



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:53 PM UTC

PDB ID : 1P7T / pdb_00001p7t
Title : Structure of Escherichia coli malate synthase G:pyruvate:acetyl-Coenzyme A abortive ternary complex at 1.95 angstrom resolution
Authors : Anstrom, D.M.; Kallio, K.; Remington, S.J.
Deposited on : 2003-05-05
Resolution : 1.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

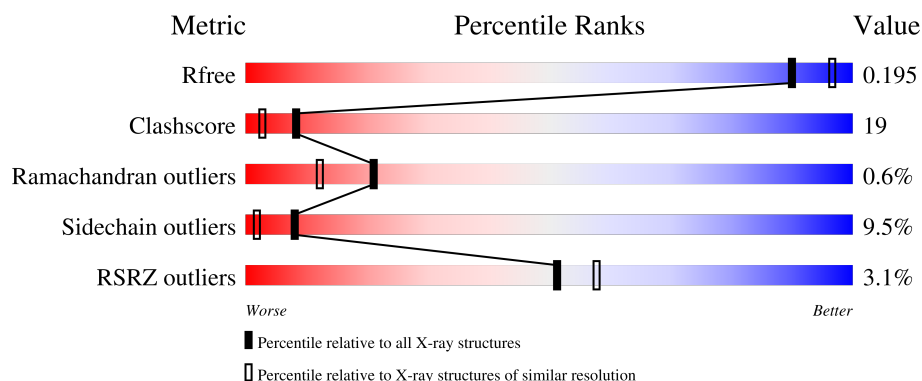
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	731	2% 52% 34% 9% ••
2	B	731	4% 58% 30% 7% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PYR	B	910	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11504 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 Malate synthase G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	0	0	0
			5414	3406	956	1025	27			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	see remark 999	UNP P37330
A	2	ALA	SER	cloning artifact	UNP P37330
A	617	CSO	CYS	modified residue	UNP P37330
A	724	LEU	-	expression tag	UNP P37330
A	725	GLU	-	expression tag	UNP P37330
A	726	HIS	-	expression tag	UNP P37330
A	727	HIS	-	expression tag	UNP P37330
A	728	HIS	-	expression tag	UNP P37330
A	729	HIS	-	expression tag	UNP P37330
A	730	HIS	-	expression tag	UNP P37330
A	731	HIS	-	expression tag	UNP P37330

- Molecule 2 is a protein called Malate synthase G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	705	Total	C	N	O	S	0	0	0
			5358	3379	944	1008	27			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	see remark 999	UNP P37330
B	2	ALA	SER	cloning artifact	UNP P37330
B	617	CSO	CYS	modified residue	UNP P37330
B	688	CSO	CYS	modified residue	UNP P37330
B	724	LEU	-	expression tag	UNP P37330

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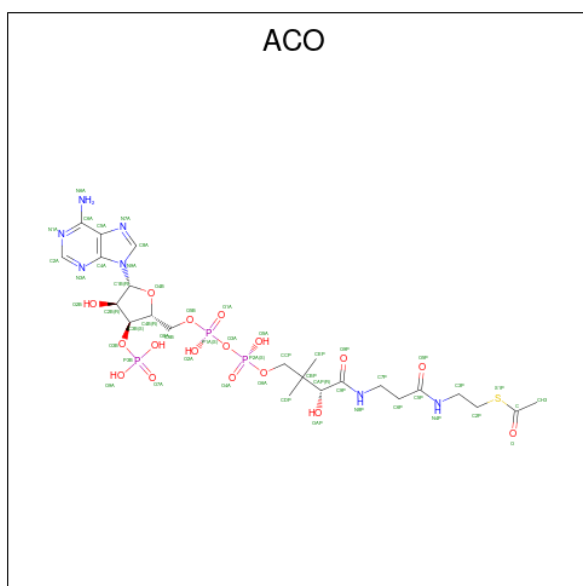
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Chain	Residue	Modelled	Actual	Comment	Reference
B	725	GLU	-	expression tag	UNP P37330
B	726	HIS	-	expression tag	UNP P37330
B	727	HIS	-	expression tag	UNP P37330
B	728	HIS	-	expression tag	UNP P37330
B	729	HIS	-	expression tag	UNP P37330
B	730	HIS	-	expression tag	UNP P37330
B	731	HIS	-	expression tag	UNP P37330

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

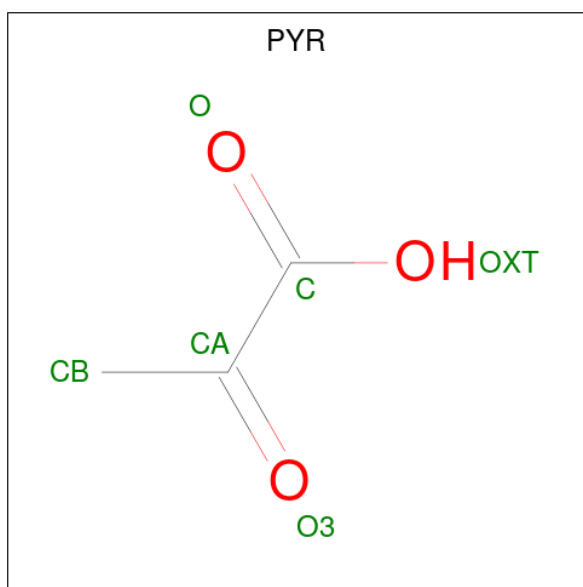
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 51 23 7 17 3 1	0	0
4	B	1	Total C N O P S 51 23 7 17 3 1	0	0

- Molecule 5 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).



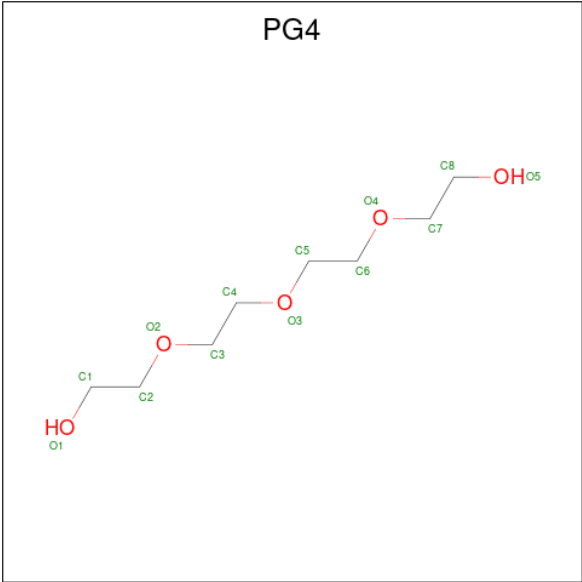
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		

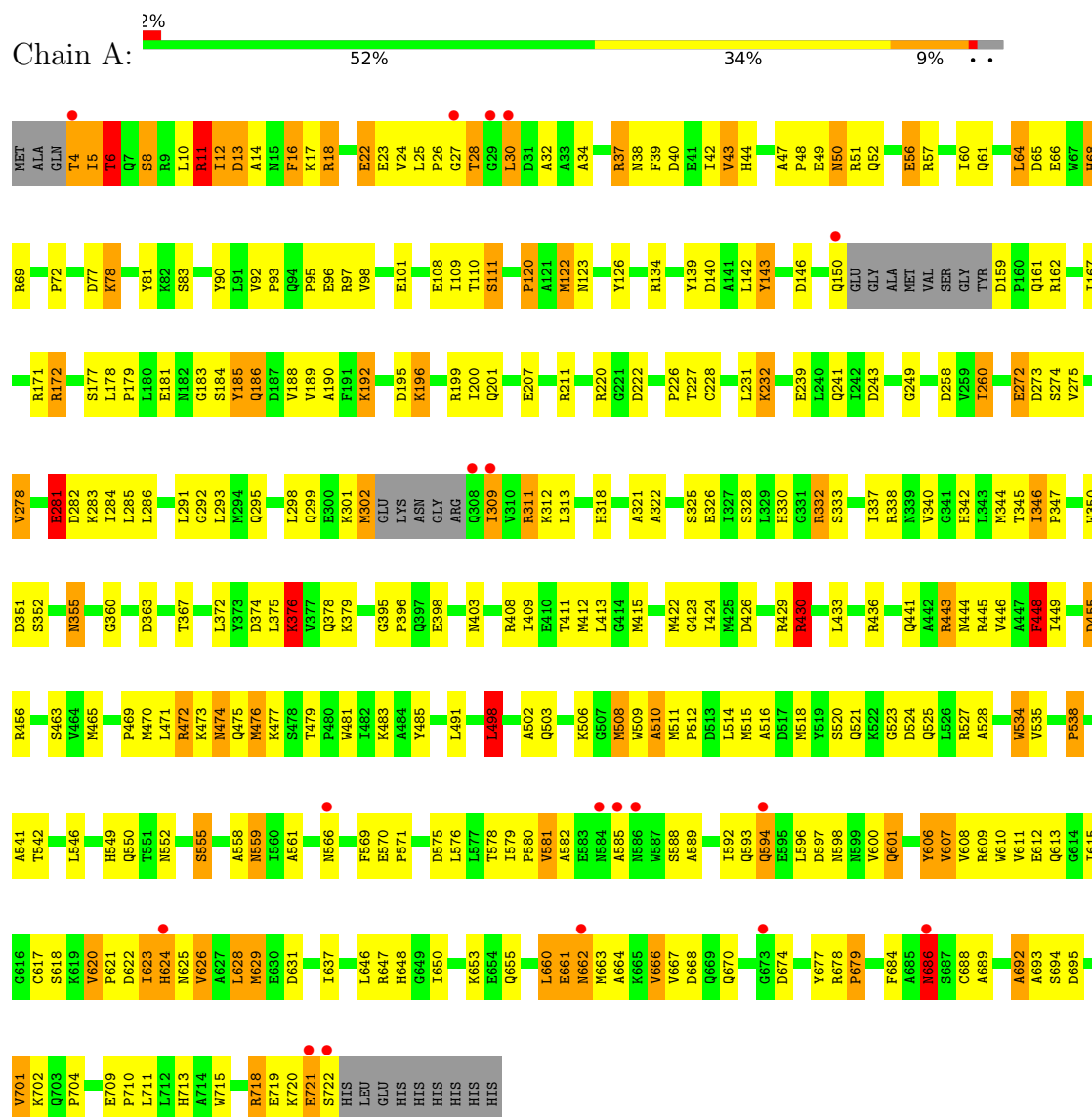
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	308	Total	O	0	0
			308	308		
8	B	275	Total	O	0	0
			275	275		

3 Residue-property plots

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

• Molecule 1: Malate synthase G



• Molecule 2: Malate synthase G





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.93Å 107.39Å 204.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.22 – 1.95 39.22 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.22-1.95) 90.0 (39.22-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 1.95Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.194 , 0.294 0.193 , 0.195	Depositor DCC
R_{free} test set	10721 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 99.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11504	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PG4, CSO, PEG, PYR, ACO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.69	45/5509 (0.8%)	1.89	100/7485 (1.3%)
2	B	1.64	29/5447 (0.5%)	1.85	89/7407 (1.2%)
All	All	1.67	74/10956 (0.7%)	1.87	189/14892 (1.3%)

