



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:48 pm BST

PDB ID : 1P7T  
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](mailto: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.

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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

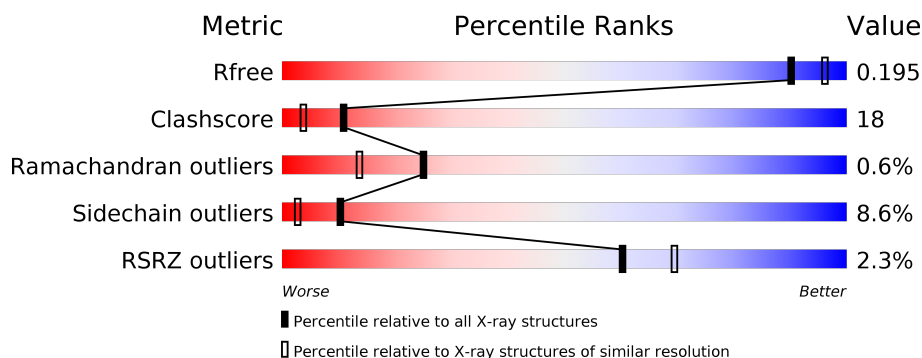
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div> <div></div> <div>57%</div> <div>30%</div> <div>8%</div> <div>• •</div> </div> <div> <div>3%</div> <div>60%</div> <div>29%</div> <div>6%</div> <div>• •</div> </div> </div>
2	B	731	<div> <div> <div></div> <div>57%</div> <div>30%</div> <div>8%</div> <div>• •</div> </div> <div> <div>3%</div> <div>60%</div> <div>29%</div> <div>6%</div> <div>• •</div> </div> </div>

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	A	810	-	-	X	-
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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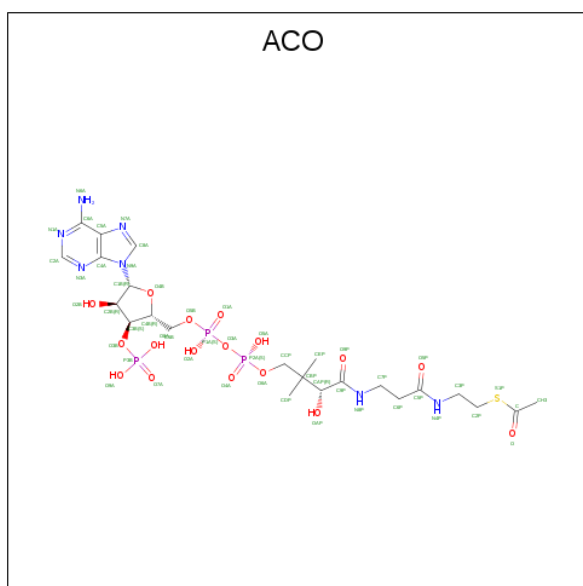
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Chain	Residue	Modelled	Actual	Comment	Reference
B	725	GLU	-	EXPRESSION TAG	UNP P37330
B	726	HIS	-	EXPRESSION TAG	UNP P37330
B	727	HIS	-	EXPRESSION TAG	UNP P37330
B	728	HIS	-	EXPRESSION TAG	UNP P37330
B	729	HIS	-	EXPRESSION TAG	UNP P37330
B	730	HIS	-	EXPRESSION TAG	UNP P37330
B	731	HIS	-	EXPRESSION TAG	UNP P37330

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

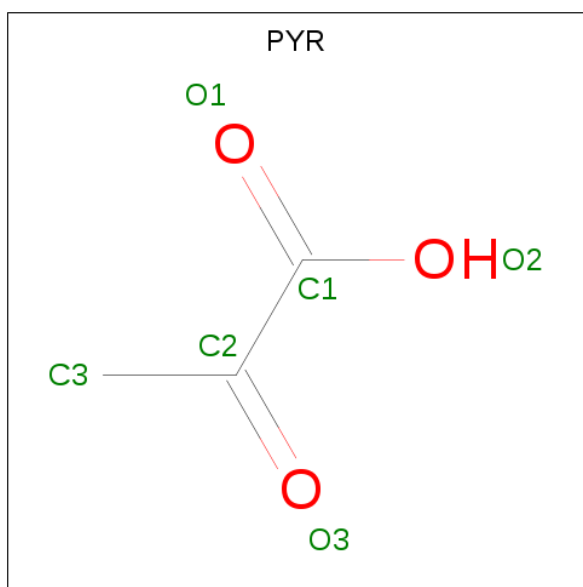
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



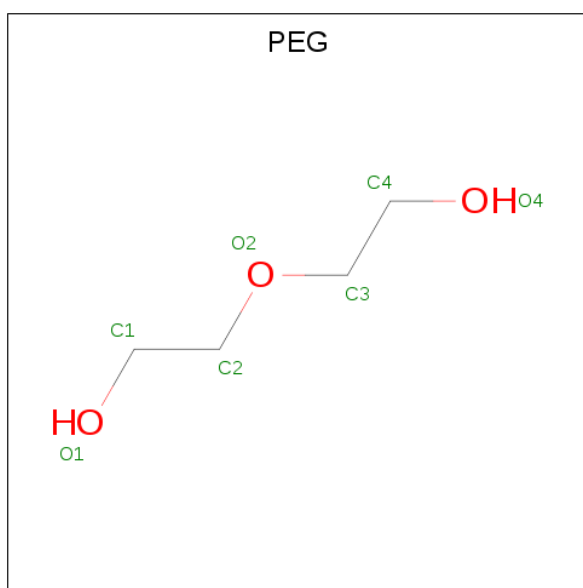
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 51 23 7 17 3 1	0	0
4	B	1	Total C N O P S 51 23 7 17 3 1	0	0

- Molecule 5 is PYRUVIC ACID (three-letter code: PYR) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>).



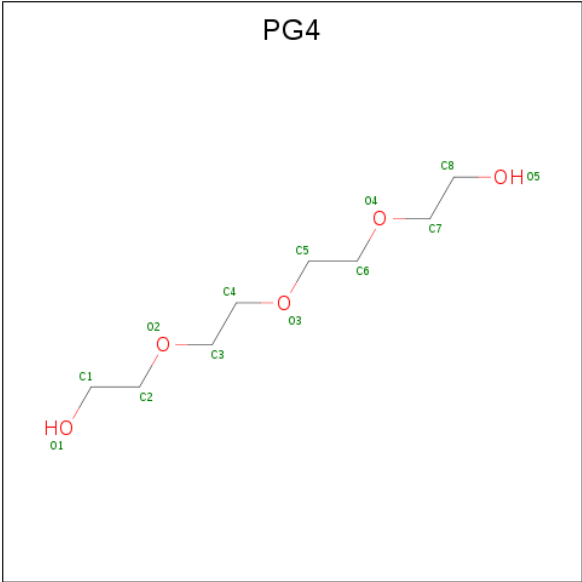
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: 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 (three-letter code: 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		

