



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 02:32 am BST

PDB ID : 3KOW
Title : Crystal Structure of ornithine 4,5 aminomutase backsoaked complex
Authors : Wolthers, K.R.; Levy, C.W.; Scrutton, N.S.; Leys, D.
Deposited on : 2009-11-14
Resolution : 2.90 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 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 : 2.11
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) : 2.11

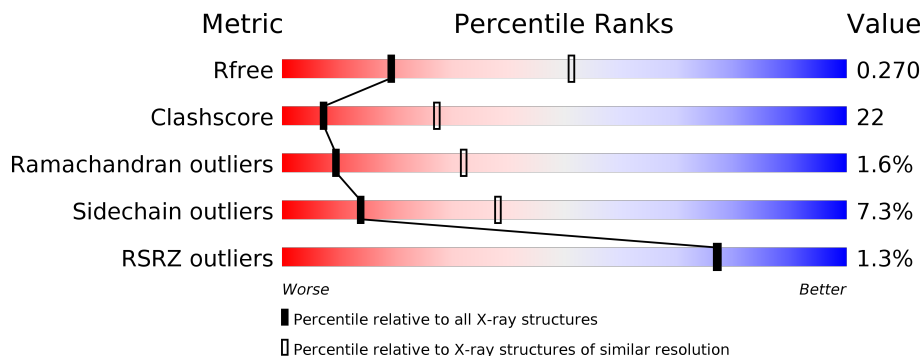
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	763	
1	B	763	
1	C	763	
1	D	763	
2	E	121	
2	F	121	

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Mol	Chain	Length	Quality of chain
2	G	121	
2	H	121	

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
3	B12	A	1801	X	-	X	-
3	B12	B	1801	X	-	X	-
3	B12	C	1801	X	-	X	-
3	B12	D	1801	X	-	-	-
5	5AD	A	1500	X	-	-	-
5	5AD	C	1500	X	-	-	-
5	5AD	D	1500	X	-	-	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 26527 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
			Total	C	N	O	S			
1	A	727	Total 5646	C 3558	N 980	O 1074	S 34	0	0	0
1	B	728	Total 5672	C 3579	N 984	O 1075	S 34	0	0	0
1	C	727	Total 5649	C 3567	N 980	O 1068	S 34	0	0	0
1	D	727	Total 5659	C 3572	N 983	O 1070	S 34	0	0	0

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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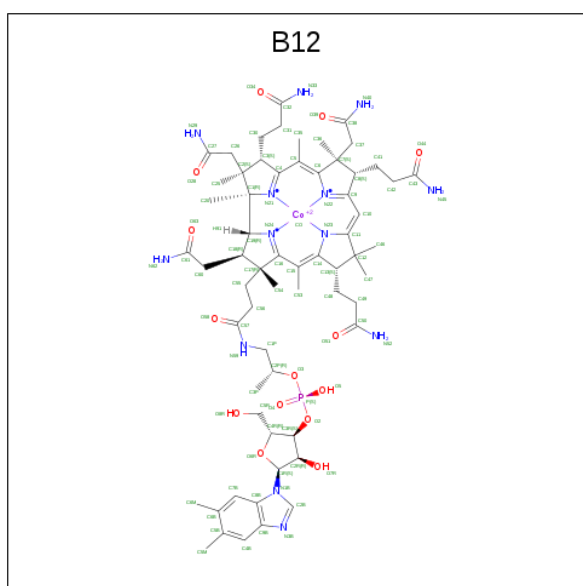
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Chain	Residue	Modelled	Actual	Comment	Reference
C	752	VAL	-	EXPRESSION TAG	UNP Q8VPJ5
C	753	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
C	754	LYS	-	EXPRESSION TAG	UNP Q8VPJ5
C	755	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
C	756	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
C	757	ALA	-	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.

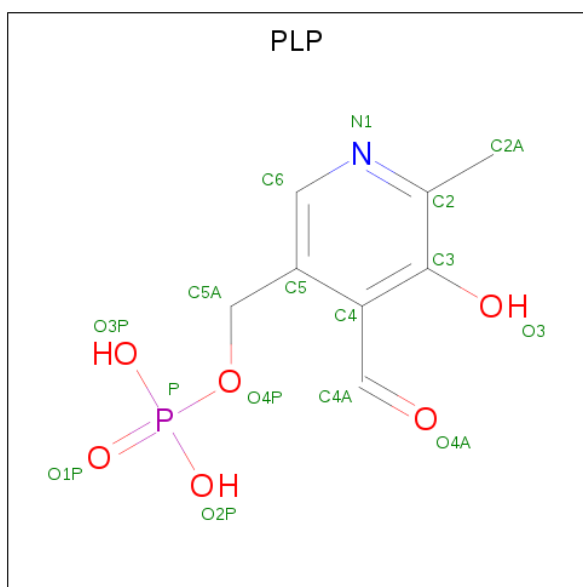
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	109	Total 855	538	152	161	4	0	0	0
2	F	109	Total 858	539	152	163	4	0	0	0
2	G	109	Total 855	538	152	161	4	0	0	0
2	H	109	Total 855	538	152	161	4	0	0	0

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



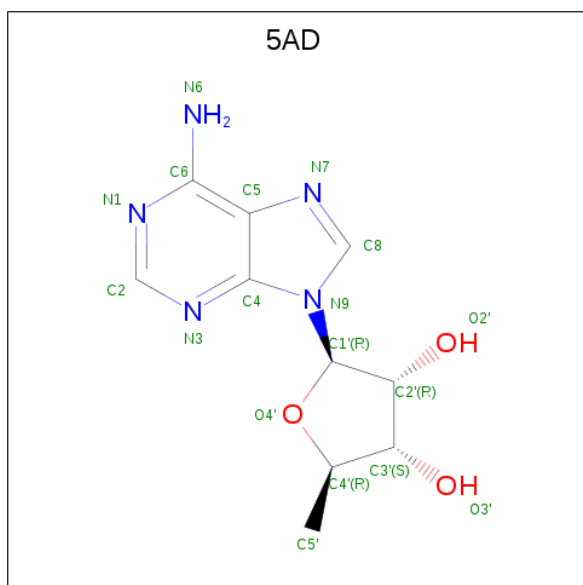
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
3	A	1	Total 91	62	1	13	14	1	0	0
3	B	1	Total 91	62	1	13	14	1	0	0
3	C	1	Total 91	62	1	13	14	1	0	0
3	D	1	Total 91	62	1	13	14	1	0	0

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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

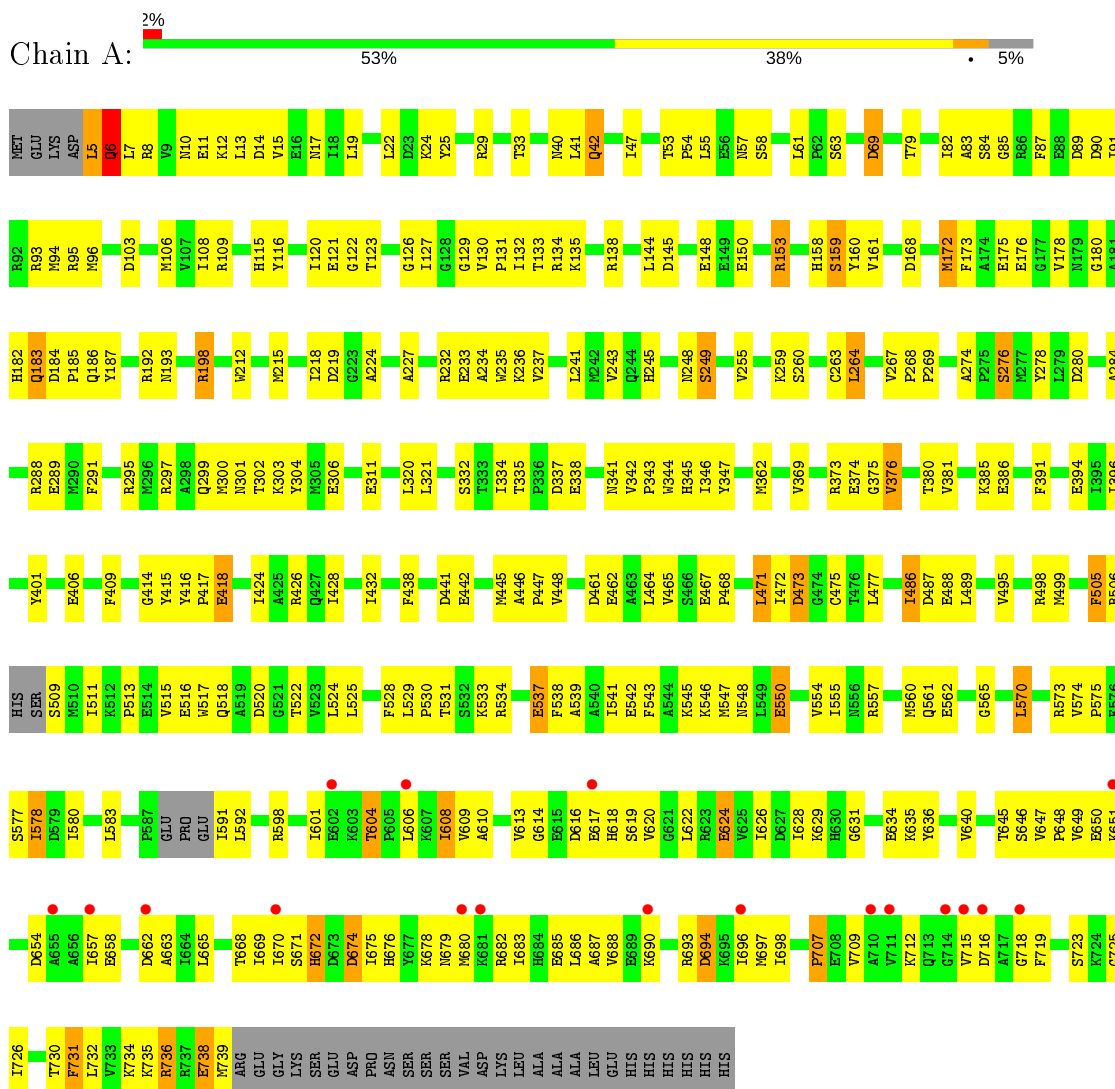


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 18	C 10	N 5	O 3	0	0
5	C	1	Total 18	C 10	N 5	O 3	0	0
5	D	1	Total 18	C 10	N 5	O 3	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



- Molecule 1: D-ornithine aminomutase E component

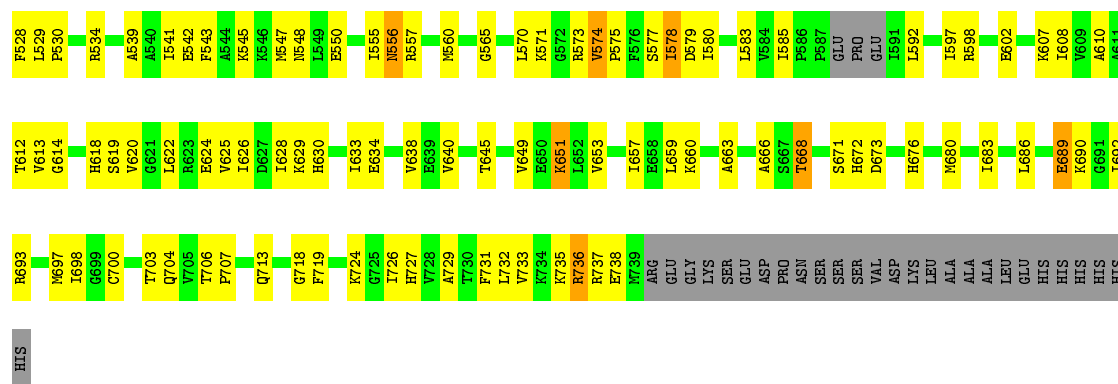


MET	GLU	LYS	ASP	L5	Q6	L7	R8	V9	M10	E11	K12	L13	D14	V15	E16	M17	I18	I19	K20	D21	T26	P27	G31	L41	Q42	M43	G44	P45	F46	D60	T63	P64	L65	S68	K65	Y66	F67	G68	D69	P72	T79	I80	E81	I82	F87	D80	I91	R92																																										
R93	M94	R95	M96	H100	H104	I105	M106	V107	L108	A111	G112	Q113	S114	H115	Y116	I120	E121	G122	T123	P124	I127	P131	I132	T133	L136	V137	R138	L147	R163	P164	S162	D168	M172	F173	E176	G177	V178	M179	G180	A181	H182	I194	M195	R196	R198	E205	S206	K207	T208	I209	A425	M210	K211	A212	M212	Q217	G223	A224	H225	M226	R232	E233	A234	K235	K236	V237	M238	P239	E240	L241	V243	Q244	A246	I250	F251	M257	K258	K259	S260	M261	I262	C263	L264	P269	T270	P273	M277	D280	L281	P282
A286	F291	Y294	M301	M305	E306	A307	R310	E311	A312	T313	G223	A224	H225	M226	R232	E233	A234	K235	K236	V237	M238	P239	E240	L241	V243	Q244	A246	I250	F251	M257	K258	K259	S260	M261	I262	C263	L264	P269	T270	P273	M277	D280	L281	F402																																														
V405	F409	Y415	Y416	P417	I424	R426	E439	R440	D441	T443	D443	Y444	M445	A446	V447	T449	A450	H451	M455	M456	V457	K458	Q459	Y460	V465	S466	E467	P468	S469	L471	G474	C475	T476	L477	V478	V479	P480	E481	K482	I483	D487	F391	M392	L489	M492	D493	M494																																											
E501	R506	HIS	SER	S509	K512	P513	L592	E514	V515	D520	G521	T522	V523	L524	L525	T526	F528	T531	S532	A533	K535	R534	V535	A536	E537	F538	I541	K545	K546	M547	E550	E551	V552	E553	I555	M556	M560	Q561	R382	E363	G565	I568	E569	L570	K571	G572	HIS	V574	P575																																									
F576	S577	I578	P587	GLU	PRO	GLU	I591	R598	K603	D694	L606	K607	L608	V609	A610	A611	T612	D616	A615	S619	V620	F731	L732	R623	E624	I628	K629	E639	V640	H641	Y642	L643	G644	T645	V649	E650	K651	D654	K660	A663	L664	L665	A666	S667	T668																																													
S671	H672	D673	D674	L675	H676	T683	H684	E685	L686	A687	V688	T692	R693	D694	K695	L696	T703	Q704	A710	W715	A729	V730	F731	L732	R733	R736	H740	GLU	GLY	LYS	SER	GLU	ASP	ASN	SER	SER	SER	VAL	ASP	LYS	LEU	ALA	ALA	ALA	LEU	GLU	HIS	HIS																																										
HIS	HIS	HIS																																																																																								

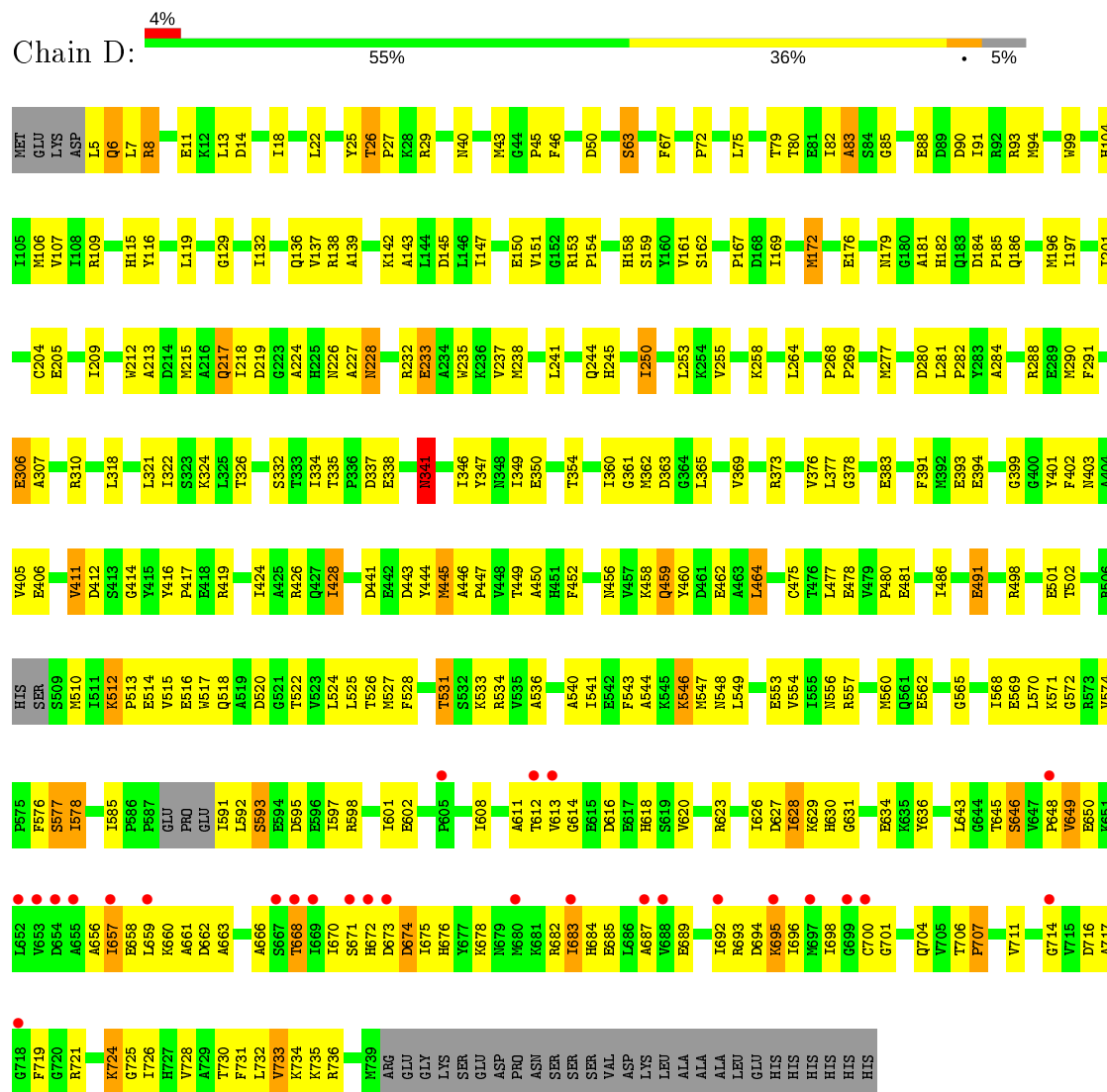
• Molecule 1: D-ornithine aminomutase E component



MET	GLU	LYS	ASP	L5	Q6	L7	R8	V9	M10	E11	K12	L13	D14	V15	E16	M17	I18	I19	K20	D21	T26	P27	K28	R29	R30	E39	M43	Y48	P54	L55	L61	T79	T80	E81	I82	R86	F87	E88	D89	D90	I91	R92	R93	M94	R95	A102	D103	H104	I105	M106	
H107	I108	H109	T110	A111	G112	H113	S114	H115	Y116	L117	I120	E121	T122	M123	H124	Q125	I128	G126	I127	V130	P131	I132	T133	R134	K135	Q136	V137	R138	M43	Q140	D145	L146	I147	R153	Y157	H158	S159	Y160	V161	S162	G163	V164	A165	D168	V171	M172	A181	H182	Q183	D184	P185
M188	V189	M196	I197	L201	C204	K207	T208	I209	W212	M210	Q217	R301	T302	K303	T304	K305	E306	A307	E311	A312	T313	H316	L320	L321	R324	E240	Q244	H245	M248	S249	I250	F251	K254	C263	L264	V267	P268	P269	T270	A271	A274	P275	S276	M277	D280						
T283	A284	V285	A286	L287	R288	E289	F291	R295	M296	Q299	M300	H301	T302	K303	T304	K305	E306	A307	E311	A312	T313	H316	L320	L321	R324	E240	Q244	H245	M248	S249	I250	F251	K254	C263	L264	V267	P268	P269	T270	A271	A274	P275	S276	M277	D280						
G381	M362	V369	Y457	R373	V376	L377	V381	R382	E386	R387	A388	F391	K392	E393	E394	I395	E478	E397	F402	V405	E406	D487	E488	L489	V411	Y416	P417	E418	G423	A425	R426	Y427	I428	M429	G430	G431	L432	G433	K434	A434	G435	V436	Y437	M348	F438	D443	T449	L450	A450	H451	
F452	G453	M456	Y457	R458	Q459	Y460	D461	A463	L464	E467	P468	S469	K470	L471	C475	T476	L477	E478	Y479	K482	Y485	L486	D487	E488	L489	N492	V495	R498	M499	F505	R506	HIS	SER	S509	M510	I511	K512	P513	E514	E514	V515	E516	W517	Q518	G521	L525	T526	M527			

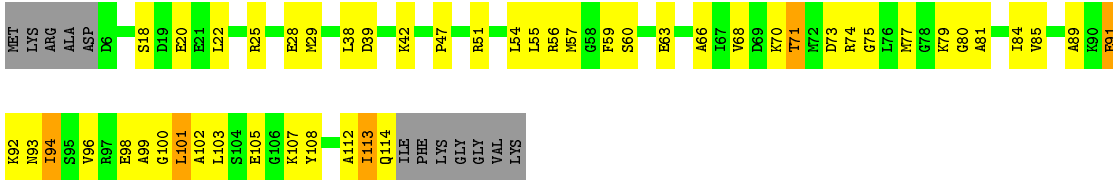


Molecule 1: D-ornithine aminomutase E component

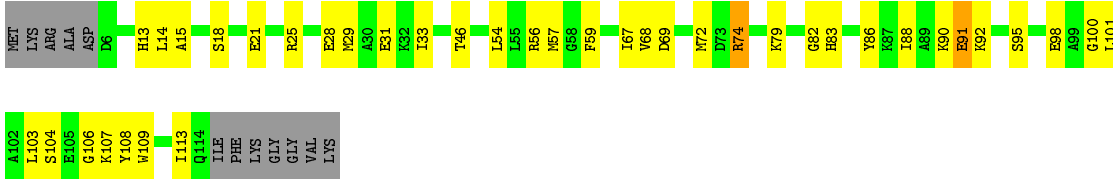


Molecule 2: D-ornithine aminomutase S component

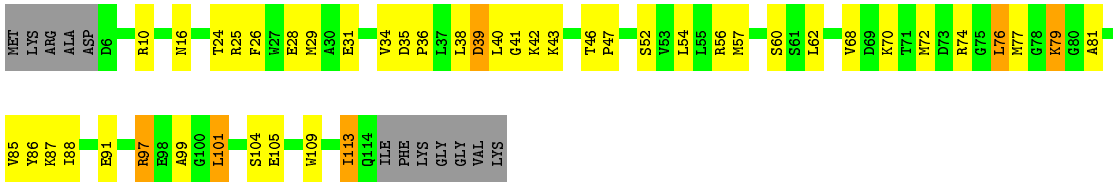




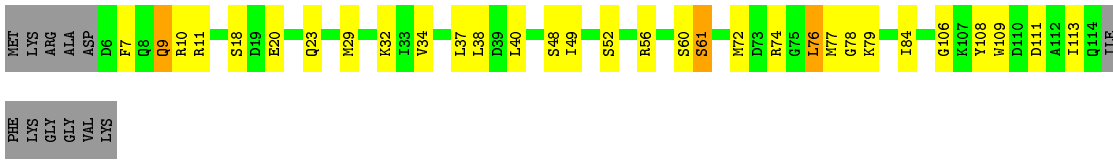
• Molecule 2: D-ornithine aminomutase S component



• Molecule 2: D-ornithine aminomutase S component



• Molecule 2: D-ornithine aminomutase S component



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.18Å 229.01Å 123.92Å 90.00° 102.76° 90.00°	Depositor
Resolution (Å)	120.86 – 2.90 62.21 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (120.86-2.90) 97.9 (62.21-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.191 , 0.279 0.181 , 0.270	Depositor DCC
R_{free} test set	3837 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtrriage
Anisotropy	0.555	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26527	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0/5751	0.60	0/7787
1	B	0.50	0/5777	0.63	0/7818
1	C	0.45	0/5754	0.59	0/7789
1	D	0.48	0/5764	0.62	0/7801
2	E	0.46	0/867	0.58	0/1163
2	F	0.53	0/870	0.64	0/1167
2	G	0.47	0/867	0.56	0/1163
2	H	0.50	0/867	0.60	0/1163
All	All	0.47	0/26517	0.61	0/35851

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5646	0	5580	256	0
1	B	5672	0	5642	242	0
1	C	5649	0	5616	282	0
1	D	5659	0	5632	260	0
2	E	855	0	863	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	858	0	865	38	0
2	G	855	0	863	44	0
2	H	855	0	863	24	0
3	A	91	0	87	25	0
3	B	91	0	87	27	0
3	C	91	0	87	29	0
3	D	91	0	87	18	0
4	A	15	0	6	2	0
4	B	15	0	7	2	0
4	C	15	0	7	0	0
4	D	15	0	6	2	0
5	A	18	0	9	3	0
5	C	18	0	9	2	0
5	D	18	0	10	2	0
All	All	26527	0	26326	1183	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 22.