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	477	LYS	C-N	-8.58	1.22	1.33
1	A	679	PRO	CA-C	-7.64	1.43	1.52
1	A	143	TYR	N-CA	-7.08	1.37	1.46
1	A	43	VAL	CA-CB	-6.98	1.46	1.54
2	B	515	MET	CA-C	-6.60	1.43	1.52
1	A	360	GLY	N-CA	6.51	1.53	1.45
1	A	524	ASP	N-CA	-6.26	1.38	1.46
2	B	642	ILE	CA-C	6.06	1.60	1.52
1	A	44	HIS	CA-C	-6.06	1.44	1.52
2	B	417	PRO	CA-C	-6.04	1.44	1.52
1	A	612	GLU	CD-OE2	6.04	1.36	1.25
2	B	394	HIS	CD2-NE2	5.93	1.44	1.37
1	A	534	TRP	CA-C	-5.92	1.45	1.52
2	B	184	SER	CA-C	-5.89	1.45	1.52
1	A	350	TRP	CA-C	-5.88	1.45	1.52
1	A	655	GLN	N-CA	-5.87	1.39	1.46
1	A	472	ARG	C-N	-5.83	1.26	1.33
1	A	511	MET	C-N	-5.80	1.27	1.34
1	A	167	ILE	CA-C	-5.79	1.45	1.52
2	B	60	ILE	CA-CB	-5.78	1.47	1.54
1	A	143	TYR	CA-C	-5.73	1.45	1.52
2	B	543	LEU	C-O	-5.66	1.17	1.24
1	A	688	CYS	CA-C	5.65	1.60	1.52
1	A	606	TYR	C-N	-5.64	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	39	PHE	C-N	-5.59	1.26	1.33
1	A	109	ILE	CA-C	-5.58	1.47	1.52
1	A	506	LYS	C-O	5.57	1.31	1.23
2	B	136	GLY	CA-C	5.57	1.57	1.51
2	B	50	ASN	N-CA	-5.54	1.39	1.46
1	A	338	ARG	NE-CZ	5.53	1.39	1.33
1	A	181	GLU	CA-C	5.52	1.59	1.52
1	A	57	ARG	NE-CZ	5.50	1.39	1.33
2	B	385	SER	CA-C	-5.49	1.46	1.52
2	B	417	PRO	N-CA	-5.49	1.40	1.47
1	A	18	ARG	C-N	5.49	1.40	1.33
1	A	692	ALA	C-O	5.45	1.30	1.24
1	A	183	GLY	C-O	5.44	1.28	1.23
2	B	615	ILE	C-N	5.43	1.41	1.33
1	A	713	HIS	C-O	-5.42	1.17	1.24
2	B	124	ALA	C-O	5.42	1.30	1.24
2	B	475	GLN	CA-C	5.42	1.60	1.52
2	B	207	GLU	CD-OE2	5.40	1.35	1.25
2	B	118	VAL	CA-C	-5.39	1.46	1.52
1	A	14	ALA	C-O	-5.38	1.18	1.24
2	B	624	HIS	CA-C	-5.34	1.45	1.52
1	A	108	GLU	CD-OE2	5.34	1.35	1.25
2	B	323	ASP	CG-OD2	5.33	1.35	1.25
2	B	468	GLY	C-N	-5.33	1.27	1.33
2	B	285	LEU	CA-C	-5.31	1.45	1.52
1	A	430	ARG	CZ-NH1	5.31	1.40	1.32
1	A	527	ARG	C-O	-5.30	1.17	1.24
2	B	510	ALA	CA-C	-5.26	1.46	1.53
1	A	283	LYS	CA-C	-5.24	1.45	1.52
1	A	535	VAL	CA-C	5.23	1.58	1.52
1	A	72	PRO	N-CA	-5.21	1.41	1.46
1	A	426	ASP	CA-CB	5.20	1.60	1.52
1	A	142	LEU	C-N	-5.18	1.27	1.33
1	A	426	ASP	CG-OD2	5.18	1.35	1.25
2	B	11	ARG	CA-C	5.15	1.59	1.52
1	A	140	ASP	CG-OD2	5.15	1.35	1.25
2	B	113	ALA	C-O	-5.10	1.18	1.23
1	A	549	HIS	CA-C	-5.09	1.45	1.52
2	B	164	GLU	CD-OE2	5.09	1.35	1.25
1	A	423	GLY	CA-C	5.09	1.59	1.51
1	A	661	GLU	N-CA	-5.08	1.40	1.46
2	B	87	GLU	CD-OE2	5.07	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	349	ILE	N-CA	-5.07	1.40	1.46
1	A	558	ALA	C-N	-5.05	1.27	1.33
1	A	111	SER	C-N	-5.05	1.26	1.33
1	A	561	ALA	C-O	-5.04	1.17	1.24
1	A	346	ILE	CA-C	5.03	1.58	1.52
2	B	350	TRP	CA-C	-5.02	1.46	1.52
1	A	56	GLU	C-O	5.02	1.30	1.24
2	B	463	SER	C-N	-5.00	1.27	1.33