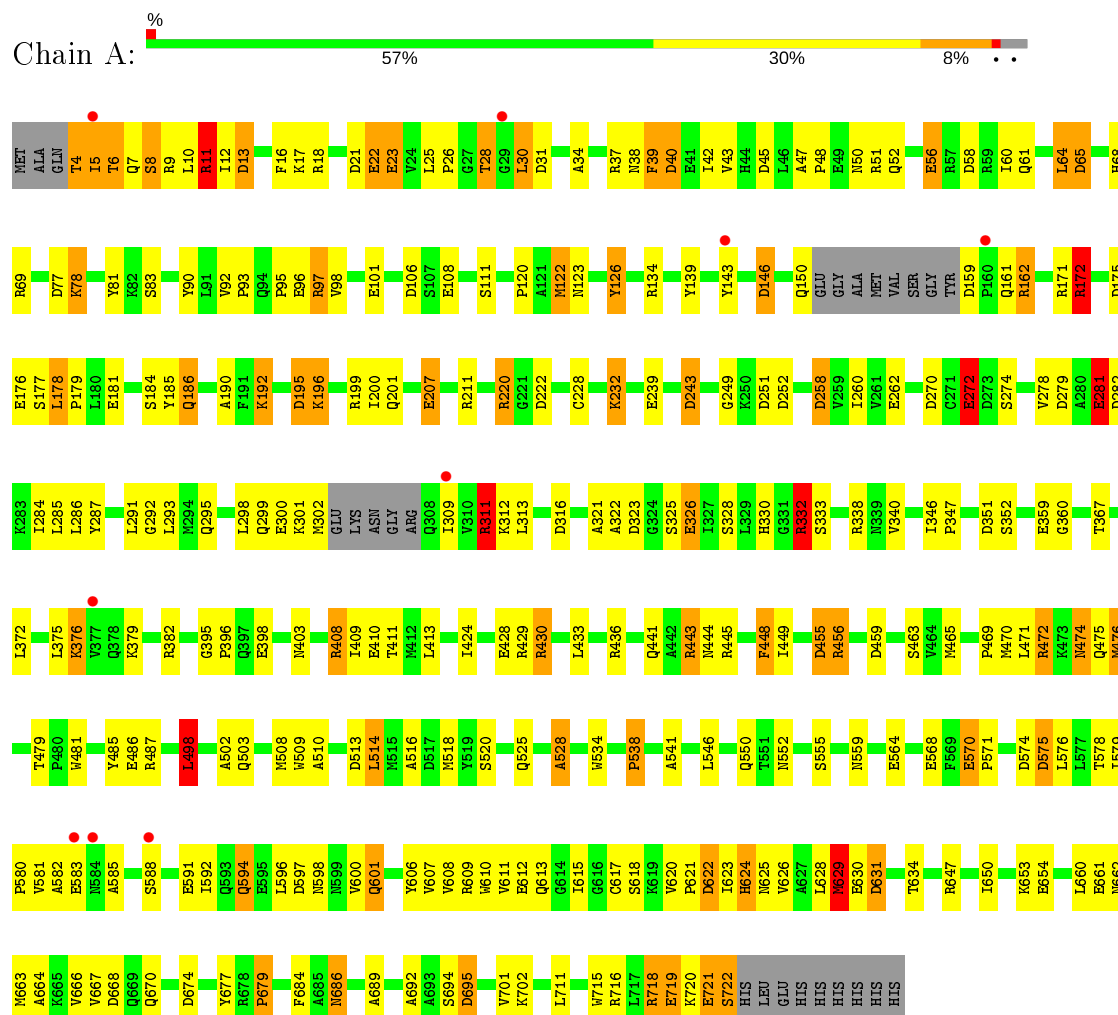
- Molecule 8 is water.

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

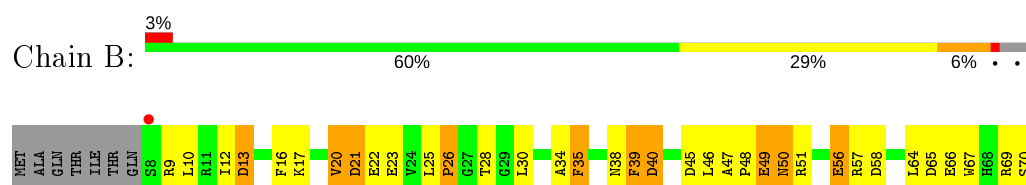
### 3 Residue-property plots

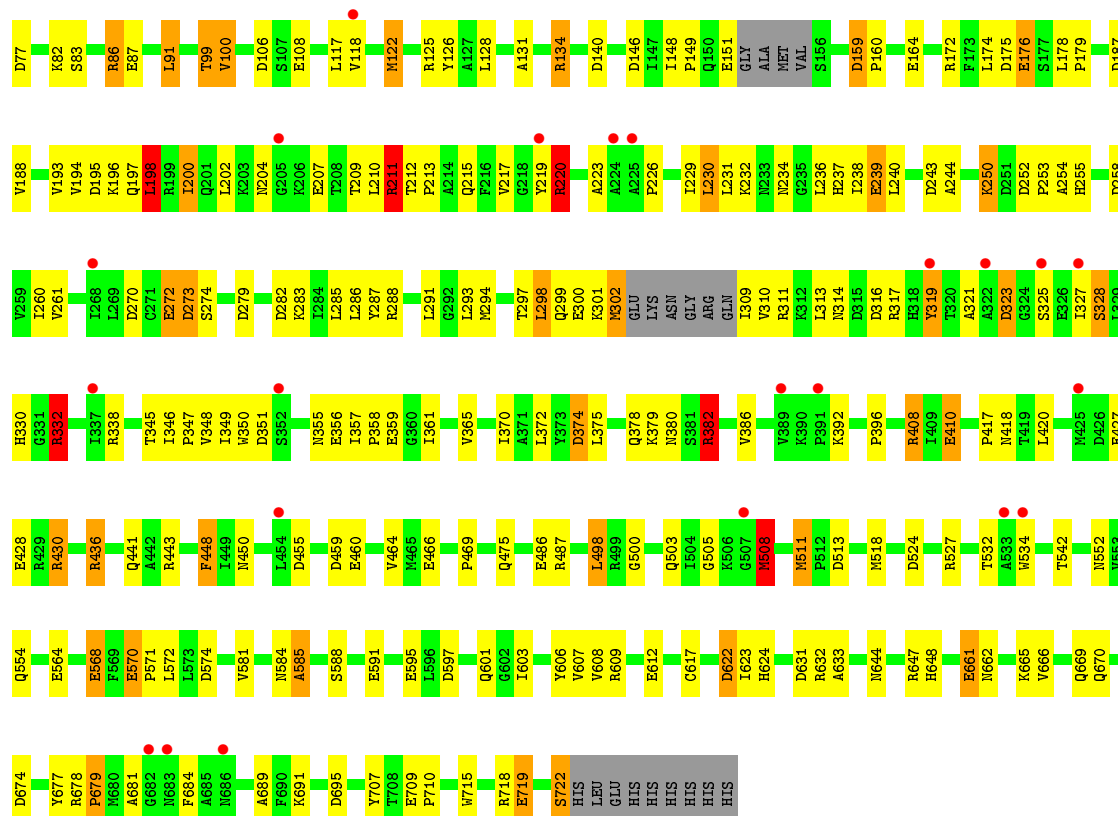
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 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, $\alpha$ , $\beta$ , $\gamma$	73.93Å 107.39Å 204.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.22 – 1.95 39.21 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.22-1.95) 90.0 (39.21-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 102.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, PYR, ACO, CSO, PG4, PEG

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	1.31	28/5509 (0.5%)	1.63	103/7485 (1.4%)
2	B	1.28	28/5447 (0.5%)	1.60	93/7407 (1.3%)
All	All	1.29	56/10956 (0.5%)	1.62	196/14892 (1.3%)

