



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:45 PM GMT

PDB ID : 1CBU
Title : ADENOSYLCOBINAMIDE KINASE/ADENOSYLCOBINAMIDE PHOSPHATE GUANYLYLTRANSFERASE (COBU) FROM SALMONELLA TYPHIMURIUM
Authors : Thompson, T.B.; Thomas, M.G.; Escalante-Semerena, J.C.; Rayment, I.
Deposited on : 1998-03-12
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

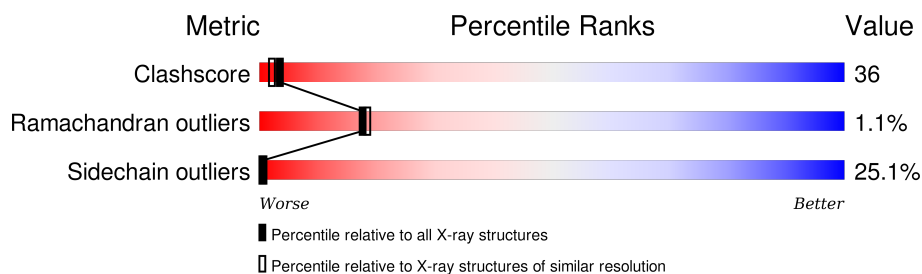
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	180	
1	B	180	
1	C	180	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	801	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	802	-	-	X	-

2 Entry composition [i](#)

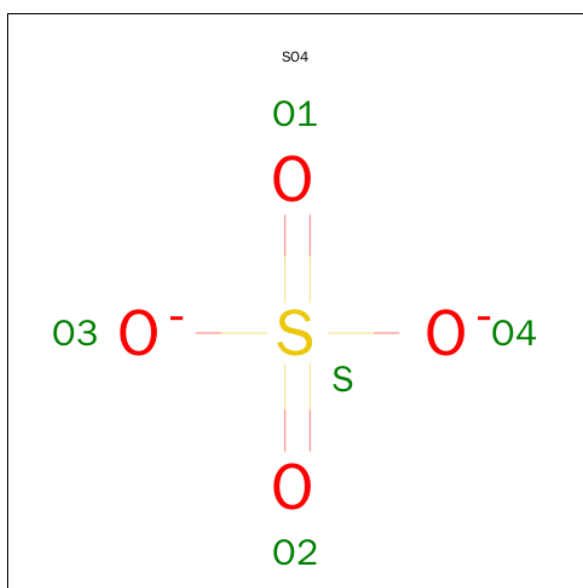
There are 3 unique types of molecules in this entry. The entry contains 4334 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ADENOSYLCOBINAMIDE KINASE/ADENOSYLCOBINAMIDE PHOSPHATE GUANYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1376	862	248	257	9			
1	B	180	Total	C	N	O	S	0	0	0
			1380	864	249	258	9			
1	C	179	Total	C	N	O	S	0	0	0
			1361	853	243	256	9			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

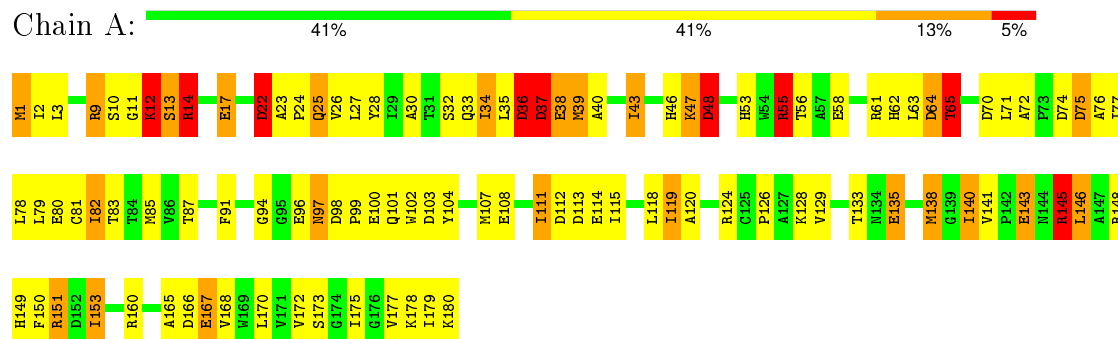
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total 72	O 72	0	0
3	B	80	Total 80	O 80	0	0
3	C	50	Total 50	O 50	0	0

3 Residue-property plots

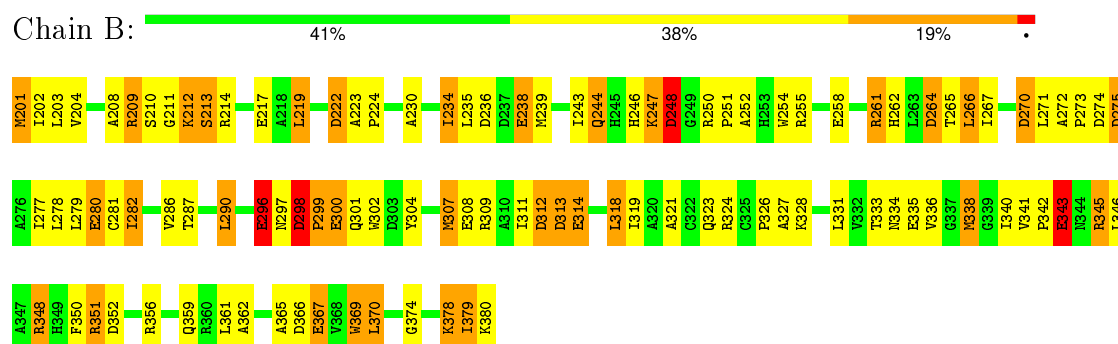
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