All (1183) 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)
2:F:74:ARG:HH11	2:F:74:ARG:HG3	0.95	1.08
1:A:82:ILE:HG12	1:A:93:ARG:HD2	1.39	1.05
1:B:528:PHE:HE1	1:B:560:MET:HG3	1.22	1.04
1:A:120:ILE:HG13	1:A:133:THR:HG22	1.48	0.96
2:F:74:ARG:CG	2:F:74:ARG:HH11	1.78	0.95
3:A:1801:B12:O28	3:A:1801:B12:H3	1.66	0.94
1:C:612:THR:HB	1:C:645:THR:HG22	1.49	0.93
2:F:74:ARG:NH1	2:F:74:ARG:HG3	1.77	0.92
5:A:1500:5AD:H5'2	3:C:1801:B12:H261	1.53	0.90
1:A:628:ILE:HG13	1:A:635:LYS:HB2	1.54	0.89
1:C:613:VAL:HG11	1:C:649:VAL:HG22	1.54	0.88
1:D:82:ILE:HG12	1:D:93:ARG:HD2	1.54	0.88
3:B:1801:B12:H601	3:B:1801:B12:H262	1.55	0.87
1:D:491:GLU:HA	1:D:491:GLU:OE2	1.72	0.87
2:E:60:SER:OG	2:E:63:GLU:HG3	1.74	0.87
3:A:1801:B12:H262	3:A:1801:B12:H601	1.56	0.86
1:C:610:ALA:HB1	1:C:622:LEU:HD21	1.57	0.85
1:D:684:HIS:CE1	1:D:693:ARG:HE	1.94	0.85
1:B:528:PHE:CE1	1:B:560:MET:HG3	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ARG:HB3	1:D:8:ARG:CZ	2.05	0.84
1:B:238:MET:CE	1:B:269:PRO:HG2	2.07	0.83
1:D:288:ARG:HG3	1:D:288:ARG:HH11	1.43	0.83
3:D:1801:B12:H351	3:D:1801:B12:H362	1.60	0.83
1:A:123:THR:HG23	1:A:135:LYS:HD3	1.61	0.81
2:F:88:ILE:HG13	2:F:103:LEU:HD11	1.60	0.81
1:A:233:GLU:HB3	1:A:235:TRP:CH2	2.15	0.81
5:A:1500:5AD:H5'3	3:C:1801:B12:C16	2.11	0.81
1:D:526:THR:HG23	1:D:569:GLU:HG2	1.60	0.81
1:D:611:ALA:HB2	1:D:643:LEU:HB2	1.60	0.81
1:C:197:ILE:HG22	1:C:437:VAL:HG21	1.61	0.81
1:D:8:ARG:HB3	1:D:8:ARG:NH1	1.96	0.81
1:A:5:LEU:O	1:A:6:GLN:HB2	1.82	0.80
1:D:592:LEU:HB2	1:D:597:ILE:HD11	1.64	0.80
1:D:161:VAL:HG22	1:D:169:ILE:HG22	1.64	0.80
1:D:132:ILE:HA	1:D:136:GLN:OE1	1.82	0.79
1:C:79:THR:HB	1:C:332:SER:HA	1.65	0.79
3:D:1801:B12:H8	3:D:1801:B12:N40	1.98	0.78
1:D:716:ASP:HB3	1:D:735:LYS:HE2	1.63	0.78
3:B:1801:B12:H552	3:B:1801:B12:H531	1.66	0.78
2:H:20:GLU:H	2:H:20:GLU:CD	1.85	0.78
1:D:406:GLU:OE2	1:D:428:ILE:HG22	1.83	0.78
1:B:534:ARG:HG3	1:B:534:ARG:HH11	1.46	0.78
1:A:218:ILE:HD13	1:A:297:ARG:HD2	1.66	0.78
1:C:264:LEU:HD21	1:C:291:PHE:CD1	2.18	0.77
3:C:1801:B12:H203	3:C:1801:B12:H302	1.63	0.77
1:B:238:MET:HE3	1:B:269:PRO:HG2	1.65	0.77
1:B:116:TYR:CE2	1:B:120:ILE:HD13	2.18	0.77
1:A:83:ALA:HB3	1:A:108:ILE:HD12	1.65	0.76
2:E:47:PRO:O	2:E:51:ARG:HG3	1.84	0.76
1:A:735:LYS:HE3	1:A:739:MET:SD	2.24	0.76
1:C:335:THR:HG21	1:C:343:PRO:HB3	1.67	0.76
1:C:120:ILE:HG13	1:C:133:THR:HG22	1.68	0.76
1:A:269:PRO:HD2	1:A:280:ASP:OD1	1.86	0.76
1:C:344:TRP:CG	1:C:515:VAL:HB	2.21	0.76
1:A:610:ALA:HB1	1:A:622:LEU:HD21	1.68	0.75
1:A:79:THR:HB	1:A:332:SER:HA	1.66	0.75
1:C:13:LEU:HD13	1:C:91:ILE:HG22	1.67	0.75
3:B:1801:B12:H471	3:B:1801:B12:H492	1.68	0.74
1:B:113:GLN:HE22	1:B:132:ILE:HB	1.52	0.74
3:C:1801:B12:H492	3:C:1801:B12:H471	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:HB	1:B:332:SER:HA	1.69	0.74
1:D:269:PRO:HD2	1:D:280:ASP:OD1	1.87	0.74
1:B:82:ILE:HG12	1:B:93:ARG:HD2	1.69	0.73
1:C:668:THR:HG23	1:C:676:HIS:HB2	1.70	0.73
1:C:495:VAL:O	1:C:499:MET:HG2	1.88	0.73
1:C:8:ARG:NH1	1:C:11:GLU:HG3	2.03	0.73
1:C:43:MET:HB2	1:C:48:TYR:CE2	2.24	0.72
1:A:424:ILE:HD11	1:C:628:ILE:HD12	1.69	0.72
1:C:633:ILE:HD12	1:C:638:VAL:HG11	1.72	0.72
3:B:1801:B12:H351	3:B:1801:B12:H362	1.70	0.72
1:A:219:ASP:HB3	1:A:248:ASN:ND2	2.04	0.72
1:A:233:GLU:OE1	1:A:236:LYS:HD2	1.90	0.72
1:B:577:SER:O	1:B:578:ILE:HD12	1.89	0.71
1:D:401:TYR:O	1:D:405:VAL:HG23	1.90	0.71
1:B:259:LYS:HA	1:B:262:ILE:HD12	1.72	0.71
3:A:1801:B12:H8	3:A:1801:B12:N40	2.05	0.71
2:E:20:GLU:H	2:E:20:GLU:CD	1.94	0.71
1:C:324:LYS:HE2	1:C:362:MET:O	1.91	0.71
1:B:623:ARG:HD3	1:D:115:HIS:CE1	2.26	0.71
1:C:607:LYS:O	1:C:608:ILE:HD12	1.90	0.70
1:D:334:ILE:HG22	1:D:335:THR:O	1.91	0.70
2:E:25:ARG:HG2	2:E:29:MET:HE2	1.73	0.70
3:C:1801:B12:N40	3:C:1801:B12:H8	2.03	0.70
1:D:597:ILE:HG23	1:D:733:VAL:HG11	1.73	0.70
1:B:172:MET:HE2	1:B:172:MET:C	2.12	0.70
1:C:5:LEU:HG	1:C:6:GLN:HB2	1.74	0.70
1:D:704:GLN:HE22	1:D:721:ARG:HH21	1.40	0.70
1:C:207:LYS:HE3	1:C:251:PHE:HD2	1.56	0.69
1:C:668:THR:CG2	1:C:676:HIS:HB2	2.22	0.69
1:D:528:PHE:HE1	1:D:560:MET:HG3	1.57	0.69
1:B:259:LYS:HE2	1:B:294:TYR:CE2	2.27	0.69
1:C:86:ARG:HB3	1:C:88:GLU:OE2	1.92	0.69
1:C:79:THR:HG21	1:C:106:MET:HE3	1.74	0.69
3:A:1801:B12:H351	3:A:1801:B12:H362	1.72	0.69
1:A:89:ASP:OD2	1:A:517:TRP:HA	1.92	0.69
1:B:113:GLN:HG3	1:B:116:TYR:CD2	2.27	0.69
1:D:186:GLN:HG2	1:D:401:TYR:OH	1.93	0.69
1:B:668:THR:HG23	1:B:676:HIS:HB2	1.74	0.69
1:C:598:ARG:O	1:C:602:GLU:HB2	1.92	0.69
1:D:531:THR:H	1:D:565:GLY:HA2	1.58	0.69
1:C:201:ILE:HG23	2:G:41:GLY:HA2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ILE:HB	1:A:580:ILE:HD11	1.73	0.68
2:E:25:ARG:HG2	2:E:29:MET:CE	2.23	0.68
1:C:511:ILE:HG13	1:C:580:ILE:HD11	1.75	0.68
1:D:531:THR:HG23	1:D:536:ALA:HB2	1.75	0.68
2:E:99:ALA:O	2:E:102:ALA:HB3	1.92	0.68
1:A:520:ASP:O	1:A:573:ARG:HD2	1.92	0.68
1:C:126:GLY:C	1:C:127:ILE:HD13	2.13	0.68
3:C:1801:B12:O28	3:C:1801:B12:H3	1.93	0.68
1:C:397:GLU:O	1:C:397:GLU:HG2	1.92	0.68
1:D:412:ASP:OD2	1:D:414:GLY:N	2.26	0.68
1:B:607:LYS:O	1:B:608:ILE:HD12	1.94	0.68
3:C:1801:B12:H362	3:C:1801:B12:H351	1.76	0.68
1:C:43:MET:HE2	1:C:54:PRO:HG3	1.74	0.68
3:A:1801:B12:H2B	3:A:1801:B12:O7R	1.94	0.68
1:A:212:TRP:CH2	1:A:477:LEU:HB3	2.28	0.68
1:C:207:LYS:HE3	1:C:251:PHE:CD2	2.29	0.68
1:B:552:VAL:HG13	1:B:570:LEU:HD23	1.75	0.67
1:D:673:ASP:O	1:D:674:ASP:HB2	1.94	0.67
1:B:238:MET:HE2	1:B:269:PRO:HG2	1.76	0.67
2:E:91:GLU:HB3	2:E:92:LYS:HD3	1.75	0.67
1:A:234:ALA:O	1:A:237:VAL:HG12	1.94	0.67
1:C:393:GLU:HG3	2:G:29:MET:SD	2.34	0.67
1:A:267:VAL:HG22	1:A:299:GLN:HB3	1.74	0.67
1:C:95:ARG:HA	1:C:147:ILE:HD13	1.77	0.66
2:G:70:LYS:O	2:G:74:ARG:HG2	1.94	0.66
1:D:445:MET:HE2	1:D:446:ALA:C	2.16	0.66
1:D:22:LEU:HD11	1:D:139:ALA:HB2	1.77	0.66
2:F:69:ASP:HA	2:F:72:MET:HE2	1.77	0.66
1:C:232:ARG:HA	1:C:232:ARG:HH11	1.61	0.66
1:C:43:MET:HB2	1:C:48:TYR:HE2	1.60	0.66
1:D:227:ALA:HB3	1:D:241:LEU:HD21	1.77	0.66
1:A:391:PHE:HD1	1:A:416:TYR:CD1	2.14	0.66
1:B:686:LEU:HD23	1:B:686:LEU:O	1.95	0.66
1:B:514:GLU:HA	1:B:520:ASP:OD1	1.96	0.66
1:C:525:LEU:HD23	1:C:570:LEU:HD13	1.77	0.66
1:B:612:THR:HG22	1:B:616:ASP:HB3	1.77	0.65
1:B:671:SER:OG	1:B:704:GLN:HG3	1.95	0.65
1:A:604:THR:HB	1:A:736:ARG:NH1	2.11	0.65
1:D:668:THR:HG23	1:D:676:HIS:HB2	1.78	0.65
1:C:254:LYS:HB2	2:G:38:LEU:HD11	1.79	0.65
1:A:289:GLU:CD	1:A:373:ARG:HH21	2.00	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:PHE:CE1	1:D:560:MET:HG3	2.30	0.65
1:A:608:ILE:HD11	1:A:663:ALA:HB3	1.77	0.65
1:C:460:TYR:CE1	2:G:86:TYR:HE2	2.13	0.65
3:B:1801:B12:C60	3:B:1801:B12:H262	2.26	0.64
1:B:41:LEU:HD21	1:B:54:PRO:HG3	1.79	0.64
2:F:67:ILE:HG13	2:F:104:SER:HB3	1.78	0.64
1:C:161:VAL:HG23	1:C:181:ALA:HB1	1.79	0.64
1:A:109:ARG:O	1:A:129:GLY:HA3	1.96	0.64
1:B:161:VAL:HG23	1:B:181:ALA:HB1	1.79	0.64
2:F:54:LEU:HD23	2:F:57:MET:CE	2.28	0.64
1:A:698:ILE:O	1:A:716:ASP:HB2	1.98	0.64
1:D:510:MET:HE3	1:D:577:SER:HB2	1.79	0.64
1:C:250:ILE:HG23	2:G:34:VAL:HG21	1.79	0.64
1:B:50:ASP:HB2	1:B:363:ASP:OD1	1.98	0.64
1:A:126:GLY:C	1:A:127:ILE:HD13	2.19	0.64
3:A:1801:B12:O7R	3:A:1801:B12:C2B	2.46	0.64
1:D:104:HIS:HE2	1:D:158:HIS:CG	2.15	0.64
2:G:52:SER:OG	2:G:56:ARG:NH2	2.29	0.64
1:B:534:ARG:HG3	1:B:534:ARG:NH1	2.13	0.64
1:D:648:PRO:C	1:D:650:GLU:H	2.00	0.64
1:A:610:ALA:HA	1:A:665:LEU:O	1.99	0.63
1:B:537:GLU:HG3	1:B:554:VAL:HG21	1.79	0.63
1:D:132:ILE:HG22	1:D:132:ILE:O	1.97	0.63
1:C:228:ASN:O	1:C:303:LYS:HD2	1.98	0.63
1:C:277:MET:CE	1:C:321:LEU:HD23	2.28	0.63
1:A:243:VAL:HG21	1:A:391:PHE:CD2	2.32	0.63
1:B:217:GLN:O	1:B:263:CYS:HB2	1.97	0.63
1:B:233:GLU:HG2	1:B:235:TRP:CH2	2.33	0.63
1:B:607:LYS:HE2	1:B:639:GLU:OE2	1.98	0.63
2:G:88:ILE:HG22	2:G:99:ALA:HB1	1.80	0.63
1:B:168:ASP:N	1:B:168:ASP:OD2	2.32	0.63
1:C:443:ASP:OD2	2:G:79:LYS:HE3	1.99	0.63
1:A:245:HIS:O	1:A:249:SER:HB2	1.99	0.62
1:B:552:VAL:CG1	1:B:570:LEU:HD23	2.29	0.62
1:B:668:THR:O	1:B:668:THR:CG2	2.47	0.62
2:H:18:SER:HB2	2:H:20:GLU:OE1	1.99	0.62
1:A:264:LEU:N	1:A:264:LEU:HD12	2.14	0.62
1:B:619:SER:HB3	1:B:645:THR:HG21	1.82	0.62
1:C:541:ILE:HG22	1:C:545:LYS:NZ	2.15	0.62
1:B:205:GLU:O	1:B:209:ILE:HD12	1.99	0.62
1:D:514:GLU:HA	1:D:520:ASP:OD1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:24:THR:O	2:G:28:GLU:HG2	1.99	0.62
1:C:108:ILE:HD12	1:C:108:ILE:H	1.64	0.62
1:C:432:ILE:N	1:C:432:ILE:HD13	2.13	0.62
1:B:264:LEU:HD21	1:B:291:PHE:CD1	2.34	0.62
1:D:238:MET:CE	1:D:269:PRO:HG2	2.29	0.62
1:D:475:CYS:HB2	2:H:56:ARG:O	2.00	0.62
1:C:402:PHE:HB3	1:C:428:ILE:HD12	1.81	0.62
1:B:350:GLU:HG2	1:D:310:ARG:HD3	1.80	0.62
1:A:193:ASN:O	1:A:432:ILE:HG12	1.99	0.62
1:C:456:ASN:ND2	1:C:459:GLN:HE21	1.96	0.62
1:C:649:VAL:O	1:C:653:VAL:HG23	2.00	0.62
1:D:224:ALA:HB3	1:D:245:HIS:CE1	2.34	0.62
1:D:79:THR:HA	1:D:104:HIS:HB3	1.81	0.62
4:A:1802:PLP:H2A2	1:C:182:HIS:HB3	1.80	0.61
1:A:14:ASP:HB3	1:A:17:ASN:HB3	1.81	0.61
1:A:730:THR:O	1:A:734:LYS:HG3	2.00	0.61
1:B:693:ARG:O	1:B:693:ARG:HG3	1.99	0.61
1:D:233:GLU:HB3	1:D:235:TRP:CH2	2.35	0.61
1:A:515:VAL:HG13	1:A:522:THR:HB	1.82	0.61
1:A:415:TYR:N	1:A:418:GLU:OE1	2.33	0.61
3:B:1801:B12:C47	3:B:1801:B12:C49	2.73	0.61
1:A:198:ARG:HH11	1:A:198:ARG:HG3	1.65	0.61
1:C:284:ALA:O	1:C:288:ARG:HD2	2.00	0.61
1:C:555:ILE:HG21	1:C:571:LYS:HG2	1.82	0.61
1:D:5:LEU:HD23	1:D:5:LEU:O	2.00	0.61
2:G:97:ARG:O	2:G:101:LEU:HB2	2.01	0.61
1:A:682:ARG:O	1:A:686:LEU:HB2	1.99	0.61
1:C:133:THR:O	1:C:137:VAL:HG23	2.00	0.61
1:A:172:MET:HE2	1:A:176:GLU:HG3	1.83	0.61
3:B:1801:B12:C16	5:D:1500:5AD:H5'3	2.31	0.60
1:C:219:ASP:HB3	1:C:248:ASN:ND2	2.16	0.60
1:D:277:MET:SD	1:D:322:ILE:HD11	2.40	0.60
1:D:204:CYS:HB3	1:D:452:PHE:CD2	2.36	0.60
2:G:25:ARG:HG2	2:G:29:MET:CE	2.30	0.60
1:A:608:ILE:CD1	1:A:663:ALA:HB3	2.30	0.60
1:C:28:LYS:HE2	1:C:145:ASP:HB3	1.82	0.60
1:B:578:ILE:HD13	1:D:543:PHE:CE1	2.36	0.60
2:F:74:ARG:CG	2:F:74:ARG:NH1	2.47	0.60
1:A:159:SER:HB3	1:A:173:PHE:CZ	2.36	0.60
1:A:528:PHE:CE1	1:A:560:MET:HG3	2.35	0.60
1:A:243:VAL:HG21	1:A:391:PHE:HD2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:VAL:O	1:C:423:GLY:HA2	2.02	0.60
1:D:516:GLU:HG3	1:D:517:TRP:CD1	2.36	0.60
1:A:683:ILE:HG22	1:A:698:ILE:HD13	1.81	0.60
1:B:172:MET:HE2	1:B:173:PHE:HD1	1.66	0.60
3:C:1801:B12:C2B	3:C:1801:B12:O7R	2.49	0.60
1:C:657:ILE:HD11	1:C:692:ILE:HD13	1.82	0.60
1:A:93:ARG:HA	1:A:96:MET:HE2	1.84	0.60
1:B:116:TYR:HE2	1:B:120:ILE:HD13	1.64	0.60
3:D:1801:B12:H422	3:D:1801:B12:H10	1.84	0.60
2:E:80:GLY:O	2:E:84:ILE:HG12	2.01	0.60
1:A:109:ARG:HG2	1:A:132:ILE:CG1	2.31	0.60
1:D:341:ASN:C	1:D:341:ASN:HD22	2.05	0.60
1:B:459:GLN:HG3	1:B:460:TYR:CD2	2.37	0.59
1:B:481:GLU:H	1:B:481:GLU:CD	2.05	0.59
1:B:475:CYS:HB2	2:F:56:ARG:O	2.02	0.59
1:C:555:ILE:O	1:C:556:ASN:HB2	2.02	0.59
1:C:135:LYS:HG3	1:C:485:TYR:OH	2.02	0.59
1:C:335:THR:HG22	1:C:348:ASN:ND2	2.17	0.59
1:A:574:VAL:HG11	1:C:543:PHE:CE1	2.37	0.59
1:D:373:ARG:NH1	1:D:378:GLY:HA2	2.17	0.59
1:C:649:VAL:HG12	1:C:686:LEU:HD12	1.85	0.59
1:D:593:SER:O	1:D:597:ILE:HG12	2.02	0.59
1:B:17:ASN:HA	1:B:20:LYS:HE2	1.83	0.59
1:C:613:VAL:CG1	1:C:649:VAL:HG22	2.31	0.59
1:C:7:LEU:HD12	1:C:146:LEU:HB3	1.84	0.59
1:D:547:MET:O	1:D:548:ASN:HB2	2.02	0.59
1:D:684:HIS:CE1	1:D:693:ARG:NE	2.69	0.59
2:F:107:LYS:O	2:F:108:TYR:HB2	2.02	0.59
1:A:416:TYR:CG	1:A:417:PRO:HA	2.37	0.59
1:B:541:ILE:HD11	1:B:554:VAL:HG23	1.84	0.59
1:D:137:VAL:HG21	1:D:172:MET:HE1	1.84	0.59
1:B:688:VAL:O	1:B:688:VAL:HG13	2.03	0.59
1:D:568:ILE:HG22	1:D:570:LEU:CD1	2.32	0.59
1:A:134:ARG:NH1	1:A:175:GLU:OE2	2.29	0.59
1:B:239:PRO:O	1:B:243:VAL:HG23	2.01	0.59
3:C:1801:B12:H601	3:C:1801:B12:H262	1.84	0.59
3:D:1801:B12:H601	3:D:1801:B12:H252	1.84	0.59
1:D:416:TYR:CD1	1:D:417:PRO:HA	2.38	0.59
1:A:264:LEU:HD21	1:A:291:PHE:CD1	2.38	0.59
1:C:732:LEU:O	1:C:736:ARG:HB3	2.03	0.59
3:D:1801:B12:C35	3:D:1801:B12:H362	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:THR:HG22	1:B:450:ALA:N	2.18	0.58
1:C:197:ILE:CG2	1:C:437:VAL:HG21	2.32	0.58
1:D:233:GLU:HB3	1:D:235:TRP:CZ2	2.37	0.58
1:C:82:ILE:O	1:C:82:ILE:HG22	2.02	0.58
1:B:401:TYR:O	1:B:405:VAL:HG23	2.04	0.58
1:D:90:ASP:O	1:D:94:MET:HG3	2.02	0.58
1:A:187:TYR:OH	1:C:629:LYS:HD3	2.04	0.58
3:B:1801:B12:H552	3:B:1801:B12:C53	2.30	0.58
1:D:5:LEU:O	1:D:6:GLN:HB2	2.03	0.58
1:D:719:PHE:CD2	3:D:1801:B12:HM63	2.38	0.58
1:A:161:VAL:O	1:A:161:VAL:CG1	2.50	0.58
1:B:445:MET:HA	1:B:455:ASN:OD1	2.03	0.58
1:C:288:ARG:HD3	1:C:326:THR:HB	1.85	0.58
1:A:55:LEU:HD21	1:A:153:ARG:CZ	2.33	0.58
1:B:207:LYS:NZ	1:B:217:GLN:NE2	2.51	0.58
1:D:668:THR:HG23	1:D:668:THR:O	2.02	0.58
1:D:730:THR:O	1:D:734:LYS:HB2	2.02	0.58
1:C:110:THR:HG22	1:C:131:PRO:HA	1.86	0.58
1:C:267:VAL:HG22	1:C:299:GLN:HB3	1.86	0.58
1:A:675:ILE:HG13	1:A:675:ILE:O	2.03	0.58
2:E:28:GLU:HB2	1:D:40:ASN:ND2	2.19	0.58
1:D:533:LYS:HG3	1:D:534:ARG:N	2.19	0.58
1:D:393:GLU:HG3	2:H:29:MET:SD	2.44	0.58
1:A:237:VAL:HG22	1:A:237:VAL:O	2.04	0.57
1:A:735:LYS:HA	1:A:738:GLU:HB2	1.86	0.57
1:B:172:MET:HE2	1:B:173:PHE:N	2.19	0.57
1:B:281:LEU:HB3	1:B:282:PRO:HD3	1.86	0.57
3:C:1801:B12:C10	3:C:1801:B12:H422	2.33	0.57
1:B:392:MET:HB3	2:F:29:MET:HE3	1.85	0.57
1:B:124:PRO:O	1:B:131:PRO:HG2	2.03	0.57
1:B:668:THR:O	1:B:668:THR:HG23	2.04	0.57
4:A:1802:PLP:O3P	1:C:114:SER:HB2	2.04	0.57
1:C:689:GLU:HG2	1:C:690:LYS:N	2.18	0.57
1:D:724:LYS:HD2	1:D:726:ILE:HG22	1.84	0.57
1:A:396:ILE:HD12	2:E:29:MET:HG2	1.84	0.57
1:A:93:ARG:HA	1:A:96:MET:CE	2.34	0.57
1:B:476:THR:HB	1:B:483:ILE:HG13	1.86	0.57
1:C:550:GLU:HB2	1:C:573:ARG:HB3	1.85	0.57
1:C:697:MET:HG2	1:C:735:LYS:HG2	1.86	0.57
1:D:416:TYR:CG	1:D:417:PRO:HA	2.39	0.57
1:D:574:VAL:HG12	1:D:576:PHE:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:PHE:O	1:A:506:ARG:HB2	2.03	0.57
1:D:288:ARG:CG	1:D:288:ARG:HH11	2.17	0.57
1:D:541:ILE:HD11	1:D:554:VAL:HG23	1.87	0.57
1:D:649:VAL:HG12	1:D:649:VAL:O	2.05	0.57
3:A:1801:B12:H531	3:A:1801:B12:H552	1.85	0.57
1:D:399:GLY:HA3	1:D:403:ASN:HD22	1.69	0.57
1:A:278:TYR:OH	1:A:376:VAL:HG21	2.05	0.57
1:A:547:MET:O	1:A:548:ASN:HB2	2.04	0.57
1:A:620:VAL:HG21	1:C:116:TYR:HE1	1.68	0.57
1:C:109:ARG:HG2	1:C:132:ILE:CG1	2.35	0.57
1:C:486:ILE:CD1	2:G:62:LEU:HD12	2.35	0.57
1:A:302:THR:HG22	1:A:334:ILE:HG21	1.86	0.57
1:A:679:ASN:O	1:A:683:ILE:HG13	2.04	0.57
1:D:648:PRO:O	1:D:650:GLU:N	2.38	0.57
3:A:1801:B12:H261	5:C:1500:5AD:H5'2	1.86	0.57
3:B:1801:B12:H203	3:B:1801:B12:H301	1.86	0.57
1:B:612:THR:HA	1:B:667:SER:HB3	1.87	0.57
3:C:1801:B12:H2B	3:C:1801:B12:O7R	2.03	0.57
1:A:619:SER:HB3	1:A:645:THR:HG21	1.87	0.56
1:D:675:ILE:O	1:D:675:ILE:HG13	2.04	0.56
1:C:109:ARG:HA	1:C:130:VAL:O	2.03	0.56
1:C:134:ARG:HD3	1:C:138:ARG:HH21	1.69	0.56
1:D:269:PRO:HD2	1:D:280:ASP:CG	2.26	0.56
2:H:37:LEU:HA	2:H:40:LEU:HD12	1.86	0.56
1:A:543:PHE:O	1:A:547:MET:HG3	2.06	0.56
1:C:108:ILE:N	1:C:108:ILE:HD12	2.20	0.56
1:C:29:ARG:O	1:C:30:ARG:HG2	2.05	0.56
1:C:358:ALA:O	1:C:362:MET:HG3	2.05	0.56
1:C:479:VAL:HG12	1:C:482:LYS:HG3	1.87	0.56
1:C:578:ILE:HG23	1:C:579:ASP:N	2.19	0.56
1:D:462:GLU:CD	1:D:462:GLU:H	2.08	0.56
2:G:87:LYS:O	2:G:91:GLU:HG2	2.04	0.56
3:B:1801:B12:C47	3:B:1801:B12:H492	2.35	0.56
1:B:211:ALA:HB2	1:B:257:MET:HG2	1.88	0.56
2:E:89:ALA:HA	2:E:94:ILE:HG13	1.87	0.56
3:D:1801:B12:H531	3:D:1801:B12:H543	1.88	0.56
1:B:333:THR:HB	1:B:351:ALA:HB1	1.86	0.56
1:A:426:ARG:HH12	1:C:634:GLU:CD	2.07	0.56
1:A:233:GLU:HB3	1:A:235:TRP:CZ3	2.41	0.56
1:A:300:MET:HE2	1:A:320:LEU:HG	1.88	0.56
1:C:633:ILE:O	1:C:638:VAL:HB	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:54:LEU:HD12	2:F:68:VAL:HG23	1.87	0.56
1:C:613:VAL:HG12	1:C:614:GLY:N	2.20	0.56
1:C:95:ARG:CA	1:C:147:ILE:HD13	2.35	0.56
1:A:391:PHE:CD1	1:A:416:TYR:CD1	2.95	0.55
1:A:6:GLN:CD	1:A:7:LEU:H	2.08	0.55
1:C:204:CYS:HB3	1:C:452:PHE:CD2	2.40	0.55
1:C:212:TRP:CZ2	1:C:477:LEU:HB3	2.41	0.55
1:D:394:GLU:OE2	1:D:416:TYR:HE1	1.90	0.55
2:E:54:LEU:HD23	2:E:57:MET:HE2	1.88	0.55
1:A:95:ARG:NH2	1:A:150:GLU:OE2	2.34	0.55
3:B:1801:B12:H8	3:B:1801:B12:N40	2.21	0.55
1:C:79:THR:HG21	1:C:106:MET:CE	2.36	0.55
3:B:1801:B12:H421	3:B:1801:B12:C10	2.35	0.55
1:B:269:PRO:HD2	1:B:280:ASP:OD1	2.07	0.55
3:C:1801:B12:C49	3:C:1801:B12:C47	2.75	0.55
1:C:267:VAL:CG2	1:C:299:GLN:HB3	2.37	0.55
1:D:613:VAL:HG13	1:D:649:VAL:HG22	1.88	0.55
1:A:438:PHE:CE2	2:E:77:MET:HG3	2.41	0.55
2:F:57:MET:HE1	2:F:82:GLY:HA2	1.89	0.55
1:A:82:ILE:O	1:A:82:ILE:HG22	2.06	0.55
1:B:138:ARG:HE	1:B:176:GLU:CD	2.10	0.55
1:B:286:ALA:HB2	1:B:381:VAL:HG13	1.89	0.55
1:B:541:ILE:O	1:B:545:LYS:HG2	2.07	0.55
1:C:286:ALA:HB2	1:C:381:VAL:HG13	1.86	0.55
1:A:115:HIS:HB2	1:C:620:VAL:HG22	1.89	0.55
3:A:1801:B12:C42	3:A:1801:B12:H363	2.35	0.55
1:B:449:THR:HG22	1:B:450:ALA:H	1.70	0.55
1:C:289:GLU:OE2	1:C:373:ARG:NH2	2.40	0.55
1:D:631:GLY:O	1:D:725:GLY:HA3	2.06	0.55
1:C:626:ILE:HD13	1:C:640:VAL:HG11	1.87	0.55
1:A:448:VAL:HB	2:E:56:ARG:HD2	1.88	0.55
3:A:1801:B12:C35	3:A:1801:B12:H362	2.37	0.55
1:A:573:ARG:HB3	1:A:573:ARG:CZ	2.36	0.55
3:C:1801:B12:H422	3:C:1801:B12:H10	1.89	0.55
2:F:95:SER:OG	2:F:98:GLU:HG2	2.07	0.55
3:A:1801:B12:H351	3:A:1801:B12:H372	1.88	0.55
1:A:525:LEU:HD23	1:A:570:LEU:HD13	1.89	0.55
1:D:205:GLU:O	1:D:209:ILE:HD12	2.07	0.55
1:B:478:GLU:C	1:B:480:PRO:HD3	2.26	0.54
1:C:171:VAL:HG23	1:C:209:ILE:HD12	1.89	0.54
1:D:683:ILE:O	1:D:698:ILE:HD13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:GLU:C	1:B:551:GLU:HG3	2.26	0.54
1:C:240:GLU:OE2	1:C:244:GLN:NE2	2.40	0.54
1:A:628:ILE:O	1:A:628:ILE:HG12	2.05	0.54
1:D:441:ASP:HB2	2:H:78:GLY:O	2.07	0.54
1:A:25:TYR:OH	1:A:145:ASP:OD2	2.21	0.54
1:A:674:ASP:O	1:A:678:LYS:HG3	2.08	0.54