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	612	GLU	CD-OE2	10.15	1.36	1.25
2	B	207	GLU	CD-OE2	9.06	1.35	1.25
1	A	108	GLU	CD-OE2	8.95	1.35	1.25
2	B	164	GLU	CD-OE2	8.52	1.35	1.25
2	B	87	GLU	CD-OE2	8.48	1.34	1.25
1	A	326	GLU	CD-OE2	8.24	1.34	1.25
1	A	719	GLU	CD-OE2	8.22	1.34	1.25
2	B	56	GLU	CD-OE2	7.96	1.34	1.25
2	B	486	GLU	CD-OE2	7.78	1.34	1.25
1	A	23	GLU	CD-OE2	7.76	1.34	1.25
1	A	281	GLU	CD-OE2	7.64	1.34	1.25
2	B	564	GLU	CD-OE2	7.61	1.34	1.25
1	A	583	GLU	CD-OE2	7.42	1.33	1.25
2	B	66	GLU	CD-OE2	7.40	1.33	1.25
2	B	595	GLU	CD-OE2	7.39	1.33	1.25
1	A	300	GLU	CD-OE2	7.27	1.33	1.25
1	A	564	GLU	CD-OE2	7.25	1.33	1.25
2	B	23	GLU	CD-OE2	7.04	1.33	1.25
1	A	176	GLU	CD-OE2	6.99	1.33	1.25
1	A	486	GLU	CD-OE2	6.95	1.33	1.25
2	B	427	GLU	CD-OE2	6.86	1.33	1.25
1	A	570	GLU	CD-OE2	6.74	1.33	1.25
1	A	96	GLU	CD-OE2	6.56	1.32	1.25
2	B	719	GLU	CD-OE2	6.53	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	176	GLU	CD-OE2	6.48	1.32	1.25
2	B	570	GLU	CD-OE2	6.37	1.32	1.25
2	B	359	GLU	CD-OE1	-6.28	1.18	1.25
2	B	66	GLU	CD-OE1	-6.25	1.18	1.25
1	A	410	GLU	CD-OE2	6.11	1.32	1.25
1	A	568	GLU	CD-OE2	6.07	1.32	1.25
1	A	428	GLU	CD-OE2	6.02	1.32	1.25
1	A	630	GLU	CD-OE2	5.93	1.32	1.25
2	B	428	GLU	CD-OE2	5.89	1.32	1.25
1	A	207	GLU	CD-OE2	5.88	1.32	1.25
2	B	661	GLU	CD-OE2	5.84	1.32	1.25
1	A	262	GLU	CD-OE2	5.77	1.31	1.25
1	A	654	GLU	CD-OE2	5.74	1.31	1.25
2	B	49	GLU	CD-OE2	5.66	1.31	1.25
1	A	410	GLU	CD-OE1	-5.60	1.19	1.25
1	A	181	GLU	CD-OE2	5.58	1.31	1.25
2	B	151	GLU	CD-OE2	5.56	1.31	1.25
1	A	56	GLU	CD-OE2	5.55	1.31	1.25
2	B	410	GLU	CD-OE2	5.54	1.31	1.25
1	A	591	GLU	CD-OE2	5.51	1.31	1.25
1	A	272	GLU	CD-OE2	5.50	1.31	1.25
1	A	430	ARG	CZ-NH1	5.48	1.40	1.33
2	B	22	GLU	CD-OE2	5.39	1.31	1.25
2	B	466	GLU	CD-OE2	5.35	1.31	1.25
2	B	356	GLU	CD-OE1	-5.31	1.19	1.25
2	B	108	GLU	CD-OE2	5.30	1.31	1.25
2	B	568	GLU	CD-OE2	5.30	1.31	1.25
2	B	300	GLU	CD-OE2	5.28	1.31	1.25
2	B	272	GLU	CD-OE2	5.25	1.31	1.25
1	A	360	GLY	N-CA	5.21	1.53	1.46
1	A	359	GLU	CD-OE2	5.17	1.31	1.25
2	B	612	GLU	CD-OE2	5.11	1.31	1.25