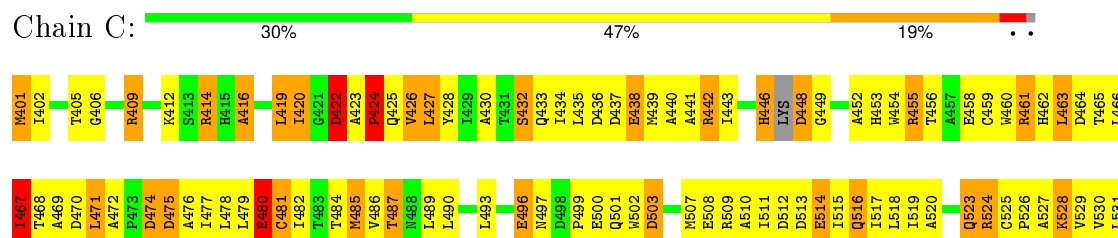
• Molecule 1: ADENOSYLCOBINAMIDE KINASE/ADENOSYLCOBINAMIDE PHOSPHATE GUANYLYLTRANSFERASE



• Molecule 1: ADENOSYLCOBINAMIDE KINASE/ADENOSYLCOBINAMIDE PHOSPHATE GUANYLYLTRANSFERASE



• Molecule 1: ADENOSYLCOBINAMIDE KINASE/ADENOSYLCOBINAMIDE PHOSPHATE GUANYLYLTRANSFERASE



Y532	Y533	Y534	E535	Y536		L540	Y541	P542	E543	Y544	R545	L546	R547	R548		D552	L553		Y557		R560	L561		A565	D566	E567	Y568	R569	L570	Y571	Y572		L575	R576	Y577	R578	L579	R580
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	96.40 Å 114.40 Å 106.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	88.5 (20.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	TNT V. 4-C	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4334	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.12	11/1399 (0.8%)	1.47	31/1901 (1.6%)
1	B	1.10	11/1403 (0.8%)	1.51	34/1906 (1.8%)
1	C	1.14	11/1383 (0.8%)	1.50	36/1880 (1.9%)
All	All	1.12	33/4185 (0.8%)	1.49	101/5687 (1.8%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	335	GLU	CD-OE1	8.70	1.35	1.25
1	C	458	GLU	CD-OE2	8.57	1.35	1.25
1	C	496	GLU	CD-OE2	8.05	1.34	1.25
1	A	100	GLU	CD-OE1	7.70	1.34	1.25
1	A	96	GLU	CD-OE1	7.64	1.34	1.25
1	C	438	GLU	CD-OE1	7.54	1.33	1.25
1	A	108	GLU	CD-OE1	7.32	1.33	1.25
1	B	296	GLU	CD-OE1	7.31	1.33	1.25
1	C	543	GLU	CD-OE2	6.99	1.33	1.25
1	B	238	GLU	CD-OE1	6.91	1.33	1.25
1	C	480	GLU	CD-OE1	6.90	1.33	1.25
1	C	535	GLU	CD-OE2	6.77	1.33	1.25
1	A	38	GLU	CD-OE1	6.74	1.33	1.25
1	A	58	GLU	CD-OE1	6.61	1.32	1.25
1	B	367	GLU	CD-OE1	6.59	1.32	1.25
1	B	314	GLU	CD-OE1	6.58	1.32	1.25
1	A	81	CYS	CB-SG	-6.48	1.71	1.82
1	A	167	GLU	CD-OE1	6.39	1.32	1.25
1	A	135	GLU	CD-OE2	6.39	1.32	1.25
1	B	280	GLU	CD-OE1	6.33	1.32	1.25
1	A	80	GLU	CD-OE1	6.29	1.32	1.25
1	B	300	GLU	CD-OE2	6.29	1.32	1.25
1	A	143	GLU	CD-OE2	6.12	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	343	GLU	CD-OE2	6.03	1.32	1.25
1	C	458	GLU	CD-OE1	-5.94	1.19	1.25
1	C	500	GLU	CD-OE2	5.83	1.32	1.25
1	C	567	GLU	CD-OE2	5.72	1.31	1.25
1	C	508	GLU	CD-OE1	5.68	1.31	1.25
1	B	217	GLU	CD-OE2	5.67	1.31	1.25
1	C	514	GLU	CD-OE1	5.45	1.31	1.25
1	B	308	GLU	CD-OE1	5.39	1.31	1.25
1	B	258	GLU	CD-OE1	5.34	1.31	1.25
1	A	17	GLU	CD-OE1	5.21	1.31	1.25