1:C:197:ILE:O	1:C:201:ILE:HG13	2.06	0.54
1:B:115:HIS:CE1	1:D:623:ARG:HD3	2.41	0.54
2:G:74:ARG:CB	2:G:76:LEU:HD22	2.37	0.54
1:A:604:THR:HB	1:A:736:ARG:HH12	1.72	0.54
1:D:119:LEU:HD12	2:H:61:SER:HB3	1.90	0.54
1:B:207:LYS:NZ	1:B:217:GLN:HE22	2.06	0.54
1:D:449:THR:HG22	1:D:450:ALA:N	2.23	0.54
1:C:651:LYS:HB2	1:C:651:LYS:HZ3	1.73	0.54
1:D:394:GLU:OE1	1:D:419:ARG:NH2	2.38	0.54
1:A:369:VAL:HG13	1:C:369:VAL:CG1	2.38	0.53
1:A:406:GLU:OE2	1:A:428:ILE:HG22	2.08	0.53
1:A:5:LEU:O	1:A:6:GLN:CB	2.56	0.53
1:B:444:TYR:HA	2:F:79:LYS:O	2.07	0.53
1:D:591:ILE:HG22	1:D:591:ILE:O	2.08	0.53
2:H:20:GLU:N	2:H:20:GLU:CD	2.59	0.53
1:A:130:VAL:HG12	1:A:131:PRO:O	2.08	0.53
1:B:246:ALA:O	1:B:250:ILE:HG22	2.08	0.53
1:D:394:GLU:OE2	1:D:416:TYR:CE1	2.61	0.53
2:E:107:LYS:O	2:E:108:TYR:HB2	2.07	0.53
1:C:608:ILE:HG13	1:C:663:ALA:HB3	1.90	0.53
1:A:109:ARG:HG2	1:A:132:ILE:HG13	1.88	0.53
1:B:108:ILE:HA	1:B:160:TYR:HE2	1.73	0.53
3:C:1801:B12:H531	3:C:1801:B12:H543	1.90	0.53
1:C:377:LEU:O	1:C:381:VAL:HG23	2.08	0.53
1:D:25:TYR:OH	1:D:145:ASP:OD2	2.26	0.53
1:D:684:HIS:CD2	1:D:714:GLY:HA3	2.44	0.53
2:F:67:ILE:CG1	2:F:104:SER:HB3	2.38	0.53
1:A:186:GLN:HG2	1:A:401:TYR:OH	2.08	0.53
1:A:524:LEU:CD1	1:A:555:ILE:HD11	2.38	0.53
1:B:391:PHE:HA	1:B:416:TYR:CZ	2.44	0.53
1:C:436:THR:O	2:G:47:PRO:HD3	2.09	0.53
4:B:1802:PLP:N1	1:D:162:SER:OG	2.37	0.53
1:A:116:TYR:CE1	1:C:620:VAL:HG21	2.43	0.53
1:C:676:HIS:O	1:C:680:MET:HG3	2.08	0.53
1:D:628:ILE:HG12	1:D:628:ILE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:PHE:HE1	1:A:560:MET:HG3	1.73	0.53
1:A:85:GLY:HA2	1:A:129:GLY:O	2.09	0.53
1:C:302:THR:HG22	1:C:334:ILE:HG13	1.91	0.53
1:A:577:SER:O	1:A:578:ILE:HD12	2.09	0.53
3:C:1801:B12:C31	3:C:1801:B12:H353	2.39	0.53
1:D:264:LEU:HD21	1:D:291:PHE:CD1	2.43	0.53
1:D:512:LYS:HB2	1:D:513:PRO:HD2	1.91	0.53
1:D:79:THR:HB	1:D:332:SER:HA	1.90	0.53
1:C:168:ASP:N	1:C:168:ASP:OD2	2.41	0.52
3:B:1801:B12:H261	5:D:1500:5AD:H5'2	1.90	0.52
1:C:61:LEU:HD13	1:C:357:GLN:HG3	1.91	0.52
1:C:391:PHE:HD1	1:C:416:TYR:CG	2.27	0.52
1:C:578:ILE:CG2	1:C:579:ASP:N	2.72	0.52
4:B:1802:PLP:H2A2	1:D:182:HIS:HB3	1.90	0.52
1:D:228:ASN:OD1	1:D:228:ASN:N	2.42	0.52
2:E:18:SER:HB2	2:E:20:GLU:OE1	2.09	0.52
2:G:25:ARG:HG2	2:G:29:MET:HE1	1.92	0.52
1:A:126:GLY:HA3	1:A:131:PRO:HD3	1.91	0.52
1:A:693:ARG:HG3	1:A:693:ARG:O	2.10	0.52
1:A:161:VAL:HG12	1:A:183:GLN:HG2	1.91	0.52
1:A:284:ALA:O	1:A:288:ARG:HD2	2.08	0.52
1:B:479:VAL:HG12	1:B:482:LYS:HG3	1.92	0.52
1:B:642:TYR:C	1:B:643:LEU:HD23	2.30	0.52
1:B:250:ILE:HD11	2:F:31:GLU:HG2	1.90	0.52
1:B:568:ILE:HG22	1:B:570:LEU:CD1	2.39	0.52
1:D:14:ASP:O	1:D:18:ILE:HG13	2.10	0.52
1:A:650:GLU:HG3	1:A:686:LEU:HD21	1.90	0.52
1:B:445:MET:HE1	1:B:447:PRO:HB3	1.90	0.52
3:A:1801:B12:H531	3:A:1801:B12:H543	1.92	0.52
1:A:626:ILE:HD13	1:A:640:VAL:HG11	1.92	0.52
1:B:445:MET:O	2:F:83:HIS:HB2	2.10	0.52
2:G:35:ASP:N	2:G:36:PRO:HD2	2.25	0.52
1:C:109:ARG:HG2	1:C:132:ILE:HG13	1.91	0.52
1:D:406:GLU:HG2	1:D:426:ARG:O	2.10	0.52
2:G:25:ARG:HG2	2:G:29:MET:HE2	1.92	0.52
1:B:378:GLY:O	1:B:381:VAL:HB	2.09	0.52
1:C:719:PHE:CD2	3:C:1801:B12:HM63	2.45	0.52
1:B:258:LYS:HB2	1:B:261:ASN:HD22	1.75	0.51
3:A:1801:B12:C26	3:A:1801:B12:H601	2.34	0.51
1:D:445:MET:HE2	1:D:447:PRO:N	2.24	0.51
2:F:109:TRP:O	2:F:113:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:PHE:CD2	2:G:77:MET:HG3	2.44	0.51
1:B:620:VAL:HG21	1:D:116:TYR:HE1	1.75	0.51
1:D:456:ASN:ND2	1:D:459:GLN:HG2	2.25	0.51
1:B:111:ALA:HB2	1:B:127:ILE:HG22	1.92	0.51
3:B:1801:B12:H531	3:B:1801:B12:C55	2.33	0.51
1:D:321:LEU:HD13	1:D:362:MET:HE2	1.93	0.51
1:D:491:GLU:OE2	1:D:491:GLU:CA	2.50	0.51
1:D:592:LEU:HB2	1:D:597:ILE:CD1	2.38	0.51
1:C:13:LEU:HD13	1:C:91:ILE:CG2	2.40	0.51
1:D:264:LEU:HD21	1:D:291:PHE:CE1	2.45	0.51
1:D:510:MET:CE	1:D:577:SER:HB2	2.41	0.51
1:A:424:ILE:HG21	1:A:426:ARG:CZ	2.41	0.51
1:B:445:MET:HE1	1:B:447:PRO:CB	2.41	0.51
5:A:1500:5AD:C5'	3:C:1801:B12:C16	2.88	0.51
1:C:93:ARG:HD3	1:C:348:ASN:OD1	2.09	0.51
1:B:207:LYS:HZ3	1:B:217:GLN:NE2	2.09	0.51
1:C:269:PRO:HD2	1:C:280:ASP:OD2	2.11	0.51
1:C:649:VAL:HG12	1:C:686:LEU:CD1	2.40	0.51
1:D:649:VAL:HG13	1:D:683:ILE:CG1	2.41	0.51
1:A:41:LEU:HD12	1:A:42:GLN:N	2.26	0.51
1:A:122:GLY:HA2	1:A:487:ASP:O	2.11	0.51
1:B:478:GLU:O	1:B:480:PRO:HD3	2.11	0.51
1:C:668:THR:CG2	1:C:668:THR:O	2.59	0.51
1:A:198:ARG:NH1	1:A:198:ARG:HG3	2.26	0.51
1:A:224:ALA:HB3	1:A:245:HIS:CE1	2.46	0.51
1:A:541:ILE:HD11	1:A:554:VAL:HG23	1.91	0.51
1:C:13:LEU:CD2	1:C:18:ILE:HD11	2.41	0.51
2:G:68:VAL:O	2:G:72:MET:HE2	2.11	0.51
1:A:345:HIS:CE1	1:A:516:GLU:HA	2.45	0.51
1:A:613:VAL:CG1	1:A:614:GLY:N	2.73	0.51
1:B:172:MET:CE	1:B:173:PHE:HD1	2.24	0.51
1:B:710:ALA:O	1:B:715:VAL:HG22	2.11	0.51
1:B:606:LEU:HD13	1:B:736:ARG:NH2	2.26	0.51
1:C:13:LEU:HD22	1:C:18:ILE:HD11	1.93	0.51
1:C:706:THR:O	1:C:707:PRO:C	2.48	0.51
3:D:1801:B12:H8	3:D:1801:B12:H401	1.75	0.51
1:D:26:THR:HG22	1:D:27:PRO:HD2	1.92	0.51
1:D:568:ILE:HG22	1:D:570:LEU:HD11	1.93	0.51
3:A:1801:B12:C49	3:A:1801:B12:H471	2.40	0.50
1:A:90:ASP:O	1:A:94:MET:HG3	2.11	0.50
1:C:528:PHE:HE1	1:C:560:MET:HG3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:MET:HE3	1:D:72:PRO:HG3	1.92	0.50
1:D:668:THR:CG2	1:D:668:THR:O	2.59	0.50
1:A:193:ASN:HB2	1:A:426:ARG:CZ	2.42	0.50
1:B:223:GLY:O	1:B:226:ASN:HB2	2.11	0.50
1:B:224:ALA:HB3	1:B:245:HIS:CE1	2.46	0.50
1:B:692:ILE:C	1:B:694:ASP:H	2.15	0.50
2:G:54:LEU:HD23	2:G:57:MET:CE	2.41	0.50
1:B:207:LYS:HZ2	1:B:217:GLN:HE22	1.59	0.50
1:B:90:ASP:O	1:B:94:MET:HG3	2.11	0.50
1:D:238:MET:HE2	1:D:269:PRO:HG2	1.91	0.50
2:E:20:GLU:N	2:E:20:GLU:CD	2.64	0.50
1:D:201:ILE:HG22	2:H:49:ILE:HD11	1.93	0.50
1:A:161:VAL:O	1:A:161:VAL:HG12	2.11	0.50
1:B:132:ILE:HA	1:B:136:GLN:OE1	2.11	0.50
1:D:591:ILE:N	1:D:591:ILE:HD12	2.26	0.50
1:B:8:ARG:NH1	1:B:11:GLU:HG3	2.26	0.50
1:B:692:ILE:O	1:B:694:ASP:N	2.44	0.50
1:D:672:HIS:O	1:D:675:ILE:HG22	2.12	0.50
1:A:461:ASP:CG	1:A:464:LEU:HD13	2.32	0.50
1:A:123:THR:O	1:A:498:ARG:NH2	2.45	0.50
1:B:310:ARG:HD2	1:D:354:THR:OG1	2.11	0.50
1:B:447:PRO:O	1:B:469:SER:HA	2.12	0.50
1:C:233:GLU:HB3	1:C:235:TRP:CH2	2.46	0.50
1:C:479:VAL:CG1	1:C:482:LYS:HG3	2.41	0.50
1:C:527:MET:SD	1:C:529:LEU:HD11	2.52	0.50
1:C:729:ALA:O	1:C:733:VAL:HG13	2.11	0.50
1:C:736:ARG:HG2	1:C:737:ARG:N	2.26	0.50
1:A:608:ILE:CG2	1:A:640:VAL:HG13	2.41	0.50
1:B:467:GLU:N	1:B:468:PRO:HD3	2.26	0.50
1:C:649:VAL:HG13	1:C:683:ILE:HG12	1.94	0.50
1:A:608:ILE:HG22	1:A:640:VAL:HA	1.93	0.50
1:C:406:GLU:HG2	1:C:426:ARG:O	2.12	0.50
1:D:456:ASN:CG	1:D:459:GLN:HG2	2.32	0.50
1:C:117:ASP:HA	1:C:164:VAL:HG23	1.94	0.50
1:D:106:MET:HG3	1:D:158:HIS:CD2	2.47	0.49
1:A:671:SER:HG	3:A:1801:B12:H332	1.56	0.49
1:D:238:MET:HE3	1:D:269:PRO:HG2	1.93	0.49
1:D:50:ASP:HB2	1:D:363:ASP:OD1	2.12	0.49
1:A:467:GLU:N	1:A:468:PRO:HD3	2.27	0.49
1:C:651:LYS:HB2	1:C:651:LYS:NZ	2.27	0.49
2:H:7:PHE:O	2:H:11:ARG:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1801:B12:H421	3:A:1801:B12:H363	1.94	0.49
1:A:624:GLU:OE2	1:C:111:ALA:HB1	2.12	0.49
1:B:528:PHE:O	1:B:528:PHE:CD2	2.65	0.49
1:D:648:PRO:C	1:D:650:GLU:N	2.65	0.49
2:G:113:ILE:CG2	2:G:113:ILE:O	2.60	0.49
1:B:608:ILE:HG22	1:B:640:VAL:HG13	1.95	0.49
1:C:16:GLU:O	1:C:20:LYS:HG3	2.12	0.49
1:D:172:MET:O	1:D:172:MET:HE2	2.13	0.49
3:D:1801:B12:C10	3:D:1801:B12:C42	2.91	0.49
1:A:415:TYR:O	1:A:418:GLU:HB3	2.13	0.49
1:A:608:ILE:HG22	1:A:640:VAL:HG13	1.95	0.49
1:A:646:SER:O	1:A:648:PRO:HD3	2.12	0.49
1:B:14:ASP:O	1:B:18:ILE:HG13	2.12	0.49
1:B:277:MET:HE3	1:D:365:LEU:HD11	1.95	0.49
1:D:613:VAL:CG1	1:D:649:VAL:HG22	2.41	0.49
1:D:670:ILE:O	1:D:676:HIS:HB3	2.12	0.49
1:A:685:GLU:HA	1:A:688:VAL:HB	1.94	0.49
3:A:1801:B12:H1P1	1:C:127:ILE:HG13	1.94	0.49
1:C:209:ILE:O	1:C:212:TRP:HB3	2.13	0.49
2:F:98:GLU:OE1	2:F:98:GLU:HA	2.11	0.49
1:A:219:ASP:HB3	1:A:248:ASN:HD22	1.78	0.49
3:B:1801:B12:C35	3:B:1801:B12:H362	2.40	0.49
1:B:207:LYS:HE3	1:B:251:PHE:HD2	1.78	0.49
3:C:1801:B12:C49	3:C:1801:B12:H471	2.32	0.49
1:C:376:VAL:HG13	1:C:377:LEU:N	2.28	0.49
2:E:28:GLU:HB2	1:D:40:ASN:HD21	1.78	0.49
1:D:568:ILE:HG22	1:D:570:LEU:HD12	1.94	0.49
1:A:264:LEU:N	1:A:264:LEU:CD1	2.76	0.48
1:A:396:ILE:CD1	2:E:29:MET:HG2	2.43	0.48
1:B:182:HIS:HB3	4:D:1802:PLP:H2A2	1.94	0.48
1:D:524:LEU:HD12	1:D:570:LEU:O	2.13	0.48
1:C:122:GLY:O	1:C:133:THR:HG21	2.13	0.48
1:C:158:HIS:CD2	1:C:159:SER:N	2.82	0.48
1:A:173:PHE:CD1	1:A:178:VAL:HG21	2.48	0.48
1:B:479:VAL:CG1	1:B:482:LYS:HG3	2.43	0.48
1:C:456:ASN:ND2	1:C:459:GLN:NE2	2.61	0.48
1:C:123:THR:O	1:C:498:ARG:NH2	2.46	0.48
1:A:134:ARG:HG3	1:A:176:GLU:OE2	2.14	0.48
1:A:374:GLU:HG3	1:A:375:GLY:N	2.28	0.48
1:A:550:GLU:CG	1:A:575:PRO:HG3	2.43	0.48
1:B:598:ARG:NH2	1:D:232:ARG:NH2	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLU:OE1	1:B:108:ILE:HD11	2.13	0.48
1:C:250:ILE:HD12	1:C:250:ILE:HA	1.75	0.48
1:A:616:ASP:OD1	1:A:669:ILE:HB	2.14	0.48
1:B:668:THR:CG2	1:B:676:HIS:HB2	2.43	0.48
1:D:197:ILE:HD11	1:D:428:ILE:CG1	2.43	0.48
1:A:94:MET:SD	1:A:144:LEU:HD21	2.53	0.48
1:B:55:LEU:HD12	1:B:58:SER:HB3	1.95	0.48
1:C:449:THR:HG22	1:C:450:ALA:N	2.28	0.48
1:C:700:CYS:O	1:C:718:GLY:HA2	2.13	0.48
1:D:45:PRO:HD2	1:D:46:PHE:CD2	2.48	0.48
2:G:74:ARG:HB3	2:G:76:LEU:HD22	1.94	0.48
2:H:74:ARG:HG3	2:H:74:ARG:HH11	1.79	0.48
1:A:135:LYS:HE2	1:A:495:VAL:HG11	1.94	0.48
1:B:21:ASP:N	1:B:21:ASP:OD1	2.46	0.48
1:C:196:MET:SD	1:C:402:PHE:CD1	3.06	0.48
1:A:441:ASP:OD2	2:E:79:LYS:HE3	2.14	0.48
1:A:103:ASP:HB3	1:A:153:ARG:NH1	2.28	0.48
1:A:394:GLU:HG2	1:A:409:PHE:CE2	2.48	0.48
1:A:606:LEU:HD12	1:A:662:ASP:OD2	2.14	0.48
3:B:1801:B12:C42	3:B:1801:B12:C10	2.92	0.48
3:D:1801:B12:H353	3:D:1801:B12:H311	1.96	0.48
1:D:601:ILE:HD12	1:D:636:TYR:HB3	1.96	0.48
1:D:656:ALA:HA	1:D:661:ALA:CB	2.43	0.48
1:A:631:GLY:HA2	1:A:635:LYS:HD3	1.95	0.48
1:B:447:PRO:HG2	2:F:57:MET:SD	2.54	0.48
1:C:55:LEU:HD21	1:C:153:ARG:CZ	2.43	0.48
3:C:1801:B12:H362	3:C:1801:B12:C35	2.42	0.48
1:D:213:ALA:HB3	1:D:215:MET:HG3	1.96	0.48
1:D:671:SER:HB2	1:D:676:HIS:CE1	2.49	0.48
2:E:103:LEU:C	2:E:105:GLU:H	2.17	0.48
1:A:6:GLN:O	1:A:7:LEU:HB2	2.14	0.48
1:B:612:THR:CG2	1:B:616:ASP:HB3	2.44	0.48
1:C:183:GLN:OE1	1:C:207:LYS:HE2	2.13	0.48
1:C:300:MET:HB2	1:C:334:ILE:HG12	1.95	0.48
1:D:218:ILE:HG22	1:D:219:ASP:O	2.14	0.48
2:F:29:MET:O	2:F:33:ILE:HD12	2.13	0.48
1:C:438:PHE:CE2	2:G:77:MET:HG3	2.48	0.48
2:H:108:TYR:O	2:H:111:ASP:HB2	2.14	0.48
1:A:693:ARG:CG	1:A:693:ARG:O	2.63	0.47
1:B:301:ASN:O	1:B:305:MET:HE3	2.14	0.47
1:B:525:LEU:HD12	1:B:526:THR:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:ILE:CD1	1:B:663:ALA:HB3	2.44	0.47
2:F:74:ARG:HE	2:F:109:TRP:CB	2.27	0.47
1:C:121:GLU:HG3	1:C:486:ILE:HD12	1.97	0.47
1:C:238:MET:HG3	1:C:283:TYR:CD1	2.48	0.47
2:E:66:ALA:O	2:E:70:LYS:HD2	2.14	0.47
1:A:180:GLY:HA2	1:A:215:MET:HB3	1.96	0.47
1:A:505:PHE:O	1:A:506:ARG:CB	2.62	0.47
1:A:609:VAL:HG23	1:A:609:VAL:O	2.14	0.47
1:B:665:LEU:HB3	3:B:1801:B12:HM52	1.96	0.47
1:B:311:GLU:CD	1:D:63:SER:HG	2.17	0.47
1:B:597:ILE:HG23	1:B:733:VAL:HG11	1.97	0.47
1:C:460:TYR:O	1:C:461:ASP:HB2	2.14	0.47
1:A:538:PHE:CD2	1:C:585:ILE:HG23	2.49	0.47
1:D:288:ARG:NH1	1:D:288:ARG:HG3	2.20	0.47
1:D:324:LYS:HE2	1:D:362:MET:O	2.14	0.47
1:A:116:TYR:HE1	1:C:620:VAL:HG21	1.80	0.47
1:A:303:LYS:HD3	1:A:304:TYR:CE2	2.49	0.47
1:A:346:ILE:HG13	1:A:347:TYR:N	2.30	0.47
1:B:236:LYS:O	1:B:415:TYR:HD1	1.98	0.47
1:B:313:THR:O	1:B:317:VAL:HG23	2.14	0.47
1:B:424:ILE:HD13	1:B:424:ILE:HA	1.76	0.47
1:A:533:LYS:HG3	1:A:534:ARG:N	2.28	0.47
1:C:618:HIS:NE2	3:C:1801:B12:N22	2.63	0.47
1:A:517:TRP:O	1:A:518:GLN:C	2.51	0.47
1:B:396:ILE:CD1	2:F:29:MET:HB3	2.44	0.47
1:B:531:THR:H	1:B:565:GLY:HA2	1.79	0.47
1:C:396:ILE:HG22	1:C:397:GLU:N	2.30	0.47
1:C:550:GLU:HG3	1:C:575:PRO:HB3	1.96	0.47
1:D:728:VAL:O	1:D:732:LEU:HG	2.14	0.47
2:F:86:TYR:CZ	2:F:90:LYS:HD3	2.49	0.47
1:A:172:MET:O	1:A:176:GLU:HG2	2.14	0.47
1:A:414:GLY:CA	1:A:418:GLU:OE1	2.62	0.47
1:A:645:THR:C	1:A:647:VAL:H	2.18	0.47
1:A:663:ALA:HB1	1:A:697:MET:O	2.15	0.47
1:A:694:ASP:N	1:A:694:ASP:OD1	2.45	0.47
1:B:307:ALA:HB3	1:B:556:ASN:OD1	2.14	0.47
1:C:8:ARG:O	1:C:10:ASN:N	2.48	0.47
1:C:8:ARG:HH11	1:C:11:GLU:HG3	1.75	0.47
1:C:618:HIS:CE1	3:C:1801:B12:N22	2.83	0.47
1:C:344:TRP:CD1	1:C:515:VAL:HB	2.47	0.47
1:D:693:ARG:O	1:D:693:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ILE:HD11	2:F:31:GLU:CG	2.44	0.47
1:B:277:MET:SD	1:B:322:ILE:HD11	2.55	0.47
1:B:386:GLU:O	1:B:390:LEU:HG	2.14	0.47
1:C:574:VAL:HG12	1:C:574:VAL:O	2.13	0.47
1:D:394:GLU:CD	1:D:419:ARG:HH22	2.17	0.47
1:A:505:PHE:CD1	1:A:505:PHE:N	2.83	0.47
1:A:650:GLU:HG3	1:A:686:LEU:HD11	1.95	0.47
1:A:654:ASP:O	1:A:658:GLU:N	2.43	0.47
1:C:224:ALA:HB3	1:C:245:HIS:CE1	2.50	0.47
1:A:583:LEU:HD11	1:C:539:ALA:HA	1.96	0.47
1:A:620:VAL:HG23	3:A:1801:B12:O51	2.15	0.47
1:A:268:PRO:HA	1:A:269:PRO:HD3	1.62	0.47
1:A:416:TYR:CD2	1:A:417:PRO:HA	2.50	0.47
1:B:115:HIS:HB3	1:D:623:ARG:HH11	1.80	0.47
1:C:231:ALA:O	1:C:303:LYS:HE2	2.15	0.47
1:C:416:TYR:HA	1:C:417:PRO:C	2.35	0.47
3:D:1801:B12:H351	3:D:1801:B12:H372	1.96	0.47
1:C:254:LYS:HE2	2:G:31:GLU:HG3	1.96	0.47
1:B:311:GLU:OE2	1:D:63:SER:OG	2.32	0.47
1:C:607:LYS:C	1:C:608:ILE:HD12	2.35	0.47
1:D:288:ARG:HD2	1:D:326:THR:HB	1.96	0.47
1:D:734:LYS:C	1:D:736:ARG:H	2.19	0.47
1:A:158:HIS:HE2	1:A:182:HIS:CE1	2.32	0.46
1:A:505:PHE:O	1:A:506:ARG:HD3	2.15	0.46
1:B:106:MET:HE3	1:B:106:MET:HB2	1.85	0.46
3:B:1801:B12:H481	3:B:1801:B12:H473	1.11	0.46
1:B:224:ALA:CB	1:B:245:HIS:CE1	2.99	0.46
1:C:342:VAL:HG12	1:C:343:PRO:HD2	1.97	0.46
1:D:85:GLY:HA2	1:D:129:GLY:O	2.15	0.46
1:B:65:LYS:HD3	1:D:306:GLU:OE2	2.15	0.46
1:D:556:ASN:HB3	1:D:569:GLU:HB2	1.98	0.46
2:E:38:LEU:O	2:E:42:LYS:HG3	2.15	0.46
1:A:10:ASN:N	1:A:10:ASN:OD1	2.48	0.46
1:A:447:PRO:HG2	2:E:57:MET:SD	2.55	0.46
1:B:212:TRP:CE3	1:B:477:LEU:HD13	2.51	0.46
1:B:578:ILE:HD13	1:D:543:PHE:CD1	2.50	0.46
1:C:320:LEU:HD13	1:C:358:ALA:HB3	1.97	0.46
1:C:88:GLU:HG2	1:C:89:ASP:N	2.30	0.46
2:G:76:LEU:HD23	2:G:109:TRP:HZ3	1.79	0.46
2:H:52:SER:OG	2:H:56:ARG:NH2	2.48	0.46
1:A:178:VAL:HG12	1:A:215:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:GLU:HG3	1:A:554:VAL:HG21	1.96	0.46
1:B:122:GLY:O	1:B:133:THR:HG21	2.15	0.46
1:B:157:TYR:CD2	1:B:178:VAL:HG22	2.50	0.46
1:B:172:MET:CE	1:B:172:MET:C	2.83	0.46
1:C:668:THR:HG23	1:C:668:THR:O	2.16	0.46
1:D:611:ALA:CB	1:D:643:LEU:HB2	2.38	0.46
1:D:685:GLU:C	1:D:687:ALA:H	2.18	0.46
2:F:69:ASP:HA	2:F:72:MET:CE	2.44	0.46
1:A:541:ILE:O	1:A:545:LYS:HG2	2.16	0.46
1:B:116:TYR:CD2	1:B:120:ILE:HD13	2.49	0.46
3:B:1801:B12:O2	3:B:1801:B12:H2B	2.14	0.46
1:B:578:ILE:O	1:B:578:ILE:HG22	2.15	0.46
1:C:163:GLY:O	1:C:165:ALA:N	2.49	0.46
1:D:153:ARG:HG2	1:D:154:PRO:HD2	1.97	0.46
1:A:274:ALA:O	1:A:276:SER:N	2.49	0.46
1:B:449:THR:O	2:F:56:ARG:NH1	2.48	0.46
1:D:109:ARG:HG2	1:D:132:ILE:HD13	1.96	0.46
1:B:321:LEU:HD21	1:D:321:LEU:HD13	1.97	0.46
1:B:96:MET:SD	1:D:560:MET:HB3	2.56	0.46
1:D:666:ALA:HB3	1:D:700:CYS:SG	2.56	0.46
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.80	0.46
1:A:687:ALA:C	1:A:693:ARG:HB2	2.36	0.46
1:C:382:ARG:NE	1:C:386:GLU:OE2	2.48	0.46
2:E:113:ILE:HG22	2:E:113:ILE:O	2.16	0.46
1:A:697:MET:HG2	1:A:735:LYS:HG2	1.97	0.46
1:A:79:THR:HG21	1:A:106:MET:HE3	1.97	0.46
1:B:157:TYR:HD2	1:B:178:VAL:HG22	1.79	0.46
1:A:542:GLU:O	1:A:546:LYS:HG2	2.16	0.46
1:A:8:ARG:NH1	1:A:11:GLU:OE2	2.49	0.46
1:B:8:ARG:HB2	1:B:11:GLU:HB2	1.97	0.46
1:D:549:LEU:HD13	1:D:572:GLY:HA3	1.97	0.46
1:A:542:GLU:O	1:A:545:LYS:HB2	2.16	0.46
1:A:631:GLY:HA2	1:A:635:LYS:CD	2.46	0.46
1:A:84:SER:HB2	1:A:516:GLU:OE1	2.16	0.46
1:B:13:LEU:HD13	1:B:91:ILE:HG22	1.98	0.46
1:C:237:VAL:O	1:C:237:VAL:HG13	2.15	0.46
1:C:529:LEU:HA	1:C:530:PRO:HD3	1.68	0.46
1:D:541:ILE:CD1	1:D:554:VAL:HG23	2.45	0.46
1:A:178:VAL:HG12	1:A:215:MET:CE	2.46	0.46
1:B:160:TYR:CD1	1:B:182:HIS:HB2	2.51	0.46
1:C:543:PHE:O	1:C:547:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:GLN:HG2	1:D:136:GLN:O	2.15	0.46
1:A:730:THR:CG2	1:A:734:LYS:HD2	2.46	0.45
1:B:610:ALA:HB1	1:B:622:LEU:HD21	1.97	0.45
1:B:684:HIS:O	1:B:688:VAL:HB	2.16	0.45
1:C:276:SER:O	1:C:280:ASP:OD1	2.33	0.45
1:C:668:THR:HG23	1:C:676:HIS:CB	2.42	0.45
1:D:268:PRO:HA	1:D:269:PRO:HD3	1.64	0.45
1:B:277:MET:HE3	1:D:365:LEU:CD1	2.46	0.45
2:E:81:ALA:O	2:E:85:VAL:HG23	2.15	0.45
2:F:25:ARG:O	2:F:29:MET:HG3	2.16	0.45
1:B:224:ALA:C	1:B:226:ASN:H	2.20	0.45
1:C:592:LEU:HB2	1:C:597:ILE:HD11	1.98	0.45
1:D:99:TRP:NE1	1:D:150:GLU:OE1	2.48	0.45
2:F:106:GLY:O	2:F:109:TRP:HD1	1.99	0.45
1:A:472:ILE:O	1:A:473:ASP:HB2	2.16	0.45
1:A:709:VAL:HA	1:A:712:LYS:HE2	1.99	0.45
1:B:340:ARG:NH2	1:B:347:TYR:CE2	2.85	0.45
1:B:606:LEU:HA	1:B:606:LEU:HD12	1.74	0.45
1:B:608:ILE:HD11	1:B:663:ALA:HB3	1.98	0.45
1:C:417:PRO:O	1:C:418:GLU:C	2.54	0.45
1:C:432:ILE:N	1:C:432:ILE:CD1	2.79	0.45
1:D:288:ARG:NH1	1:D:288:ARG:CG	2.77	0.45
1:D:546:LYS:HD2	1:D:546:LYS:HA	1.82	0.45
1:D:614:GLY:O	1:D:646:SER:HA	2.16	0.45
1:A:580:ILE:HG22	1:A:580:ILE:O	2.16	0.45
1:A:628:ILE:O	1:A:629:LYS:C	2.54	0.45
1:B:95:ARG:HA	1:B:147:ILE:HD13	1.98	0.45
1:C:619:SER:HB3	1:C:645:THR:HG21	1.99	0.45
3:D:1801:B12:C2B	3:D:1801:B12:O7R	2.64	0.45
1:D:224:ALA:C	1:D:226:ASN:N	2.69	0.45
1:B:629:LYS:HE3	1:D:226:ASN:OD1	2.15	0.45
1:D:79:THR:HG21	1:D:106:MET:CE	2.47	0.45
2:E:74:ARG:O	2:E:75:GLY:C	2.52	0.45
2:G:76:LEU:HD23	2:G:109:TRP:CZ3	2.52	0.45
1:A:233:GLU:HB3	1:A:235:TRP:CZ2	2.50	0.45
1:B:26:THR:O	1:B:27:PRO:C	2.55	0.45
1:B:610:ALA:HA	1:B:665:LEU:O	2.16	0.45
1:D:13:LEU:HD22	1:D:18:ILE:HD11	1.97	0.45