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	ARG	NE-CZ-NH2	-14.30	113.15	120.30
1	A	316	ASP	CB-CG-OD2	-11.49	107.96	118.30
1	A	436	ARG	NE-CZ-NH1	11.41	126.01	120.30
2	B	382	ARG	NE-CZ-NH2	-11.23	114.69	120.30
2	B	678	ARG	NE-CZ-NH2	-11.20	114.70	120.30
1	A	258	ASP	CB-CG-OD1	10.70	127.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	ARG	NE-CZ-NH1	10.17	125.38	120.30
1	A	631	ASP	CB-CG-OD2	-9.95	109.34	118.30
2	B	382	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	A	311	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	172	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	574	ASP	CB-CG-OD2	-9.37	109.86	118.30
2	B	13	ASP	CB-CG-OD2	-9.26	109.97	118.30
2	B	40	ASP	CB-CG-OD2	-9.20	110.02	118.30
1	A	456	ARG	NE-CZ-NH2	-9.19	115.70	120.30
2	B	258	ASP	CB-CG-OD1	8.99	126.39	118.30
1	A	668	ASP	CB-CG-OD1	8.98	126.38	118.30
1	A	172	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	A	243	ASP	CB-CG-OD2	-8.90	110.29	118.30
1	A	222	ASP	CB-CG-OD1	8.83	126.25	118.30
2	B	408	ARG	NE-CZ-NH1	8.81	124.71	120.30
2	B	58	ASP	CB-CG-OD2	-8.80	110.38	118.30
2	B	524	ASP	CB-CG-OD2	-8.77	110.41	118.30
2	B	134	ARG	NE-CZ-NH2	-8.70	115.95	120.30
2	B	243	ASP	CB-CG-OD2	-8.66	110.50	118.30
2	B	622	ASP	CB-CG-OD2	-8.66	110.51	118.30
1	A	258	ASP	CB-CG-OD2	-8.64	110.52	118.30
2	B	146	ASP	CB-CG-OD2	-8.55	110.60	118.30
1	A	195	ASP	CB-CG-OD2	-8.53	110.62	118.30
1	A	77	ASP	CB-CG-OD2	-8.47	110.67	118.30
2	B	51	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	A	323	ASP	CB-CG-OD2	-8.34	110.80	118.30
1	A	668	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	A	408	ARG	NE-CZ-NH1	8.32	124.46	120.30
2	B	622	ASP	CB-CG-OD1	8.30	125.77	118.30
1	A	443	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	351	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	A	222	ASP	CB-CG-OD2	-8.17	110.95	118.30
1	A	97	ARG	NE-CZ-NH1	8.06	124.33	120.30
2	B	13	ASP	CB-CG-OD1	8.05	125.55	118.30
2	B	125	ARG	NE-CZ-NH1	7.92	124.26	120.30
2	B	316	ASP	CB-CG-OD2	-7.88	111.20	118.30
1	A	316	ASP	CB-CG-OD1	7.81	125.33	118.30
2	B	674	ASP	CB-CG-OD1	7.81	125.33	118.30
1	A	97	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	455	ASP	CB-CG-OD2	-7.79	111.29	118.30
2	B	243	ASP	CB-CG-OD1	7.74	125.27	118.30
1	A	45	ASP	CB-CG-OD1	7.71	125.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	574	ASP	CB-CG-OD1	7.71	125.24	118.30
2	B	678	ARG	NE-CZ-NH1	7.71	124.16	120.30
2	B	279	ASP	CB-CG-OD1	7.67	125.20	118.30
1	A	11	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	A	411	THR	CA-CB-CG2	-7.64	101.70	112.40
2	B	140	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	A	146	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	A	58	ASP	CB-CG-OD2	-7.58	111.47	118.30
2	B	106	ASP	CB-CG-OD2	-7.58	111.48	118.30
2	B	159	ASP	CB-CG-OD2	-7.53	111.52	118.30
2	B	258	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	A	175	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	A	459	ASP	CB-CG-OD2	-7.43	111.61	118.30
2	B	597	ASP	CB-CG-OD2	-7.41	111.64	118.30
2	B	273	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	195	ASP	CB-CG-OD1	7.34	124.90	118.30
2	B	508	MET	CG-SD-CE	-7.34	88.46	100.20
1	A	252	ASP	CB-CG-OD1	7.30	124.87	118.30
2	B	21	ASP	CB-CG-OD1	7.28	124.86	118.30
2	B	220	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	459	ASP	CB-CG-OD1	7.28	124.85	118.30
2	B	597	ASP	CB-CG-OD1	7.21	124.78	118.30
1	A	351	ASP	CB-CG-OD1	7.12	124.71	118.30
2	B	51	ARG	NE-CZ-NH2	-7.12	116.74	120.30
2	B	279	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	323	ASP	CB-CG-OD1	6.96	124.56	118.30
2	B	374	ASP	CB-CG-OD1	6.95	124.55	118.30
2	B	282	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	126	TYR	CB-CG-CD1	6.84	125.10	121.00
2	B	695	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	45	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	220	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	106	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	A	243	ASP	CB-CG-OD1	6.75	124.38	118.30
2	B	58	ASP	CB-CG-OD1	6.75	124.38	118.30
2	B	273	ASP	CB-CG-OD2	-6.75	112.23	118.30
2	B	524	ASP	CB-CG-OD1	6.71	124.34	118.30
2	B	459	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	13	ASP	CB-CG-OD1	6.70	124.33	118.30
2	B	674	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	126	TYR	CB-CG-CD2	-6.69	116.99	121.00
1	A	192	LYS	N-CA-CB	6.67	122.60	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	282	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	A	106	ASP	CB-CG-OD1	6.55	124.19	118.30
2	B	239	GLU	N-CA-CB	6.52	122.34	110.60
1	A	251	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	40	ASP	CB-CG-OD1	6.47	124.13	118.30
2	B	631	ASP	CB-CG-OD2	-6.47	112.48	118.30
2	B	21	ASP	CB-CG-OD2	-6.45	112.49	118.30
2	B	695	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	A	332	ARG	NE-CZ-NH2	-6.41	117.09	120.30
2	B	65	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	11	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	175	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	476	MET	CG-SD-CE	6.38	110.41	100.20
1	A	622	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	A	631	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	332	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	40	ASP	CB-CG-OD2	-6.33	112.61	118.30
2	B	609	ARG	NE-CZ-NH2	-6.31	117.15	120.30
2	B	159	ASP	CB-CG-OD1	6.25	123.93	118.30
2	B	211	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	674	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	674	ASP	CB-CG-OD2	-6.23	112.69	118.30
2	B	316	ASP	CB-CG-OD1	6.20	123.88	118.30
2	B	459	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	211	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	575	ASP	CB-CG-OD2	-6.18	112.74	118.30
2	B	57	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	498	LEU	N-CA-CB	6.08	122.55	110.40
1	A	58	ASP	CB-CG-OD1	6.07	123.76	118.30
2	B	487	ARG	NE-CZ-NH2	-6.06	117.27	120.30
2	B	57	ARG	NE-CZ-NH1	6.05	123.33	120.30
2	B	140	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	695	ASP	CB-CG-OD2	-6.01	112.89	118.30
2	B	131	ALA	N-CA-CB	-6.01	101.69	110.10
1	A	21	ASP	CB-CG-OD2	-5.99	112.91	118.30
2	B	631	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	513	ASP	CB-CG-OD2	-5.98	112.92	118.30
2	B	146	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	379	LYS	N-CA-CB	5.95	121.31	110.60
2	B	527	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	178	LEU	C-N-CD	-5.94	107.53	120.60
1	A	162	ARG	NE-CZ-NH2	-5.93	117.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	679	PRO	N-CA-CB	5.93	110.42	103.30
1	A	4	THR	N-CA-CB	5.92	121.54	110.30
2	B	436	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	159	ASP	CB-CG-OD1	5.90	123.61	118.30
2	B	677	TYR	CB-CG-CD1	-5.89	117.47	121.00
2	B	511	MET	CG-SD-CE	-5.88	90.79	100.20
1	A	716	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	622	ASP	CB-CG-OD1	5.82	123.53	118.30
2	B	187	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	31	ASP	CB-CG-OD2	-5.80	113.08	118.30
2	B	117	LEU	CB-CG-CD2	-5.80	101.14	111.00
2	B	40	ASP	CB-CG-OD1	5.80	123.52	118.30
2	B	430	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	81	TYR	N-CA-CB	-5.78	100.20	110.60
2	B	175	ASP	CB-CG-OD2	-5.75	113.12	118.30
2	B	69	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	634	THR	CA-CB-CG2	-5.72	104.39	112.40
2	B	487	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	A	9	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	279	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	629	MET	CG-SD-CE	-5.68	91.11	100.20
1	A	695	ASP	CB-CG-OD1	5.68	123.41	118.30
2	B	270	ASP	CB-CG-OD2	-5.68	113.19	118.30
2	B	175	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	22	GLU	CG-CD-OE2	-5.57	107.16	118.30
2	B	20	VAL	CA-CB-CG1	-5.57	102.55	110.90
2	B	134	ARG	NE-CZ-NH1	5.53	123.06	120.30
2	B	574	ASP	CB-CG-OD2	-5.51	113.34	118.30
2	B	332	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	270	ASP	CB-CG-OD1	5.48	123.23	118.30
2	B	198	LEU	N-CA-CB	5.48	121.36	110.40
1	A	159	ASP	N-CA-CB	5.47	120.45	110.60
2	B	513	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	472	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	514	LEU	CB-CG-CD2	-5.42	101.79	111.00
2	B	338	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	B	455	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	513	ASP	CB-CG-OD1	5.38	123.14	118.30
2	B	436	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	367	THR	CA-CB-CG2	-5.37	104.89	112.40
2	B	323	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	287	TYR	CB-CG-CD1	5.26	124.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	ASN	N-CA-CB	5.22	120.00	110.60
1	A	77	ASP	CA-CB-CG	-5.22	101.92	113.40
1	A	279	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	338	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	674	ASP	CB-CA-C	5.17	120.74	110.40
2	B	374	ASP	CB-CG-OD2	-5.16	113.65	118.30
2	B	319	TYR	CB-CG-CD2	-5.12	117.93	121.00
2	B	648	HIS	CA-CB-CG	-5.11	104.92	113.60
2	B	518	MET	CA-CB-CG	-5.11	104.62	113.30
1	A	311	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	B	287	TYR	CB-CG-CD1	5.09	124.05	121.00
2	B	172	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	B	606	TYR	CB-CG-CD1	5.08	124.05	121.00
1	A	11	ARG	N-CA-CB	5.08	119.73	110.60
2	B	647	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	B	77	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	65	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	408	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	528	ALA	N-CA-CB	-5.05	103.03	110.10
2	B	527	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	465	MET	N-CA-CB	-5.04	101.54	110.60
1	A	716	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5414	0	5271	192	0
2	B	5358	0	5172	188	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	51	0	34	10	0
4	B	51	0	34	13	0
5	A	6	0	3	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	3	9	0
6	A	7	0	10	1	0
7	B	26	0	36	8	0
8	A	308	0	0	10	0
8	B	275	0	0	10	0
All	All	11504	0	10563	391	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (391) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:MET:HE1	1:A:481:TRP:HE1	1.15	1.10
1:A:476:MET:HE3	1:A:479:THR:HG21	1.32	1.10
2:B:86:ARG:HH11	2:B:86:ARG:HB2	1.21	1.05
2:B:86:ARG:NH1	2:B:86:ARG:HB2	1.81	0.95
2:B:534:TRP:CZ3	5:B:910:PYR:H31	2.03	0.94
1:A:470:MET:HE1	1:A:581:VAL:HG12	1.46	0.94