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	ARG	C-N-CD	-17.39	82.33	120.60
1	C	422	ASP	CB-CG-OD1	10.66	127.90	118.30
1	C	422	ASP	CB-CG-OD2	-9.99	109.31	118.30
1	C	512	ASP	CB-CG-OD2	9.40	126.76	118.30
1	C	512	ASP	CB-CG-OD1	-9.28	109.95	118.30
1	A	145	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	B	356	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	C	509	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	B	236	ASP	CB-CG-OD2	8.25	125.73	118.30
1	A	36	ASP	CB-CG-OD1	-7.70	111.37	118.30
1	C	544	ASN	CB-CA-C	7.63	125.66	110.40
1	B	236	ASP	CB-CG-OD1	-7.62	111.44	118.30
1	A	36	ASP	CB-CG-OD2	7.45	125.00	118.30
1	A	166	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	B	222	ASP	CB-CG-OD1	-7.26	111.77	118.30
1	C	464	ASP	CB-CG-OD1	-7.15	111.86	118.30
1	A	112	ASP	CB-CG-OD1	-7.10	111.91	118.30
1	B	370	LEU	CB-CA-C	7.07	123.64	110.20
1	C	503	ASP	CB-CG-OD1	-7.07	111.94	118.30
1	B	255	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	A	81	CYS	N-CA-CB	-6.94	98.10	110.60
1	B	351	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	103	ASP	CB-CG-OD1	-6.88	112.11	118.30
1	B	270	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	B	356	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	C	481	CYS	N-CA-CB	-6.62	98.69	110.60
1	A	55	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	48	ASP	CB-CG-OD1	-6.57	112.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	566	ASP	CB-CG-OD1	6.53	124.18	118.30
1	C	424	PRO	N-CA-CB	6.52	111.13	103.30
1	A	75	ASP	CB-CG-OD2	6.47	124.12	118.30
1	C	513	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	A	70	ASP	CB-CG-OD1	-6.42	112.53	118.30
1	A	64	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	C	566	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	B	366	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	C	464	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	75	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	B	366	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	74	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	151	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	437	ASP	CB-CG-OD1	-6.22	112.70	118.30
1	B	222	ASP	CB-CG-OD2	6.18	123.86	118.30
1	B	312	ASP	CB-CG-OD1	-6.14	112.77	118.30
1	B	214	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	509	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	C	513	ASP	CB-CG-OD2	6.10	123.79	118.30
1	B	255	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	113	ASP	CB-CG-OD1	-6.04	112.86	118.30
1	C	436	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	541	VAL	CB-CA-C	-5.98	100.04	111.40
1	C	474	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	248	ASP	CB-CG-OD2	5.94	123.65	118.30
1	B	275	ASP	CB-CG-OD1	-5.93	112.97	118.30
1	A	14	ARG	CB-CA-C	5.93	122.25	110.40
1	B	248	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	C	475	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	A	46	HIS	CB-CA-C	-5.84	98.73	110.40
1	B	281	CYS	N-CA-CB	-5.83	100.10	110.60
1	B	270	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	166	ASP	CB-CG-OD1	5.79	123.51	118.30
1	C	448	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	C	448	ASP	CB-CG-OD1	5.74	123.46	118.30
1	B	274	ASP	CB-CG-OD1	-5.71	113.17	118.30
1	B	264	ASP	CB-CG-OD2	5.62	123.35	118.30
1	B	370	LEU	N-CA-CB	5.62	121.63	110.40
1	C	437	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	275	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	474	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	552	ASP	CB-CG-OD2	5.56	123.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	22	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	C	503	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	264	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	C	560	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	64	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	552	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	B	356	ARG	CD-NE-CZ	5.42	131.19	123.60
1	A	70	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	436	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	A	55	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	48	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	103	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	351	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	369	TRP	CB-CA-C	-5.29	99.82	110.40
1	A	14	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	313	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	A	145	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	12	LYS	N-CA-CB	5.22	120.00	110.60
1	C	536	VAL	CB-CA-C	-5.19	101.55	111.40
1	B	313	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	423	ALA	N-CA-C	-5.17	97.05	111.00
1	B	298	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	567	GLU	N-CA-CB	5.15	119.86	110.60
1	A	37	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	B	298	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	A	65	THR	CA-CB-CG2	5.11	119.56	112.40
1	C	416	ALA	N-CA-CB	5.11	117.25	110.10
1	C	461	ARG	CB-CA-C	-5.08	100.23	110.40
1	B	274	ASP	CB-CG-OD2	5.00	122.80	118.30
1	C	470	ASP	CB-CG-OD1	-5.00	113.80	118.30

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	1376	0	1376	103	1
1	B	1380	0	1379	85	1
1	C	1361	0	1348	123	0
2	A	5	0	0	2	0
2	B	5	0	0	3	0
2	C	5	0	0	0	0
3	A	72	0	0	6	0
3	B	80	0	0	6	0
3	C	50	0	0	6	0
All	All	4334	0	4103	299	1

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 36.