1:D:307:ALA:HB3	1:D:556:ASN:OD1	2.16	0.45
1:D:694:ASP:CG	1:D:695:LYS:HE2	2.37	0.45
1:A:528:PHE:CZ	1:A:565:GLY:HA3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:HA	1:B:104:HIS:HB3	1.98	0.45
1:A:161:VAL:CG1	1:A:183:GLN:HG2	2.47	0.45
3:B:1801:B12:O28	3:B:1801:B12:H3	2.17	0.45
1:B:273:PRO:HD2	1:D:67:PHE:CD2	2.52	0.45
1:B:693:ARG:CG	1:B:693:ARG:O	2.64	0.45
1:C:512:LYS:HB2	1:C:513:PRO:HD2	1.99	0.45
1:D:104:HIS:HE2	1:D:158:HIS:CB	2.29	0.45
1:D:107:VAL:HG12	1:D:107:VAL:O	2.15	0.45
1:D:335:THR:HB	1:D:337:ASP:OD1	2.17	0.45
3:A:1801:B12:H203	3:A:1801:B12:C30	2.46	0.45
1:B:277:MET:HE1	1:B:321:LEU:CD2	2.47	0.45
1:B:337:ASP:HB3	1:B:347:TYR:CD2	2.51	0.45
1:C:185:PRO:O	1:C:188:ASN:HB2	2.16	0.45
1:C:183:GLN:O	1:C:217:GLN:NE2	2.49	0.45
1:C:264:LEU:HD21	1:C:291:PHE:CE1	2.50	0.45
1:D:184:ASP:HA	1:D:185:PRO:HD2	1.81	0.45
1:D:196:MET:SD	1:D:402:PHE:CD1	3.09	0.45
1:D:411:VAL:HB	1:D:424:ILE:HG12	1.98	0.45
1:D:540:ALA:CB	1:D:568:ILE:HG21	2.47	0.45
1:A:373:ARG:NH1	1:A:373:ARG:HG3	2.31	0.45
1:B:241:LEU:HD23	1:B:241:LEU:HA	1.73	0.45
1:C:335:THR:HB	1:C:337:ASP:OD1	2.16	0.45
2:G:54:LEU:HD23	2:G:57:MET:HE3	1.97	0.45
2:H:106:GLY:O	2:H:109:TRP:HD1	2.00	0.45
1:B:277:MET:HE1	1:B:321:LEU:HD23	1.98	0.45
2:E:112:ALA:O	2:E:114:GLN:N	2.50	0.45
2:E:55:LEU:HD23	2:E:59:PHE:O	2.17	0.45
2:E:70:LYS:O	2:E:73:ASP:N	2.50	0.45
1:A:19:LEU:HD12	1:A:499:MET:HE3	1.99	0.44
1:A:57:ASN:O	1:A:58:SER:HB3	2.15	0.44
1:B:87:PHE:O	1:B:91:ILE:HG13	2.17	0.44
1:C:514:GLU:OE2	1:C:518:GLN:HA	2.17	0.44
1:D:227:ALA:HB3	1:D:241:LEU:CD2	2.46	0.44
1:D:678:LYS:CB	1:D:682:ARG:HH21	2.30	0.44
2:F:91:GLU:O	2:F:92:LYS:HD3	2.17	0.44
2:G:113:ILE:O	2:G:113:ILE:HG22	2.17	0.44
1:A:172:MET:CE	1:A:176:GLU:HG3	2.45	0.44
1:A:631:GLY:O	1:A:725:GLY:HA3	2.16	0.44
1:B:212:TRP:CD2	1:B:477:LEU:HD13	2.52	0.44
1:B:441:ASP:OD2	2:F:79:LYS:HE3	2.17	0.44
1:C:14:ASP:CG	1:C:17:ASN:HB2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:ILE:HG22	1:C:545:LYS:HZ1	1.81	0.44
1:C:545:LYS:O	1:C:548:ASN:N	2.50	0.44
1:C:307:ALA:HB3	1:C:556:ASN:OD1	2.17	0.44
1:D:224:ALA:C	1:D:226:ASN:H	2.20	0.44
1:A:13:LEU:HD13	1:A:91:ILE:HG22	1.98	0.44
1:B:14:ASP:OD1	1:B:16:GLU:HB3	2.17	0.44
1:B:467:GLU:O	1:B:469:SER:N	2.51	0.44
1:C:20:LYS:O	1:C:21:ASP:HB2	2.17	0.44
1:C:462:GLU:C	1:C:464:LEU:H	2.21	0.44
1:D:512:LYS:HB2	1:D:513:PRO:CD	2.47	0.44
3:B:1801:B12:H471	3:B:1801:B12:C49	2.35	0.44
1:B:624:GLU:HA	1:B:624:GLU:OE2	2.18	0.44
3:C:1801:B12:H312	3:C:1801:B12:H353	2.00	0.44
1:C:683:ILE:HG22	1:C:698:ILE:HD13	1.99	0.44
1:D:598:ARG:O	1:D:602:GLU:CB	2.66	0.44
2:F:13:HIS:CD2	2:F:14:LEU:HG	2.52	0.44
3:A:1801:B12:N23	5:C:1500:5AD:C4'	2.80	0.44
1:C:263:CYS:SG	1:C:295:ARG:HB2	2.57	0.44
1:C:492:ASN:HA	1:C:492:ASN:HD22	1.63	0.44
3:D:1801:B12:H301	3:D:1801:B12:H253	1.63	0.44
1:D:692:ILE:HD12	1:D:696:ILE:HD12	1.99	0.44
2:H:32:LYS:HB3	2:H:32:LYS:HE2	1.79	0.44
2:H:72:MET:HG2	2:H:77:MET:HG3	1.99	0.44
1:A:15:VAL:HG22	1:A:15:VAL:O	2.17	0.44
1:A:337:ASP:OD2	1:A:347:TYR:CD2	2.71	0.44
1:B:672:HIS:O	1:B:673:ASP:HB3	2.18	0.44
1:C:196:MET:HE2	1:C:405:VAL:HG11	2.00	0.44
3:D:1801:B12:H351	3:D:1801:B12:C36	2.33	0.44
1:D:88:GLU:OE1	1:D:498:ARG:NH1	2.50	0.44
1:D:578:ILE:HA	1:D:578:ILE:HD13	1.66	0.44
2:G:10:ARG:HB3	2:G:10:ARG:HE	1.56	0.44
1:A:488:GLU:O	1:A:489:LEU:HD23	2.17	0.44
1:B:521:GLY:O	1:B:573:ARG:HA	2.17	0.44
1:C:693:ARG:O	1:C:693:ARG:NH1	2.50	0.44
1:C:81:GLU:O	1:C:82:ILE:HG13	2.18	0.44
1:D:284:ALA:O	1:D:288:ARG:HG3	2.18	0.44
2:E:25:ARG:HG2	2:E:29:MET:HE1	1.98	0.44
2:F:18:SER:OG	2:F:21:GLU:HG3	2.17	0.44
1:C:486:ILE:HD13	2:G:62:LEU:HD12	1.99	0.44
1:A:123:THR:CG2	1:A:135:LYS:HD3	2.40	0.44
1:A:22:LEU:HD23	1:A:22:LEU:HA	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:THR:HA	1:A:54:PRO:HD3	1.82	0.44
1:C:109:ARG:NH2	1:C:162:SER:HB2	2.33	0.44
1:C:335:THR:HG22	1:C:348:ASN:HD22	1.80	0.44
1:C:406:GLU:OE2	1:C:428:ILE:HG22	2.17	0.44
1:C:459:GLN:O	1:C:459:GLN:HG3	2.18	0.44
1:C:467:GLU:N	1:C:468:PRO:HD3	2.32	0.44
1:D:346:ILE:O	1:D:350:GLU:HG3	2.18	0.44
1:D:373:ARG:HA	1:D:377:LEU:HD23	2.00	0.44
1:D:250:ILE:HG23	2:H:34:VAL:HG21	1.99	0.44
2:H:9:GLN:HG2	2:H:10:ARG:N	2.32	0.44
1:C:346:ILE:HG13	1:C:347:TYR:N	2.33	0.44
1:C:666:ALA:O	1:C:700:CYS:HA	2.17	0.44
1:D:444:TYR:HA	2:H:79:LYS:O	2.17	0.44
1:D:689:GLU:HG2	1:D:689:GLU:O	2.17	0.44
2:G:101:LEU:HA	2:G:101:LEU:HD12	1.86	0.44
2:H:76:LEU:HG	2:H:84:ILE:HD11	1.99	0.44
1:A:446:ALA:HA	1:A:447:PRO:HD3	1.82	0.43
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.63	0.43
3:C:1801:B12:H252	3:C:1801:B12:H601	2.00	0.43
1:C:394:GLU:CG	1:C:409:PHE:CE2	3.01	0.43
1:C:671:SER:OG	1:C:704:GLN:HG3	2.18	0.43
1:D:264:LEU:N	1:D:264:LEU:HD12	2.32	0.43
1:D:525:LEU:HD21	1:D:547:MET:HE3	2.00	0.43
1:D:8:ARG:NH1	1:D:8:ARG:CB	2.73	0.43
2:G:54:LEU:HA	2:G:57:MET:HE3	2.01	0.43
1:A:475:CYS:HB2	2:E:56:ARG:O	2.18	0.43
1:B:568:ILE:HG22	1:B:570:LEU:HD12	1.99	0.43
3:C:1801:B12:H561	3:C:1801:B12:H18	1.73	0.43
1:C:392:MET:O	1:C:395:ILE:HB	2.18	0.43
1:C:345:HIS:CE1	1:C:516:GLU:O	2.70	0.43
1:C:659:LEU:O	1:C:660:LYS:C	2.56	0.43
1:C:8:ARG:NH1	1:C:10:ASN:OD1	2.51	0.43
1:B:162:SER:OG	4:D:1802:PLP:N1	2.43	0.43
1:D:612:THR:HB	1:D:645:THR:HA	2.00	0.43
1:D:656:ALA:HA	1:D:661:ALA:HB3	2.00	0.43
2:E:92:LYS:N	2:E:92:LYS:HD3	2.32	0.43
1:C:250:ILE:CG2	2:G:34:VAL:HG21	2.48	0.43
1:A:241:LEU:HD23	1:A:241:LEU:HA	1.63	0.43
1:A:461:ASP:O	1:A:462:GLU:C	2.56	0.43
1:B:541:ILE:CD1	1:B:552:VAL:HG12	2.47	0.43
1:C:264:LEU:HD13	1:C:296:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:GLU:CG	1:C:517:TRP:N	2.81	0.43
1:C:633:ILE:CD1	1:C:638:VAL:HG11	2.47	0.43
1:D:608:ILE:HG13	1:D:663:ALA:HB3	1.99	0.43
1:A:160:TYR:N	1:A:160:TYR:CD2	2.87	0.43
1:B:534:ARG:CG	1:B:534:ARG:NH1	2.80	0.43
1:A:63:SER:HB2	1:C:311:GLU:OE2	2.18	0.43
1:C:456:ASN:CG	1:C:459:GLN:HE21	2.21	0.43
1:D:626:ILE:O	1:D:634:GLU:HB2	2.18	0.43
1:D:683:ILE:O	1:D:683:ILE:HG22	2.18	0.43
1:A:386:GLU:HG3	2:E:22:LEU:HD21	1.99	0.43
2:E:51:ARG:HG2	2:E:68:VAL:HG21	2.01	0.43
2:F:54:LEU:HD23	2:F:57:MET:HE1	1.99	0.43
1:A:391:PHE:HD1	1:A:416:TYR:CG	2.36	0.43
1:B:108:ILE:HA	1:B:160:TYR:CE2	2.53	0.43
1:B:116:TYR:CE1	3:D:1801:B12:H491	2.54	0.43
1:C:79:THR:HA	1:C:104:HIS:HB3	1.99	0.43
1:C:189:VAL:HG22	1:C:196:MET:HA	2.00	0.43
1:C:348:ASN:HD22	1:C:348:ASN:HA	1.66	0.43
1:C:516:GLU:HG2	1:C:517:TRP:H	1.82	0.43
1:B:547:MET:HB3	1:D:547:MET:HB3	2.00	0.43
3:B:1801:B12:O7R	3:B:1801:B12:C2B	2.65	0.43
1:B:688:VAL:HG23	1:B:693:ARG:HG2	2.01	0.43
1:C:17:ASN:O	1:C:20:LYS:HB2	2.19	0.43
1:D:612:THR:CG2	1:D:616:ASP:HB3	2.49	0.43
2:E:63:GLU:OE1	2:E:101:LEU:HD11	2.18	0.43
1:D:255:VAL:HG23	2:H:38:LEU:HD21	2.00	0.43
1:A:539:ALA:HB2	1:C:583:LEU:HD11	2.01	0.43
1:A:657:ILE:CD1	1:A:690:LYS:HD2	2.49	0.43
1:B:643:LEU:N	1:B:643:LEU:HD23	2.33	0.43
1:D:464:LEU:HA	1:D:464:LEU:HD12	1.68	0.43
2:E:25:ARG:O	2:E:29:MET:HE2	2.19	0.43
1:A:134:ARG:HD3	1:A:138:ARG:HH21	1.83	0.43
1:A:232:ARG:HD3	1:A:232:ARG:HA	1.75	0.43
1:A:381:VAL:HG12	1:A:385:LYS:HE3	2.01	0.43
1:B:277:MET:O	1:B:281:LEU:HB2	2.19	0.43
1:B:489:LEU:HA	1:B:489:LEU:HD23	1.83	0.43
3:C:1801:B12:N40	3:C:1801:B12:C8	2.77	0.43
1:C:653:VAL:HG21	1:C:686:LEU:HB3	1.99	0.43
1:D:613:VAL:HG11	1:D:683:ILE:HD11	2.01	0.43
1:B:115:HIS:HB3	1:D:623:ARG:NH1	2.34	0.43
1:A:416:TYR:CD1	1:A:417:PRO:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:VAL:HG13	1:D:369:VAL:HG13	2.00	0.43
1:B:196:MET:SD	1:B:402:PHE:CD1	3.11	0.43
1:B:561:GLN:O	1:B:562:GLU:C	2.57	0.43
1:C:340:ARG:O	1:C:341:ASN:HB3	2.18	0.43
1:C:464:LEU:HG	1:C:470:LYS:HB2	2.01	0.43
1:C:668:THR:HG21	1:C:676:HIS:HB2	2.00	0.43
1:D:186:GLN:OE1	1:D:244:GLN:HG2	2.18	0.43
1:A:547:MET:O	1:A:548:ASN:CB	2.67	0.43
1:A:682:ARG:O	1:A:686:LEU:CB	2.65	0.43
1:C:93:ARG:NH1	1:C:348:ASN:OD1	2.52	0.43
1:C:471:LEU:HA	1:C:471:LEU:HD12	1.67	0.43
1:D:657:ILE:C	1:D:659:LEU:H	2.22	0.43
1:A:561:GLN:O	1:A:562:GLU:C	2.57	0.42
1:A:13:LEU:HD13	1:A:91:ILE:CG2	2.49	0.42
1:B:100:HIS:CD2	1:B:349:ILE:HG13	2.54	0.42
1:B:570:LEU:N	1:B:570:LEU:HD12	2.34	0.42
1:B:593:SER:O	1:B:596:GLU:N	2.52	0.42
1:B:6:GLN:CG	1:B:7:LEU:H	2.30	0.42
1:D:253:LEU:HD12	1:D:253:LEU:HA	1.86	0.42
2:G:81:ALA:O	2:G:85:VAL:HG23	2.18	0.42
1:A:321:LEU:HD13	1:A:362:MET:HE1	2.01	0.42
1:A:618:HIS:CD2	3:A:1801:B12:N24	2.87	0.42
1:B:522:THR:HA	1:B:572:GLY:O	2.19	0.42
1:B:619:SER:HB3	1:B:645:THR:CG2	2.48	0.42
1:C:271:ALA:O	1:C:274:ALA:HB3	2.19	0.42
1:C:360:ILE:HA	1:C:360:ILE:HD13	1.69	0.42
1:C:394:GLU:HG3	1:C:409:PHE:CE2	2.54	0.42
1:D:662:ASP:O	1:D:696:ILE:HA	2.19	0.42
1:A:13:LEU:O	1:A:15:VAL:N	2.52	0.42
1:A:87:PHE:CD1	1:A:87:PHE:C	2.92	0.42
1:B:43:MET:HE1	1:B:72:PRO:HA	2.01	0.42
1:B:538:PHE:CE2	1:D:585:ILE:HG23	2.55	0.42
1:B:597:ILE:HG21	1:B:729:ALA:HB1	2.00	0.42
1:C:8:ARG:HH12	1:C:11:GLU:HG3	1.83	0.42
3:D:1801:B12:C10	3:D:1801:B12:H422	2.48	0.42
1:D:277:MET:CE	1:D:321:LEU:HD23	2.48	0.42
2:E:100:GLY:C	2:E:102:ALA:N	2.73	0.42
1:A:583:LEU:HD21	1:C:542:GLU:HG2	2.02	0.42
1:A:616:ASP:OD2	1:A:670:ILE:HG12	2.19	0.42
1:B:53:THR:HA	1:B:54:PRO:HD3	1.78	0.42
1:A:620:VAL:HG13	1:C:112:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1801:B12:H412	3:C:1801:B12:H363	1.58	0.42
1:D:91:ILE:HD13	1:D:143:ALA:CB	2.49	0.42
1:D:458:LYS:C	1:D:460:TYR:H	2.23	0.42
1:D:82:ILE:O	1:D:83:ALA:HB2	2.19	0.42
1:C:28:LYS:HG3	1:C:145:ASP:OD2	2.20	0.42
1:C:207:LYS:NZ	1:C:217:GLN:NE2	2.67	0.42
1:D:138:ARG:NE	1:D:176:GLU:OE1	2.49	0.42
1:A:335:THR:HB	1:A:337:ASP:OD1	2.19	0.42
1:B:344:TRP:CG	1:B:515:VAL:HB	2.55	0.42
1:C:102:ALA:HB2	1:C:352:CYS:SG	2.59	0.42
1:C:251:PHE:CE1	2:G:38:LEU:HD23	2.55	0.42
1:D:147:ILE:O	1:D:151:VAL:HG22	2.20	0.42
1:D:217:GLN:HG2	1:D:218:ILE:N	2.33	0.42
1:D:22:LEU:HD22	1:D:138:ARG:HB3	2.00	0.42
2:G:46:THR:HB	2:G:47:PRO:HD2	2.02	0.42
1:B:123:THR:O	1:B:494:ASN:HA	2.20	0.42
3:B:1801:B12:C25	3:B:1801:B12:H312	2.49	0.42
1:B:660:LYS:HG3	1:B:660:LYS:O	2.20	0.42
1:C:388:ALA:HB1	2:G:26:PHE:HE1	1.85	0.42
1:D:335:THR:O	1:D:338:GLU:HB2	2.20	0.42
1:A:438:PHE:CD2	2:E:77:MET:HG3	2.54	0.42
1:B:46:PHE:HE2	1:B:67:PHE:CD1	2.38	0.42
1:D:159:SER:O	1:D:181:ALA:HA	2.20	0.42
2:G:39:ASP:O	2:G:40:LEU:C	2.57	0.42
1:A:227:ALA:HB3	1:A:241:LEU:HD21	2.01	0.42
1:A:121:GLU:HG3	1:A:486:ILE:HB	2.02	0.42
1:A:650:GLU:HG2	1:A:654:ASP:OD2	2.19	0.42
1:B:79:THR:CB	1:B:332:SER:HA	2.46	0.42
1:B:416:TYR:CD1	1:B:417:PRO:HA	2.55	0.42
1:B:426:ARG:HH22	1:D:634:GLU:CD	2.23	0.42
1:C:424:ILE:HG21	1:C:426:ARG:CZ	2.50	0.42
1:C:577:SER:O	1:C:578:ILE:HD12	2.20	0.42
1:D:25:TYR:CE1	1:D:142:LYS:HB2	2.55	0.42
1:D:629:LYS:HG3	1:D:630:HIS:CD2	2.55	0.42
1:A:626:ILE:O	1:A:634:GLU:HB2	2.20	0.42
1:A:726:ILE:HA	1:A:726:ILE:HD12	1.89	0.42
1:B:194:ILE:O	1:B:195:ASN:C	2.58	0.42
1:B:44:GLY:HA3	1:B:45:PRO:HD3	1.79	0.42
1:B:465:VAL:O	1:B:465:VAL:HG12	2.19	0.42
1:C:134:ARG:O	1:C:138:ARG:HG3	2.19	0.42
1:C:488:GLU:O	1:C:489:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:ILE:HA	1:D:360:ILE:HD13	1.90	0.42
1:D:481:GLU:CD	1:D:481:GLU:H	2.22	0.42
1:D:734:LYS:HE2	1:D:734:LYS:HB3	1.87	0.42
3:A:1801:B12:C3	3:A:1801:B12:O28	2.49	0.41
1:A:513:PRO:HA	1:C:528:PHE:O	2.20	0.41
1:A:671:SER:O	1:A:672:HIS:C	2.57	0.41
1:C:476:THR:HG23	2:G:56:ARG:O	2.20	0.41
1:D:8:ARG:HG3	1:D:11:GLU:OE1	2.20	0.41
1:D:167:PRO:HD2	2:H:48:SER:HB2	2.02	0.41
1:D:441:ASP:HB3	1:D:443:ASP:OD1	2.20	0.41
2:F:90:LYS:HB3	2:F:90:LYS:HE2	1.69	0.41
1:A:471:LEU:HA	1:A:471:LEU:HD13	1.93	0.41
1:B:322:ILE:HD13	1:B:322:ILE:HA	1.85	0.41
1:C:234:ALA:O	1:C:237:VAL:HG12	2.20	0.41
1:D:281:LEU:HB3	1:D:282:PRO:HD3	2.02	0.41
1:D:318:LEU:HD23	1:D:318:LEU:HA	1.79	0.41
2:G:38:LEU:O	2:G:42:LYS:HG3	2.20	0.41
2:H:74:ARG:HD3	2:H:113:ILE:HD11	2.01	0.41
2:H:37:LEU:O	2:H:40:LEU:HB2	2.21	0.41
1:A:533:LYS:HE3	1:A:533:LYS:HB2	1.55	0.41
1:B:111:ALA:O	1:D:620:VAL:HG11	2.20	0.41
1:B:172:MET:CE	1:B:172:MET:O	2.68	0.41
1:B:224:ALA:C	1:B:226:ASN:N	2.73	0.41
1:B:232:ARG:HD3	1:B:232:ARG:HA	1.80	0.41
1:B:512:LYS:HE3	1:B:512:LYS:HB2	1.75	0.41
1:C:505:PHE:CD1	1:C:505:PHE:N	2.88	0.41
1:D:623:ARG:HB3	1:D:627:ASP:OD2	2.20	0.41
1:D:704:GLN:NE2	1:D:721:ARG:HH21	2.13	0.41
1:A:663:ALA:HB2	1:A:697:MET:HB2	2.02	0.41
1:A:636:TYR:OH	1:A:726:ILE:HD13	2.21	0.41
1:B:26:THR:HG22	1:B:27:PRO:O	2.20	0.41
1:B:651:LYS:O	1:B:654:ASP:HB2	2.20	0.41
1:C:306:GLU:HB3	1:C:307:ALA:H	1.66	0.41
1:C:300:MET:CE	1:C:316:HIS:HB3	2.51	0.41
1:C:458:LYS:C	1:C:460:TYR:H	2.24	0.41
1:C:86:ARG:HB3	1:C:88:GLU:CD	2.41	0.41
1:D:138:ARG:HE	1:D:176:GLU:CD	2.22	0.41
1:D:335:THR:CB	1:D:337:ASP:OD1	2.67	0.41
1:D:82:ILE:CG2	1:D:90:ASP:HB3	2.51	0.41
2:G:74:ARG:HB2	2:G:76:LEU:HD22	2.01	0.41
1:A:731:PHE:CD2	1:A:732:LEU:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLN:NE2	1:B:132:ILE:HB	2.29	0.41
1:D:347:TYR:HA	1:D:350:GLU:HB2	2.03	0.41
1:D:553:GLU:OE2	1:D:571:LYS:HE3	2.20	0.41
1:D:711:VAL:CG2	1:D:717:ALA:HA	2.50	0.41
2:F:59:PHE:CE1	2:F:100:GLY:HA3	2.56	0.41
1:A:617:GLU:HB2	3:A:1801:B12:O44	2.20	0.41
1:A:609:VAL:HG22	1:A:663:ALA:O	2.20	0.41
1:A:730:THR:HG22	1:A:731:PHE:N	2.35	0.41
1:B:531:THR:HG23	1:B:536:ALA:HB2	2.03	0.41
1:B:592:LEU:HD12	1:B:730:THR:HG23	2.02	0.41
1:C:171:VAL:HG12	1:C:172:MET:N	2.36	0.41
3:C:1801:B12:H473	3:C:1801:B12:H481	1.07	0.41
1:C:264:LEU:HD13	1:C:296:MET:HE1	2.01	0.41
1:C:430:GLY:O	1:C:434:ALA:HB2	2.21	0.41
1:C:521:GLY:O	1:C:573:ARG:HA	2.20	0.41
1:C:624:GLU:OE1	1:C:630:HIS:ND1	2.53	0.41
1:D:399:GLY:CA	1:D:403:ASN:HD22	2.32	0.41
1:A:344:TRP:CG	1:A:515:VAL:HB	2.56	0.41
1:A:731:PHE:CE2	1:A:732:LEU:HD23	2.55	0.41
1:B:31:GLY:O	1:B:179:ASN:ND2	2.49	0.41
1:B:575:PRO:HD2	1:B:576:PHE:CD2	2.55	0.41
1:C:137:VAL:HG13	1:C:157:TYR:HE2	1.86	0.41
1:C:475:CYS:HB2	2:G:56:ARG:O	2.20	0.41
1:C:713:GLN:NE2	1:C:713:GLN:N	2.68	0.41
1:D:255:VAL:O	1:D:255:VAL:CG1	2.68	0.41
1:D:478:GLU:O	1:D:480:PRO:HD3	2.20	0.41
1:D:701:GLY:HA3	3:D:1801:B12:C9B	2.50	0.41
1:A:373:ARG:HA	1:A:373:ARG:HD2	1.88	0.41
3:B:1801:B12:H312	3:B:1801:B12:H251	2.03	0.41
1:B:620:VAL:HG12	3:B:1801:B12:H3P3	2.02	0.41
1:C:335:THR:CG2	1:C:348:ASN:ND2	2.82	0.41
1:D:515:VAL:HG13	1:D:522:THR:HB	2.02	0.41
1:B:523:VAL:HG11	1:D:527:MET:HE1	2.03	0.41
1:B:198:ARG:HD2	2:F:46:THR:HG21	2.02	0.41
1:B:233:GLU:OE1	1:B:235:TRP:CZ2	2.74	0.41
1:B:555:ILE:CG2	1:B:571:LYS:HG2	2.50	0.41
1:B:55:LEU:CD1	1:B:58:SER:HB3	2.49	0.41
1:C:726:ILE:HG23	1:C:727:HIS:N	2.36	0.41
1:C:7:LEU:HA	1:C:7:LEU:HD23	1.75	0.41
1:D:678:LYS:HB2	1:D:682:ARG:HH21	1.86	0.41
1:A:263:CYS:HA	1:A:295:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ARG:HA	1:B:154:PRO:HD3	1.90	0.41
1:B:439:GLU:HG2	1:B:440:ARG:N	2.35	0.41
1:B:649:VAL:HG13	1:B:683:ILE:HG12	2.02	0.41
1:C:184:ASP:HA	1:C:185:PRO:HD2	1.90	0.41
1:C:649:VAL:HG13	1:C:683:ILE:CG1	2.51	0.41
1:D:197:ILE:O	1:D:201:ILE:HD12	2.21	0.41
1:D:516:GLU:HG2	1:D:517:TRP:N	2.36	0.41
1:D:568:ILE:CG2	1:D:570:LEU:HD11	2.51	0.41
1:D:706:THR:HA	1:D:707:PRO:HD3	1.87	0.41
1:D:8:ARG:HG2	1:D:8:ARG:H	1.48	0.41
2:E:70:LYS:O	2:E:71:THR:C	2.58	0.41
1:A:464:LEU:HD12	1:A:464:LEU:N	2.36	0.41
1:A:676:HIS:O	1:A:680:MET:HG3	2.21	0.41
3:B:1801:B12:H412	3:B:1801:B12:H363	1.62	0.41
1:B:409:PHE:N	1:B:409:PHE:HD1	2.19	0.41
1:B:479:VAL:HG12	1:B:479:VAL:O	2.21	0.41
2:E:94:ILE:HG13	2:E:99:ALA:HB2	2.03	0.41
1:A:698:ILE:HG21	1:A:715:VAL:HG12	2.02	0.40
1:B:196:MET:SD	1:B:402:PHE:HD1	2.45	0.40
1:C:316:HIS:CE1	1:C:334:ILE:HB	2.56	0.40
1:C:619:SER:HB3	1:C:645:THR:CG2	2.51	0.40
1:D:458:LYS:O	1:D:460:TYR:N	2.54	0.40
1:D:544:ALA:HB2	1:D:570:LEU:HD22	2.03	0.40
3:A:1801:B12:H492	3:A:1801:B12:H471	2.02	0.40
1:A:613:VAL:HG12	1:A:679:ASN:HD22	1.86	0.40
3:B:1801:B12:H601	3:B:1801:B12:C26	2.38	0.40
1:B:409:PHE:N	1:B:409:PHE:CD1	2.89	0.40
1:B:528:PHE:C	1:B:528:PHE:CD2	2.94	0.40
3:C:1801:B12:H541	3:C:1801:B12:H602	1.82	0.40
1:C:462:GLU:O	1:C:464:LEU:N	2.54	0.40
1:C:528:PHE:CZ	1:C:565:GLY:HA3	2.55	0.40
1:C:613:VAL:CG1	1:C:614:GLY:N	2.84	0.40
1:D:613:VAL:HG21	1:D:683:ILE:CD1	2.52	0.40
2:E:98:GLU:HA	2:E:101:LEU:HB2	2.03	0.40
1:A:445:MET:HG2	1:A:446:ALA:N	2.37	0.40
1:B:467:GLU:N	1:B:468:PRO:CD	2.85	0.40
1:B:672:HIS:O	1:B:675:ILE:HG22	2.20	0.40
1:C:618:HIS:CE1	3:C:1801:B12:H421	2.56	0.40
1:D:212:TRP:CZ2	1:D:477:LEU:HB3	2.56	0.40
2:E:18:SER:CB	2:E:20:GLU:OE1	2.68	0.40
1:A:192:ARG:HD3	1:A:192:ARG:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:PRO:HG3	1:A:718:GLY:O	2.22	0.40
1:A:719:PHE:HB3	1:A:723:SER:OG	2.21	0.40
1:B:42:GLN:HA	1:B:46:PHE:O	2.22	0.40
1:A:598:ARG:NH1	1:C:232:ARG:HD2	2.37	0.40
1:C:672:HIS:O	1:C:673:ASP:HB3	2.21	0.40
1:C:713:GLN:HE21	1:C:713:GLN:N	2.18	0.40
1:D:618:HIS:NE2	3:D:1801:B12:N22	2.69	0.40
2:E:63:GLU:OE1	2:E:101:LEU:CD1	2.69	0.40
3:A:1801:B12:H473	3:A:1801:B12:H481	0.98	0.40
1:A:184:ASP:HA	1:A:185:PRO:HD2	1.82	0.40
1:A:342:VAL:O	1:A:343:PRO:C	2.59	0.40
1:B:205:GLU:OE2	1:B:451:HIS:HA	2.22	0.40
1:C:94:MET:CE	1:C:140:GLN:NE2	2.85	0.40
1:C:305:MET:HE2	1:C:305:MET:HB2	1.92	0.40
1:C:424:ILE:CG2	1:C:426:ARG:CZ	2.99	0.40
1:C:463:ALA:C	1:C:464:LEU:HD13	2.42	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	721/763 (94%)	633 (88%)	75 (10%)	13 (2%)	8	29
1	B	722/763 (95%)	658 (91%)	56 (8%)	8 (1%)	14	42
1	C	721/763 (94%)	629 (87%)	79 (11%)	13 (2%)	8	29
1	D	721/763 (94%)	643 (89%)	64 (9%)	14 (2%)	8	28
2	E	107/121 (88%)	93 (87%)	11 (10%)	3 (3%)	5	19
2	F	107/121 (88%)	95 (89%)	11 (10%)	1 (1%)	17	48
2	G	107/121 (88%)	97 (91%)	9 (8%)	1 (1%)	17	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	107/121 (88%)	102 (95%)	5 (5%)	0	100	100
All	All	3313/3536 (94%)	2950 (89%)	310 (9%)	53 (2%)	9	32

