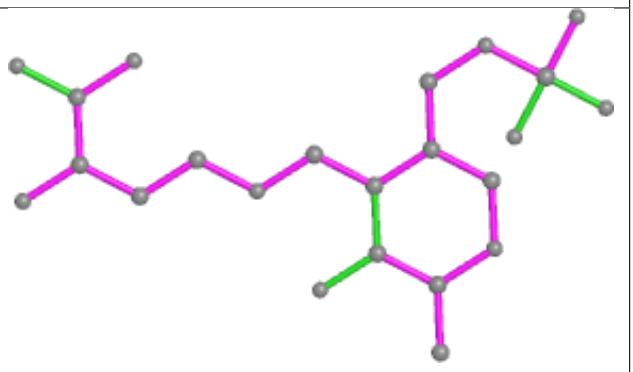

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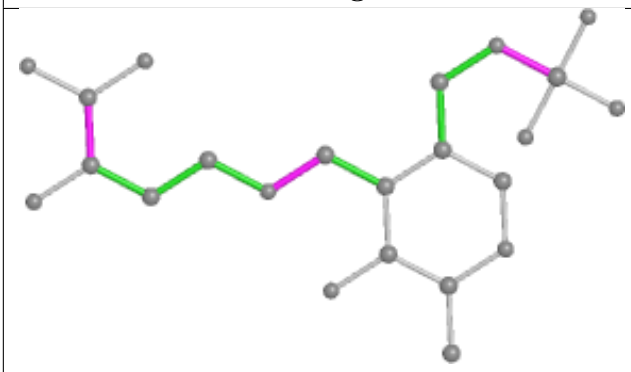

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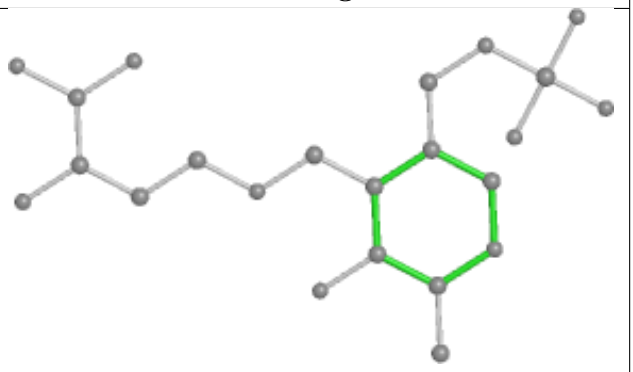
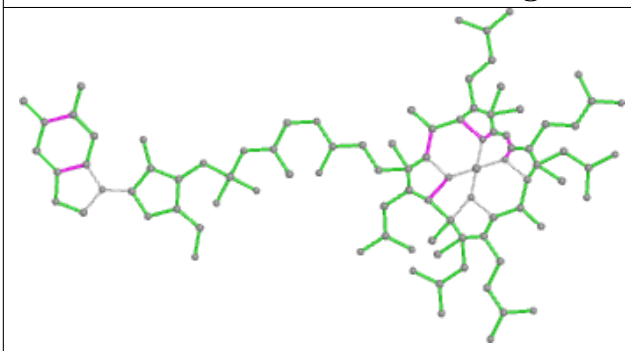


Rings

Ligand B12 C 1801



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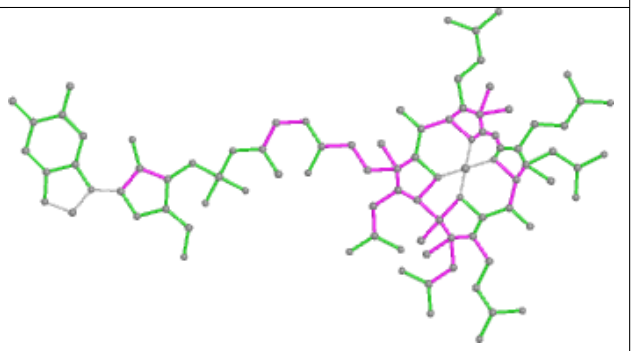
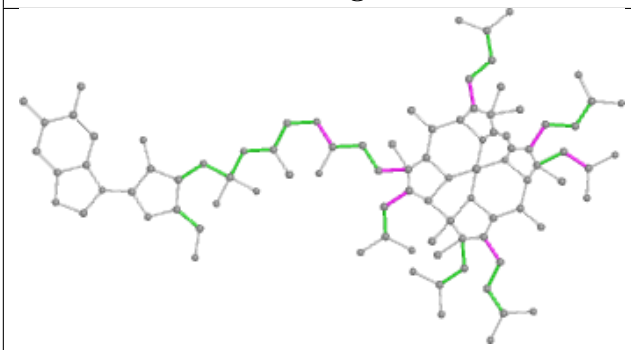