All (299) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ILE:HG12	1:C:567:GLU:HG3	1.14	1.07
1:A:14:ARG:HH11	1:A:14:ARG:HG2	1.26	1.01
1:B:234:ILE:HD12	1:B:234:ILE:H	1.30	0.95
1:A:145:ARG:H	1:A:145:ARG:HD3	1.34	0.92
1:B:379:ILE:HG13	1:C:575:ILE:HG21	1.51	0.91
1:C:479:LEU:HB3	1:C:531:LEU:HD22	1.54	0.89
1:A:25:GLN:NE2	1:A:53:HIS:HB3	1.88	0.88
1:A:1:MET:HG2	1:A:2:ILE:N	1.90	0.85
1:A:26:VAL:HG22	1:A:76:ALA:HB3	1.58	0.84
1:C:434:ILE:HD12	1:C:434:ILE:H	1.41	0.84
1:A:145:ARG:H	1:A:145:ARG:CD	1.89	0.83
1:C:560:ARG:HH11	1:C:560:ARG:HG3	1.45	0.82
1:A:55:ARG:HH11	1:A:55:ARG:HG3	1.45	0.81
1:A:34:ILE:H	1:A:34:ILE:HD13	1.46	0.81
1:C:425:GLN:NE2	1:C:453:HIS:HB3	1.96	0.81
1:B:265:THR:HG22	1:B:266:LEU:HD13	1.63	0.80
1:C:402:ILE:HG12	1:C:567:GLU:CG	2.04	0.79
1:A:115:ILE:HG22	1:A:119:ILE:CD1	2.12	0.79
1:C:402:ILE:CG1	1:C:567:GLU:HG3	2.07	0.79
1:C:463:LEU:HD23	1:C:518:LEU:HD22	1.65	0.78
1:C:439:MET:HG3	1:C:443:ILE:HD11	1.65	0.78
1:A:34:ILE:O	1:A:38:GLU:HG3	1.83	0.77
1:B:201:MET:HG2	1:B:202:ILE:N	1.98	0.77
1:B:307:MET:O	1:B:311:ILE:HG13	1.85	0.77
1:A:62:HIS:O	1:A:65:THR:HB	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:TRP:CZ3	1:C:489:LEU:HD23	2.21	0.76
1:B:261:ARG:CB	1:B:261:ARG:HH11	2.00	0.75
1:C:426:VAL:HG11	1:C:454:TRP:CD2	2.22	0.75
1:C:425:GLN:HB3	1:C:455:ARG:HH12	1.49	0.75
1:A:150:PHE:CE2	1:C:540:ILE:HD11	2.22	0.74
1:A:107:MET:O	1:A:111:ILE:HG13	1.87	0.74
1:A:3:LEU:HD11	1:A:133:THR:HG22	1.69	0.74
1:A:34:ILE:H	1:A:34:ILE:CD1	1.97	0.74
1:C:442:ARG:O	1:C:446:HIS:HB2	1.88	0.73
1:B:345:ARG:HH11	1:B:345:ARG:HG2	1.53	0.73
1:B:345:ARG:NH1	1:B:345:ARG:HG2	2.02	0.73
1:A:10:SER:OG	1:A:12:LYS:HG2	1.88	0.73
1:C:530:VAL:C	1:C:531:LEU:HD23	2.08	0.73
1:C:460:TRP:HZ3	1:C:489:LEU:HD23	1.52	0.73
1:C:568:VAL:HG12	1:C:579:ILE:CG1	2.18	0.73
1:A:40:ALA:HB1	3:A:776:HOH:O	1.88	0.73
1:C:530:VAL:O	1:C:531:LEU:HD23	1.89	0.73
1:A:115:ILE:O	1:A:119:ILE:HD12	1.89	0.72
1:C:471:LEU:O	1:C:526:PRO:HG2	1.89	0.72
1:A:145:ARG:HH11	1:A:145:ARG:HG2	1.53	0.72
1:A:150:PHE:CD2	1:C:540:ILE:HD11	2.26	0.71
1:C:465:THR:HG22	1:C:466:LEU:HD13	1.72	0.71
1:A:1:MET:HB2	1:A:129:VAL:HB	1.73	0.70
1:C:568:VAL:HG12	1:C:579:ILE:HG13	1.71	0.70
1:A:25:GLN:HE21	1:A:53:HIS:HB3	1.55	0.70
1:C:520:ALA:O	1:C:523:GLN:HG3	1.91	0.70
1:C:493:LEU:HD11	1:C:510:ALA:HB3	1.73	0.70
1:C:570:LEU:O	1:C:577:VAL:HG23	1.93	0.69
1:C:412:LYS:HE2	1:C:534:ASN:ND2	2.08	0.69
1:C:471:LEU:HD12	1:C:525:CYS:SG	2.33	0.68
1:A:115:ILE:HG22	1:A:119:ILE:HD11	1.75	0.67
1:C:465:THR:HG22	1:C:466:LEU:CD1	2.23	0.67
1:B:234:ILE:O	1:B:238:GLU:HB2	1.94	0.67
1:A:33:GLN:HB3	1:A:34:ILE:HD13	1.77	0.66
1:A:64:ASP:OD1	1:A:64:ASP:N	2.27	0.66
1:A:94:GLY:N	1:A:107:MET:HE3	2.10	0.66
1:C:493:LEU:CD1	1:C:510:ALA:HB3	2.26	0.66
1:A:11:GLY:N	2:A:801:SO4:O4	2.28	0.66
1:B:287:THR:HG23	1:B:350:PHE:CE1	2.31	0.66
1:B:379:ILE:HG13	1:C:575:ILE:CG2	2.26	0.66
1:C:499:PRO:HB3	1:C:546:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASN:OD1	1:A:97:ASN:N	2.29	0.65
1:B:212:LYS:NZ	2:B:802:SO4:O4	2.30	0.65
1:B:362:ALA:O	1:B:380:LYS:NZ	2.30	0.65
1:A:119:ILE:HG22	1:A:120:ALA:N	2.12	0.65
1:B:341:VAL:HG22	1:B:351:ARG:NH2	2.12	0.64
1:A:82:ILE:O	1:A:85:MET:HB3	1.97	0.64
1:A:173:SER:HA	3:C:650:HOH:O	1.96	0.64
1:B:342:PRO:O	1:B:348:ARG:NE	2.26	0.64
1:B:271:LEU:O	1:B:326:PRO:HG2	1.98	0.64
1:B:359:GLN:OE1	1:C:414:ARG:NH1	2.31	0.64
1:C:416:ALA:O	1:C:419:LEU:HB2	1.98	0.64