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ASP	CA-CB-CG	-10.68	101.92	112.60
1	A	674	ASP	CB-CA-C	10.68	120.74	110.17
2	B	147	ILE	CA-C-N	-10.30	113.57	123.04
2	B	147	ILE	C-N-CA	-10.30	113.57	123.04
1	A	448	PHE	CA-CB-CG	9.80	123.60	113.80
2	B	648	HIS	CA-CB-CG	-8.88	104.92	113.80
1	A	510	ALA	N-CA-C	8.50	122.96	112.59
1	A	679	PRO	N-CA-CB	8.45	110.42	103.32
1	A	226	PRO	CA-C-N	8.35	133.00	120.31
1	A	226	PRO	C-N-CA	8.35	133.00	120.31
2	B	16	PHE	CA-CB-CG	-8.31	105.49	113.80
2	B	200	ILE	N-CA-C	7.82	119.16	107.75
1	A	24	VAL	N-CA-C	7.80	117.84	110.74
1	A	566	ASN	CA-CB-CG	-7.71	104.89	112.60
1	A	686	ASN	CA-CB-CG	7.70	120.30	112.60
1	A	32	ALA	N-CA-C	7.55	119.14	111.07
1	A	581	VAL	N-CA-CB	7.51	120.92	110.56
2	B	239	GLU	N-CA-CB	7.50	122.34	110.65
2	B	713	HIS	CA-CB-CG	-7.49	106.31	113.80
2	B	549	HIS	CA-CB-CG	-7.41	106.39	113.80
2	B	418	ASN	CA-CB-CG	-7.41	105.19	112.60
1	A	376	LYS	CA-C-N	7.22	132.11	120.55
1	A	376	LYS	C-N-CA	7.22	132.11	120.55
1	A	379	LYS	N-CA-CB	7.15	121.31	110.30
2	B	395	GLY	CA-C-N	7.13	126.75	119.19
2	B	395	GLY	C-N-CA	7.13	126.75	119.19
1	A	355	ASN	CA-CB-CG	-7.09	105.51	112.60
2	B	227	THR	N-CA-C	-7.01	104.53	113.23
2	B	703	GLN	CA-C-O	7.00	125.99	119.76
1	A	342	HIS	N-CA-C	6.98	121.05	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	179	PRO	CB-CA-C	-6.96	102.72	111.56
2	B	446	VAL	N-CA-C	6.96	118.00	109.30
1	A	498	LEU	N-CA-CB	6.95	122.55	110.39
2	B	169	TRP	CA-C-O	6.95	127.91	120.55
1	A	110	THR	CA-C-N	-6.92	110.59	122.14
1	A	110	THR	C-N-CA	-6.92	110.59	122.14
2	B	624	HIS	CA-CB-CG	-6.91	106.89	113.80
1	A	549	HIS	CA-CB-CG	-6.83	106.97	113.80
2	B	198	LEU	N-CA-CB	6.79	121.36	110.16
1	A	81	TYR	N-CA-CB	-6.75	100.20	110.12
1	A	16	PHE	CA-CB-CG	-6.75	107.05	113.80
1	A	436	ARG	NE-CZ-NH2	-6.72	113.15	119.20
1	A	443	ARG	N-CA-C	6.64	120.84	112.87
1	A	111	SER	N-CA-C	6.59	121.26	112.30
1	A	192	LYS	N-CA-CB	6.55	122.60	111.66
1	A	607	VAL	CA-C-N	-6.54	112.32	120.56
1	A	607	VAL	C-N-CA	-6.54	112.32	120.56
2	B	442	ALA	CA-C-N	6.53	129.91	120.38
2	B	442	ALA	C-N-CA	6.53	129.91	120.38
2	B	517	ASP	CA-CB-CG	-6.46	106.14	112.60
1	A	701	VAL	CA-C-N	-6.43	111.93	122.54
1	A	701	VAL	C-N-CA	-6.43	111.93	122.54
1	A	363	ASP	CA-C-N	-6.43	112.81	119.94
1	A	363	ASP	C-N-CA	-6.43	112.81	119.94
1	A	542	THR	CA-CB-OG1	-6.42	99.97	109.60
2	B	157	GLY	N-CA-C	-6.37	101.30	110.60
1	A	446	VAL	N-CA-C	6.35	117.51	108.93
1	A	374	ASP	CA-CB-CG	-6.34	106.26	112.60
2	B	600	VAL	CA-C-O	6.33	127.56	120.85
1	A	491	LEU	CA-C-O	6.31	127.24	120.55
2	B	148	ILE	CA-C-O	6.26	123.26	119.19
2	B	345	THR	N-CA-C	-6.24	100.97	110.14
1	A	668	ASP	CA-CB-CG	6.23	118.83	112.60
2	B	241	GLN	CA-C-O	6.21	127.39	120.43
2	B	623	ILE	CA-C-N	-6.15	113.36	122.83
2	B	623	ILE	C-N-CA	-6.15	113.36	122.83
1	A	181	GLU	O-C-N	-6.13	115.75	122.07
2	B	668	ASP	CA-CB-CG	-6.13	106.47	112.60
2	B	522	LYS	N-CA-C	6.13	118.76	111.71
1	A	344	MET	N-CA-C	6.12	118.68	110.35
2	B	579	ILE	N-CA-C	6.12	114.72	109.02
1	A	646	LEU	N-CA-C	-6.08	104.34	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	85	LEU	CA-C-O	6.01	126.93	120.55
1	A	628	LEU	CA-C-N	-5.99	112.86	121.42
1	A	628	LEU	C-N-CA	-5.99	112.86	121.42
2	B	223	ALA	CA-C-N	5.98	128.29	120.28
2	B	223	ALA	C-N-CA	5.98	128.29	120.28
2	B	662	ASN	N-CA-C	5.96	117.58	111.14
1	A	68	HIS	CA-CB-CG	-5.94	107.86	113.80
1	A	227	THR	N-CA-CB	-5.93	101.08	110.28
1	A	626	VAL	N-CA-CB	5.93	118.75	110.56
2	B	705	ASN	CA-CB-CG	-5.93	106.67	112.60
1	A	108	GLU	CA-C-N	-5.93	116.91	122.66
1	A	108	GLU	C-N-CA	-5.93	116.91	122.66
2	B	47	ALA	CA-C-O	5.92	124.09	118.34
2	B	469	PRO	CB-CA-C	-5.92	104.30	111.46
1	A	474	ASN	N-CA-CB	5.91	120.00	110.42
1	A	4	THR	N-CA-CB	5.91	121.54	111.50
2	B	672	ALA	CA-C-N	-5.89	115.13	123.08
2	B	672	ALA	C-N-CA	-5.89	115.13	123.08
1	A	660	LEU	CA-C-N	-5.88	112.40	120.28
1	A	660	LEU	C-N-CA	-5.88	112.40	120.28
1	A	159	ASP	N-CA-CB	5.85	120.45	110.50
1	A	345	THR	N-CA-C	-5.85	100.61	109.85
1	A	11	ARG	N-CA-CB	5.82	119.73	110.65
2	B	57	ARG	CA-C-O	5.80	126.70	120.55
2	B	613	GLN	N-CA-CB	5.80	118.64	110.98
1	A	569	PHE	N-CA-C	5.79	117.59	111.28
1	A	96	GLU	CB-CG-CD	-5.76	102.81	112.60
1	A	704	PRO	N-CA-CB	5.75	108.29	103.17
2	B	131	ALA	N-CA-CB	-5.74	101.69	110.12
2	B	669	GLN	N-CA-C	-5.71	105.06	111.28
1	A	56	GLU	CA-C-N	-5.68	113.06	120.44
1	A	56	GLU	C-N-CA	-5.68	113.06	120.44
1	A	422	MET	N-CA-C	5.67	117.66	108.41
2	B	508	MET	CG-SD-CE	-5.65	88.46	100.90
2	B	322	ALA	N-CA-C	-5.62	104.85	110.97
1	A	188	VAL	N-CA-C	5.62	116.85	109.21
1	A	521	GLN	N-CA-C	5.60	120.12	113.12
2	B	38	ASN	CA-CB-CG	-5.60	107.00	112.60
2	B	242	ILE	N-CA-C	5.59	115.85	107.51
2	B	417	PRO	O-C-N	5.59	129.79	123.03
2	B	671	ASN	CA-CB-CG	-5.59	107.01	112.60
2	B	161	GLN	N-CA-CB	5.58	118.10	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	392	LYS	N-CA-C	5.57	119.26	111.90
1	A	367	THR	CA-C-O	5.56	126.66	120.82
2	B	75	VAL	CA-C-N	-5.55	111.88	121.66
2	B	75	VAL	C-N-CA	-5.55	111.88	121.66
1	A	620	VAL	CA-C-N	5.54	125.86	119.93
1	A	620	VAL	C-N-CA	5.54	125.86	119.93
2	B	575	ASP	O-C-N	5.54	129.08	122.27
1	A	508	MET	N-CA-CB	-5.54	101.83	109.97
2	B	678	ARG	CA-CB-CG	-5.53	103.03	114.10
2	B	336	PHE	CB-CA-C	-5.53	100.52	110.36
2	B	518	MET	CA-C-O	5.51	126.60	120.82
2	B	570	GLU	CA-C-O	5.49	124.11	118.73
1	A	273	ASP	N-CA-C	5.48	119.07	112.38
1	A	12	ILE	N-CA-C	5.48	115.78	108.11
2	B	625	ASN	CA-CB-CG	-5.46	107.14	112.60
2	B	501	LYS	CB-CA-C	-5.45	100.63	109.13
1	A	337	ILE	CA-C-N	-5.43	115.20	122.42
1	A	337	ILE	C-N-CA	-5.43	115.20	122.42
1	A	648	HIS	CA-CB-CG	-5.41	108.39	113.80
1	A	222	ASP	N-CA-CB	5.40	117.94	109.69
1	A	57	ARG	CA-C-O	5.39	126.48	120.82
2	B	537	SER	N-CA-C	5.39	113.07	108.22
2	B	95	PRO	N-CA-CB	5.39	108.04	103.35
1	A	646	LEU	CB-CA-C	-5.37	102.69	110.96
2	B	713	HIS	CA-C-O	5.37	126.65	120.90
2	B	322	ALA	CB-CA-C	-5.35	102.72	110.96
2	B	531	ASN	CA-C-O	5.34	125.89	119.59
2	B	25	LEU	N-CA-C	5.34	120.19	113.25
1	A	211	ARG	N-CA-C	-5.33	105.47	111.28
2	B	417	PRO	N-CA-CB	5.31	108.04	103.31
1	A	278	VAL	N-CA-CB	-5.31	106.01	112.33
1	A	589	ALA	N-CA-C	-5.30	105.50	111.28
1	A	22	GLU	CB-CG-CD	-5.30	103.60	112.60
1	A	465	MET	N-CA-CB	-5.30	101.54	110.49
2	B	124	ALA	O-C-N	5.29	127.73	122.12
2	B	243	ASP	N-CA-C	5.29	116.20	107.20
2	B	222	ASP	N-CA-CB	5.28	117.78	110.17
1	A	318	HIS	CA-CB-CG	-5.27	108.53	113.80
1	A	241	GLN	CA-CB-CG	-5.26	103.57	114.10
1	A	6	THR	CA-CB-OG1	5.26	117.49	109.60
1	A	56	GLU	CA-C-O	5.25	126.01	119.97
1	A	455	ASP	CA-C-O	5.25	126.11	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	580	PRO	N-CA-CB	5.23	106.24	102.79
2	B	275	VAL	N-CA-CB	-5.23	102.86	111.44
1	A	278	VAL	N-CA-C	5.21	118.73	113.47
1	A	120	PRO	N-CA-CB	5.20	107.46	103.30
2	B	300	GLU	N-CA-C	5.18	117.04	108.13
1	A	411	THR	CA-CB-CG2	-5.17	101.70	110.50
2	B	161	GLN	N-CA-C	-5.16	105.55	111.07
1	A	666	VAL	N-CA-CB	-5.16	105.21	110.62
1	A	376	LYS	O-C-N	5.14	129.83	122.28
2	B	381	SER	CA-C-N	-5.13	114.59	122.60
2	B	381	SER	C-N-CA	-5.13	114.59	122.60
2	B	273	ASP	N-CA-C	5.13	118.31	111.75
2	B	375	LEU	N-CA-C	-5.11	105.89	111.82
1	A	637	ILE	N-CA-CB	-5.11	105.05	110.62
1	A	37	ARG	N-CA-CB	5.09	117.78	110.20
2	B	59	ARG	CA-C-O	5.08	125.94	120.55
2	B	99	THR	O-C-N	-5.08	117.33	123.27
1	A	13	ASP	CA-CB-CG	-5.08	107.52	112.60
1	A	227	THR	OG1-CB-CG2	5.08	119.45	109.30
2	B	201	GLN	CB-CA-C	5.08	118.12	109.75
1	A	281	GLU	CA-C-O	5.06	125.91	120.55
1	A	662	ASN	N-CA-CB	5.06	117.65	110.16
1	A	185	TYR	CA-C-O	5.05	125.61	119.49
2	B	78	LYS	CA-C-O	5.05	126.08	120.63
2	B	402	ALA	CA-C-O	5.05	125.91	120.55
1	A	6	THR	CB-CA-C	5.04	118.06	109.75
2	B	12	ILE	CB-CA-C	-5.03	103.13	110.62
1	A	593	GLN	CA-C-O	5.02	126.59	121.07
2	B	201	GLN	N-CA-CB	5.02	118.61	110.43
2	B	382	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	A	523	GLY	CA-C-O	5.01	125.41	119.50
2	B	359	GLU	N-CA-C	5.01	116.74	111.28
2	B	678	ARG	NE-CZ-NH2	-5.00	114.70	119.20

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	5414	0	5271	209	0
2	B	5358	0	5172	197	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	51	0	34	8	0
4	B	51	0	34	11	0
5	A	6	0	0	3	0
5	B	6	0	0	4	0
6	A	7	0	10	1	0
7	B	26	0	36	8	0
8	A	308	0	0	9	0
8	B	275	0	0	9	0
All	All	11504	0	10557	412	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 19.