Bond angles



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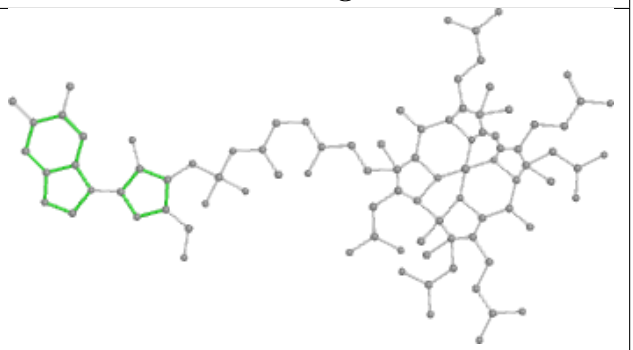
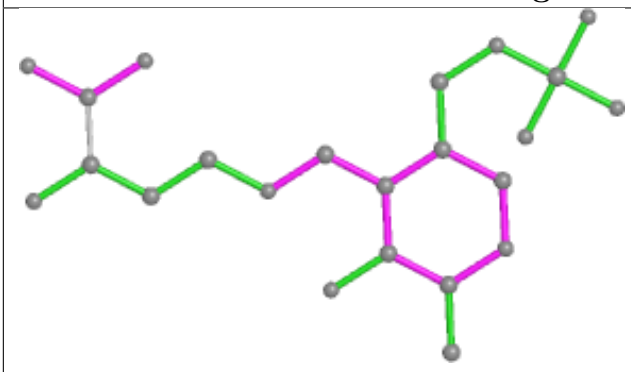


Rings

Ligand Z98 B 767



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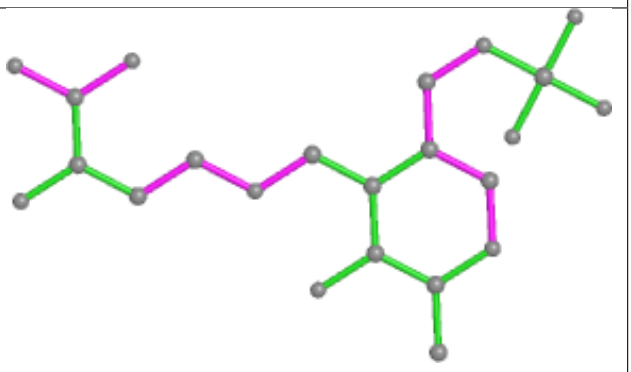
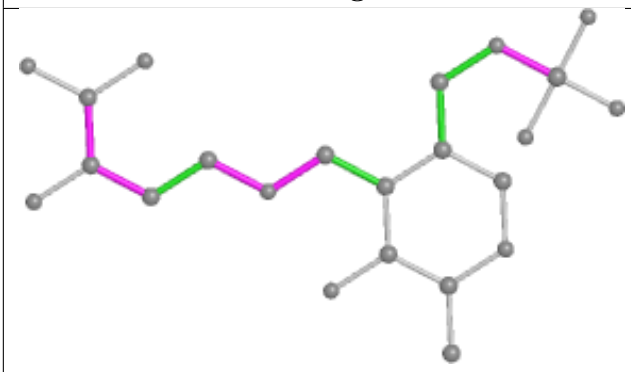
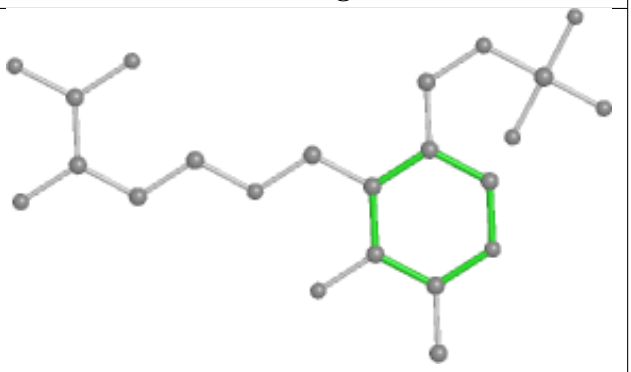