2:B:217:VAL:HG23	2:B:230:LEU:HD23	1.49	0.91
1:A:470:MET:CE	1:A:581:VAL:HG12	2.00	0.90
1:A:11:ARG:HH11	1:A:11:ARG:HG3	1.38	0.88
1:A:143:TYR:CE2	1:A:162:ARG:HG2	2.08	0.87
2:B:346:ILE:HG13	2:B:347:PRO:HD2	1.56	0.87
2:B:76:LYS:HB2	2:B:76:LYS:HZ3	1.38	0.86
1:A:476:MET:CE	1:A:481:TRP:HE1	1.87	0.86
2:B:508:MET:HG2	2:B:534:TRP:HB3	1.59	0.85
1:A:534:TRP:CZ3	5:A:810:PYR:H31	2.12	0.84
2:B:302:MET:HE3	2:B:311:ARG:HB2	1.60	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
1:A:546:LEU:O	1:A:550:GLN:HG3	1.78	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:8:SER:HB3	1:A:40:ASP:OD2	1.81	0.80
2:B:534:TRP:HZ3	5:B:910:PYR:H31	1.46	0.79
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
1:A:18:ARG:O	1:A:22:GLU:HG2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:SER:O	1:A:592:ILE:HG13	1.85	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
2:B:122:MET:HA	2:B:122:MET:HE3	1.66	0.76
1:A:534:TRP:HZ3	5:A:810:PYR:H31	1.49	0.76
1:A:122:MET:HE1	1:A:286:LEU:N	2.01	0.75
1:A:302:MET:HE3	1:A:311:ARG:HB2	1.68	0.75
1:A:609:ARG:HH12	1:A:615:ILE:HG21	1.52	0.73
1:A:302:MET:HE3	1:A:311:ARG:CB	2.17	0.73
6:A:1001:PEG:H31	8:A:2448:HOH:O	1.88	0.73
1:A:172:ARG:NH1	8:A:2070:HOH:O	2.24	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
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
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: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: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
1:A:476:MET:CE	1:A:479:THR:HG21	2.19	0.67
2:B:448:PHE:CB	2:B:503:GLN:HB2	2.25	0.67
1:A:195:ASP:C	1:A:196:LYS:HG2	2.15	0.66
2:B:288:ARG:O	2:B:291:LEU:HB3	1.96	0.66
1:A:122:MET:HA	1:A:122:MET:HE3	1.76	0.66
1:A:594:GLN:NE2	1:A:594:GLN:HA	2.12	0.65
2:B:122:MET:HE1	2:B:285:LEU:HB2	1.78	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
2:B:475:GLN:NE2	8:B:2154:HOH:O	2.29	0.65
1:A:122:MET:HE1	1:A:285:LEU:HB2	1.79	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:629:MET:O	1:A:629:MET:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:800:ACO:S1P	5:A:810:PYR:H33	2.38	0.64
2:B:302:MET:HE3	2:B:311:ARG:CB	2.27	0.64
1:A:623:ILE:HD11	1:A:624:HIS:NE2	2.13	0.63
4:B:900:ACO:S1P	5:B:910:PYR:H33	2.38	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:193:VAL:O	2:B:194:VAL:HG23	1.99	0.62
2:B:83:SER:CA	2:B:86:ARG:HH12	2.11	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: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:508:MET:HE3	4:A:800:ACO:H21	1.81	0.60
2:B:302:MET:CE	2:B:311:ARG:HB2	2.30	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
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
2:B:16:PHE:O	2:B:20:VAL:HG23	2.03	0.59
1:A:470:MET:HE1	1:A:581:VAL:CG1	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:B:910:PYR:H32	8:B:2224:HOH:O	2.04	0.58
2:B:10:LEU:HD23	2:B:351:ASP:HA	1.86	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
1:A:122:MET:HE1	1:A:285:LEU:C	2.26	0.56
2:B:633:ALA:HB3	4:B:900:ACO:CH3	2.35	0.56
1:A:476:MET:HE1	1:A:481:TRP:NE1	2.01	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
2:B:122:MET:HA	2:B:122:MET:CE	2.35	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:NH1	1:A:11:ARG:HG3	2.13	0.55
1:A:663:MET:O	1:A:666:VAL:HB	2.06	0.55
1:A:190:ALA:HB3	1:A:201:GLN:HE21	1.71	0.55
1:A:122:MET:HE3	1:A:286:LEU:HA	1.88	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:349:ILE:HG22	2:B:350:TRP:N	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
1:A:621:PRO:HA	1:A:626:VAL:O	2.07	0.54
1:A:122:MET:HA	1:A:122:MET:CE	2.38	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
5:A:810:PYR:H32	8:A:2171:HOH:O	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:PHE:HA	1:A:284:ILE:HD11	1.91	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
2:B:252:ASP:CG	2:B:253:PRO:HD2	2.29	0.53
2:B:35:PHE:O	2:B:39:PHE:HB2	2.08	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
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
1:A:122:MET:HE1	1:A:285:LEU:CB	2.38	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
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
1:A:64:LEU:HD22	1:A:68:HIS:CD2	2.45	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
7:B:1002:PG4:H32	8:B:2279:HOH:O	2.08	0.52
2:B:661:GLU:HG2	2:B:684:PHE:CE2	2.45	0.52
2:B:302:MET:HE3	2:B:311:ARG:CD	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
2:B:392:LYS:HD3	2:B:707:TYR:CE1	2.45	0.51
2:B:261:VAL:HG22	2:B:542:THR:HG23	1.92	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:O	2:B:198:LEU:HD23	2.10	0.51
1:A:311:ARG:HD3	8:A:2277:HOH:O	2.10	0.51
1:A:660:LEU:O	1:A:664:ALA:HB2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:476:MET:CE	1:A:580:PRO:HB3	2.43	0.49
2:B:273:ASP:CG	2:B:632:ARG:HB2	2.33	0.49
1:A:470:MET:HE2	1:A:581:VAL:HG12	1.87	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:244:ALA:HB2	2:B:255:HIS:CD2	2.47	0.49
2:B:30:LEU:HD11	2:B:372:LEU:HD11	1.92	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:379:LYS:HB3	8:B:2532:HOH:O	2.13	0.49
2:B:76:LYS:NZ	8:B:2034:HOH:O	2.46	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:122:MET:HE1	2:B:285:LEU:CB	2.43	0.48
1:A:579:ILE:HD12	1:A:581:VAL:HG13	1.95	0.48
1:A:298:LEU:C	1:A:299:GLN:HG3	2.33	0.48
1:A:123:ASN:ND2	1:A:126:TYR:CD2	2.81	0.48
1:A:42:ILE:HD12	1:A:408:ARG:HB3	1.94	0.48
2:B:357:ILE:CG1	2:B:358:PRO:HD2	2.43	0.48
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:196:LYS:HB3	1:A:322:ALA:O	2.14	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
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:596:LEU:CD1	1:A:600:VAL:HG23	2.45	0.47
1:A:92:VAL:HB	1:A:93:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:LEU:C	2:B:198:LEU:HD23	2.35	0.47
2:B:349:ILE:CG2	2:B:350:TRP:N	2.77	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
1:A:596:LEU:HD12	1:A:596:LEU:C	2.35	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: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:12:ILE:O	1:A:13:ASP:C	2.54	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
1:A:260:ILE:N	1:A:260:ILE:HD13	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:476:MET:CE	1:A:476:MET:HA	2.45	0.45
1:A:663:MET:O	1:A:667:VAL:HG23	2.16	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:552:ASN:OD1	2:B:552:ASN:C	2.55	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
2:B:534:TRP:CE3	5:B:910:PYR:H31	2.51	0.45
1:A:552:ASN:O	1:A:555:SER:OG	2.32	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
1:A:647:ARG:O	1:A:647:ARG:HG3	2.12	0.45
2:B:238:ILE:HD13	2:B:261:VAL:HG12	1.99	0.45
2:B:25:LEU:N	2:B:26:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:ALA:N	2:B:325:SER:O	2.38	0.45
1:A:220:ARG:NH1	1:A:239:GLU:OE1	2.50	0.45
1:A:38:ASN:HD22	1:A:38:ASN:HA	1.52	0.45
2:B:570:GLU:N	2:B:571:PRO:CD	2.80	0.45
2:B:159:ASP:OD1	2:B:159:ASP:C	2.55	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
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:302:MET:HE3	1:A:311:ARG:NE	2.32	0.44
1:A:372:LEU:HD23	1:A:372:LEU:HA	1.68	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
1:A:28:THR:HA	1:A:376:LYS:HZ3	1.79	0.44
2:B:588:SER:OG	2:B:591:GLU:HG3	2.17	0.44
2:B:448:PHE:C	2:B:448:PHE:CD1	2.90	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:254:ALA:O	2:B:255:HIS:HB2	2.18	0.43
2:B:134:ARG:NH1	2:B:332:ARG:O	2.50	0.43
2:B:49:GLU:O	2:B:50:ASN:C	2.54	0.43
1:A:232:LYS:HE3	1:A:232:LYS:HB3	1.79	0.43
2:B:302:MET:CE	2:B:311:ARG:CB	2.94	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:661:GLU:O	1:A:664:ALA:HB3	2.18	0.43
2:B:718:ARG:O	2:B:719:GLU:C	2.54	0.43
1:A:525:GLN:O	1:A:528:ALA:HB3	2.19	0.43
1:A:92:VAL:HB	1:A:93:PRO:CD	2.49	0.43
1:A:292:GLY:HA3	1:A:298:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:TYR:CE2	1:A:679:PRO:HA	2.54	0.43
4:A:800:ACO:S1P	5:A:810:PYR:C3	3.05	0.43
2:B:134:ARG:O	2:B:134:ARG:HG3	2.19	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:HD23	2:B:25:LEU:HA	1.65	0.43
2:B:410:GLU:CD	2:B:418:ASN:H	2.21	0.43
1:A:692:ALA:HA	1:A:715:TRP:CD1	2.53	0.43
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:10:LEU:HD21	1:A:40:ASP:HA	2.00	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:HD21	2.33	0.42
1:A:101:GLU:CG	1:A:444:ASN:ND2	2.83	0.42
2:B:194:VAL:HG12	2:B:194:VAL:O	2.20	0.42
1:A:301:LYS:HA	1:A:309:ILE:O	2.19	0.42
1:A:487:ARG:O	1:A:487:ARG:HG3	2.19	0.42
1:A:510:ALA:HB1	1:A:629:MET:HG2	2.01	0.42
2:B:572:LEU:HA	2:B:572:LEU:HD23	1.88	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
2:B:219:TYR:O	2:B:220:ARG:HG3	2.19	0.42
2:B:35:PHE:CE2	2:B:39:PHE:HD2	2.37	0.42
2:B:283:LYS:HD3	2:B:346:ILE:CD1	2.49	0.42
2:B:49:GLU:HB2	8:B:2488:HOH:O	2.19	0.42
2:B:76:LYS:HB2	2:B:76:LYS:NZ	1.96	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:611:VAL:O	1:A:719:GLU:HG2	2.20	0.42
1:A:95:PRO:CG	1:A:98:VAL:CG2	2.97	0.42
2:B:298:LEU:CD2	2:B:299:GLN:N	2.83	0.42
2:B:118:VAL:HG11	4:B:900:ACO:C3P	2.50	0.42
4:B:900:ACO:C	5:B:910:PYR:C3	2.98	0.42
4:B:900:ACO:C	5:B:910:PYR:H33	2.50	0.42
2:B:86:ARG:HD3	2:B:91:LEU:HD12	2.03	0.41
1:A:476:MET:CE	1:A:580:PRO:CB	2.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:LEU:HA	2:B:174:LEU:HD23	1.76	0.41
2:B:288:ARG:HD2	2:B:288:ARG:HH11	1.69	0.41
2:B:330:HIS:HE1	2:B:379:LYS:O	2.03	0.41
2:B:148:ILE:HA	2:B:149:PRO:HD3	1.91	0.41
2:B:261:VAL:HG21	2:B:542:THR:HG23	1.97	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
2:B:73:GLY:HA3	2:B:74:PRO:HD2	1.91	0.41
4:B:900:ACO:C	5:B:910:PYR:C2	2.99	0.41
2:B:159:ASP:HA	2:B:160:PRO:HD2	1.97	0.41
2:B:45:ASP:OD2	2:B:408:ARG:NH1	2.45	0.41
2:B:64:LEU:HA	2:B:64:LEU:HD23	1.81	0.41
1:A:281:GLU:O	1:A:285:LEU:HG	2.20	0.41
1:A:607:VAL:O	1:A:608:VAL:C	2.57	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:302:MET:CE	1:A:311:ARG:CB	2.94	0.41
1:A:65:ASP:O	1:A:69:ARG:HB2	2.21	0.41
2:B:298:LEU:HD23	2:B:299:GLN:H	1.86	0.41
1:A:134:ARG:HB2	1:A:333:SER:N	2.36	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:C1	2.51	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:508:MET:HE2	4:A:800:ACO:H21	2.03	0.40
2:B:215:GLN:O	2:B:231:LEU:HA	2.21	0.40
1:A:403:ASN:OD1	1:A:445:ARG:HD2	2.21	0.40
1:A:718:ARG:HD3	1:A:718:ARG:HA	1.50	0.40
2:B:82:LYS:C	2:B:86:ARG:HH12	2.24	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
5:A:810:PYR:H32	8:A:2231:HOH:O	2.21	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%)	34	22
2	B	697/731 (95%)	665 (95%)	27 (4%)	5 (1%)	22	11
All	All	1396/1462 (96%)	1331 (95%)	57 (4%)	8 (1%)	25	14