All (412) 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:B:86:ARG:HH11	2:B:86:ARG:HB2	1.21	1.05
2:B:302:MET:HE3	2:B:311:ARG:HB2	1.41	0.99
1:A:476:MET:HE3	1:A:479:THR:HG21	1.46	0.97
2:B:86:ARG:HB2	2:B:86:ARG:NH1	1.81	0.95
1:A:470:MET:CE	1:A:581:VAL:HG12	2.00	0.91
2:B:217:VAL:HG23	2:B:230:LEU:HD23	1.49	0.91
1:A:476:MET:HE1	1:A:580:PRO:HB3	1.53	0.90
1:A:11:ARG:HG3	1:A:11:ARG:HH11	1.38	0.88
1:A:143:TYR:CE2	1:A:162:ARG:HG2	2.08	0.87
1:A:476:MET:CE	1:A:481:TRP:HE1	1.87	0.87
2:B:346:ILE:HG13	2:B:347:PRO:HD2	1.56	0.87
2:B:122:MET:HA	2:B:122:MET:HE3	1.57	0.86
2:B:508:MET:HG2	2:B:534:TRP:HB3	1.59	0.85
1:A:470:MET:HE1	1:A:581:VAL:HG12	1.58	0.84
1:A:609:ARG:NH1	1:A:615:ILE:HG21	1.93	0.83
1:A:346:ILE:HG13	1:A:347:PRO:HD2	1.58	0.83
2:B:83:SER:HA	2:B:86:ARG:HH12	1.43	0.83
2:B:302:MET:HE3	2:B:311:ARG:CB	2.09	0.82
1:A:546:LEU:O	1:A:550:GLN:HG3	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:MET:HE3	1:A:311:ARG:CB	2.08	0.82
2:B:12:ILE:HD12	2:B:17:LYS:HE2	1.60	0.81
2:B:261:VAL:CG2	2:B:542:THR:HG23	2.09	0.81
1:A:302:MET:HE3	1:A:311:ARG:HB2	1.63	0.81
1:A:122:MET:HE1	1:A:286:LEU:N	1.95	0.80
1:A:8:SER:HB3	1:A:40:ASP:OD2	1.81	0.80
1:A:476:MET:HE1	1:A:580:PRO:CB	2.11	0.80
1:A:97:ARG:HG2	2:B:70:SER:OG	1.83	0.79
2:B:314:ASN:O	2:B:332:ARG:HD3	1.83	0.78
2:B:666:VAL:O	2:B:670:GLN:HG3	1.84	0.78
2:B:76:LYS:HB2	2:B:76:LYS:NZ	1.96	0.78
1:A:18:ARG:O	1:A:22:GLU:HG2	1.84	0.78
1:A:588:SER:O	1:A:592:ILE:HG13	1.85	0.77
1:A:122:MET:HE3	1:A:122:MET:HA	1.65	0.77
2:B:346:ILE:HG12	2:B:348:VAL:HG23	1.66	0.77
1:A:28:THR:OG1	1:A:30:LEU:HB2	1.86	0.76
1:A:42:ILE:HD13	1:A:408:ARG:NH2	2.01	0.76
1:A:609:ARG:HH12	1:A:615:ILE:HG21	1.52	0.73
1:A:476:MET:HE2	1:A:481:TRP:HE1	1.52	0.73
6:A:1001:PEG:H31	8:A:2448:HOH:O	1.88	0.73
1:A:476:MET:CE	1:A:479:THR:HG21	2.19	0.72
1:A:172:ARG:NH1	8:A:2070:HOH:O	2.24	0.71
1:A:195:ASP:C	1:A:196:LYS:HG2	2.15	0.71
2:B:681:ALA:HA	2:B:684:PHE:CE1	2.26	0.71
2:B:617:CSO:SG	4:B:900:ACO:H131	2.31	0.70
1:A:476:MET:HE3	1:A:476:MET:HA	1.73	0.70
2:B:508:MET:HG2	2:B:534:TRP:CB	2.22	0.70
2:B:372:LEU:HA	2:B:375:LEU:HD12	1.74	0.69
2:B:662:ASN:O	2:B:665:LYS:HG3	1.91	0.69
1:A:302:MET:HE1	1:A:311:ARG:NE	2.07	0.69
2:B:12:ILE:HG22	2:B:13:ASP:O	1.91	0.69
2:B:100:VAL:HG11	2:B:498:LEU:HD22	1.72	0.69
2:B:234:ASN:HA	7:B:1002:PG4:H81	1.72	0.69
1:A:476:MET:HE1	1:A:481:TRP:HE1	1.56	0.69
1:A:686:ASN:ND2	8:A:2496:HOH:O	2.25	0.68
1:A:299:GLN:HG2	1:A:312:LYS:HB3	1.76	0.68
1:A:470:MET:HE2	1:A:581:VAL:HG12	1.74	0.68
1:A:56:GLU:HG3	1:A:60:ILE:HD12	1.76	0.67
1:A:372:LEU:HA	1:A:375:LEU:HD12	1.76	0.67
2:B:448:PHE:CB	2:B:503:GLN:HB2	2.25	0.67
1:A:375:LEU:HD11	1:A:415:MET:HE2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:ARG:O	2:B:291:LEU:HB3	1.96	0.66
1:A:594:GLN:NE2	1:A:594:GLN:HA	2.12	0.65
2:B:21:ASP:O	2:B:26:PRO:HD3	1.96	0.65
1:A:28:THR:HA	1:A:376:LYS:NZ	2.11	0.65
1:A:291:LEU:O	1:A:295:GLN:HG3	1.97	0.65
2:B:448:PHE:HB3	2:B:503:GLN:HB2	1.77	0.65
1:A:476:MET:HE3	1:A:479:THR:CG2	2.25	0.65
2:B:475:GLN:NE2	8:B:2154:HOH:O	2.29	0.65
1:A:647:ARG:NE	8:A:2501:HOH:O	2.30	0.65
2:B:217:VAL:HG23	2:B:230:LEU:CD2	2.26	0.65
2:B:244:ALA:O	2:B:250:LYS:HA	1.98	0.65
1:A:508:MET:HE3	4:A:800:ACO:H21	1.78	0.64
1:A:623:ILE:HD11	1:A:624:HIS:NE2	2.13	0.63
2:B:317:ARG:O	2:B:328:SER:HA	1.98	0.63
2:B:83:SER:HA	2:B:86:ARG:NH1	2.13	0.63
2:B:239:GLU:HG2	2:B:260:ILE:HB	1.81	0.63
2:B:358:PRO:HG2	2:B:361:ILE:HD12	1.80	0.63
1:A:508:MET:CE	4:A:800:ACO:H21	2.30	0.62
1:A:472:ARG:HB2	1:A:475:GLN:OE1	1.98	0.62
1:A:720:LYS:O	1:A:722:SER:N	2.30	0.62
2:B:83:SER:CA	2:B:86:ARG:HH12	2.11	0.62
2:B:193:VAL:O	2:B:194:VAL:HG23	1.99	0.62
1:A:120:PRO:HD3	4:A:800:ACO:H71	1.81	0.61
1:A:243:ASP:O	1:A:249:GLY:HA3	2.00	0.61
1:A:498:LEU:CB	1:A:502:ALA:HB3	2.30	0.61
1:A:538:PRO:O	1:A:541:ALA:HB3	1.99	0.61
2:B:202:LEU:HB2	2:B:204:ASN:OD1	2.00	0.61
2:B:12:ILE:CG2	2:B:17:LYS:HB2	2.30	0.61
2:B:76:LYS:HB2	2:B:76:LYS:HZ3	1.66	0.61
2:B:198:LEU:HD23	8:B:2504:HOH:O	2.01	0.61
2:B:198:LEU:HD21	2:B:200:ILE:HD11	1.82	0.61
2:B:10:LEU:HD11	2:B:40:ASP:HA	1.82	0.61
2:B:294:MET:HG3	2:B:370:ILE:HG22	1.83	0.60
1:A:608:VAL:HA	1:A:689:ALA:HB1	1.83	0.60
2:B:460:GLU:O	2:B:464:VAL:HG22	2.01	0.60
1:A:122:MET:HE1	1:A:285:LEU:C	2.26	0.60
1:A:596:LEU:HD12	1:A:600:VAL:HG23	1.83	0.60
2:B:25:LEU:N	2:B:26:PRO:HD2	2.16	0.60
2:B:350:TRP:HA	2:B:355:ASN:O	2.00	0.60
1:A:575:ASP:OD2	1:A:575:ASP:N	2.32	0.60
2:B:436:ARG:NH2	7:B:1003:PG4:H72	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ALA:N	1:A:48:PRO:HD2	2.17	0.60
2:B:633:ALA:CB	4:B:900:ACO:HH31	2.32	0.59
1:A:143:TYR:CD2	1:A:162:ARG:HG2	2.37	0.59
1:A:42:ILE:HD13	1:A:408:ARG:HH21	1.66	0.59
2:B:239:GLU:OE1	2:B:317:ARG:NH2	2.29	0.59
1:A:448:PHE:HB2	1:A:503:GLN:HB2	1.85	0.59
1:A:5:ILE:HG12	1:A:17:LYS:CD	2.33	0.59
1:A:302:MET:HE3	1:A:311:ARG:HB3	1.84	0.59
2:B:16:PHE:O	2:B:20:VAL:HG23	2.03	0.59
2:B:232:LYS:HD2	2:B:237:HIS:NE2	2.19	0.58
1:A:139:TYR:HB2	1:A:258:ASP:OD1	2.03	0.58
2:B:56:GLU:HA	2:B:56:GLU:OE1	2.03	0.58
2:B:252:ASP:CG	2:B:253:PRO:HD2	2.29	0.58
2:B:10:LEU:HD23	2:B:351:ASP:HA	1.86	0.57
2:B:122:MET:HE1	2:B:285:LEU:HB2	1.87	0.57
2:B:436:ARG:HH21	7:B:1003:PG4:H72	1.68	0.57
1:A:509:TRP:CE2	1:A:518:MET:HB2	2.39	0.57
2:B:82:LYS:O	2:B:86:ARG:NH1	2.37	0.57
1:A:199:ARG:NH1	1:A:207:GLU:OE2	2.37	0.57
1:A:321:ALA:HB3	1:A:325:SER:OG	2.05	0.57
1:A:47:ALA:O	1:A:51:ARG:HG3	2.05	0.56
2:B:633:ALA:HB3	4:B:900:ACO:CH3	2.35	0.56
2:B:17:LYS:HZ1	2:B:36:TRP:CD1	2.24	0.56
1:A:598:ASN:ND2	1:A:623:ILE:HG12	2.21	0.56
1:A:498:LEU:HB2	1:A:502:ALA:HB3	1.88	0.56
1:A:39:PHE:O	1:A:43:VAL:HG23	2.05	0.56
1:A:620:VAL:CG1	1:A:621:PRO:HD2	2.36	0.56
1:A:11:ARG:HG3	1:A:11:ARG:NH1	2.13	0.55
1:A:629:MET:O	1:A:629:MET:HG3	1.98	0.55
1:A:663:MET:O	1:A:666:VAL:HB	2.06	0.55
1:A:122:MET:HE1	1:A:285:LEU:HB2	1.88	0.55
1:A:190:ALA:HB3	1:A:201:GLN:HE21	1.71	0.55
2:B:310:VAL:HG12	2:B:310:VAL:O	2.07	0.55
1:A:95:PRO:HG2	1:A:98:VAL:CG2	2.37	0.55
2:B:12:ILE:HG21	2:B:17:LYS:HB2	1.89	0.55
2:B:12:ILE:CD1	2:B:17:LYS:HE2	2.34	0.54
2:B:273:ASP:CG	2:B:632:ARG:HB2	2.33	0.54
2:B:349:ILE:HG22	2:B:350:TRP:N	2.22	0.54
1:A:476:MET:HE2	1:A:481:TRP:NE1	2.22	0.54
