



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:27 PM UTC

PDB ID : 1CBU / pdb_00001cbu
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

<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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

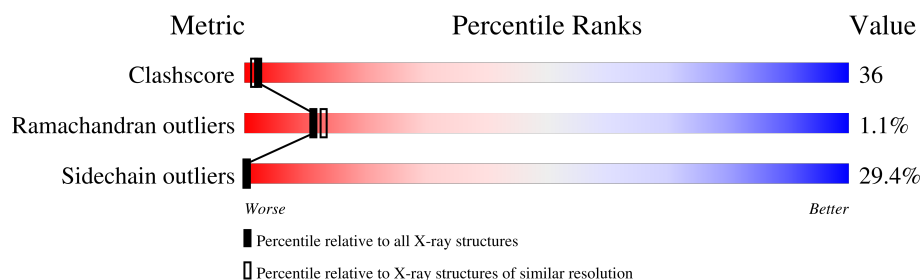
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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 $\leq 5\%$.

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	-
2	SO4	B	802	-	-	X	-

2 Entry composition [i](#)

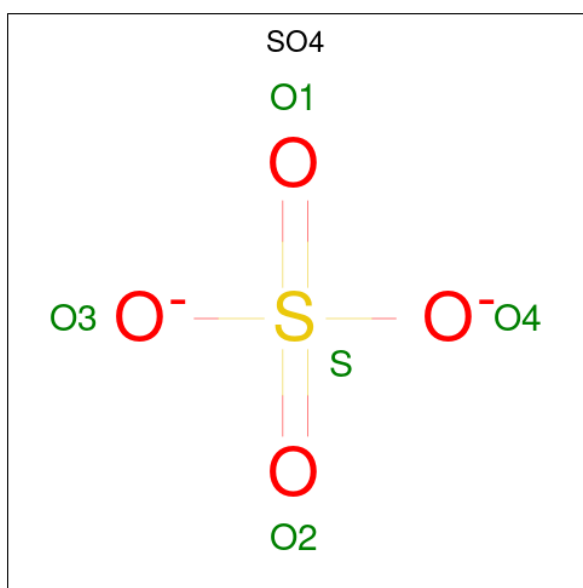
There are 3 unique types of molecules in this entry. The entry contains 4334 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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.

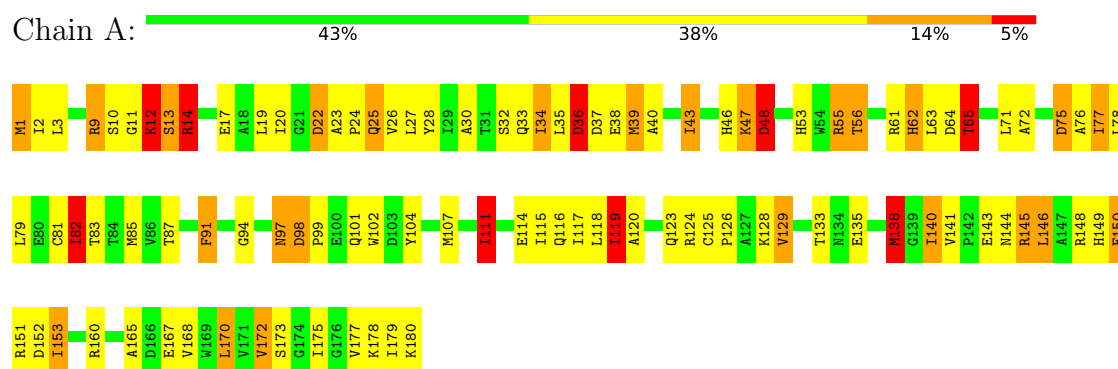
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total 72	O 72	0	0
3	B	80	Total 80	O 80	0	0
3	C	50	Total 50	O 50	0	0