1:A:1:MET:HE1	1:A:165:ALA:HB2	1.79	0.63
1:C:477:ILE:HB	1:C:529:VAL:HG22	1.80	0.63
1:A:13:SER:O	1:A:17:GLU:HG3	1.98	0.63
1:A:141:VAL:HG22	1:A:151:ARG:HH22	1.63	0.63
1:C:560:ARG:CG	1:C:560:ARG:HH11	2.11	0.63
1:B:213:SER:HB3	1:B:280:GLU:OE2	1.98	0.63
1:C:497:ASN:HB2	1:C:502:TRP:HE1	1.63	0.63
1:A:145:ARG:N	1:A:145:ARG:HD3	2.10	0.63
1:B:309:ARG:HA	1:B:312:ASP:OD2	1.99	0.63
1:C:432:SER:OG	1:C:435:LEU:HD12	1.99	0.62
1:B:264:ASP:N	1:B:264:ASP:OD1	2.28	0.62
1:A:145:ARG:CG	1:A:145:ARG:HH11	2.13	0.62
1:C:452:ALA:HB1	1:C:454:TRP:HD1	1.63	0.62
1:C:452:ALA:HB1	1:C:454:TRP:CD1	2.33	0.62
1:B:304:TYR:HA	1:B:307:MET:HG3	1.80	0.62
1:A:135:GLU:HG3	3:A:639:HOH:O	1.98	0.62
1:B:247:LYS:HG3	1:B:248:ASP:OD1	2.00	0.62
1:C:440:ALA:HA	1:C:443:ILE:HD12	1.81	0.62
1:C:493:LEU:HD11	1:C:510:ALA:CB	2.29	0.61
1:A:145:ARG:HA	1:A:148:ARG:NH2	2.14	0.61
1:A:71:LEU:O	1:A:126:PRO:HG2	2.00	0.61
1:A:178:LYS:HE3	1:A:180:LYS:OXT	2.00	0.61
1:C:499:PRO:CB	1:C:546:LEU:HD12	2.29	0.61
1:B:262:HIS:O	1:B:265:THR:HB	2.01	0.61
1:C:475:ASP:O	1:C:527:ALA:HB1	2.01	0.60
1:A:14:ARG:HG2	1:A:14:ARG:NH1	2.02	0.60
1:B:352:ASP:OD1	1:C:409:ARG:HD3	2.01	0.60
1:A:115:ILE:HG22	1:A:119:ILE:HD12	1.82	0.60
1:B:243:ILE:O	1:B:247:LYS:HB3	2.02	0.59
1:B:235:LEU:O	1:B:238:GLU:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:LYS:HE2	1:C:533:THR:O	2.03	0.59
1:C:439:MET:HA	1:C:439:MET:HE2	1.85	0.59
1:C:553:ILE:O	1:C:557:VAL:HG23	2.03	0.59
1:A:140:ILE:CD1	1:B:351:ARG:HG3	2.33	0.58
1:A:82:ILE:HB	1:A:133:THR:HB	1.84	0.58
1:C:580:LYS:HE3	3:C:665:HOH:O	2.02	0.58
1:A:175:ILE:HD13	1:C:580:LYS:HB2	1.83	0.58
1:A:141:VAL:HG22	1:A:151:ARG:NH2	2.18	0.58
1:B:244:GLN:HA	1:B:244:GLN:NE2	2.16	0.57
1:A:48:ASP:OD1	1:A:48:ASP:N	2.35	0.57
1:C:516:GLN:HB3	3:C:765:HOH:O	2.02	0.57
1:A:1:MET:CE	1:A:165:ALA:HB2	2.33	0.57
1:B:247:LYS:HE2	3:B:685:HOH:O	2.05	0.57
1:C:477:ILE:N	1:C:528:LYS:O	2.32	0.57
1:A:55:ARG:HH11	1:A:55:ARG:CG	2.15	0.57
1:B:271:LEU:CD1	1:B:277:ILE:HD11	2.34	0.57
1:B:211:GLY:N	2:B:802:SO4:O2	2.28	0.56
1:C:401:MET:CE	1:C:531:LEU:HG	2.36	0.56
1:A:47:LYS:HD2	1:A:48:ASP:OD2	2.05	0.56
1:A:83:THR:HG22	3:A:701:HOH:O	2.05	0.56
1:A:149:HIS:O	1:A:153:ILE:HG13	2.05	0.56
1:C:472:ALA:HB3	1:C:475:ASP:OD2	2.05	0.56
1:B:296:GLU:HG2	1:B:296:GLU:O	2.03	0.56
1:A:3:LEU:HD11	1:A:133:THR:CG2	2.35	0.56
1:A:76:ALA:O	1:A:77:ILE:HG12	2.06	0.56
1:B:282:ILE:O	1:B:286:VAL:HG23	2.06	0.56
1:A:177:VAL:O	1:A:179:ILE:HG23	2.06	0.55
1:C:425:GLN:HE21	1:C:453:HIS:HB3	1.71	0.55
1:A:27:LEU:HD12	1:A:28:TYR:N	2.20	0.55
1:C:479:LEU:HD23	1:C:479:LEU:C	2.26	0.55
1:C:405:THR:HB	1:C:533:THR:HG22	1.88	0.55
1:A:98:ASP:O	1:A:101:GLN:HG2	2.05	0.55
1:B:261:ARG:HB2	1:B:261:ARG:HH11	1.71	0.55
1:B:261:ARG:HB3	1:B:261:ARG:HH11	1.72	0.55
1:C:460:TRP:HB2	1:C:485:MET:HG2	1.89	0.55
1:A:138:MET:HG2	1:B:338:MET:HG3	1.88	0.54
1:C:515:ILE:O	1:C:519:ILE:HG13	2.07	0.54
1:C:434:ILE:CD1	1:C:434:ILE:H	2.16	0.54
1:C:565:ALA:O	1:C:580:LYS:NZ	2.27	0.54
1:B:342:PRO:HG2	1:B:348:ARG:HA	1.88	0.54
1:B:324:ARG:O	1:B:326:PRO:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:C	1:A:119:ILE:HD12	2.28	0.54
1:B:210:SER:OG	1:B:212:LYS:HG2	2.08	0.54
1:B:279:LEU:HD23	1:B:279:LEU:C	2.27	0.54
1:B:210:SER:O	1:B:374:GLY:N	2.41	0.53
1:A:39:MET:O	1:A:43:ILE:HD12	2.08	0.53
1:C:426:VAL:HG12	1:C:454:TRP:HA	1.90	0.53
1:B:212:LYS:HG3	2:B:802:SO4:O1	2.07	0.53
1:A:150:PHE:HE2	1:C:540:ILE:HD11	1.73	0.53