1:A:90:TYR:HE2	1:A:433:LEU:HD12	1.71	0.54
1:A:330:HIS:HE1	8:A:2020:HOH:O	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:PRO:HA	1:A:626:VAL:O	2.07	0.54
1:A:617:CSO:SG	4:A:800:ACO:H131	2.48	0.54
1:A:274:SER:HB2	1:A:617:CSO:HB3	1.89	0.53
1:A:184:SER:OG	1:A:186:GLN:HB2	2.09	0.53
1:A:471:LEU:HG	1:A:580:PRO:O	2.08	0.53
1:A:597:ASP:O	1:A:601:GLN:HB3	2.09	0.53
1:A:293:LEU:HG	1:A:298:LEU:HD23	1.90	0.53
2:B:128:LEU:HD23	2:B:313:LEU:CD2	2.38	0.53
2:B:195:ASP:O	2:B:196:LYS:HB2	2.08	0.53
1:A:16:PHE:HA	1:A:284:ILE:HD11	1.91	0.53
2:B:35:PHE:O	2:B:39:PHE:HB2	2.08	0.53
2:B:179:PRO:O	2:B:211:ARG:HB2	2.08	0.53
2:B:217:VAL:CG2	2:B:230:LEU:HD23	2.33	0.53
1:A:598:ASN:HD22	1:A:623:ILE:HG23	1.73	0.53
2:B:311:ARG:NH2	4:B:900:ACO:O8A	2.38	0.53
1:A:97:ARG:HD2	2:B:67:TRP:HA	1.91	0.53
1:A:298:LEU:C	1:A:299:GLN:HG3	2.33	0.53
2:B:374:ASP:O	2:B:378:GLN:N	2.37	0.53
1:A:456:ARG:HG2	1:A:485:TYR:CE1	2.44	0.53
2:B:200:ILE:HD12	2:B:209:THR:HA	1.90	0.53
2:B:633:ALA:HB3	4:B:900:ACO:HH31	1.91	0.53
1:A:631:ASP:OD1	4:A:800:ACO:HH32	2.09	0.52
1:A:409:ILE:O	1:A:413:LEU:HG	2.09	0.52
2:B:128:LEU:HD23	2:B:313:LEU:HD21	1.90	0.52
1:A:95:PRO:HG2	1:A:98:VAL:HG21	1.89	0.52
2:B:302:MET:HE1	2:B:311:ARG:HD2	1.91	0.52
1:A:64:LEU:HD22	1:A:68:HIS:CD2	2.45	0.52
1:A:313:LEU:HB3	1:A:332:ARG:HD2	1.91	0.52
1:A:346:ILE:HG13	1:A:347:PRO:CD	2.35	0.52
2:B:570:GLU:N	2:B:571:PRO:HD2	2.24	0.52
1:A:631:ASP:OD2	4:A:800:ACO:H32	2.09	0.52
2:B:661:GLU:HG2	2:B:684:PHE:CE2	2.45	0.52
7:B:1002:PG4:H32	8:B:2279:HOH:O	2.08	0.52
1:A:122:MET:HA	1:A:122:MET:CE	2.38	0.52
1:A:302:MET:HE1	1:A:311:ARG:CZ	2.39	0.52
2:B:302:MET:HE1	2:B:311:ARG:CZ	2.40	0.52
1:A:498:LEU:HB3	1:A:502:ALA:HB3	1.92	0.52
2:B:298:LEU:O	2:B:299:GLN:HG2	2.10	0.51
2:B:469:PRO:HA	2:B:644:ASN:OD1	2.10	0.51
1:A:596:LEU:HD12	1:A:596:LEU:C	2.35	0.51
2:B:261:VAL:HG22	2:B:542:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:LYS:HD3	2:B:707:TYR:CE1	2.45	0.51
2:B:293:LEU:HG	2:B:298:LEU:HD12	1.92	0.51
1:A:171:ARG:HD2	1:A:185:TYR:HB3	1.92	0.51
1:A:90:TYR:OH	1:A:429:ARG:HD3	2.11	0.51
2:B:198:LEU:HD23	2:B:198:LEU:O	2.10	0.51
1:A:311:ARG:HD3	8:A:2277:HOH:O	2.10	0.51
2:B:534:TRP:CZ3	5:B:910:PYR:CB	2.94	0.51
1:A:12:ILE:O	1:A:13:ASP:C	2.54	0.50
1:A:660:LEU:O	1:A:664:ALA:HB2	2.12	0.50
2:B:198:LEU:HD23	2:B:198:LEU:C	2.35	0.50
2:B:448:PHE:HB2	2:B:503:GLN:HB2	1.94	0.50
2:B:357:ILE:HG12	2:B:358:PRO:N	2.26	0.50
1:A:5:ILE:HG12	1:A:17:LYS:HD3	1.93	0.50
1:A:622:ASP:OD2	1:A:628:LEU:HD11	2.12	0.50
1:A:606:TYR:CZ	1:A:610:TRP:HD1	2.30	0.50
2:B:358:PRO:HB3	8:B:2052:HOH:O	2.11	0.50
2:B:500:GLY:HA2	7:B:1002:PG4:O2	2.12	0.49
2:B:508:MET:HE1	2:B:536:PRO:HA	1.94	0.49
2:B:159:ASP:OD1	2:B:159:ASP:C	2.55	0.49
2:B:188:VAL:O	2:B:254:ALA:HB2	2.12	0.49
1:A:299:GLN:HB3	1:A:311:ARG:O	2.12	0.49
2:B:30:LEU:HD11	2:B:372:LEU:HD11	1.92	0.49
2:B:244:ALA:HB2	2:B:255:HIS:CD2	2.47	0.49
1:A:620:VAL:HG13	1:A:621:PRO:HD2	1.94	0.49
2:B:396:PRO:O	2:B:441:GLN:HG3	2.13	0.49
2:B:34:ALA:O	2:B:38:ASN:ND2	2.45	0.49
2:B:709:GLU:HB2	2:B:710:PRO:HD3	1.94	0.49
1:A:200:ILE:HD12	1:A:200:ILE:N	2.28	0.49
2:B:76:LYS:NZ	8:B:2034:HOH:O	2.46	0.49
2:B:379:LYS:HB3	8:B:2532:HOH:O	2.13	0.49
2:B:198:LEU:HD21	2:B:210:LEU:HG	1.95	0.49
1:A:594:GLN:OE1	1:A:594:GLN:O	2.31	0.49
1:A:5:ILE:HD12	1:A:6:THR:N	2.27	0.48
2:B:234:ASN:CA	7:B:1002:PG4:H81	2.42	0.48
2:B:448:PHE:CD1	2:B:448:PHE:C	2.90	0.48
1:A:579:ILE:HD12	1:A:581:VAL:HG13	1.95	0.48
2:B:49:GLU:O	2:B:50:ASN:C	2.54	0.48
2:B:718:ARG:O	2:B:719:GLU:C	2.54	0.48
1:A:42:ILE:HD12	1:A:408:ARG:HB3	1.94	0.48
1:A:123:ASN:ND2	1:A:126:TYR:CD2	2.81	0.48
2:B:357:ILE:CG1	2:B:358:PRO:HD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:508:MET:HA	2:B:534:TRP:O	2.14	0.48
2:B:386:VAL:HB	2:B:420:LEU:HD23	1.95	0.48
1:A:278:VAL:HG22	1:A:282:ASP:OD2	2.14	0.48
1:A:433:LEU:HD23	1:A:576:LEU:HD13	1.95	0.48
2:B:311:ARG:HH22	4:B:900:ACO:P3B	2.36	0.48
1:A:122:MET:HE3	1:A:286:LEU:HA	1.96	0.47
1:A:196:LYS:HB3	1:A:322:ALA:O	2.14	0.47
1:A:470:MET:HE1	1:A:581:VAL:CG1	2.38	0.47
2:B:410:GLU:CD	2:B:418:ASN:H	2.21	0.47
1:A:28:THR:HA	1:A:376:LYS:HZ1	1.80	0.47
1:A:42:ILE:CD1	1:A:408:ARG:HB3	2.44	0.47
1:A:623:ILE:HG13	1:A:624:HIS:CE1	2.50	0.47
2:B:122:MET:HA	2:B:122:MET:CE	2.35	0.47
1:A:126:TYR:CZ	4:A:800:ACO:H2B	2.49	0.47
2:B:584:ASN:O	2:B:585:ALA:HB3	2.14	0.47
1:A:139:TYR:CD2	1:A:258:ASP:HA	2.50	0.47
1:A:661:GLU:HG2	1:A:684:PHE:CE2	2.50	0.47
1:A:92:VAL:HB	1:A:93:PRO:HD2	1.95	0.47
1:A:596:LEU:CD1	1:A:600:VAL:HG23	2.45	0.47
2:B:349:ILE:CG2	2:B:350:TRP:N	2.77	0.47
2:B:552:ASN:C	2:B:552:ASN:OD1	2.55	0.47
2:B:568:GLU:O	2:B:572:LEU:HG	2.15	0.47
2:B:47:ALA:N	2:B:48:PRO:CD	2.77	0.47
1:A:471:LEU:HD23	1:A:582:ALA:HB2	1.96	0.47
1:A:47:ALA:N	1:A:48:PRO:CD	2.77	0.47
2:B:99:THR:HG22	2:B:443:ARG:HH21	1.80	0.46
2:B:100:VAL:HG11	2:B:498:LEU:CD2	2.43	0.46
1:A:64:LEU:HD13	1:A:463:SER:O	2.16	0.46
1:A:552:ASN:O	1:A:555:SER:OG	2.32	0.46
1:A:25:LEU:N	1:A:26:PRO:CD	2.79	0.46
2:B:12:ILE:HG22	2:B:17:LYS:HB2	1.97	0.46
2:B:252:ASP:OD1	2:B:253:PRO:HD2	2.15	0.46
2:B:317:ARG:HB3	2:B:319:TYR:CE1	2.51	0.46
2:B:505:GLY:HA2	2:B:532:THR:O	2.14	0.46
1:A:396:PRO:O	1:A:441:GLN:HG3	2.16	0.46
1:A:430:ARG:HD2	8:A:2078:HOH:O	2.16	0.46
1:A:469:PRO:HG3	1:A:650:ILE:HD11	1.97	0.46
2:B:39:PHE:CE2	2:B:365:VAL:HG11	2.51	0.46
1:A:299:GLN:HG2	1:A:312:LYS:CB	2.43	0.46
1:A:623:ILE:CD1	1:A:624:HIS:CD2	2.99	0.46
2:B:436:ARG:HH21	7:B:1003:PG4:C7	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:HD13	1:A:260:ILE:N	2.31	0.46
1:A:272:GLU:HG3	1:A:340:VAL:HA	1.98	0.46
2:B:239:GLU:CG	2:B:260:ILE:HB	2.46	0.46
1:A:663:MET:O	1:A:667:VAL:HG23	2.16	0.45
2:B:82:LYS:C	2:B:86:ARG:HH12	2.24	0.45
1:A:607:VAL:O	1:A:608:VAL:C	2.57	0.45
1:A:609:ARG:HD3	1:A:618:SER:OG	2.16	0.45
2:B:178:LEU:N	2:B:179:PRO:CD	2.78	0.45
2:B:193:VAL:HB	2:B:223:ALA:HB1	1.98	0.45
2:B:718:ARG:O	2:B:722:SER:N	2.48	0.45
1:A:701:VAL:HG23	1:A:702:LYS:HG2	1.97	0.45
1:A:311:ARG:HG3	1:A:312:LYS:N	2.31	0.45
1:A:613:GLN:HG3	8:A:2535:HOH:O	2.16	0.45
2:B:25:LEU:N	2:B:26:PRO:CD	2.80	0.45
2:B:238:ILE:HD13	2:B:261:VAL:HG12	1.99	0.45
2:B:321:ALA:N	2:B:325:SER:O	2.38	0.45
1:A:476:MET:CE	1:A:476:MET:HA	2.45	0.45