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 [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	555/606 (92%)	501 (90%)	54 (10%)	8	2
2	B	538/605 (89%)	498 (93%)	40 (7%)	13	4
All	All	1093/1211 (90%)	999 (91%)	94 (9%)	10	3

All (94) 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	7	GLN
1	A	8	SER
1	A	11	ARG
1	A	23	GLU
1	A	30	LEU
1	A	39	PHE
1	A	50	ASN
1	A	52	GLN
1	A	64	LEU
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	192	LYS
1	A	196	LYS
1	A	228	CYS
1	A	232	LYS
1	A	272	GLU
1	A	281	GLU
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	382	ARG
1	A	443	ARG
1	A	448	PHE
1	A	455	ASP
1	A	474	ASN
1	A	498	LEU
1	A	520	SER
1	A	538	PRO
1	A	559	ASN
1	A	594	GLN

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Mol	Chain	Res	Type
1	A	601	GLN
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
1	A	722	SER
2	B	28	THR
2	B	35	PHE
2	B	39	PHE
2	B	46	LEU
2	B	50	ASN
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	176	GLU
2	B	197	GLN
2	B	198	LEU
2	B	200	ILE
2	B	211	ARG
2	B	212	THR
2	B	220	ARG
2	B	230	LEU
2	B	250	LYS
2	B	286	LEU
2	B	298	LEU
2	B	302	MET
2	B	323	ASP
2	B	327	ILE
2	B	328	SER
2	B	332	ARG
2	B	382	ARG
2	B	430	ARG
2	B	448	PHE
2	B	450	ASN

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Mol	Chain	Res	Type
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	669	GLN
2	B	679	PRO
2	B	722	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
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	233	ASN
1	A	299	GLN
1	A	314	ASN
1	A	339	ASN
1	A	444	ASN
1	A	521	GLN
1	A	559	ASN
1	A	598	ASN
1	A	683	ASN
1	A	703	GLN
2	B	38	ASN
2	B	197	GLN
2	B	299	GLN
2	B	450	ASN
2	B	683	ASN

### 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
2	CSO	B	617	2	3,6,7	0.63	0	0,6,8	0.00	-
1	CSO	A	617	1	3,6,7	1.22	0	0,6,8	0.00	-
2	CSO	B	688	2	3,6,7	2.28	1 (33%)	0,6,8	0.00	-