Bond angles

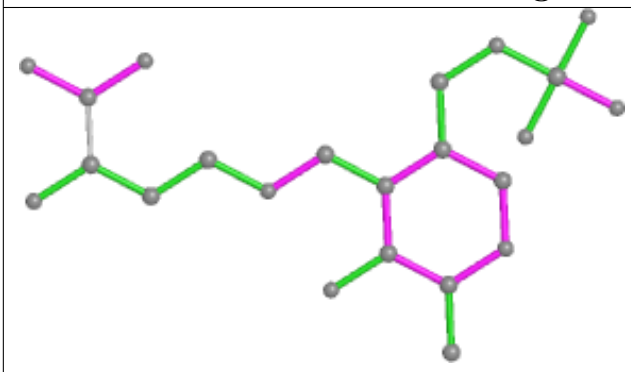


Torsions

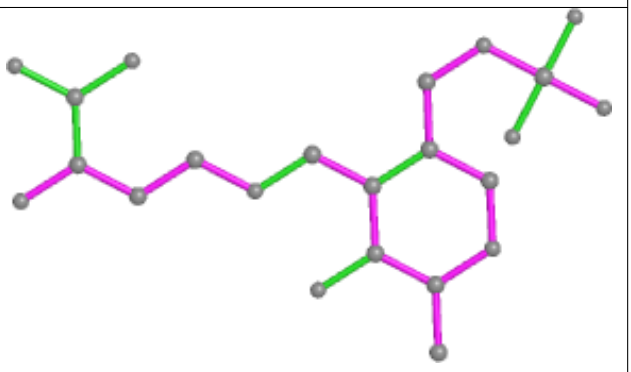


Rings

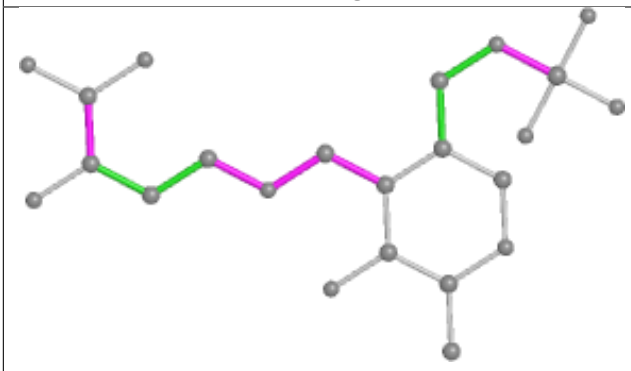
Ligand Z98 C 767



Bond lengths



Bond angles



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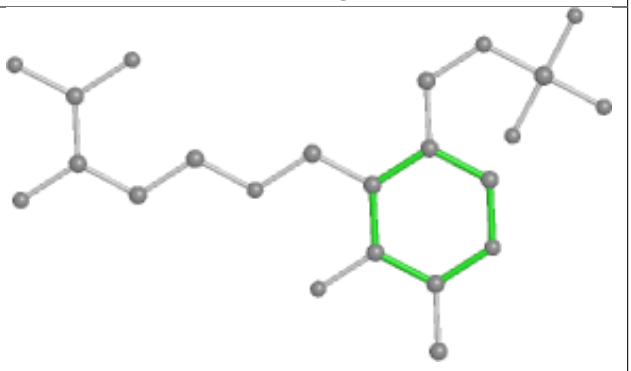
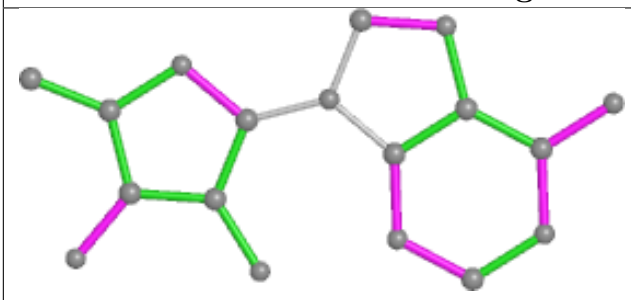
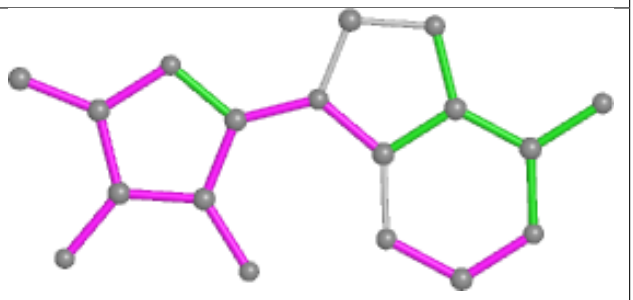