2:B:178:LEU:O	2:B:185:TYR:OH	2.34	0.45
2:B:302:MET:HE1	2:B:311:ARG:CD	2.46	0.45
1:A:38:ASN:HD22	1:A:38:ASN:HA	1.52	0.45
1:A:220:ARG:NH1	1:A:239:GLU:OE1	2.50	0.45
2:B:570:GLU:N	2:B:571:PRO:CD	2.80	0.45
2:B:226:PRO:HG2	2:B:229:ILE:HD11	1.99	0.45
2:B:417:PRO:O	2:B:418:ASN:HB2	2.17	0.45
1:A:534:TRP:CZ3	5:A:810:PYR:CB	3.01	0.44
4:A:800:ACO:S1P	5:A:810:PYR:CB	3.05	0.44
2:B:603:ILE:O	2:B:607:VAL:HG23	2.18	0.44
2:B:12:ILE:HG21	2:B:12:ILE:HD13	1.75	0.44
2:B:608:VAL:HA	2:B:689:ALA:HB1	1.99	0.44
1:A:498:LEU:HD23	1:A:498:LEU:N	2.33	0.44
2:B:623:ILE:CG2	2:B:624:HIS:CE1	3.01	0.44
1:A:78:LYS:NZ	1:A:578:THR:OG1	2.47	0.44
1:A:623:ILE:CD1	1:A:624:HIS:NE2	2.81	0.44
1:A:721:GLU:O	1:A:722:SER:HB3	2.17	0.44
2:B:297:THR:O	2:B:299:GLN:HG3	2.17	0.44
2:B:357:ILE:HG13	2:B:358:PRO:HD2	1.99	0.44
1:A:372:LEU:HA	1:A:372:LEU:HD23	1.68	0.44
1:A:26:PRO:O	1:A:27:GLY:C	2.59	0.44
1:A:372:LEU:O	1:A:376:LYS:HG2	2.18	0.44
2:B:622:ASP:OD1	2:B:624:HIS:N	2.51	0.44
2:B:681:ALA:HA	2:B:684:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:THR:HA	1:A:376:LYS:HZ3	1.79	0.44
1:A:351:ASP:CG	1:A:355:ASN:HB2	2.43	0.44
2:B:588:SER:OG	2:B:591:GLU:HG3	2.17	0.44
1:A:678:ARG:O	1:A:679:PRO:C	2.61	0.43
1:A:5:ILE:HG12	1:A:17:LYS:HD2	1.98	0.43
1:A:346:ILE:CG1	1:A:347:PRO:HD2	2.38	0.43
2:B:134:ARG:NH1	2:B:332:ARG:O	2.50	0.43
2:B:254:ALA:O	2:B:255:HIS:HB2	2.18	0.43
1:A:232:LYS:HE3	1:A:232:LYS:HB3	1.79	0.43
1:A:709:GLU:O	1:A:710:PRO:C	2.56	0.43
2:B:283:LYS:HD3	2:B:346:ILE:HD13	2.00	0.43
2:B:448:PHE:HB2	2:B:503:GLN:O	2.19	0.43
2:B:623:ILE:HG22	2:B:624:HIS:CE1	2.53	0.43
1:A:146:ASP:OD1	1:A:516:ALA:N	2.43	0.43
1:A:510:ALA:C	1:A:512:PRO:HD3	2.43	0.43
1:A:661:GLU:O	1:A:664:ALA:HB3	2.18	0.43
1:A:92:VAL:HB	1:A:93:PRO:CD	2.49	0.43
1:A:525:GLN:O	1:A:528:ALA:HB3	2.19	0.43
1:A:292:GLY:HA3	1:A:298:LEU:HB2	2.01	0.43
1:A:677:TYR:CE2	1:A:679:PRO:HA	2.54	0.43
1:A:570:GLU:N	1:A:571:PRO:HD2	2.33	0.43
2:B:10:LEU:CD1	2:B:40:ASP:HA	2.46	0.43
2:B:25:LEU:HA	2:B:25:LEU:HD23	1.65	0.43
2:B:82:LYS:C	2:B:86:ARG:NH1	2.76	0.43
1:A:122:MET:HE1	1:A:285:LEU:CB	2.48	0.43
1:A:448:PHE:CD1	1:A:448:PHE:C	2.96	0.43
1:A:692:ALA:HA	1:A:715:TRP:CD1	2.53	0.43
2:B:302:MET:HE1	2:B:311:ARG:NH1	2.34	0.43
1:A:10:LEU:HD21	1:A:40:ASP:HA	2.00	0.42
1:A:16:PHE:CA	1:A:284:ILE:HD11	2.48	0.42
1:A:395:GLY:O	1:A:398:GLU:HB2	2.19	0.42
1:A:34:ALA:HA	1:A:37:ARG:CG	2.48	0.42
1:A:101:GLU:CG	1:A:444:ASN:ND2	2.83	0.42
1:A:101:GLU:CG	1:A:444:ASN:HD21	2.33	0.42
2:B:194:VAL:O	2:B:194:VAL:HG12	2.20	0.42
1:A:301:LYS:HA	1:A:309:ILE:O	2.19	0.42
1:A:510:ALA:HB1	1:A:629:MET:HG2	2.01	0.42
2:B:572:LEU:HD23	2:B:572:LEU:HA	1.88	0.42
2:B:43:VAL:O	2:B:44:HIS:C	2.60	0.42
2:B:210:LEU:HB2	2:B:213:PRO:HA	2.01	0.42
1:A:514:LEU:HA	1:A:514:LEU:HD23	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:PHE:CD2	2:B:35:PHE:C	2.98	0.42
2:B:35:PHE:CE2	2:B:39:PHE:HD2	2.37	0.42
2:B:219:TYR:O	2:B:220:ARG:HG3	2.19	0.42
1:A:647:ARG:O	1:A:647:ARG:HG3	2.12	0.42
2:B:49:GLU:HB2	8:B:2488:HOH:O	2.19	0.42
2:B:283:LYS:HD3	2:B:346:ILE:CD1	2.49	0.42
2:B:301:LYS:HA	2:B:309:ILE:O	2.19	0.42
2:B:330:HIS:CE1	2:B:379:LYS:O	2.72	0.42
2:B:552:ASN:HA	8:B:2185:HOH:O	2.19	0.42
1:A:695:ASP:HB3	1:A:711:LEU:HD13	2.01	0.42
1:A:95:PRO:CG	1:A:98:VAL:CG2	2.97	0.42
1:A:611:VAL:O	1:A:719:GLU:HG2	2.20	0.42
2:B:118:VAL:HG11	4:B:900:ACO:C3P	2.50	0.42
2:B:298:LEU:CD2	2:B:299:GLN:N	2.83	0.42
4:B:900:ACO:C	5:B:910:PYR:CB	2.98	0.42
1:A:122:MET:HE1	1:A:286:LEU:CA	2.49	0.41
1:A:472:ARG:O	1:A:473:LYS:C	2.62	0.41
2:B:86:ARG:HD3	2:B:91:LEU:HD12	2.03	0.41
1:A:620:VAL:HA	1:A:621:PRO:HD3	1.63	0.41
7:B:1002:PG4:H82	7:B:1002:PG4:H61	1.61	0.41
1:A:61:GLN:OE1	1:A:463:SER:HA	2.20	0.41
1:A:515:MET:HA	1:A:515:MET:HE2	2.02	0.41
2:B:174:LEU:HD23	2:B:174:LEU:HA	1.76	0.41
1:A:472:ARG:HB2	1:A:475:GLN:CD	2.45	0.41
1:A:720:LYS:C	1:A:722:SER:N	2.78	0.41
5:A:810:PYR:CB	8:A:2171:HOH:O	2.68	0.41
2:B:288:ARG:HH11	2:B:288:ARG:HD2	1.69	0.41
2:B:330:HIS:HE1	2:B:379:LYS:O	2.03	0.41
2:B:600:VAL:O	2:B:601:GLN:C	2.63	0.41
1:A:49:GLU:O	1:A:50:ASN:C	2.63	0.41
2:B:148:ILE:HA	2:B:149:PRO:HD3	1.91	0.41
2:B:196:LYS:C	2:B:197:GLN:NE2	2.78	0.41
2:B:261:VAL:HG21	2:B:542:THR:HG23	1.97	0.41
2:B:25:LEU:O	2:B:26:PRO:C	2.63	0.41
2:B:73:GLY:HA3	2:B:74:PRO:HD2	1.91	0.41
2:B:126:TYR:CZ	4:B:900:ACO:H2B	2.55	0.41
2:B:229:ILE:HB	2:B:240:LEU:HB2	2.01	0.41
4:B:900:ACO:C	5:B:910:PYR:CA	2.99	0.41
2:B:45:ASP:OD2	2:B:408:ARG:NH1	2.45	0.41
2:B:64:LEU:HD23	2:B:64:LEU:HA	1.81	0.41
2:B:159:ASP:HA	2:B:160:PRO:HD2	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLU:O	1:A:285:LEU:HG	2.20	0.41
1:A:606:TYR:CZ	1:A:610:TRP:CD1	3.07	0.41
2:B:232:LYS:HA	2:B:236:LEU:O	2.20	0.41
2:B:274:SER:HB2	2:B:617:CSO:HB3	2.02	0.41
2:B:345:THR:HA	2:B:358:PRO:HA	2.02	0.41
1:A:65:ASP:O	1:A:69:ARG:HB2	2.21	0.41
1:A:134:ARG:HB2	1:A:333:SER:N	2.36	0.41
2:B:259:VAL:C	2:B:260:ILE:HD13	2.46	0.41
2:B:298:LEU:HD23	2:B:299:GLN:H	1.86	0.41
2:B:380:ASN:O	2:B:382:ARG:HD3	2.21	0.41
4:B:900:ACO:HH33	5:B:910:PYR:C	2.51	0.41
2:B:371:ALA:O	2:B:372:LEU:C	2.64	0.41
2:B:418:ASN:O	2:B:419:THR:C	2.60	0.41
2:B:691:LYS:HE3	2:B:715:TRP:CZ3	2.56	0.41
1:A:122:MET:CE	1:A:286:LEU:CA	2.99	0.40
1:A:559:ASN:ND2	1:A:559:ASN:C	2.79	0.40
2:B:215:GLN:O	2:B:231:LEU:HA	2.21	0.40
1:A:351:ASP:CG	1:A:355:ASN:HD22	2.29	0.40
1:A:403:ASN:OD1	1:A:445:ARG:HD2	2.21	0.40
1:A:718:ARG:HA	1:A:718:ARG:HD3	1.50	0.40
1:A:692:ALA:O	1:A:693:ALA:C	2.62	0.40
1:A:178:LEU:N	1:A:179:PRO:CD	2.84	0.40
1:A:424:ILE:O	1:A:449:ILE:HA	2.22	0.40
2:B:380:ASN:HA	8:B:2075:HOH:O	2.21	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	699/731 (96%)	666 (95%)	30 (4%)	3 (0%)	30 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	697/731 (95%)	665 (95%)	27 (4%)	5 (1%)	18	10
All	All	1396/1462 (96%)	1331 (95%)	57 (4%)	8 (1%)	21	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	ARG
1	A	28	THR
2	B	585	ALA
2	B	26	PRO
1	A	585	ALA
2	B	272	GLU
1	A	721	GLU
2	B	679	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	555/606 (92%)	491 (88%)	64 (12%)	5	1
2	B	538/605 (89%)	498 (93%)	40 (7%)	13	4
All	All	1093/1211 (90%)	989 (90%)	104 (10%)	8	2