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	12	LYS
1	A	69	ASP
1	B	162	SER
1	D	6	GLN
1	A	255	VAL
1	A	473	ASP
2	E	113	ILE
1	B	6	GLN
1	B	66	TYR
1	B	693	ARG
1	C	6	GLN
1	C	21	ASP
1	C	461	ASP
1	C	556	ASN
1	D	649	VAL
1	B	225	HIS
1	C	738	GLU
1	D	63	SER
1	D	83	ALA
1	D	361	GLY
1	D	459	GLN
1	A	40	ASN
1	A	672	HIS
1	A	738	GLU
2	E	71	THR
2	E	93	ASN
1	B	195	ASN
1	B	474	GLY
1	C	39	GLU
1	C	164	VAL
1	C	505	PHE
2	G	113	ILE
1	D	674	ASP
1	A	649	VAL
1	A	694	ASP

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Mol	Chain	Res	Type
1	B	487	ASP
2	F	15	ALA
1	D	562	GLU
1	D	593	SER
1	D	658	GLU
1	D	683	ILE
1	A	537	GLU
1	A	601	ILE
1	C	189	VAL
1	C	463	ALA
1	D	341	ASN
1	A	707	PRO
1	C	9	VAL
1	D	411	VAL
1	D	707	PRO
1	C	453	GLY
1	C	417	PRO