Rings

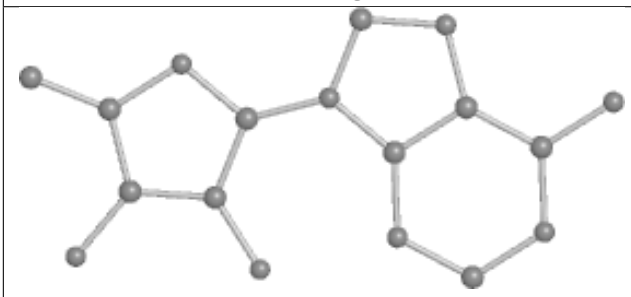
Ligand 5AD A 1500



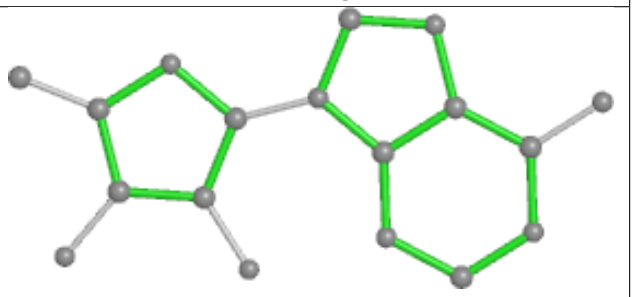
Bond lengths



Bond angles



Torsions



Rings

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	578/763 (75%)	-0.61	2 (0%) 94 93	17, 31, 57, 84	0
1	B	728/763 (95%)	-0.51	2 (0%) 94 93	18, 34, 61, 80	0
1	C	728/763 (95%)	-0.48	4 (0%) 91 88	19, 38, 62, 85	0
1	D	578/763 (75%)	-0.68	0 100 100	15, 27, 51, 74	0
2	E	109/121 (90%)	-0.40	0 100 100	22, 40, 60, 67	0
2	F	109/121 (90%)	-0.34	0 100 100	23, 35, 52, 58	0
2	G	109/121 (90%)	-0.29	1 (0%) 84 80	32, 44, 61, 75	0
2	H	109/121 (90%)	-0.47	0 100 100	21, 34, 56, 74	0
All	All	3048/3536 (86%)	-0.54	9 (0%) 94 93	15, 34, 60, 85	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	492	ASN	2.3
1	A	230	THR	2.3
1	C	112	GLY	2.3
1	C	489	LEU	2.3
1	C	116	TYR	2.2
1	A	587	PRO	2.2
1	B	231	ALA	2.1
2	G	108	TYR	2.1
1	B	116	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

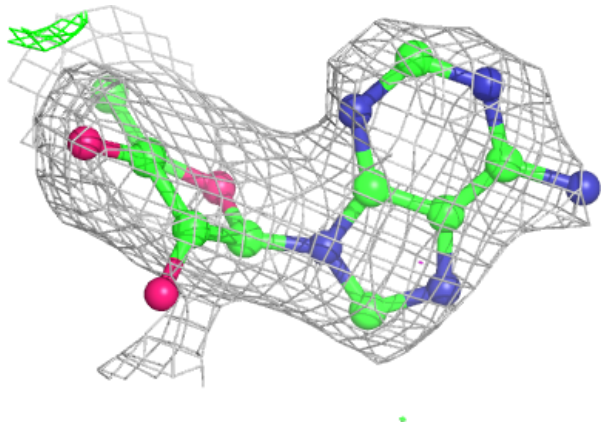
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