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	ILE
1	A	6	THR
1	A	8	SER
1	A	11	ARG
1	A	23	GLU
1	A	30	LEU
1	A	50	ASN

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Mol	Chain	Res	Type
1	A	52	GLN
1	A	64	LEU
1	A	66	GLU
1	A	78	LYS
1	A	83	SER
1	A	111	SER
1	A	122	MET
1	A	150	GLN
1	A	161	GLN
1	A	172	ARG
1	A	177	SER
1	A	186	GLN
1	A	189	VAL
1	A	192	LYS
1	A	196	LYS
1	A	228	CYS
1	A	231	LEU
1	A	232	LYS
1	A	260	ILE
1	A	272	GLU
1	A	275	VAL
1	A	281	GLU
1	A	302	MET
1	A	309	ILE
1	A	311	ARG
1	A	326	GLU
1	A	328	SER
1	A	332	ARG
1	A	352	SER
1	A	376	LYS
1	A	378	GLN
1	A	412	MET
1	A	430	ARG
1	A	443	ARG
1	A	448	PHE
1	A	455	ASP
1	A	474	ASN
1	A	476	MET
1	A	483	LYS
1	A	498	LEU
1	A	520	SER
1	A	538	PRO

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Mol	Chain	Res	Type
1	A	555	SER
1	A	559	ASN
1	A	594	GLN
1	A	601	GLN
1	A	623	ILE
1	A	624	HIS
1	A	625	ASN
1	A	629	MET
1	A	653	LYS
1	A	662	ASN
1	A	670	GLN
1	A	686	ASN
1	A	694	SER
1	A	718	ARG
2	B	28	THR
2	B	46	LEU
2	B	76	LYS
2	B	86	ARG
2	B	91	LEU
2	B	99	THR
2	B	100	VAL
2	B	122	MET
2	B	147	ILE
2	B	148	ILE
2	B	161	GLN
2	B	176	GLU
2	B	194	VAL
2	B	197	GLN
2	B	198	LEU
2	B	200	ILE
2	B	212	THR
2	B	220	ARG
2	B	230	LEU
2	B	242	ILE
2	B	250	LYS
2	B	275	VAL
2	B	286	LEU
2	B	298	LEU
2	B	302	MET
2	B	323	ASP
2	B	327	ILE
2	B	332	ARG

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Mol	Chain	Res	Type
2	B	412	MET
2	B	430	ARG
2	B	441	GLN
2	B	498	LEU
2	B	508	MET
2	B	511	MET
2	B	554	GLN
2	B	581	VAL
2	B	601	GLN
2	B	625	ASN
2	B	669	GLN
2	B	722	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	38	ASN
1	A	52	GLN
1	A	129	ASN
1	A	150	GLN
1	A	197	GLN
1	A	201	GLN
1	A	241	GLN
1	A	299	GLN
1	A	314	ASN
1	A	339	ASN
1	A	355	ASN
1	A	444	ASN
1	A	521	GLN
1	A	559	ASN
1	A	598	ASN
1	A	683	ASN
2	B	38	ASN
2	B	50	ASN
2	B	52	GLN
2	B	197	GLN
2	B	255	HIS
2	B	403	ASN
2	B	418	ASN
2	B	450	ASN
2	B	474	ASN

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Mol	Chain	Res	Type
2	B	521	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSO	A	617	1	3,6,7	1.19	0	1,6,8	0.14	0
2	CSO	B	617	2	3,6,7	0.64	0	1,6,8	0.22	0
2	CSO	B	688	2	3,6,7	2.21	1 (33%)	1,6,8	1.28	0

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
1	CSO	A	617	1	-	0/1/5/7	-
2	CSO	B	617	2	-	0/1/5/7	-
2	CSO	B	688	2	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	688	CSO	CB-CA	3.62	1.62	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	617	CSO	2	0
2	B	617	CSO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	PG4	B	1002	-	12,12,12	1.16	1 (8%)	11,11,11	0.55	0
4	ACO	B	900	-	51,53,53	1.46	6 (11%)	73,79,79	1.18	6 (8%)
4	ACO	A	800	-	51,53,53	1.56	4 (7%)	73,79,79	1.09	6 (8%)
6	PEG	A	1001	-	6,6,6	0.79	0	5,5,5	0.33	0
5	PYR	A	810	3	5,5,5	1.85	2 (40%)	3,6,6	1.77	1 (33%)
7	PG4	B	1003	-	12,12,12	0.59	0	11,11,11	0.47	0
5	PYR	B	910	3	5,5,5	1.46	1 (20%)	3,6,6	2.00	1 (33%)

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
7	PG4	B	1002	-	-	6/10/10/10	-
4	ACO	B	900	-	-	14/51/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACO	A	800	-	-	13/51/67/67	0/3/3/3
6	PEG	A	1001	-	-	2/4/4/4	-
5	PYR	A	810	3	-	0/4/4/4	-
7	PG4	B	1003	-	-	4/10/10/10	-
5	PYR	B	910	3	-	0/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	ACO	P2A-O3A	-6.23	1.52	1.59
4	A	800	ACO	P1A-O3A	-5.22	1.53	1.59
4	B	900	ACO	P1A-O3A	-4.79	1.54	1.59
4	B	900	ACO	P2A-O3A	-4.53	1.54	1.59
4	A	800	ACO	P3B-O3B	-4.47	1.51	1.59
5	A	810	PYR	O-C	2.88	1.29	1.22
4	B	900	ACO	C6P-C5P	2.76	1.56	1.51
5	A	810	PYR	CB-CA	-2.58	1.45	1.50
4	B	900	ACO	P1A-O5B	-2.45	1.49	1.59
5	B	910	PYR	OXT-C	-2.39	1.24	1.30
4	B	900	ACO	P2A-O6A	-2.33	1.50	1.59
7	B	1002	PG4	O4-C7	2.23	1.51	1.42
4	B	900	ACO	C7P-N8P	2.19	1.51	1.46
4	A	800	ACO	C-S1P	2.02	1.86	1.75

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	900	ACO	C4A-N9A-C1B	-3.81	117.72	126.63
4	B	900	ACO	C1B-N9A-C8A	3.68	135.27	127.09
4	B	900	ACO	P3B-O3B-C3B	-3.57	113.89	123.43
4	A	800	ACO	C6P-C5P-N4P	-3.08	110.72	116.34
5	A	810	PYR	OXT-C-CA	3.06	122.06	113.59
5	B	910	PYR	OXT-C-CA	3.03	121.99	113.59
4	B	900	ACO	O6A-CCP-CBP	2.62	114.76	110.55
4	B	900	ACO	C7P-C6P-C5P	2.61	116.74	112.39
4	A	800	ACO	O9A-P3B-O8A	2.54	117.32	107.80
4	B	900	ACO	C7P-N8P-C9P	2.47	126.98	122.55
4	A	800	ACO	C4A-N9A-C1B	-2.30	121.25	126.63
4	A	800	ACO	O6A-CCP-CBP	2.17	114.03	110.55
4	A	800	ACO	CAP-C9P-N8P	-2.03	112.62	116.48
4	A	800	ACO	C2A-N1A-C6A	2.02	122.06	118.73

There are no chirality outliers.

All (39) torsion outliers are listed below:

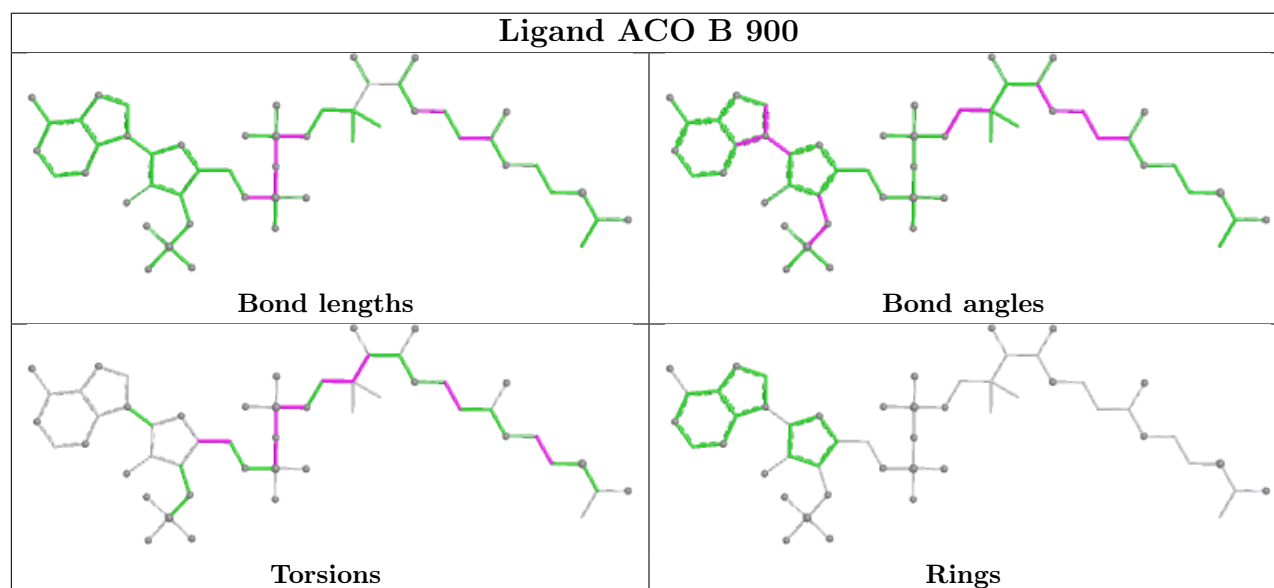
Mol	Chain	Res	Type	Atoms
4	A	800	ACO	C5B-O5B-P1A-O1A
4	A	800	ACO	C5B-O5B-P1A-O3A
4	A	800	ACO	P1A-O3A-P2A-O6A
4	A	800	ACO	CCP-O6A-P2A-O3A
4	A	800	ACO	CCP-O6A-P2A-O5A
4	A	800	ACO	CDP-CBP-CCP-O6A
4	A	800	ACO	CEP-CBP-CCP-O6A
4	A	800	ACO	CAP-CBP-CCP-O6A
4	A	800	ACO	S1P-C2P-C3P-N4P
4	B	900	ACO	P1A-O3A-P2A-O6A
4	B	900	ACO	CCP-O6A-P2A-O3A
4	B	900	ACO	CCP-O6A-P2A-O5A
4	B	900	ACO	CDP-CBP-CCP-O6A
4	B	900	ACO	CEP-CBP-CCP-O6A
4	B	900	ACO	CAP-CBP-CCP-O6A
4	B	900	ACO	C9P-CAP-CBP-CCP
4	B	900	ACO	C9P-CAP-CBP-CDP
4	B	900	ACO	C5P-C6P-C7P-N8P
4	B	900	ACO	S1P-C2P-C3P-N4P
7	B	1002	PG4	C8-C7-O4-C6
4	B	900	ACO	C3B-C4B-C5B-O5B
7	B	1002	PG4	C4-C3-O2-C2
6	A	1001	PEG	O1-C1-C2-O2
4	B	900	ACO	O4B-C4B-C5B-O5B
7	B	1002	PG4	O4-C7-C8-O5
7	B	1003	PG4	C3-C4-O3-C5
7	B	1003	PG4	C1-C2-O2-C3
4	A	800	ACO	CBP-CCP-O6A-P2A
7	B	1003	PG4	O1-C1-C2-O2
4	A	800	ACO	O-C-S1P-C2P
7	B	1002	PG4	O1-C1-C2-O2
6	A	1001	PEG	C1-C2-O2-C3
7	B	1003	PG4	O3-C5-C6-O4
4	A	800	ACO	CH3-C-S1P-C2P
4	B	900	ACO	C9P-CAP-CBP-CEP
7	B	1002	PG4	C6-C5-O3-C4
4	A	800	ACO	C5P-C6P-C7P-N8P
7	B	1002	PG4	O2-C3-C4-O3
4	B	900	ACO	P2A-O3A-P1A-O2A