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
2	CSO	B	617	2	-	0/1/5/7	-
1	CSO	A	617	1	-	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	3.75	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
2	B	617	CSO	2	0
1	A	617	CSO	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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
5	PYR	B	910	3	2,5,5	0.50	0	2,6,6	1.89	1 (50%)
4	ACO	A	800	-	45,53,53	1.08	1 (2%)	56,79,79	1.22	5 (8%)
4	ACO	B	900	-	45,53,53	1.19	5 (11%)	56,79,79	1.26	5 (8%)
6	PEG	A	1001	-	6,6,6	0.79	0	5,5,5	0.34	0
7	PG4	B	1002	-	12,12,12	1.16	1 (8%)	11,11,11	0.56	0
5	PYR	A	810	3	2,5,5	1.08	0	2,6,6	1.25	0
7	PG4	B	1003	-	12,12,12	0.59	0	11,11,11	0.48	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
5	PYR	B	910	3	-	0/0/4/4	-
4	ACO	A	800	-	-	12/47/67/67	0/3/3/3
4	ACO	B	900	-	-	13/47/67/67	0/3/3/3
6	PEG	A	1001	-	-	2/4/4/4	-
7	PG4	B	1002	-	-	6/10/10/10	-
5	PYR	A	810	3	-	0/0/4/4	-
7	PG4	B	1003	-	-	4/10/10/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	ACO	P3B-O3B	-4.03	1.51	1.59
4	B	900	ACO	C6P-C5P	2.90	1.56	1.51
4	B	900	ACO	P1A-O5B	-2.34	1.49	1.59
4	B	900	ACO	O4B-C1B	2.34	1.44	1.41
7	B	1002	PG4	O4-C7	2.24	1.51	1.42
4	B	900	ACO	P2A-O6A	-2.23	1.50	1.59
4	B	900	ACO	C7P-N8P	2.16	1.51	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	900	ACO	C1B-N9A-C4A	-5.08	117.72	126.64
4	A	800	ACO	C6P-C5P-N4P	-3.39	110.72	116.42
4	A	800	ACO	C1B-N9A-C4A	-3.07	121.25	126.64
4	A	800	ACO	C5A-C6A-N6A	2.74	124.52	120.35
4	B	900	ACO	C7P-C6P-C5P	2.63	116.74	112.36
4	B	900	ACO	O6A-CCP-CBP	2.62	114.76	110.55
4	A	800	ACO	O9A-P3B-O8A	2.53	117.32	107.64
4	B	900	ACO	C7P-N8P-C9P	2.46	126.98	122.59
5	B	910	PYR	C3-C2-C1	-2.30	113.37	120.24
4	B	900	ACO	C5A-C6A-N6A	2.18	123.66	120.35
4	A	800	ACO	O6A-CCP-CBP	2.17	114.03	110.55

There are no chirality outliers.

All (37) 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	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	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

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Mol	Chain	Res	Type	Atoms
4	A	800	ACO	CDP-CBP-CCP-O6A
4	A	800	ACO	CEP-CBP-CCP-O6A
4	B	900	ACO	CDP-CBP-CCP-O6A
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
4	B	900	ACO	CEP-CBP-CCP-O6A
7	B	1003	PG4	C3-C4-O3-C5
4	A	800	ACO	CCP-O6A-P2A-O3A
7	B	1003	PG4	C1-C2-O2-C3
4	A	800	ACO	CBP-CCP-O6A-P2A
4	A	800	ACO	CCP-O6A-P2A-O5A
7	B	1003	PG4	O1-C1-C2-O2
6	A	1001	PEG	C1-C2-O2-C3
7	B	1003	PG4	O3-C5-C6-O4
7	B	1002	PG4	O1-C1-C2-O2
4	A	800	ACO	O-C-S1P-C2P
4	A	800	ACO	CH3-C-S1P-C2P
4	B	900	ACO	C9P-CAP-CBP-CEP
7	B	1002	PG4	O2-C3-C4-O3
7	B	1002	PG4	C6-C5-O3-C4

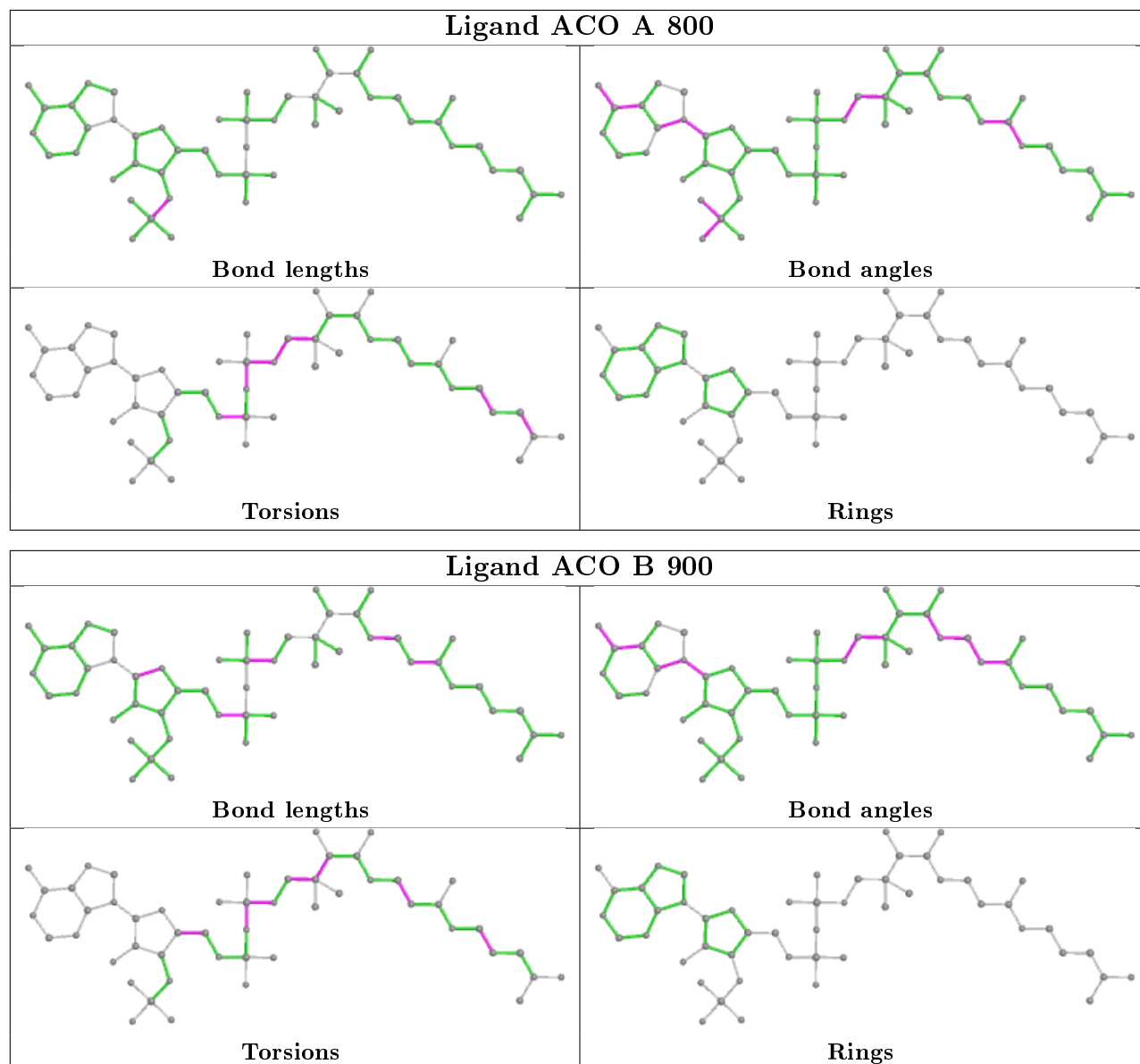
There are no ring outliers.

7 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	910	PYR	9	0
4	A	800	ACO	10	0
4	B	900	ACO	13	0
6	A	1001	PEG	1	0
7	B	1002	PG4	5	0
5	A	810	PYR	6	0
7	B	1003	PG4	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	705/731 (96%)	-0.08	9 (1%) 77 83	14, 26, 53, 100	0
2	B	703/731 (96%)	0.08	23 (3%) 46 56	14, 27, 58, 99	0
All	All	1408/1462 (96%)	-0.00	32 (2%) 60 69	14, 26, 56, 100	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	682	GLY	6.3
1	A	309	ILE	4.2
2	B	683	ASN	3.8
1	A	584	ASN	2.9
2	B	352	SER	2.9
1	A	5	ILE	2.9
2	B	389	VAL	2.7
2	B	224	ALA	2.7
2	B	534	TRP	2.6
1	A	377	VAL	2.6
2	B	454	LEU	2.6
2	B	327	ILE	2.6
2	B	391	PRO	2.4
2	B	8	SER	2.4
2	B	219	TYR	2.3
2	B	337	ILE	2.3
2	B	686	ASN	2.3
1	A	160	PRO	2.2
2	B	205	GLY	2.2
1	A	143	TYR	2.2
2	B	319	TYR	2.2
2	B	322	ALA	2.2
2	B	118	VAL	2.2
2	B	268	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	588	SER	2.1
1	A	29	GLY	2.1
2	B	225	ALA	2.1
2	B	325	SER	2.1
2	B	533	ALA	2.1
2	B	507	GLY	2.0
2	B	425	MET	2.0
1	A	583	GLU	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CSO	B	688	7/8	0.95	0.12	22,24,45,47	0
1	CSO	A	617	7/8	0.96	0.10	23,26,45,85	0
2	CSO	B	617	7/8	0.98	0.07	16,24,30,35	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