1:A:168:VAL:HB	1:A:180:LYS:HB3	1.90	0.52
1:A:72:ALA:O	1:A:75:ASP:N	2.36	0.52
1:C:438:GLU:HB2	3:C:752:HOH:O	2.10	0.52
1:C:568:VAL:CG1	1:C:579:ILE:HG13	2.39	0.52
1:B:272:ALA:O	1:B:275:ASP:HB2	2.09	0.52
1:C:446:HIS:O	1:C:449:GLY:N	2.29	0.52
1:C:401:MET:HG2	1:C:402:ILE:N	2.24	0.51
1:B:301:GLN:HG2	3:B:771:HOH:O	2.09	0.51
1:C:503:ASP:O	1:C:507:MET:HG3	2.10	0.51
1:B:201:MET:HE1	1:B:365:ALA:HB2	1.93	0.51
1:A:34:ILE:N	1:A:34:ILE:HD13	2.20	0.51
1:C:463:LEU:O	1:C:467:ILE:HG13	2.09	0.51
1:A:79:LEU:C	1:A:79:LEU:HD23	2.31	0.51
1:B:212:LYS:HE2	1:B:334:ASN:OD1	2.10	0.51
1:B:273:PRO:HA	1:B:326:PRO:O	2.11	0.51
1:B:345:ARG:HH11	1:B:345:ARG:CG	2.24	0.50
1:C:402:ILE:HG23	1:C:567:GLU:O	2.11	0.50
1:A:53:HIS:ND1	3:A:708:HOH:O	2.35	0.50
1:A:99:PRO:HA	1:A:102:TRP:CG	2.46	0.50
1:C:428:TYR:CE2	1:C:430:ALA:HB2	2.45	0.50
1:A:99:PRO:HA	1:A:102:TRP:CD2	2.46	0.50
1:C:497:ASN:CB	1:C:502:TRP:HE1	2.25	0.50
1:A:14:ARG:CG	1:A:14:ARG:HH11	2.11	0.50
1:B:351:ARG:HD2	3:B:589:HOH:O	2.10	0.50
1:C:461:ARG:O	1:C:462:HIS:HB2	2.11	0.50
1:C:499:PRO:HB3	1:C:546:LEU:CD1	2.40	0.49
1:C:405:THR:HB	1:C:533:THR:CG2	2.43	0.49
1:B:279:LEU:HD23	1:B:280:GLU:N	2.27	0.49
1:A:22:ASP:OD1	1:A:22:ASP:N	2.45	0.49
1:B:204:VAL:HG22	1:B:369:TRP:HB2	1.95	0.48
1:C:426:VAL:HG12	1:C:454:TRP:CG	2.49	0.48
1:B:313:ASP:HB3	3:B:718:HOH:O	2.14	0.48
1:B:201:MET:HE3	1:B:203:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:TYR:HE1	3:A:764:HOH:O	1.95	0.48
1:C:438:GLU:O	1:C:441:ALA:HB3	2.14	0.48
1:C:524:ARG:NH1	3:C:733:HOH:O	2.32	0.48
1:C:443:ILE:HG22	1:C:443:ILE:O	2.13	0.48
1:C:401:MET:HE2	1:C:531:LEU:HG	1.96	0.47
1:C:482:ILE:O	1:C:486:VAL:HG23	2.14	0.47
1:B:267:ILE:HD12	1:B:318:LEU:HD12	1.96	0.47
1:C:479:LEU:HD23	1:C:480:GLU:N	2.30	0.47
1:B:201:MET:HG3	1:B:331:LEU:HG	1.95	0.47
1:C:426:VAL:CG1	1:C:454:TRP:CG	2.98	0.47
1:C:466:LEU:O	1:C:468:THR:HG23	2.15	0.47
1:A:12:LYS:HE3	1:A:133:THR:O	2.13	0.47
1:A:167:GLU:HG2	1:A:178:LYS:NZ	2.29	0.47
1:C:439:MET:C	1:C:441:ALA:H	2.18	0.47
1:C:446:HIS:O	1:C:448:ASP:N	2.48	0.47
1:C:471:LEU:HD12	1:C:525:CYS:HG	1.78	0.47
1:B:299:PRO:HA	1:B:302:TRP:CD1	2.49	0.47
1:A:9:ARG:HA	2:A:801:SO4:O1	2.15	0.47
1:C:401:MET:HE3	1:C:531:LEU:HG	1.97	0.47
1:C:406:GLY:O	1:C:534:ASN:HA	2.15	0.46
1:C:426:VAL:HG23	1:C:476:ALA:HB3	1.98	0.46
1:A:94:GLY:N	1:A:107:MET:CE	2.78	0.46
1:B:209:ARG:N	1:B:209:ARG:HD3	2.31	0.46
1:A:55:ARG:HD3	3:A:667:HOH:O	2.15	0.46
1:A:124:ARG:O	1:A:126:PRO:HD3	2.16	0.46
1:C:439:MET:HE3	3:C:752:HOH:O	2.15	0.46
1:B:287:THR:CG2	1:B:350:PHE:CE1	2.97	0.46
1:B:282:ILE:HD12	1:B:361:LEU:HD11	1.97	0.46
1:B:223:ALA:O	1:B:252:ALA:HB1	2.16	0.46
1:B:266:LEU:HA	1:B:266:LEU:HD12	1.60	0.46
1:C:460:TRP:CE3	1:C:489:LEU:CD2	2.99	0.46
1:B:267:ILE:HG22	1:B:321:ALA:O	2.16	0.45
1:A:32:SER:OG	1:A:35:LEU:HG	2.17	0.45
1:C:439:MET:HA	1:C:439:MET:CE	2.46	0.45
1:C:420:ILE:HG12	1:C:420:ILE:H	1.60	0.45
1:C:568:VAL:HB	1:C:580:LYS:HB3	1.98	0.45
1:A:91:PHE:CD1	1:A:102:TRP:HH2	2.34	0.45
1:A:111:ILE:O	1:A:114:GLU:HB2	2.17	0.45
1:C:507:MET:O	1:C:511:ILE:HG13	2.16	0.45
1:B:299:PRO:HA	1:B:302:TRP:CE2	2.52	0.45
1:A:63:LEU:C	1:A:65:THR:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:MET:HB3	1:B:338:MET:HB2	1.98	0.44
1:A:1:MET:HE3	1:A:3:LEU:HB2	1.99	0.44
1:C:424:PRO:O	1:C:453:HIS:N	2.48	0.44
1:B:351:ARG:HB3	3:B:679:HOH:O	2.17	0.44
1:C:419:LEU:HD12	1:C:419:LEU:HA	1.82	0.44
1:C:480:GLU:HB2	1:C:532:VAL:HB	1.99	0.44