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	598/644 (93%)	547 (92%)	51 (8%)	10	31
1	B	604/644 (94%)	561 (93%)	43 (7%)	14	40
1	C	600/644 (93%)	562 (94%)	38 (6%)	18	46
1	D	602/644 (94%)	557 (92%)	45 (8%)	13	37
2	E	89/100 (89%)	84 (94%)	5 (6%)	21	52
2	F	90/100 (90%)	86 (96%)	4 (4%)	28	61
2	G	89/100 (89%)	79 (89%)	10 (11%)	6	18
2	H	89/100 (89%)	84 (94%)	5 (6%)	21	52
All	All	2761/2976 (93%)	2560 (93%)	201 (7%)	14	38

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	GLN
1	A	24	LYS
1	A	29	ARG
1	A	33	THR
1	A	42	GLN
1	A	47	ILE
1	A	61	LEU
1	A	69	ASP
1	A	148	GLU
1	A	153	ARG
1	A	159	SER
1	A	168	ASP
1	A	172	MET
1	A	183	GLN
1	A	198	ARG
1	A	249	SER
1	A	259	LYS
1	A	260	SER
1	A	264	LEU
1	A	276	SER
1	A	301	ASN
1	A	306	GLU
1	A	311	GLU
1	A	338	GLU
1	A	341	ASN
1	A	376	VAL
1	A	380	THR
1	A	418	GLU
1	A	442	GLU
1	A	465	VAL
1	A	471	LEU
1	A	486	ILE
1	A	505	PHE
1	A	509	SER
1	A	531	THR
1	A	550	GLU
1	A	557	ARG
1	A	570	LEU
1	A	578	ILE
1	A	591	ILE
1	A	592	LEU
1	A	604	THR

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Mol	Chain	Res	Type
1	A	608	ILE
1	A	624	GLU
1	A	651	LYS
1	A	668	THR
1	A	674	ASP
1	A	696	ILE
1	A	731	PHE
1	A	736	ARG
2	E	39	ASP
2	E	91	GLU
2	E	94	ILE
2	E	96	VAL
2	E	101	LEU
1	B	6	GLN
1	B	7	LEU
1	B	9	VAL
1	B	21	ASP
1	B	69	ASP
1	B	92	ARG
1	B	127	ILE
1	B	153	ARG
1	B	162	SER
1	B	168	ASP
1	B	172	MET
1	B	232	ARG
1	B	270	THR
1	B	301	ASN
1	B	306	GLU
1	B	338	GLU
1	B	341	ASN
1	B	383	GLU
1	B	391	PHE
1	B	424	ILE
1	B	442	GLU
1	B	457	VAL
1	B	471	LEU
1	B	477	LEU
1	B	489	LEU
1	B	492	ASN
1	B	501	GLU
1	B	509	SER
1	B	525	LEU

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Mol	Chain	Res	Type
1	B	532	SER
1	B	551	GLU
1	B	591	ILE
1	B	603	LYS
1	B	616	ASP
1	B	628	ILE
1	B	651	LYS
1	B	668	THR
1	B	674	ASP
1	B	688	VAL
1	B	696	ILE
1	B	703	THR
1	B	731	PHE
1	B	736	ARG
2	F	28	GLU
2	F	74	ARG
2	F	91	GLU
2	F	101	LEU
1	C	5	LEU
1	C	6	GLN
1	C	13	LEU
1	C	15	VAL
1	C	26	THR
1	C	110	THR
1	C	125	GLN
1	C	159	SER
1	C	168	ASP
1	C	171	VAL
1	C	182	HIS
1	C	232	ARG
1	C	238	MET
1	C	280	ASP
1	C	288	ARG
1	C	289	GLU
1	C	306	GLU
1	C	313	THR
1	C	362	MET
1	C	394	GLU
1	C	396	ILE
1	C	432	ILE
1	C	464	LEU
1	C	469	SER

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Mol	Chain	Res	Type
1	C	471	LEU
1	C	526	THR
1	C	534	ARG
1	C	557	ARG
1	C	574	VAL
1	C	578	ILE
1	C	625	VAL
1	C	651	LYS
1	C	668	THR
1	C	689	GLU
1	C	703	THR
1	C	724	LYS
1	C	731	PHE
1	C	736	ARG
2	G	16	ASN
2	G	39	ASP
2	G	43	LYS
2	G	60	SER
2	G	76	LEU
2	G	79	LYS
2	G	97	ARG
2	G	101	LEU
2	G	104	SER
2	G	105	GLU
1	D	7	LEU
1	D	8	ARG
1	D	26	THR
1	D	29	ARG
1	D	75	LEU
1	D	80	THR
1	D	172	MET
1	D	179	ASN
1	D	217	GLN
1	D	228	ASN
1	D	233	GLU
1	D	237	VAL
1	D	250	ILE
1	D	258	LYS
1	D	290	MET
1	D	306	GLU
1	D	341	ASN
1	D	349	ILE

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Mol	Chain	Res	Type
1	D	376	VAL
1	D	383	GLU
1	D	391	PHE
1	D	428	ILE
1	D	445	MET
1	D	464	LEU
1	D	486	ILE
1	D	491	GLU
1	D	501	GLU
1	D	502	THR
1	D	512	LYS
1	D	518	GLN
1	D	531	THR
1	D	546	LYS
1	D	557	ARG
1	D	577	SER
1	D	578	ILE
1	D	595	ASP
1	D	628	ILE
1	D	646	SER
1	D	657	ILE
1	D	660	LYS
1	D	668	THR
1	D	695	LYS
1	D	724	LYS
1	D	731	PHE
1	D	733	VAL
2	H	9	GLN
2	H	23	GLN
2	H	60	SER
2	H	61	SER
2	H	76	LEU

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

Mol	Chain	Res	Type
1	A	17	ASN
1	A	244	GLN
1	A	248	ASN
1	A	341	ASN
1	A	456	ASN
1	A	518	GLN

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Mol	Chain	Res	Type
1	A	672	HIS
1	A	679	ASN
1	B	217	GLN
1	B	261	ASN
1	B	331	GLN
1	B	341	ASN
1	B	403	ASN
1	B	459	GLN
1	C	217	GLN
1	C	370	GLN
1	C	459	GLN
1	C	492	ASN
1	C	518	GLN
1	C	713	GLN
2	G	16	ASN
2	G	93	ASN
1	D	40	ASN
1	D	331	GLN
1	D	341	ASN
1	D	348	ASN
1	D	370	GLN
1	D	403	ASN
1	D	459	GLN
1	D	518	GLN
1	D	704	GLN
2	H	16	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 carbohydrates in this entry.

5.6 Ligand geometry i

11 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	B12	C	1801	1,5	80,101,101	1.13	5 (6%)	101,166,166	2.24	23 (22%)
5	5AD	D	1500	3	17,20,20	2.13	6 (35%)	15,30,30	4.36	8 (53%)
4	PLP	D	1802	1	15,15,16	1.43	1 (6%)	20,22,23	1.37	3 (15%)
5	5AD	C	1500	3	17,20,20	2.13	6 (35%)	15,30,30	4.30	8 (53%)
3	B12	A	1801	1,5	80,101,101	1.14	4 (5%)	101,166,166	2.12	24 (23%)
4	PLP	B	1802	1	15,15,16	1.75	3 (20%)	20,22,23	1.96	7 (35%)
4	PLP	C	1802	1	15,15,16	1.75	3 (20%)	20,22,23	1.66	2 (10%)
3	B12	B	1801	1,5	80,101,101	1.18	7 (8%)	101,166,166	2.11	24 (23%)
4	PLP	A	1802	1	15,15,16	2.00	3 (20%)	20,22,23	1.64	2 (10%)
3	B12	D	1801	1	80,101,101	1.13	4 (5%)	101,166,166	1.99	20 (19%)
5	5AD	A	1500	3	17,20,20	2.19	6 (35%)	15,30,30	3.99	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	B12	C	1801	1,5	1/1/36/38	11/51/223/223	0/3/11/11
4	PLP	A	1802	1	-	0/6/6/8	0/1/1/1
4	PLP	D	1802	1	-	0/6/6/8	0/1/1/1
5	5AD	C	1500	3	3/3/4/4	0/0/20/20	0/3/3/3
3	B12	A	1801	1,5	1/1/36/38	12/51/223/223	0/3/11/11
4	PLP	B	1802	1	-	0/6/6/8	0/1/1/1
4	PLP	C	1802	1	-	0/6/6/8	0/1/1/1
3	B12	B	1801	1,5	1/1/36/38	3/51/223/223	0/3/11/11
5	5AD	D	1500	3	3/3/4/4	0/0/20/20	0/3/3/3
3	B12	D	1801	1	1/1/36/38	19/51/223/223	0/3/11/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	5AD	A	1500	3	3/3/4/4	0/0/20/20	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1802	PLP	C6-N1	4.93	1.44	1.34
3	D	1801	B12	C11-C10	-4.85	1.32	1.40
3	B	1801	B12	C11-C10	-4.84	1.32	1.40
4	A	1802	PLP	C6-N1	4.62	1.44	1.34
4	D	1802	PLP	C6-N1	4.59	1.44	1.34
5	C	1500	5AD	C2-N3	4.40	1.39	1.32
5	D	1500	5AD	C2-N3	4.36	1.39	1.32
5	A	1500	5AD	C2-N3	4.36	1.39	1.32
3	C	1801	B12	C11-C10	-4.32	1.33	1.40
4	A	1802	PLP	C5-C4	-4.25	1.35	1.40
4	C	1802	PLP	C6-N1	4.16	1.43	1.34
3	A	1801	B12	C2-C3	-4.16	1.51	1.58
5	A	1500	5AD	C8-N7	4.00	1.41	1.34
3	A	1801	B12	C8B-C9B	3.95	1.48	1.40
5	D	1500	5AD	O4 ¹ -C1 ¹	3.94	1.46	1.41
3	D	1801	B12	C8B-C9B	3.83	1.48	1.40
3	B	1801	B12	C8B-C9B	3.82	1.48	1.40
5	C	1500	5AD	C8-N7	3.75	1.41	1.34
3	C	1801	B12	C2-C3	-3.75	1.52	1.58
3	A	1801	B12	C11-C10	-3.73	1.34	1.40
5	C	1500	5AD	O4 ¹ -C1 ¹	3.70	1.46	1.41
5	D	1500	5AD	C8-N7	3.59	1.41	1.34
5	A	1500	5AD	O4 ¹ -C1 ¹	3.52	1.46	1.41
3	D	1801	B12	C2-C3	-3.47	1.52	1.58
3	A	1801	B12	C6B-C5B	3.44	1.49	1.40
3	B	1801	B12	C2-C3	-3.35	1.52	1.58
4	C	1802	PLP	C5-C4	-3.34	1.36	1.40
3	C	1801	B12	C8B-C9B	3.23	1.47	1.40
3	D	1801	B12	C6B-C5B	3.16	1.48	1.40
5	A	1500	5AD	C4-N3	3.09	1.39	1.35
4	C	1802	PLP	C4A-C4	-2.91	1.45	1.51
3	C	1801	B12	C6B-C5B	2.81	1.47	1.40
3	B	1801	B12	C6B-C5B	2.69	1.47	1.40
4	A	1802	PLP	C4A-C4	-2.67	1.46	1.51
5	A	1500	5AD	C6-N6	2.58	1.43	1.34
5	D	1500	5AD	C6-N6	2.58	1.43	1.34
5	C	1500	5AD	C6-N6	2.58	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1802	PLP	C5-C4	-2.56	1.37	1.40
4	B	1802	PLP	C4A-C4	-2.52	1.46	1.51
5	D	1500	5AD	C4-N3	2.49	1.39	1.35
5	A	1500	5AD	C2-N1	2.43	1.38	1.33
5	C	1500	5AD	C4-N3	2.36	1.38	1.35
5	C	1500	5AD	C2-N1	2.22	1.38	1.33
3	B	1801	B12	C16-C15	-2.17	1.33	1.41
3	B	1801	B12	C1-C19	-2.16	1.50	1.55
3	C	1801	B12	C16-C15	-2.11	1.33	1.41
5	D	1500	5AD	C2-N1	2.09	1.37	1.33
3	B	1801	B12	C1-C2	-2.07	1.54	1.58

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1500	5AD	C5'-C4'-C3'	10.91	127.15	115.70
5	D	1500	5AD	C5'-C4'-C3'	10.72	126.96	115.70
5	A	1500	5AD	C5'-C4'-C3'	8.83	124.97	115.70
3	C	1801	B12	C1-C19-N24	8.73	116.06	106.24
3	A	1801	B12	C1-C19-N24	8.60	115.91	106.24
3	D	1801	B12	C1-C19-N24	8.47	115.77	106.24
3	B	1801	B12	C20-C1-C19	-7.87	101.77	109.36
3	C	1801	B12	C20-C1-C19	-7.71	101.92	109.36
3	B	1801	B12	C1-C19-N24	7.50	114.67	106.24
3	B	1801	B12	C47-C12-C46	6.97	124.33	109.73
3	A	1801	B12	C47-C12-C46	6.96	124.32	109.73
5	D	1500	5AD	N3-C2-N1	-6.84	117.99	128.68
5	D	1500	5AD	O3'-C3'-C4'	6.68	126.84	110.47
5	C	1500	5AD	O3'-C3'-C4'	6.67	126.80	110.47
3	D	1801	B12	C1-C19-C18	6.62	132.88	121.93
3	C	1801	B12	C47-C12-C46	6.35	123.05	109.73
5	A	1500	5AD	N3-C2-N1	-6.34	118.77	128.68
3	B	1801	B12	C12-C11-C10	-6.32	113.92	124.64
4	B	1802	PLP	O4P-C5A-C5	6.17	121.11	109.35
3	B	1801	B12	C1-C19-C18	6.04	131.92	121.93
5	A	1500	5AD	O3'-C3'-C4'	6.02	125.22	110.47
5	C	1500	5AD	N3-C2-N1	-6.02	119.28	128.68
3	C	1801	B12	C2P-C1P-N59	-6.01	104.07	112.93
3	A	1801	B12	C1-C19-C18	5.98	131.82	121.93
3	C	1801	B12	C1-C19-C18	5.88	131.65	121.93
3	D	1801	B12	C12-C11-C10	-5.83	114.75	124.64
3	D	1801	B12	C47-C12-C46	5.75	121.79	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1802	PLP	O4P-C5A-C5	5.64	120.09	109.35
4	A	1802	PLP	O4P-C5A-C5	5.61	120.04	109.35
3	C	1801	B12	C12-C11-C10	-5.53	115.26	124.64
3	C	1801	B12	C26-C2-C1	5.47	118.53	110.02
3	A	1801	B12	C20-C1-C19	-5.47	104.08	109.36
3	D	1801	B12	C20-C1-C19	-5.14	104.41	109.36
3	A	1801	B12	C12-C11-C10	-5.04	116.09	124.64
3	A	1801	B12	C26-C2-C1	4.71	117.34	110.02
5	A	1500	5AD	O3'-C3'-C2'	4.57	126.62	111.82
5	D	1500	5AD	O2'-C2'-C3'	4.56	126.58	111.82
5	A	1500	5AD	O2'-C2'-C3'	4.47	126.30	111.82
3	C	1801	B12	C30-C3-C2	-4.44	109.72	119.13
3	C	1801	B12	C2-C1-C19	4.39	125.53	118.60
5	A	1500	5AD	O2'-C2'-C1'	4.35	126.90	110.85
3	D	1801	B12	C16-C15-C14	-4.32	117.53	124.27
3	A	1801	B12	C19-C1-N21	4.29	106.55	102.16
5	C	1500	5AD	O2'-C2'-C1'	4.28	126.67	110.85
3	D	1801	B12	C19-C1-N21	4.24	106.51	102.16
5	C	1500	5AD	O2'-C2'-C3'	4.18	125.34	111.82
5	C	1500	5AD	O3'-C3'-C2'	4.16	125.26	111.82
3	A	1801	B12	C16-C15-C14	-4.11	117.86	124.27
3	A	1801	B12	C54-C17-C18	-4.10	106.93	112.98
5	D	1500	5AD	O2'-C2'-C1'	4.05	125.80	110.85
3	D	1801	B12	C26-C2-C1	4.02	116.26	110.02
5	D	1500	5AD	O3'-C3'-C2'	3.93	124.52	111.82
4	D	1802	PLP	O4P-C5A-C5	3.90	116.79	109.35
3	B	1801	B12	C54-C17-C18	-3.88	107.25	112.98
3	A	1801	B12	C25-C2-C3	-3.79	109.80	115.58
3	B	1801	B12	C19-C1-N21	3.72	105.97	102.16
5	C	1500	5AD	C3'-C2'-C1'	3.58	106.37	100.98
3	B	1801	B12	C25-C2-C3	-3.55	110.17	115.58
3	B	1801	B12	C2-C1-C19	3.39	123.96	118.60
3	A	1801	B12	C30-C3-C2	-3.36	112.00	119.13
5	D	1500	5AD	C3'-C2'-C1'	3.33	105.99	100.98
3	D	1801	B12	C25-C2-C3	-3.32	110.51	115.58
3	C	1801	B12	C19-C1-N21	3.29	105.54	102.16
3	A	1801	B12	C20-C1-C2	-3.20	108.02	113.32
3	B	1801	B12	C16-C15-C14	-3.20	119.28	124.27
3	D	1801	B12	C30-C3-C2	-3.11	112.54	119.13
3	C	1801	B12	C20-C1-C2	-3.10	108.19	113.32
3	A	1801	B12	C2-C26-C27	-3.10	106.52	115.22
3	A	1801	B12	C2-C1-C19	3.06	123.44	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1500	5AD	O4'-C4'-C5'	3.03	125.15	110.29
3	B	1801	B12	C55-C56-C57	-3.02	104.63	111.23
3	C	1801	B12	C16-C15-C14	-3.02	119.56	124.27
5	A	1500	5AD	O4'-C4'-C5'	3.01	125.06	110.29
3	A	1801	B12	C3-C4-C5	-2.95	120.98	131.68
3	D	1801	B12	C25-C2-C1	-2.94	109.44	113.80
5	C	1500	5AD	O4'-C4'-C5'	2.94	124.70	110.29
5	A	1500	5AD	C3'-C2'-C1'	2.94	105.40	100.98
4	A	1802	PLP	C4A-C4-C5	-2.93	117.92	120.94
3	C	1801	B12	C54-C17-C18	-2.92	108.67	112.98
3	B	1801	B12	C25-C2-C1	-2.90	109.50	113.80
3	D	1801	B12	C3-C4-C5	-2.89	121.21	131.68
3	B	1801	B12	C18-C60-C61	-2.87	106.82	113.97
3	B	1801	B12	C30-C3-C2	-2.84	113.12	119.13
3	C	1801	B12	C25-C2-C1	-2.81	109.62	113.80
4	B	1802	PLP	C5-C6-N1	-2.80	119.16	123.82
3	C	1801	B12	C25-C2-C3	-2.79	111.32	115.58
3	B	1801	B12	C2P-C1P-N59	-2.72	108.92	112.93
3	A	1801	B12	C9-C10-C11	-2.71	121.44	130.91
3	B	1801	B12	C6-C5-C4	-2.70	120.06	124.27
3	A	1801	B12	C2-C3-C4	-2.70	98.84	101.67
4	B	1802	PLP	O3P-P-O4P	2.69	113.90	106.73
3	D	1801	B12	C2-C1-C19	2.68	122.83	118.60
3	D	1801	B12	C20-C1-C2	-2.66	108.91	113.32
3	B	1801	B12	C20-C1-C2	-2.65	108.93	113.32
3	A	1801	B12	C6-C5-C4	-2.54	120.30	124.27
3	A	1801	B12	C13-C14-C15	-2.54	122.49	131.68
3	A	1801	B12	C3R-C2R-C1R	2.50	105.43	99.89
3	C	1801	B12	C2-C26-C27	-2.49	108.21	115.22
3	A	1801	B12	C2P-C1P-N59	-2.48	109.28	112.93
3	C	1801	B12	C18-C60-C61	-2.46	107.83	113.97
3	D	1801	B12	C9-C10-C11	-2.46	122.32	130.91
3	C	1801	B12	C13-C14-C15	-2.46	122.77	131.68
3	B	1801	B12	C3-C4-C5	-2.45	122.78	131.68
3	B	1801	B12	C26-C2-C1	2.45	113.83	110.02
3	D	1801	B12	C6-C5-C4	-2.43	120.48	124.27
3	C	1801	B12	C54-C17-C55	2.41	113.25	109.26
3	C	1801	B12	C3-C4-C5	-2.39	123.01	131.68
3	C	1801	B12	C55-C56-C57	-2.34	106.11	111.23
3	A	1801	B12	C8-C9-N22	2.34	114.04	111.12
3	D	1801	B12	C8-C9-N22	2.28	113.96	111.12
3	B	1801	B12	C1-C2-C3	2.27	104.43	101.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1801	B12	C2-C26-C27	-2.22	108.97	115.22
4	D	1802	PLP	C6-C5-C4	2.22	119.91	118.16
3	A	1801	B12	C1-C2-C3	2.22	104.37	101.59
3	D	1801	B12	C55-C56-C57	-2.22	106.38	111.23
4	B	1802	PLP	C3-C4-C5	2.22	121.14	118.74
3	C	1801	B12	C6-C5-C4	-2.20	120.85	124.27
4	C	1802	PLP	O2P-P-O4P	2.19	112.55	106.73
3	D	1801	B12	C3R-C2R-C1R	2.18	104.73	99.89
3	B	1801	B12	C8-C9-N22	2.16	113.81	111.12
4	B	1802	PLP	C2A-C2-C3	2.13	123.53	120.89
3	C	1801	B12	C2R-C3R-C4R	2.13	107.00	103.22
4	D	1802	PLP	C5-C6-N1	-2.13	120.27	123.82
3	D	1801	B12	C13-C14-C15	-2.11	124.02	131.68
3	A	1801	B12	C60-C18-C17	-2.08	110.73	115.74
4	B	1802	PLP	O2P-P-O4P	2.07	112.25	106.73
3	B	1801	B12	C13-C14-C15	-2.04	124.28	131.68
3	B	1801	B12	C9-C10-C11	-2.03	123.84	130.91
4	B	1802	PLP	C4A-C4-C5	-2.02	118.85	120.94