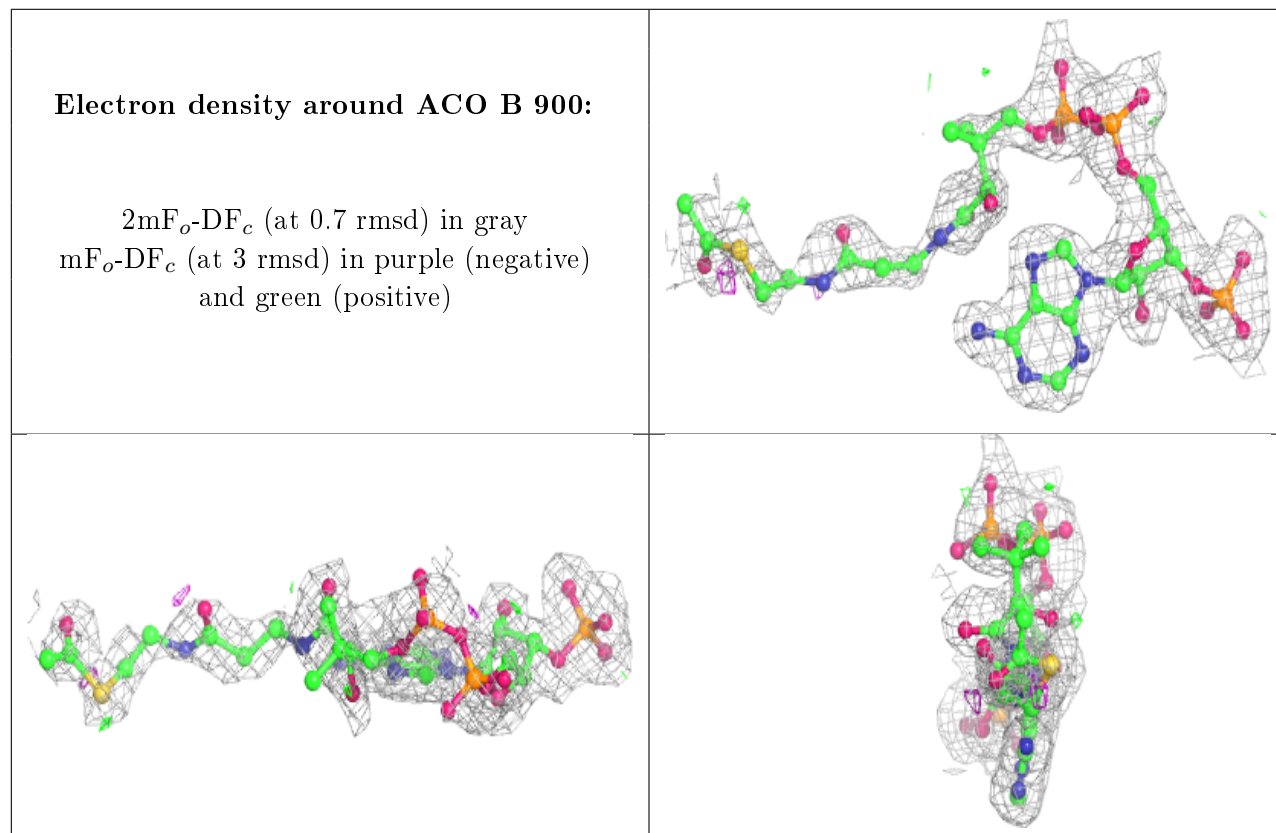
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	PG4	B	1003	13/13	0.83	0.17	44,56,68,68	0
7	PG4	B	1002	13/13	0.84	0.19	29,40,64,66	0
6	PEG	A	1001	7/7	0.85	0.20	43,44,47,48	0
4	ACO	B	900	51/51	0.92	0.15	23,53,98,100	0
4	ACO	A	800	51/51	0.92	0.14	17,50,91,96	0
5	PYR	B	910	6/6	0.98	0.19	20,23,32,32	0
5	PYR	A	810	6/6	0.98	0.14	13,20,21,44	0

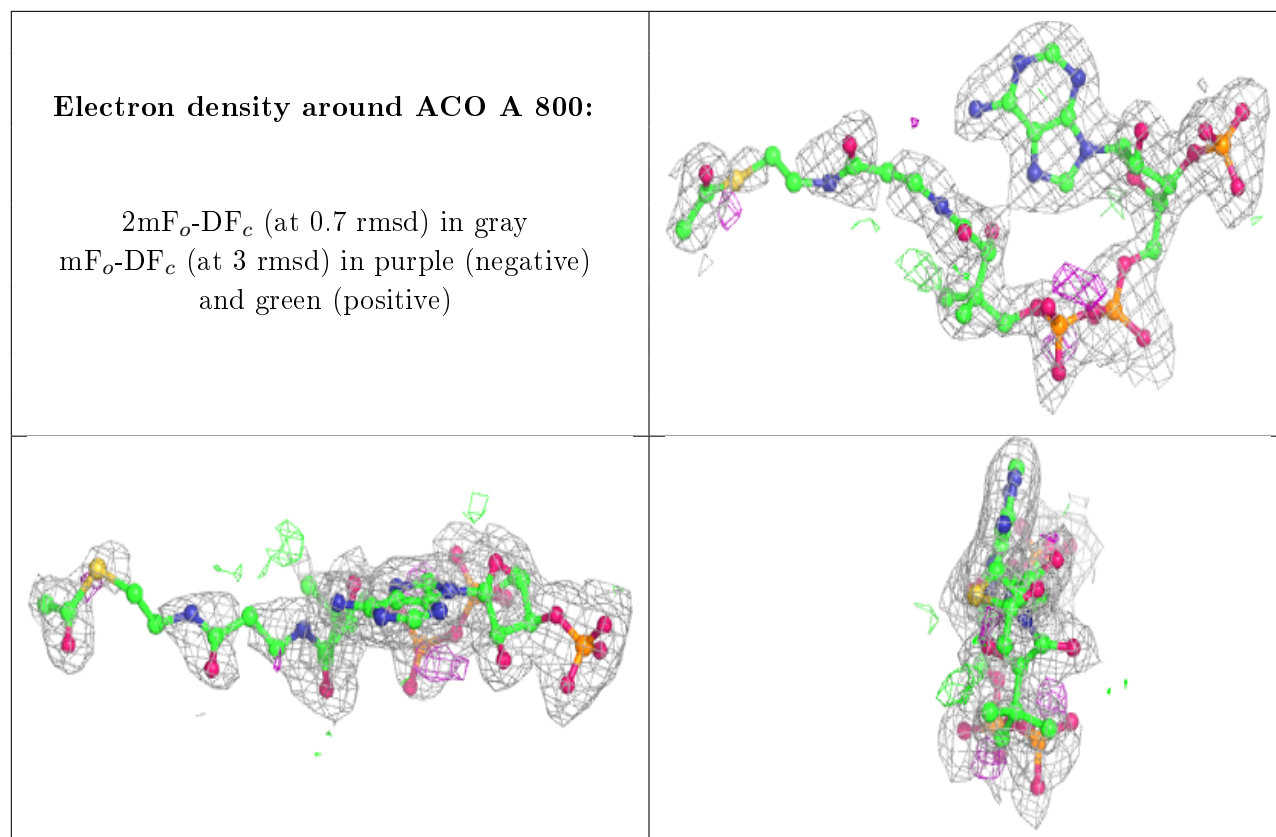
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	1000	1/1	0.98	0.09	16,16,16,16	0
3	MG	B	1001	1/1	0.99	0.11	17,17,17,17	0

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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.