1:B:234:ILE:H	1:B:234:ILE:CD1	2.04	0.44
1:B:202:ILE:HG12	1:B:367:GLU:HB3	1.99	0.44
1:A:43:ILE:O	1:A:47:LYS:N	2.50	0.44
1:C:427:LEU:HD22	1:C:428:TYR:N	2.32	0.44
1:A:28:TYR:CG	1:A:39:MET:HG2	2.52	0.44
1:A:1:MET:HE2	1:A:165:ALA:CB	2.48	0.43
1:A:167:GLU:CD	1:A:178:LYS:HZ2	2.21	0.43
1:C:557:VAL:O	1:C:561:LEU:HG	2.17	0.43
1:A:145:ARG:NH1	1:A:145:ARG:CG	2.78	0.43
1:C:405:THR:CB	1:C:533:THR:HG22	2.48	0.43
1:A:34:ILE:HA	1:A:37:ASP:HB2	2.00	0.43
1:C:471:LEU:CD1	1:C:525:CYS:SG	3.05	0.43
1:C:412:LYS:CE	1:C:534:ASN:ND2	2.79	0.43
1:B:209:ARG:CD	1:B:209:ARG:N	2.82	0.43
1:A:145:ARG:HA	1:A:148:ARG:CZ	2.47	0.43
1:B:346:LEU:HD12	1:B:346:LEU:O	2.19	0.43
1:C:426:VAL:CG1	1:C:454:TRP:CD2	2.99	0.43
1:C:487:THR:O	1:C:490:LEU:HB2	2.19	0.43
1:B:219:LEU:HD12	1:B:219:LEU:HA	1.71	0.42
1:C:480:GLU:HA	1:C:481:CYS:HA	1.79	0.42
1:A:120:ALA:O	1:A:124:ARG:HG3	2.19	0.42
1:A:35:LEU:HA	1:A:35:LEU:HD23	1.73	0.42
1:B:336:VAL:HG23	1:B:336:VAL:O	2.17	0.42
1:B:298:ASP:O	1:B:300:GLU:N	2.52	0.42
1:C:422:ASP:O	1:C:422:ASP:OD1	2.37	0.42
1:B:262:HIS:N	1:B:314:GLU:OE2	2.44	0.42
1:A:170:LEU:O	1:A:177:VAL:N	2.51	0.42
1:A:99:PRO:HB3	1:A:146:LEU:HD13	2.02	0.42
1:B:254:TRP:HB2	3:B:658:HOH:O	2.19	0.42
1:C:402:ILE:HG23	1:C:567:GLU:C	2.40	0.42
1:C:511:ILE:O	1:C:515:ILE:HG12	2.19	0.42
1:B:290:LEU:HA	1:B:290:LEU:HD12	1.87	0.42
1:B:201:MET:CE	1:B:365:ALA:HB2	2.50	0.42
1:C:490:LEU:HA	1:C:490:LEU:HD23	1.64	0.42
1:C:460:TRP:CZ3	1:C:489:LEU:CD2	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASN:O	1:A:102:TRP:NE1	2.52	0.41
1:A:99:PRO:O	1:A:102:TRP:HB2	2.21	0.41
1:C:533:THR:HG23	1:C:534:ASN:N	2.35	0.41
1:A:1:MET:CE	1:A:165:ALA:CB	2.99	0.41
1:C:460:TRP:CE3	1:C:489:LEU:HD23	2.53	0.41
1:C:460:TRP:N	1:C:460:TRP:CD1	2.89	0.41
1:B:271:LEU:HD11	1:B:277:ILE:HD11	2.02	0.41
1:C:497:ASN:HB2	1:C:502:TRP:NE1	2.34	0.41
1:B:201:MET:CG	1:B:202:ILE:N	2.78	0.41
1:C:478:LEU:CD1	1:C:530:VAL:HG12	2.51	0.41
1:C:469:ALA:HA	1:C:526:PRO:HD3	2.03	0.41
1:C:466:LEU:C	1:C:468:THR:HG23	2.41	0.41
1:B:333:THR:OG1	1:B:334:ASN:N	2.54	0.41
1:B:271:LEU:HD13	1:B:327:ALA:CB	2.51	0.41
1:A:27:LEU:HD12	1:A:27:LEU:C	2.41	0.41
1:A:79:LEU:O	1:A:79:LEU:HD23	2.21	0.41
1:A:30:ALA:HB3	1:A:36:ASP:HB2	2.03	0.41
1:C:479:LEU:HB3	1:C:531:LEU:CD2	2.39	0.40
1:A:94:GLY:HA3	1:A:102:TRP:CE2	2.56	0.40
1:A:23:ALA:HA	1:A:24:PRO:HD3	1.96	0.40
1:C:531:LEU:N	1:C:531:LEU:HD23	2.35	0.40
1:B:261:ARG:HB2	1:B:261:ARG:NH1	2.33	0.40
1:B:230:ALA:HA	1:B:280:GLU:O	2.22	0.40
1:C:517:ILE:O	1:C:520:ALA:HB3	2.22	0.40
1:B:369:TRP:CZ2	1:B:378:LYS:HG3	2.56	0.40
1:B:208:ALA:O	1:B:209:ARG:HB2	2.21	0.40
1:A:150:PHE:HD2	1:C:540:ILE:HD11	1.80	0.40
1:B:267:ILE:HD12	1:B:318:LEU:CD1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:NH2	1:B:343:GLU:OE1[3_656]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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	178/180 (99%)	171 (96%)	7 (4%)	0	100	100
1	B	178/180 (99%)	169 (95%)	6 (3%)	3 (2%)	11	10
1	C	175/180 (97%)	157 (90%)	15 (9%)	3 (2%)	11	10
All	All	531/540 (98%)	497 (94%)	28 (5%)	6 (1%)	17	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	PRO
1	C	420	ILE
1	C	424	PRO
1	C	467	ILE
1	B	299	PRO
1	B	224	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	141/143 (99%)	107 (76%)	34 (24%)	1	0
1	B	142/143 (99%)	108 (76%)	34 (24%)	1	0
1	C	139/143 (97%)	101 (73%)	38 (27%)	0	0
All	All	422/429 (98%)	316 (75%)	106 (25%)	1	0