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1801	B12	C19
5	D	1500	5AD	C2'
5	D	1500	5AD	C4'
5	D	1500	5AD	C3'
5	C	1500	5AD	C2'
5	C	1500	5AD	C4'
5	C	1500	5AD	C3'
3	A	1801	B12	C19
3	B	1801	B12	C19
3	D	1801	B12	C19
5	A	1500	5AD	C2'
5	A	1500	5AD	C4'
5	A	1500	5AD	C3'

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1801	B12	C38-C37-C7-C36
3	C	1801	B12	C38-C37-C7-C8
3	C	1801	B12	C42-C41-C8-C7

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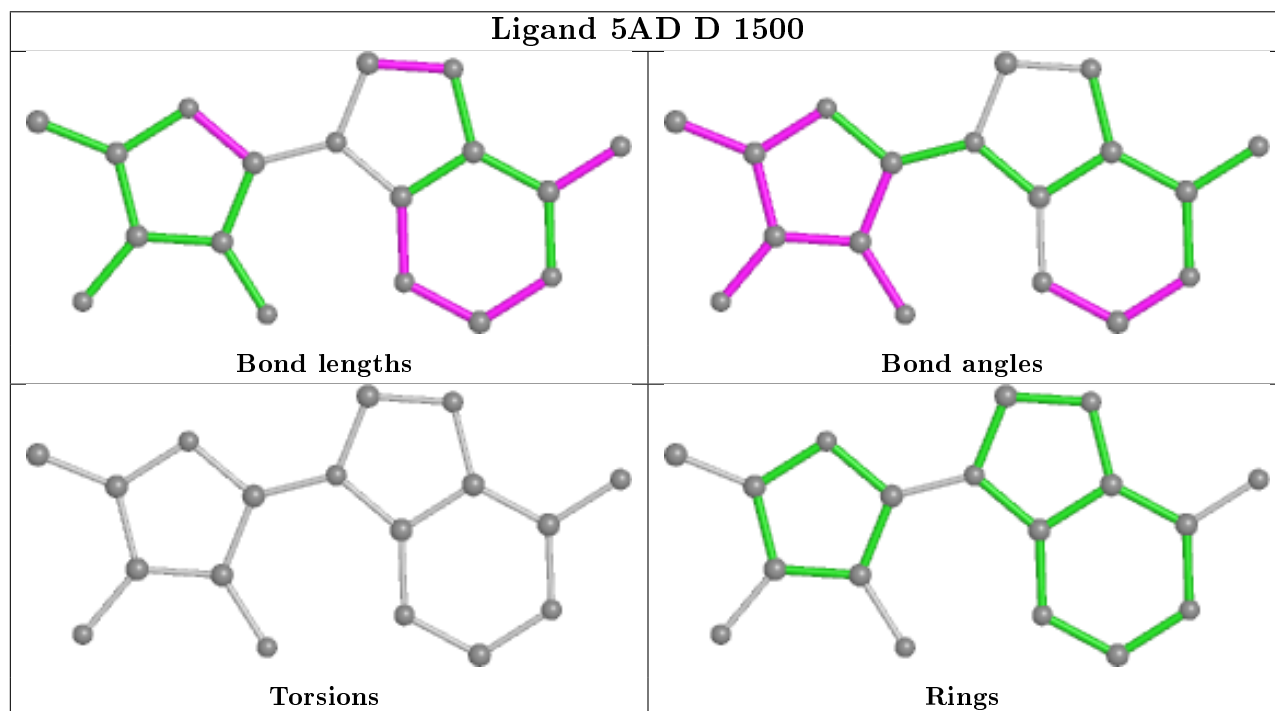
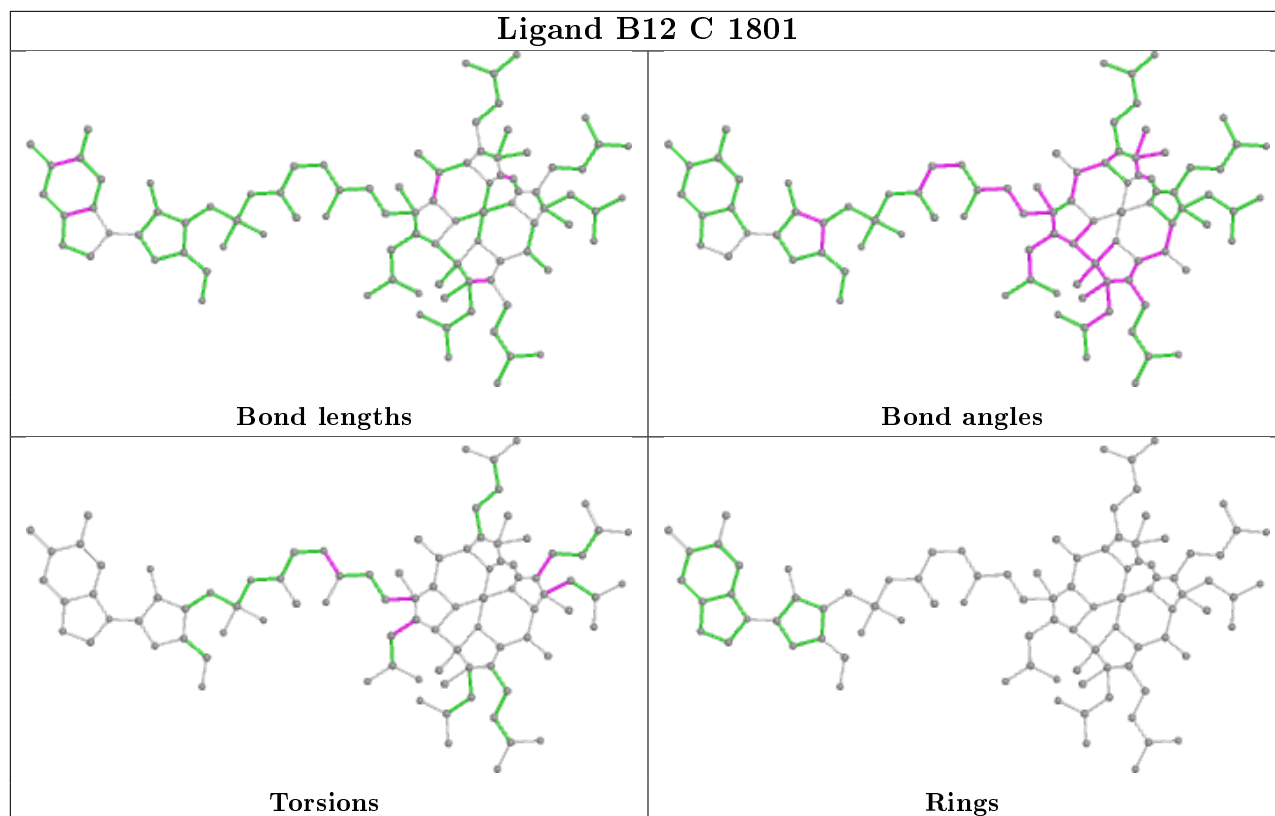
Mol	Chain	Res	Type	Atoms
3	C	1801	B12	C42-C41-C8-C9
3	C	1801	B12	C16-C17-C55-C56
3	C	1801	B12	C54-C17-C55-C56
3	C	1801	B12	C18-C17-C55-C56
3	A	1801	B12	C4-C3-C30-C31
3	A	1801	B12	C42-C41-C8-C9
3	A	1801	B12	N59-C1P-C2P-O3
3	A	1801	B12	C3R-C4R-C5R-O8R
3	A	1801	B12	O6R-C4R-C5R-O8R
3	B	1801	B12	C16-C17-C55-C56
3	B	1801	B12	C18-C17-C55-C56
3	D	1801	B12	C16-C17-C55-C56
3	D	1801	B12	C54-C17-C55-C56
3	D	1801	B12	C18-C17-C55-C56
3	D	1801	B12	C56-C57-N59-C1P
3	D	1801	B12	C1P-C2P-O3-P
3	D	1801	B12	C3P-C2P-O3-P
3	D	1801	B12	O58-C57-N59-C1P
3	A	1801	B12	C8-C41-C42-C43
3	C	1801	B12	C56-C57-N59-C1P
3	C	1801	B12	O58-C57-N59-C1P
3	A	1801	B12	C2-C3-C30-C31
3	D	1801	B12	C3-C2-C26-C27
3	D	1801	B12	C42-C41-C8-C7
3	B	1801	B12	C54-C17-C55-C56
3	D	1801	B12	C2-C3-C30-C31
3	A	1801	B12	N59-C1P-C2P-C3P
3	A	1801	B12	C41-C42-C43-O44
3	D	1801	B12	C1-C2-C26-C27
3	D	1801	B12	C38-C37-C7-C8
3	A	1801	B12	C41-C42-C43-N45
3	D	1801	B12	C42-C41-C8-C9
3	D	1801	B12	C14-C13-C48-C49
3	D	1801	B12	C18-C60-C61-O63
3	D	1801	B12	C25-C2-C26-C27
3	A	1801	B12	C38-C37-C7-C8
3	A	1801	B12	C2P-O3-P-O2
3	D	1801	B12	C2-C26-C27-N29
3	D	1801	B12	C18-C60-C61-N62
3	D	1801	B12	C2-C26-C27-O28
3	C	1801	B12	C19-C18-C60-C61
3	C	1801	B12	C17-C18-C60-C61

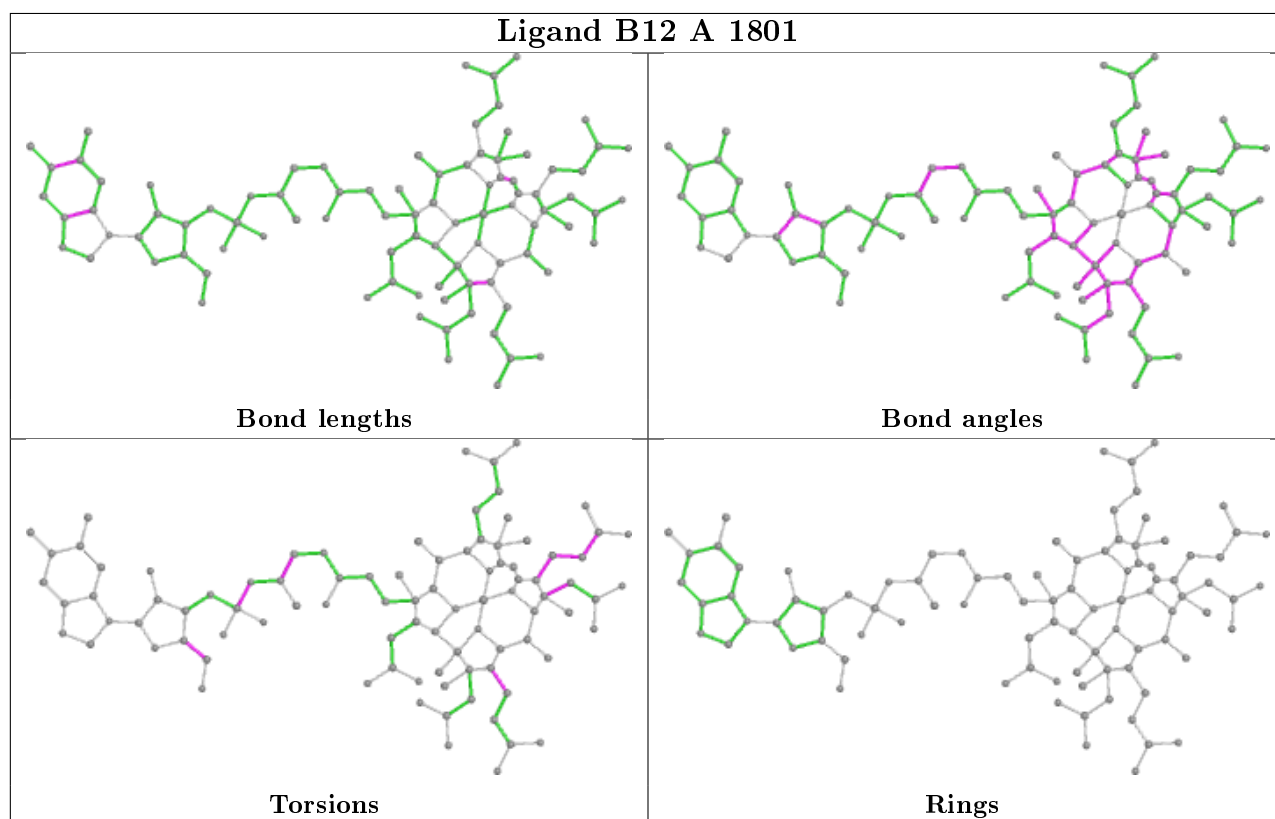
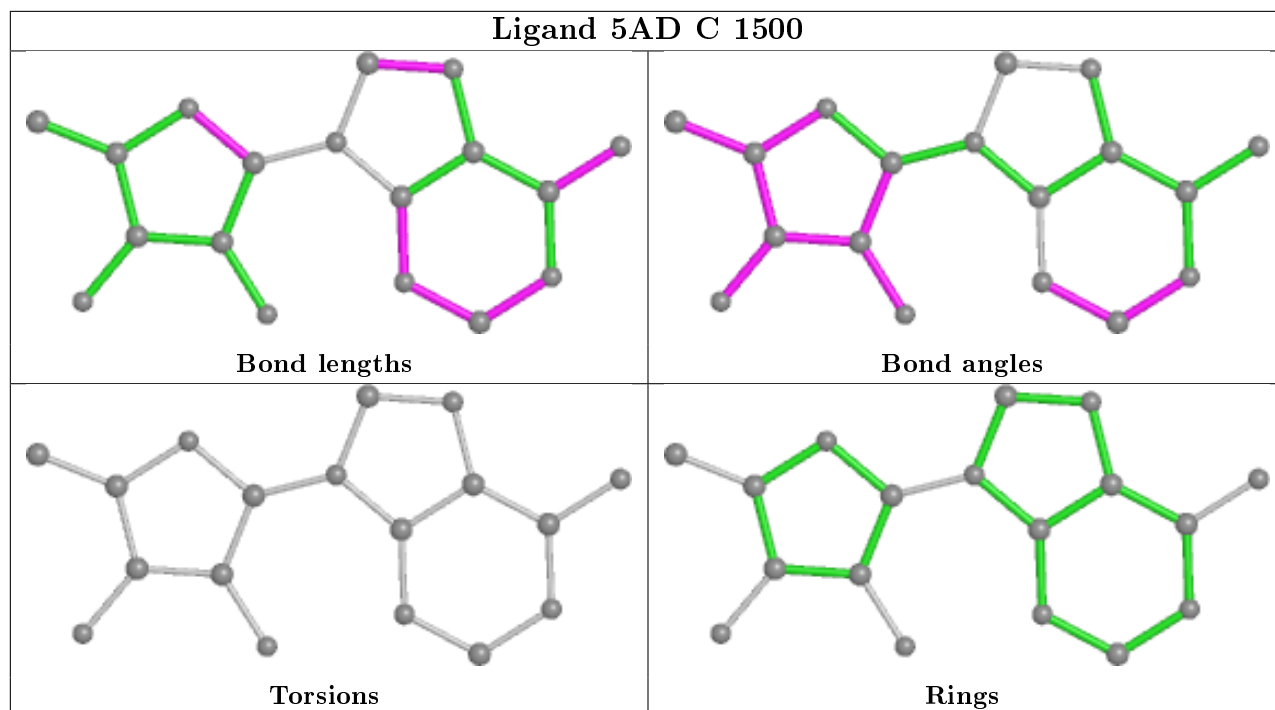
There are no ring outliers.

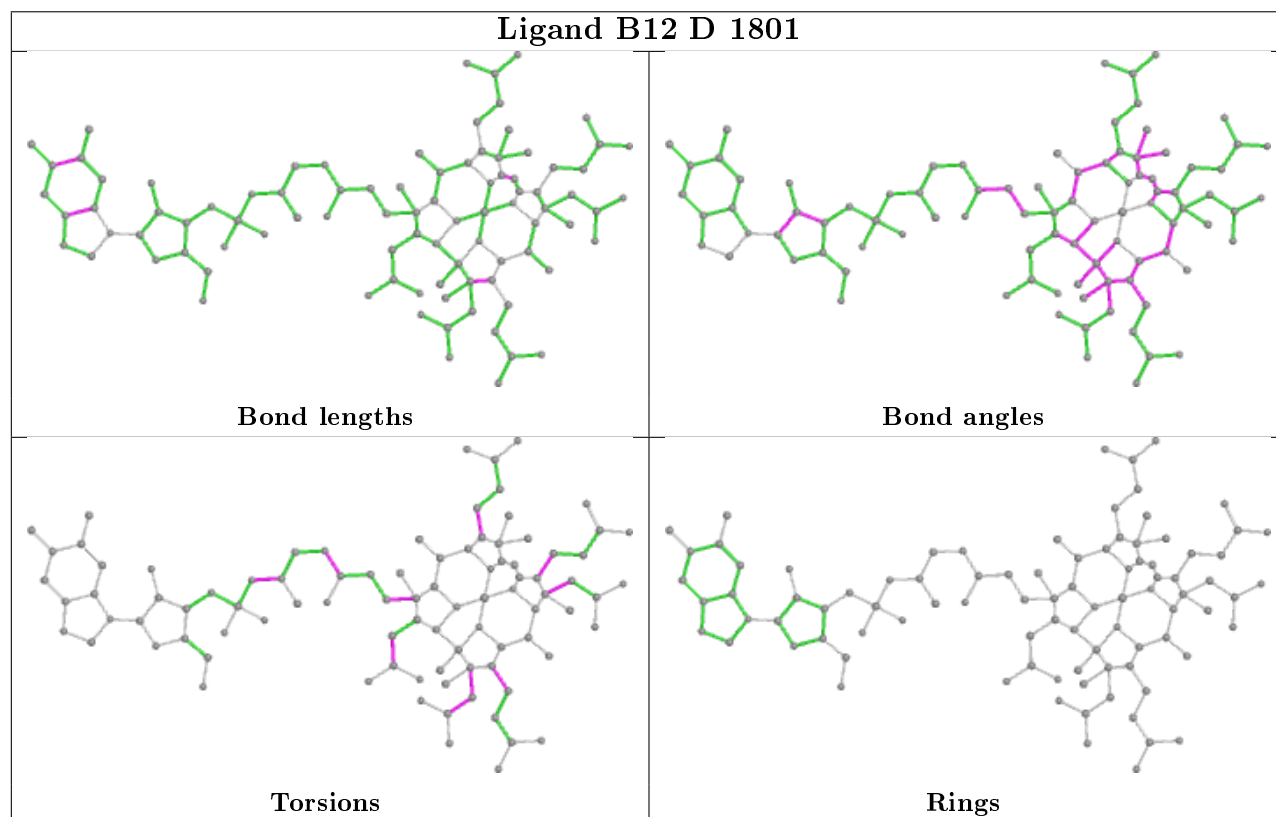
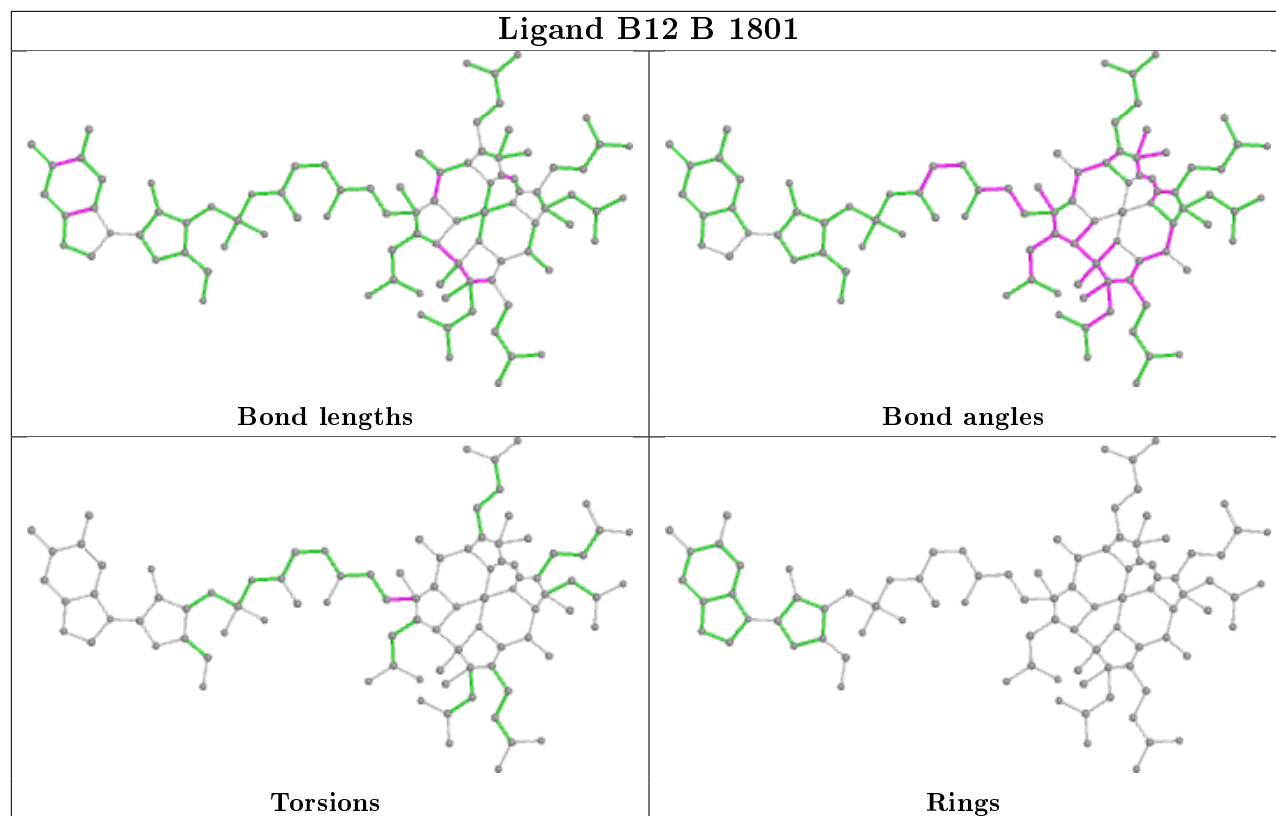
10 monomers are involved in 105 short contacts:

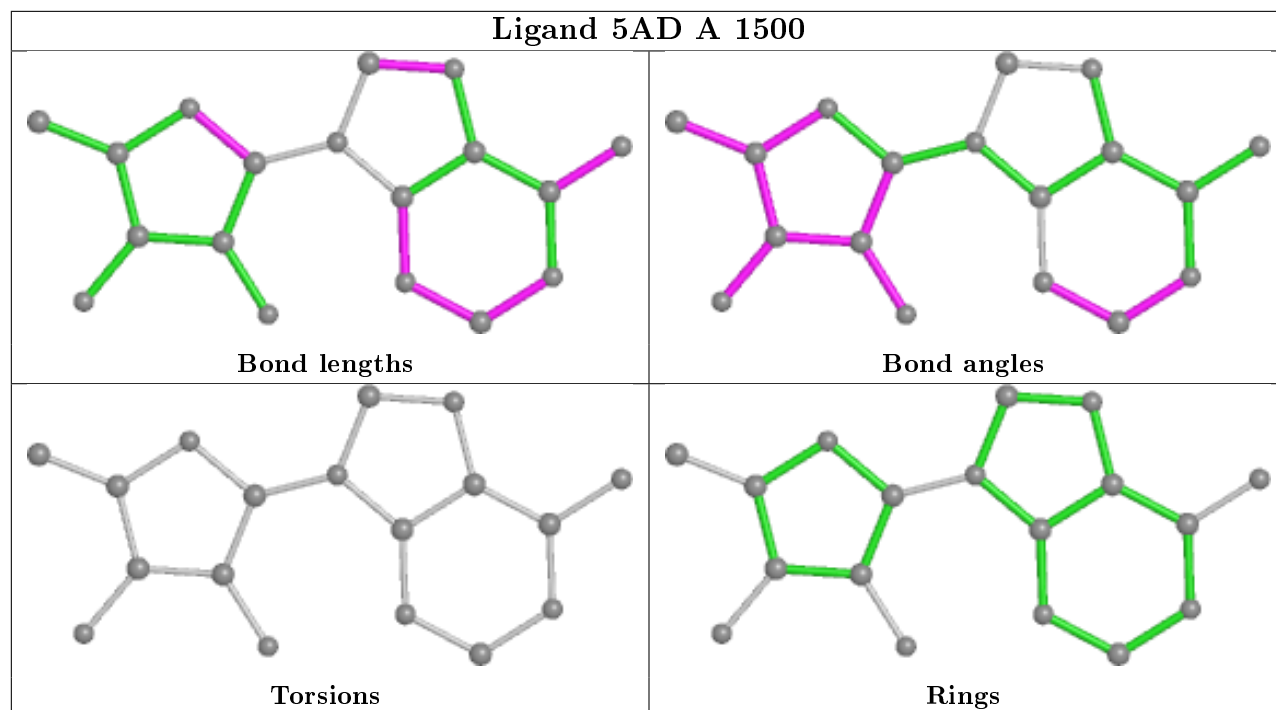
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1801	B12	29	0
5	D	1500	5AD	2	0
4	D	1802	PLP	2	0
5	C	1500	5AD	2	0
3	A	1801	B12	25	0
4	B	1802	PLP	2	0
3	B	1801	B12	27	0
4	A	1802	PLP	2	0
3	D	1801	B12	18	0
5	A	1500	5AD	3	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	727/763 (95%)	-0.15	18 (2%) 57 55	16, 37, 90, 105	0
1	B	728/763 (95%)	-0.38	0 100 100	15, 32, 54, 72	0
1	C	727/763 (95%)	-0.29	0 100 100	17, 38, 65, 84	0
1	D	727/763 (95%)	-0.14	27 (3%) 41 37	15, 30, 93, 118	0
2	E	109/121 (90%)	-0.32	0 100 100	22, 39, 59, 75	0
2	F	109/121 (90%)	-0.33	0 100 100	19, 32, 53, 69	0
2	G	109/121 (90%)	-0.22	0 100 100	25, 44, 62, 68	0
2	H	109/121 (90%)	-0.18	0 100 100	15, 31, 55, 72	0
All	All	3345/3536 (94%)	-0.24	45 (1%) 77 77	15, 35, 79, 118	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	692	ILE	5.0
1	D	652	LEU	3.6
1	D	688	VAL	3.4
1	D	671	SER	3.2
1	A	680	MET	3.2
1	D	673	ASP	3.1
1	D	683	ILE	3.1
1	D	699	GLY	3.0
1	D	672	HIS	2.8
1	D	718	GLY	2.8
1	A	696	ILE	2.8
1	D	714	GLY	2.8
1	D	680	MET	2.7
1	A	657	ILE	2.7
1	A	662	ASP	2.7
1	A	714	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	667	SER	2.6
1	A	602	GLU	2.5
1	D	695	LYS	2.5
1	D	655	ALA	2.4
1	A	715	VAL	2.4
1	D	669	ILE	2.4
1	A	690	LYS	2.4
1	A	617	GLU	2.4
1	A	718	GLY	2.3
1	D	613	VAL	2.3
1	D	653	VAL	2.3
1	D	612	THR	2.3
1	D	648	PRO	2.3
1	D	657	ILE	2.3
1	A	716	ASP	2.2
1	A	711	VAL	2.2
1	D	697	MET	2.2
1	A	710	ALA	2.2
1	D	654	ASP	2.2
1	A	681	LYS	2.1
1	D	687	ALA	2.1
1	D	605	PRO	2.1
1	D	668	THR	2.1
1	A	670	ILE	2.1
1	D	659	LEU	2.1
1	A	655	ALA	2.1
1	A	651	LYS	2.1
1	D	700	CYS	2.0
1	A	606	LEU	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

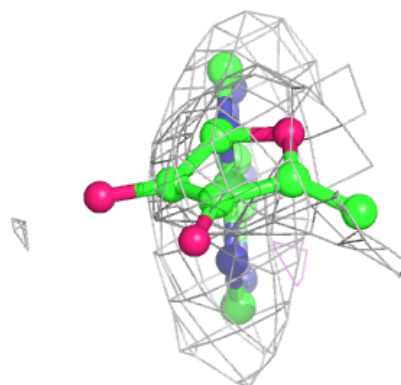
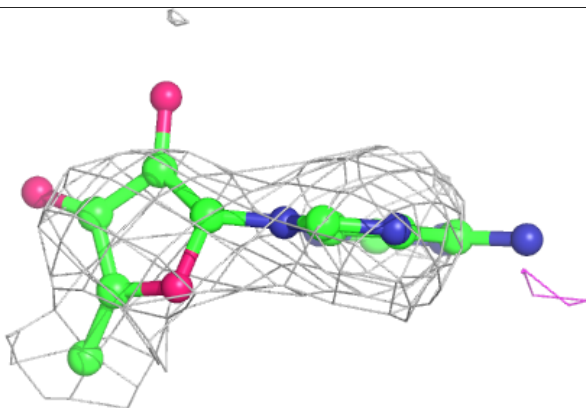
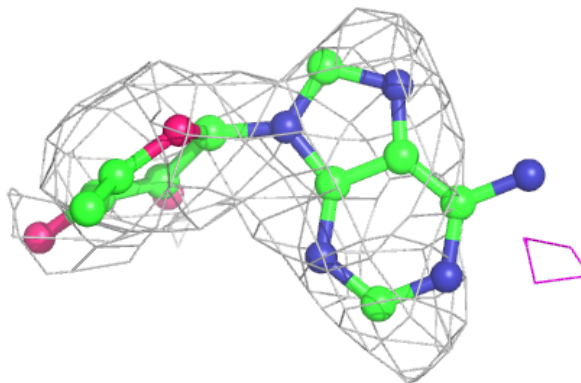
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	5AD	C	1500	18/18	0.85	0.28	68,80,83,86	0
5	5AD	D	1500	18/18	0.93	0.19	27,44,50,51	0
3	B12	D	1801	91/91	0.94	0.24	37,56,69,77	0
5	5AD	A	1500	18/18	0.94	0.23	37,56,61,65	0
3	B12	A	1801	91/91	0.95	0.20	41,65,75,82	0
4	PLP	C	1802	15/16	0.97	0.14	27,29,36,37	0
3	B12	B	1801	91/91	0.97	0.16	16,28,35,38	0
4	PLP	A	1802	15/16	0.97	0.15	30,37,49,52	0
3	B12	C	1801	91/91	0.97	0.17	17,35,43,50	0
4	PLP	D	1802	15/16	0.97	0.12	25,32,38,43	0
4	PLP	B	1802	15/16	0.98	0.13	18,27,36,37	0

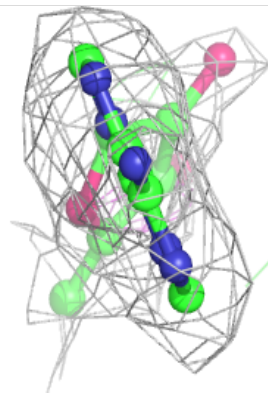
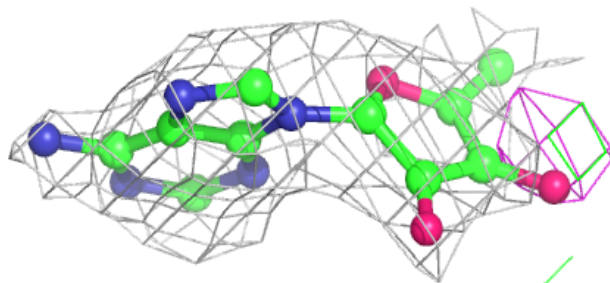
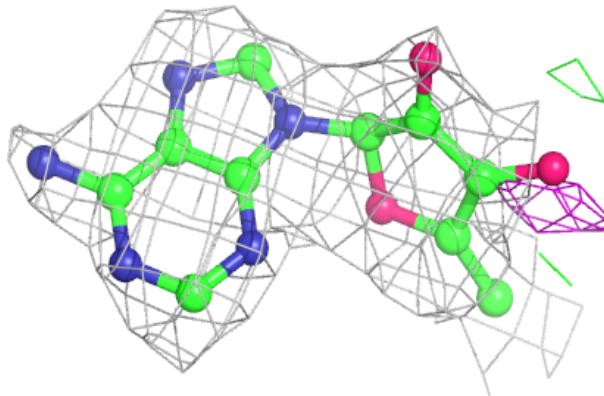
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5AD C 1500:

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

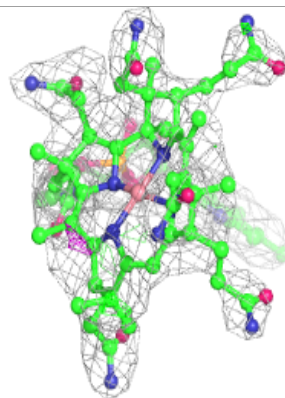
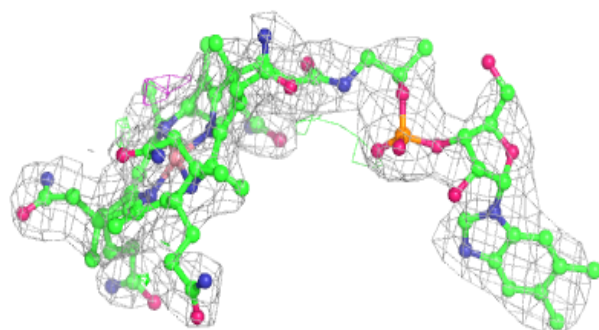
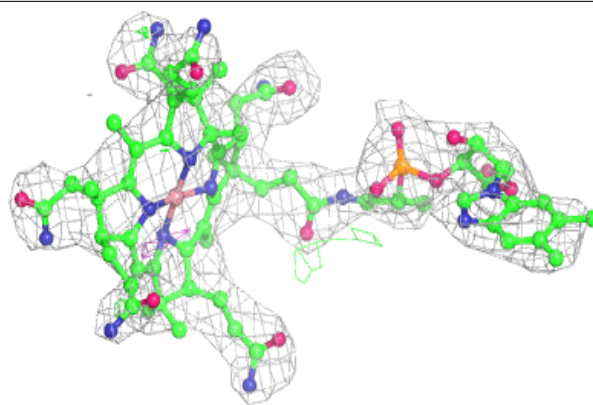
**Electron density around 5AD D 1500:**

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



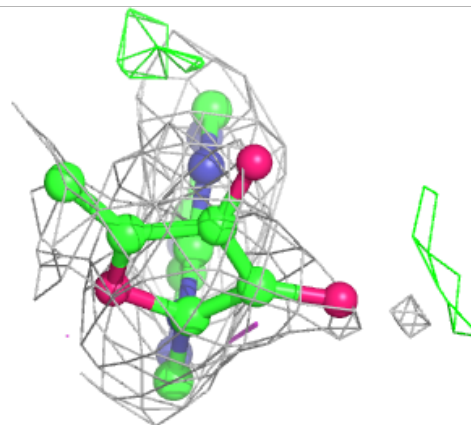
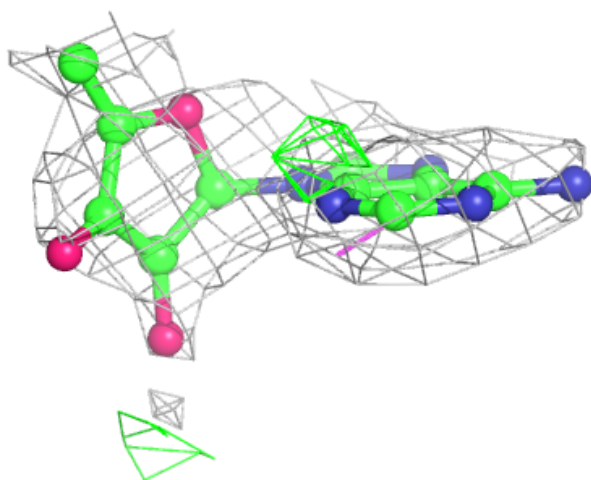
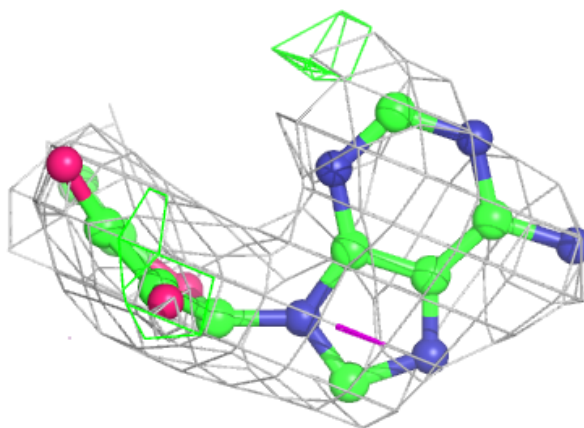
Electron density around B12 D 1801:

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



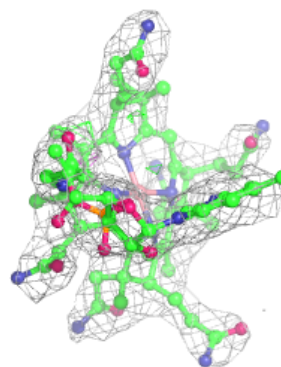
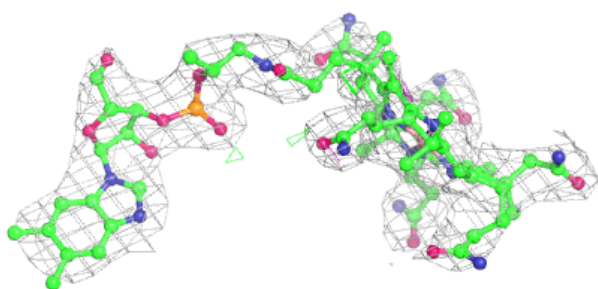
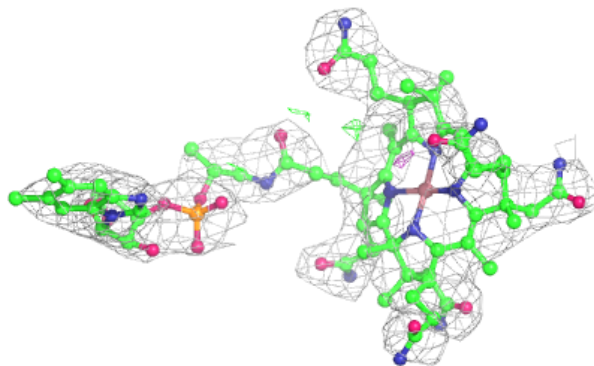
Electron density around 5AD A 1500:

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

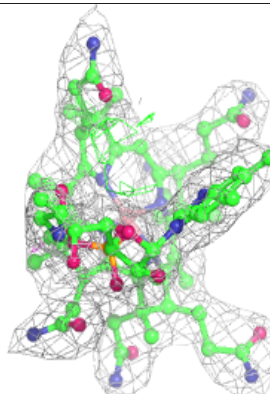
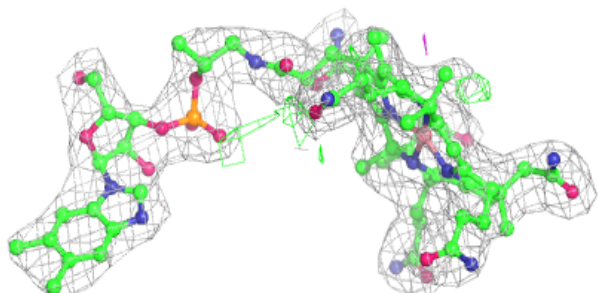
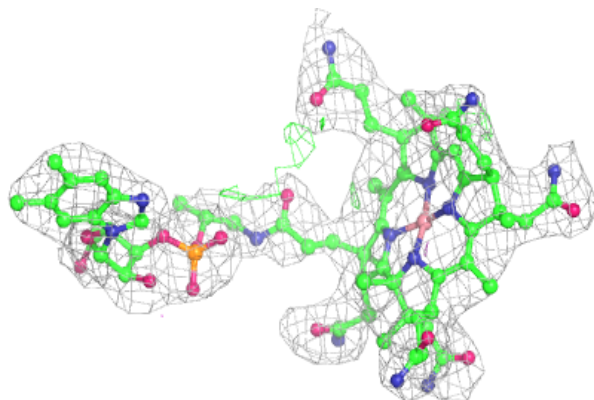


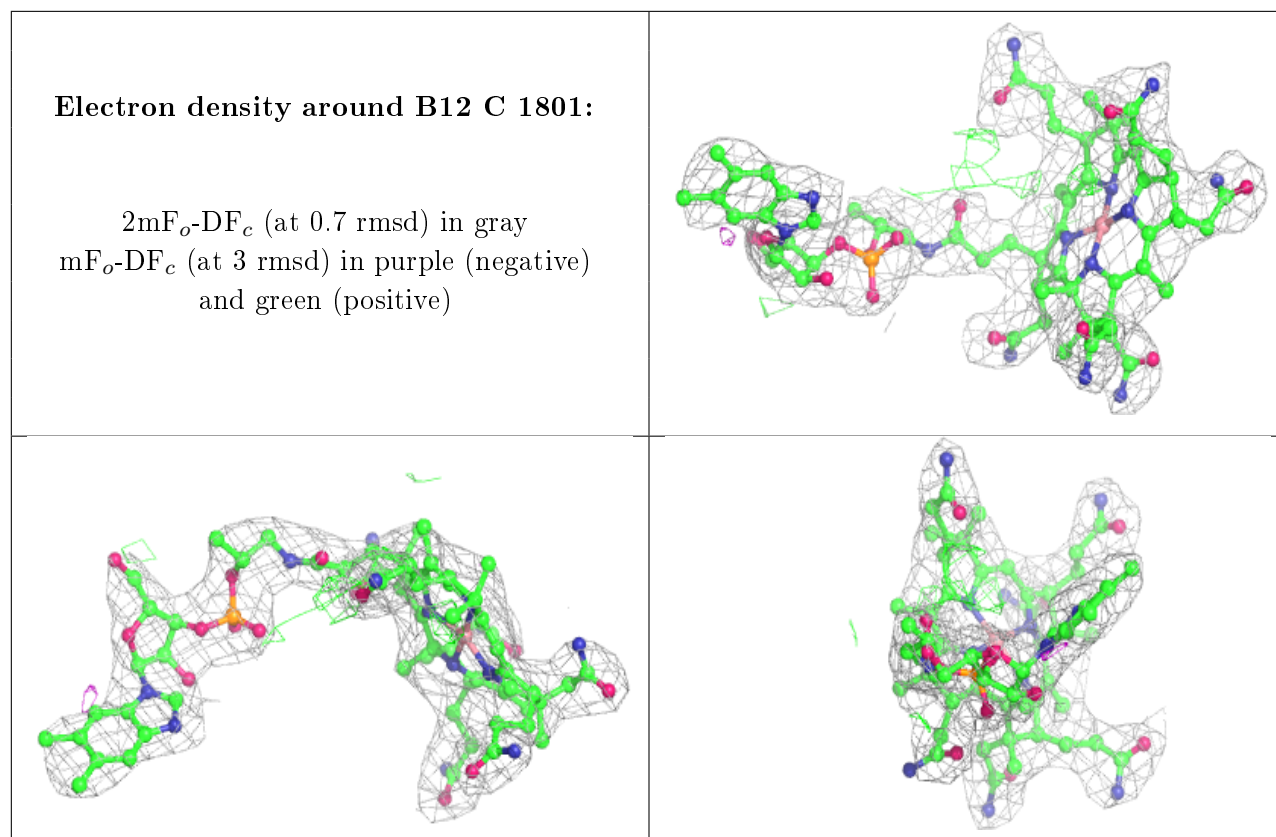
Electron density around B12 A 1801:

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

**Electron density around B12 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.