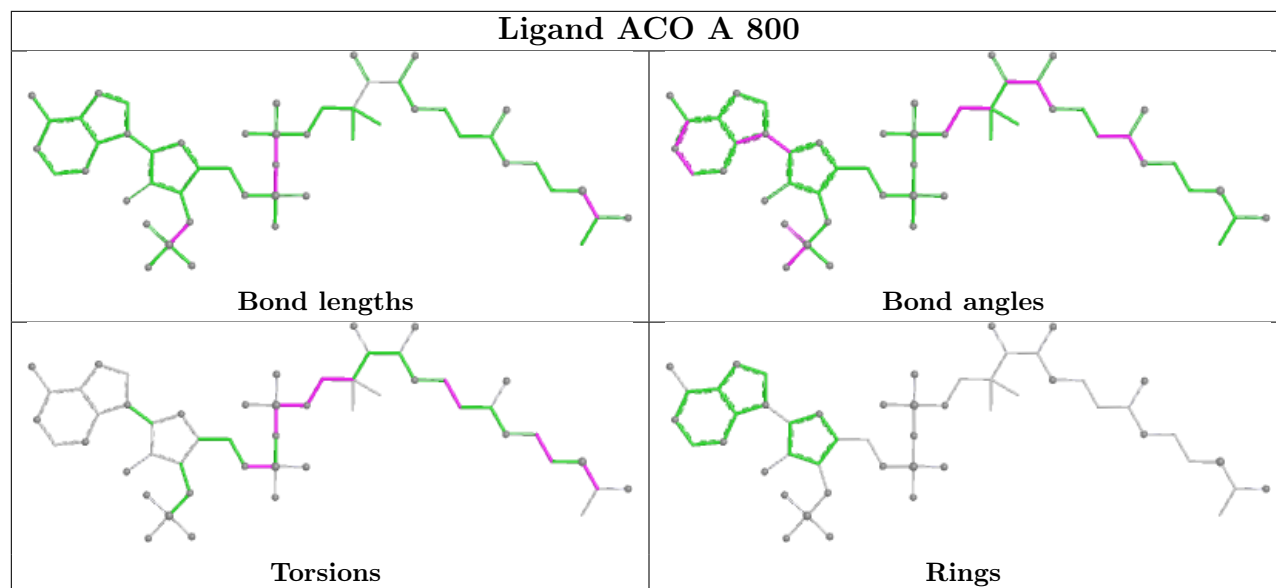
There are no ring outliers.

7 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1002	PG4	5	0
4	B	900	ACO	11	0
4	A	800	ACO	8	0
6	A	1001	PEG	1	0
5	A	810	PYR	3	0
7	B	1003	PG4	3	0
5	B	910	PYR	4	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	705/731 (96%)	-0.17	18 (2%) 57 64	14, 26, 53, 100	0
2	B	703/731 (96%)	-0.01	26 (3%) 45 52	14, 27, 58, 99	0
All	All	1408/1462 (96%)	-0.09	44 (3%) 51 58	14, 26, 56, 100	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	585	ALA	4.5
2	B	8	SER	3.7
1	A	584	ASN	3.6
2	B	682	GLY	3.6
2	B	352	SER	3.5
1	A	585	ALA	3.3
2	B	86	ARG	3.2
2	B	309	ILE	3.0
2	B	584	ASN	2.8
2	B	205	GLY	2.8
2	B	373	TYR	2.8
1	A	722	SER	2.8
1	A	624	HIS	2.7
1	A	308	GLN	2.7
1	A	662	ASN	2.7
2	B	326	GLU	2.6
1	A	566	ASN	2.6
2	B	27	GLY	2.6
1	A	150	GLN	2.6
2	B	684	PHE	2.6
2	B	222	ASP	2.6
2	B	629	MET	2.5
1	A	27	GLY	2.4
1	A	4	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	29	GLY	2.4
1	A	30	LEU	2.4
2	B	224	ALA	2.3
2	B	586	ASN	2.3
1	A	686	ASN	2.3
2	B	625	ASN	2.3
1	A	586	ASN	2.3
2	B	686	ASN	2.3
1	A	673	GLY	2.2
2	B	230	LEU	2.2
2	B	245	ASN	2.1
1	A	721	GLU	2.1
2	B	9	ARG	2.1
2	B	583	GLU	2.1
2	B	296	GLY	2.1
1	A	594	GLN	2.1
1	A	309	ILE	2.0
2	B	250	LYS	2.0
2	B	194	VAL	2.0
2	B	44	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CSO	B	688	7/8	0.95	0.08	22,24,45,47	0
1	CSO	A	617	7/8	0.96	0.09	23,26,45,85	0
2	CSO	B	617	7/8	0.97	0.05	16,24,30,35	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

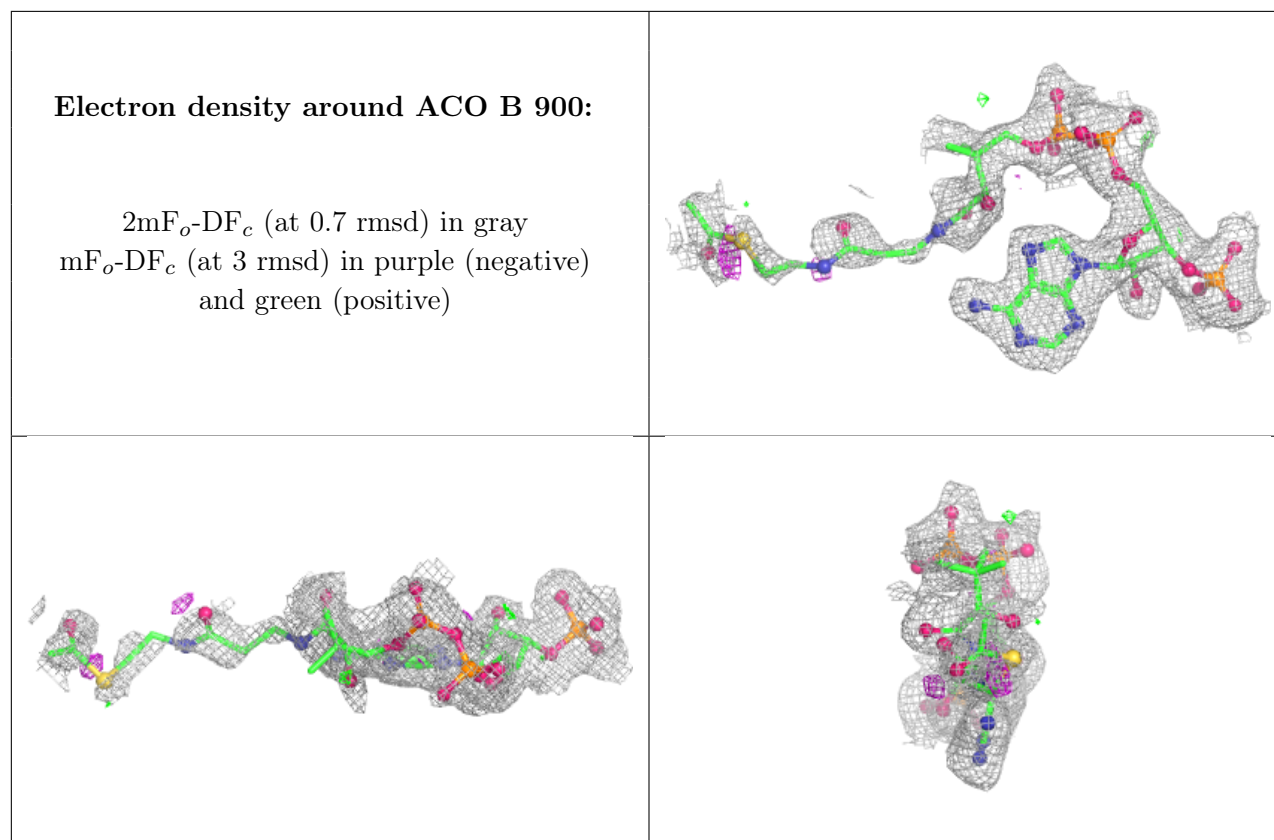
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

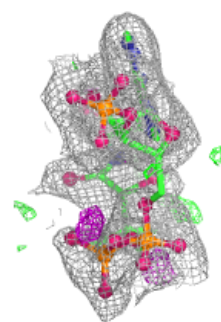
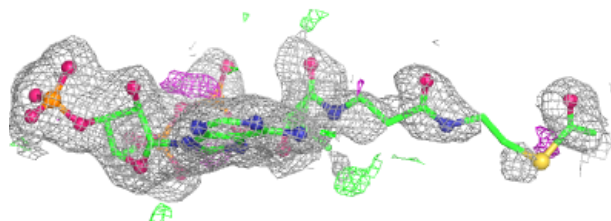
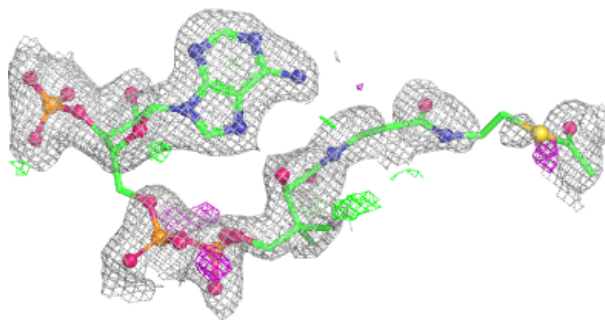
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PG4	B	1002	13/13	0.86	0.14	29,40,64,66	0
6	PEG	A	1001	7/7	0.87	0.12	43,44,47,48	0
7	PG4	B	1003	13/13	0.89	0.13	44,56,68,68	0
4	ACO	B	900	51/51	0.93	0.14	23,53,98,100	0
4	ACO	A	800	51/51	0.93	0.11	17,50,91,96	0
5	PYR	B	910	6/6	0.96	0.08	20,23,32,32	0
5	PYR	A	810	6/6	0.97	0.07	13,20,21,44	0
3	MG	B	1001	1/1	0.99	0.03	17,17,17,17	0
3	MG	A	1000	1/1	0.99	0.02	16,16,16,16	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 ACO A 800:

$2mF_o-DF_c$ (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.