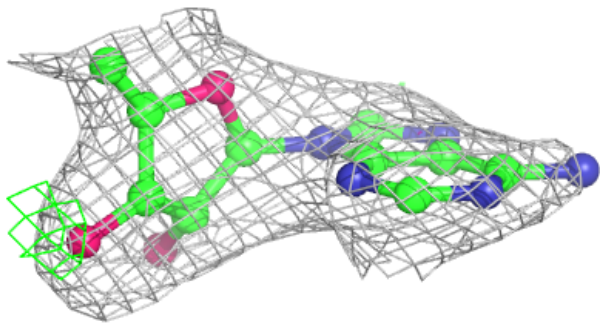
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	5AD	A	1500	18/18	0.93	0.19	34,48,54,57	0
4	Z98	C	767	23/23	0.93	0.20	28,40,48,56	0
3	5AD	D	1500	18/18	0.94	0.15	33,41,46,50	0
4	Z98	A	767	23/23	0.95	0.17	21,30,37,40	0
4	Z98	D	767	23/23	0.96	0.17	22,31,42,44	0
4	Z98	B	767	23/23	0.97	0.18	21,34,38,43	0
5	B12	B	1801	91/91	0.97	0.17	15,37,45,47	0
5	B12	C	1801	91/91	0.97	0.16	22,38,46,51	0

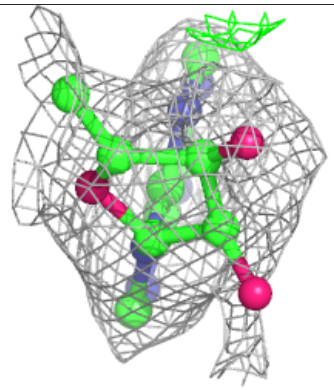
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5AD A 1500:

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

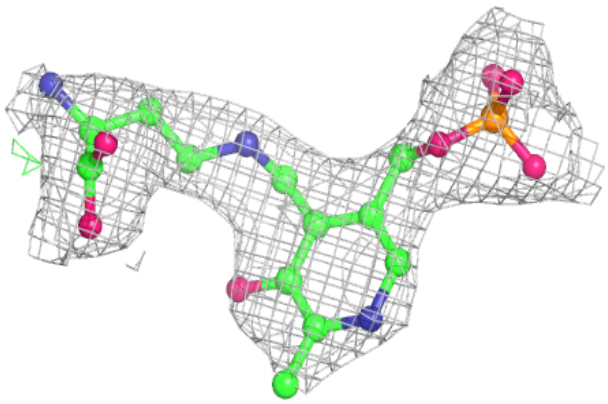


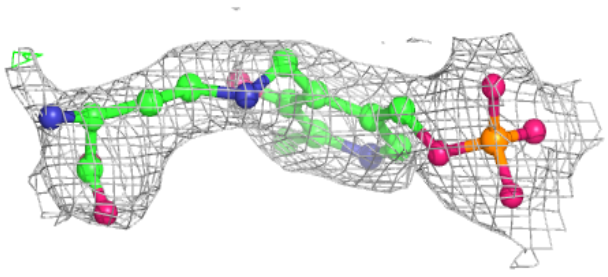


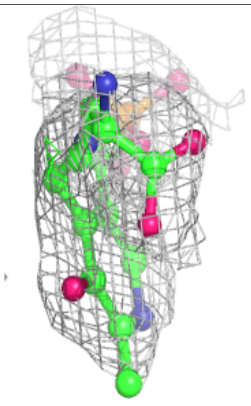


Electron density around Z98 C 767:

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

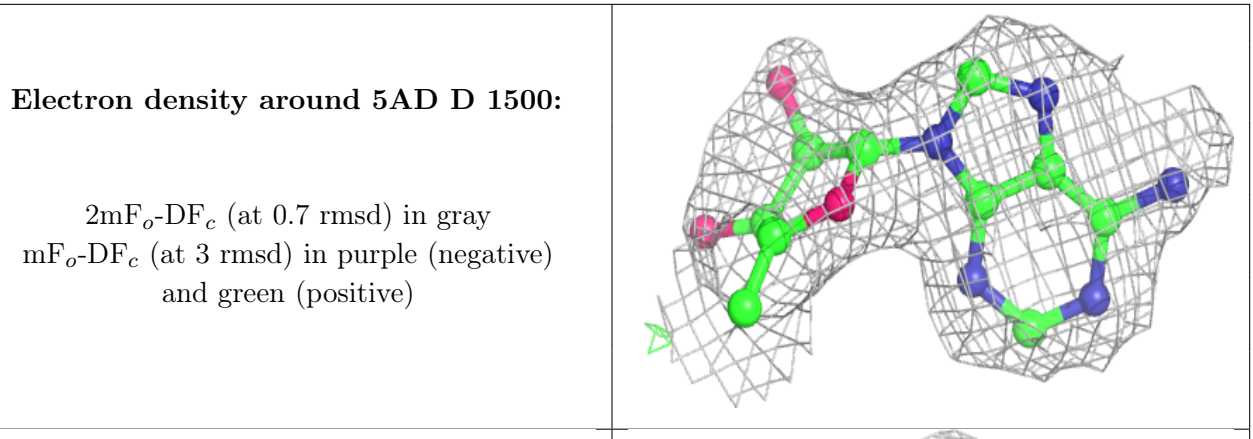






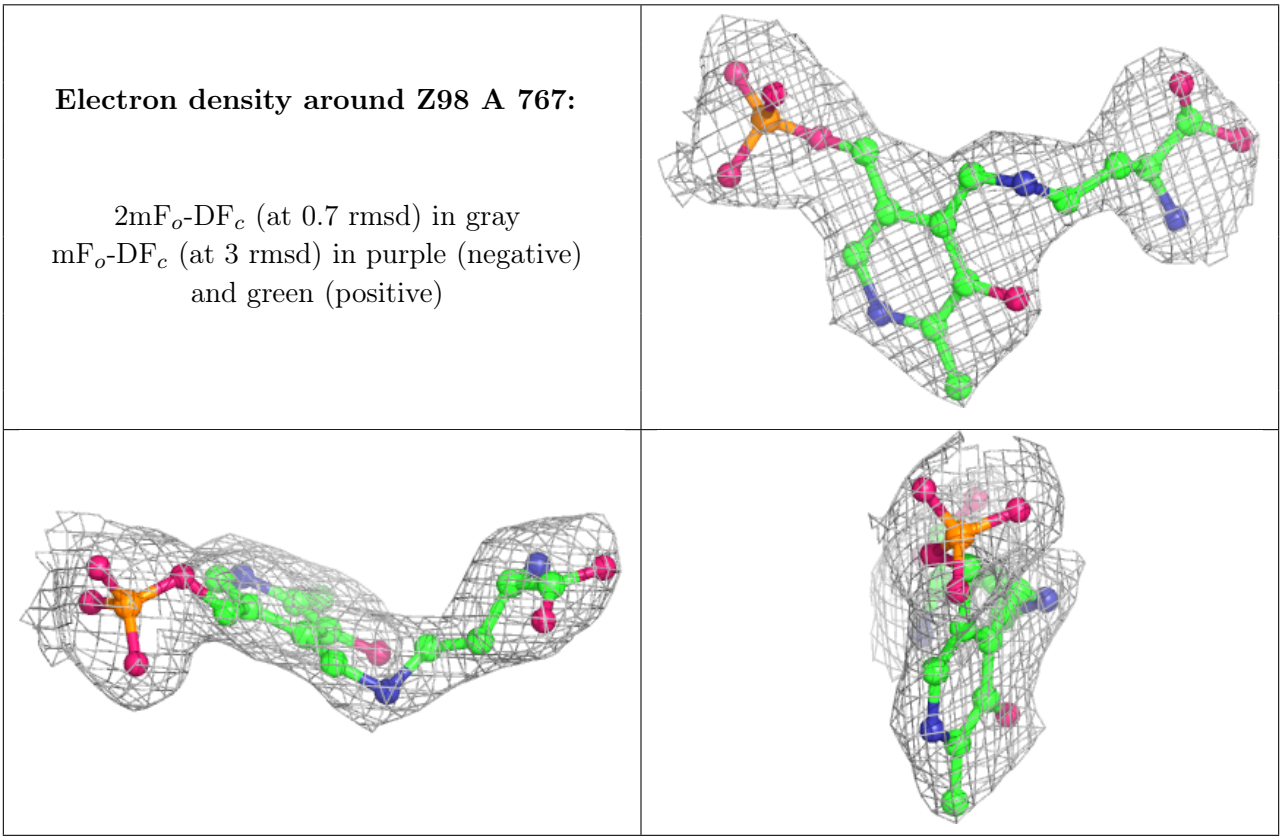
Electron density around 5AD D 1500:

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



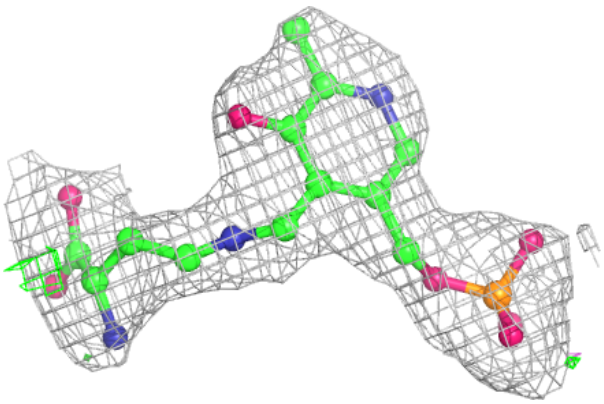
Electron density around Z98 A 767:

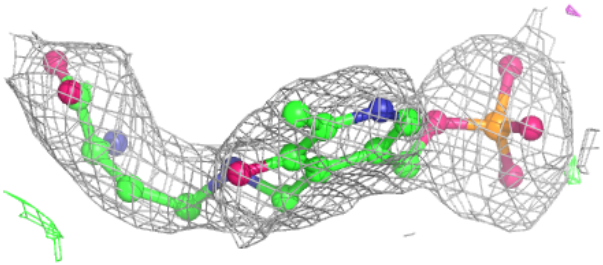
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

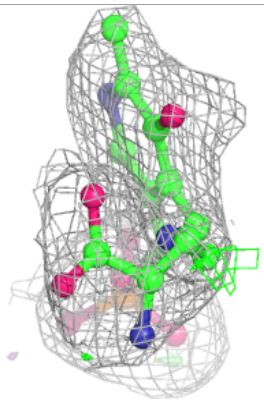


Electron density around Z98 D 767:

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

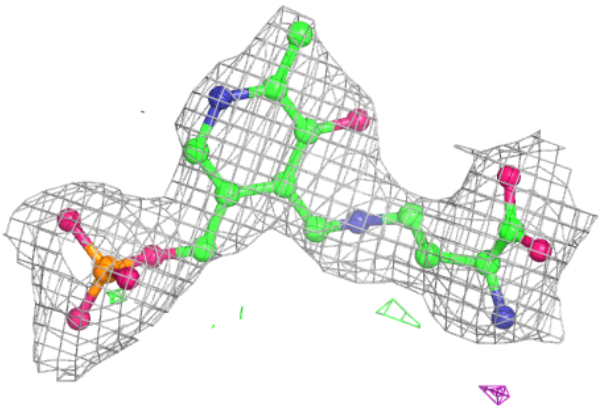


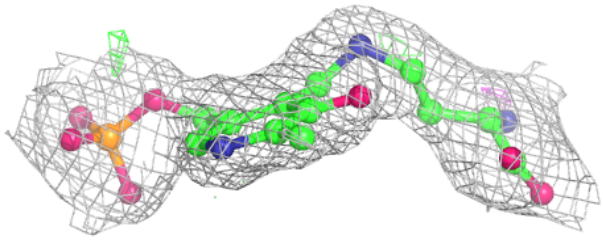


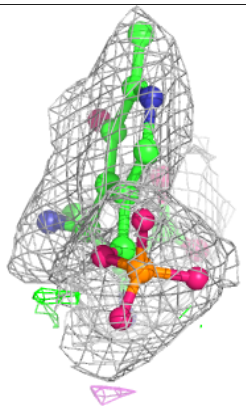


Electron density around Z98 B 767:

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

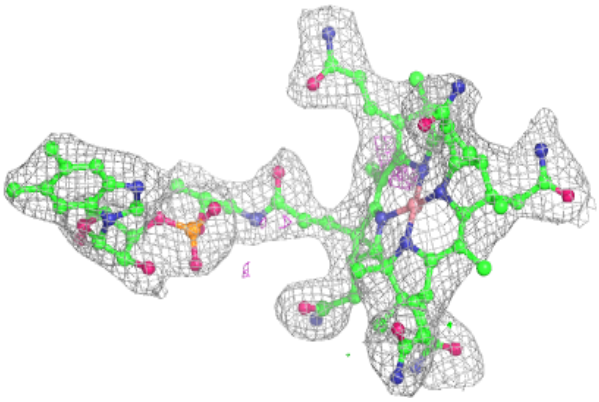


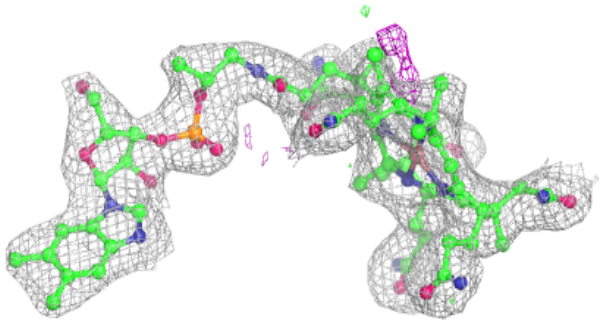


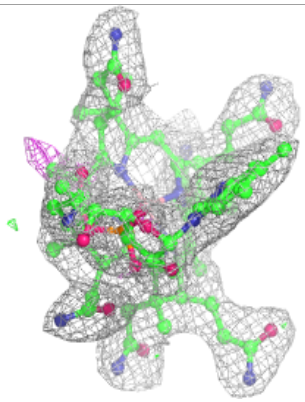


Electron density around B12 B 1801:

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







Electron density around B12 C 1801:

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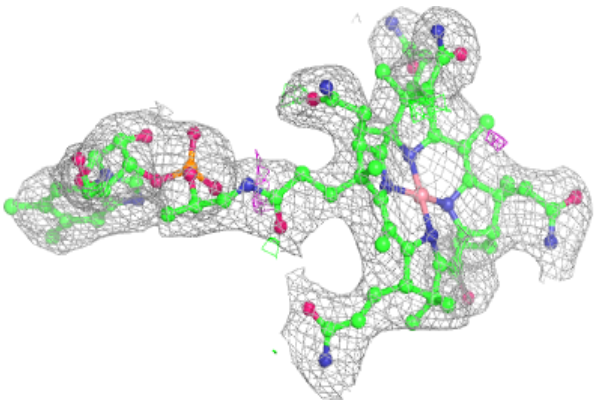
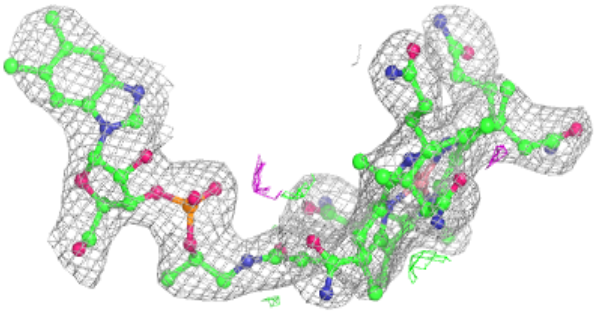
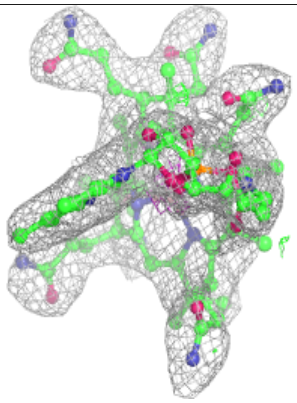
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.