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	ARG
1	A	12	LYS
1	A	13	SER
1	A	14	ARG
1	A	22	ASP
1	A	25	GLN
1	A	34	ILE
1	A	36	ASP
1	A	37	ASP
1	A	39	MET
1	A	43	ILE
1	A	47	LYS
1	A	48	ASP
1	A	55	ARG
1	A	56	THR
1	A	61	ARG
1	A	65	THR
1	A	78	LEU
1	A	82	ILE
1	A	87	THR
1	A	97	ASN
1	A	111	ILE
1	A	118	LEU
1	A	119	ILE
1	A	128	LYS
1	A	138	MET
1	A	140	ILE
1	A	143	GLU
1	A	145	ARG
1	A	146	LEU
1	A	153	ILE
1	A	160	ARG
1	A	172	VAL
1	B	201	MET
1	B	209	ARG
1	B	212	LYS
1	B	213	SER
1	B	219	LEU
1	B	222	ASP
1	B	234	ILE
1	B	239	MET

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Mol	Chain	Res	Type
1	B	244	GLN
1	B	246	HIS
1	B	247	LYS
1	B	248	ASP
1	B	261	ARG
1	B	266	LEU
1	B	270	ASP
1	B	278	LEU
1	B	282	ILE
1	B	290	LEU
1	B	296	GLU
1	B	297	ASN
1	B	298	ASP
1	B	307	MET
1	B	318	LEU
1	B	319	ILE
1	B	323	GLN
1	B	328	LYS
1	B	338	MET
1	B	340	ILE
1	B	343	GLU
1	B	345	ARG
1	B	348	ARG
1	B	370	LEU
1	B	378	LYS
1	B	379	ILE
1	C	401	MET
1	C	409	ARG
1	C	414	ARG
1	C	419	LEU
1	C	422	ASP
1	C	426	VAL
1	C	427	LEU
1	C	432	SER
1	C	433	GLN
1	C	442	ARG
1	C	446	HIS
1	C	455	ARG
1	C	456	THR
1	C	459	CYS
1	C	463	LEU
1	C	467	ILE

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Mol	Chain	Res	Type
1	C	471	LEU
1	C	474	ASP
1	C	480	GLU
1	C	484	THR
1	C	485	MET
1	C	487	THR
1	C	496	GLU
1	C	501	GLN
1	C	514	GLU
1	C	516	GLN
1	C	523	GLN
1	C	524	ARG
1	C	528	LYS
1	C	533	THR
1	C	540	ILE
1	C	544	ASN
1	C	546	LEU
1	C	548	ARG
1	C	560	ARG
1	C	566	ASP
1	C	567	GLU
1	C	572	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	123	GLN
1	B	215	HIS
1	B	225	GLN
1	C	501	GLN
1	C	516	GLN
1	C	534	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	801	-	4,4,4	0.45	0	6,6,6	0.16	0
2	SO4	B	802	-	4,4,4	0.53	0	6,6,6	0.08	0
2	SO4	C	803	-	4,4,4	0.45	0	6,6,6	0.09	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
2	SO4	A	801	-	-	0/0/0/0	0/0/0/0
2	SO4	B	802	-	-	0/0/0/0	0/0/0/0
2	SO4	C	803	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

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 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	SO4	2	0
2	B	802	SO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.