3 Residue-property plots [i](#)

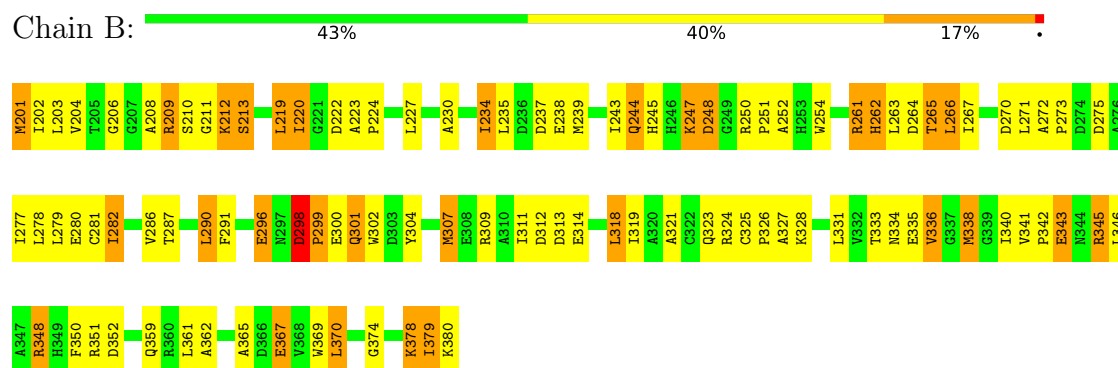
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

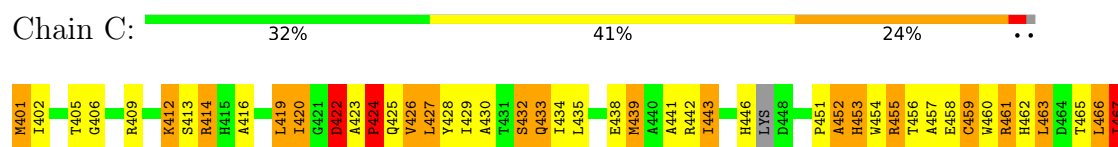
• Molecule 1: ADENOSYLCOBINAMIDE KINASE/ADENOSYLCOBINAMIDE PHOSPHATE GUANYLYLTRANSFERASE

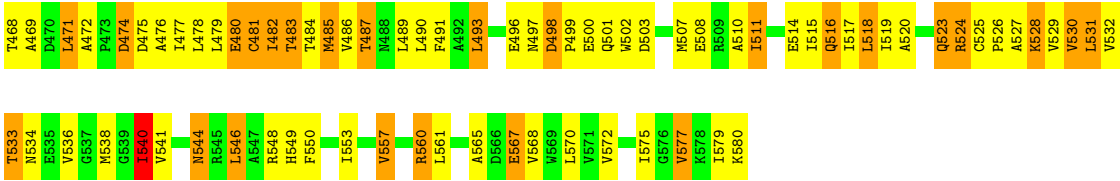


• Molecule 1: ADENOSYLCOBINAMIDE KINASE/ADENOSYLCOBINAMIDE PHOSPHATE GUANYLYLTRANSFERASE



• Molecule 1: ADENOSYLCOBINAMIDE KINASE/ADENOSYLCOBINAMIDE PHOSPHATE GUANYLYLTRANSFERASE





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 4C	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	1.32	3/1399 (0.2%)	1.63	24/1901 (1.3%)
1	B	1.27	1/1403 (0.1%)	1.62	15/1906 (0.8%)
1	C	1.34	6/1383 (0.4%)	1.69	26/1880 (1.4%)
All	All	1.31	10/4185 (0.2%)	1.65	65/5687 (1.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	ILE	CA-CB	-7.45	1.45	1.54
1	C	458	GLU	CA-CB	6.47	1.61	1.53
1	C	511	ILE	CA-CB	-6.18	1.46	1.54
1	A	117	ILE	CA-CB	-5.39	1.48	1.54
1	A	129	VAL	CA-CB	-5.24	1.48	1.54
1	B	335	GLU	CD-OE1	5.20	1.35	1.25
1	C	458	GLU	CD-OE2	5.12	1.35	1.25
1	C	498	ASP	CG-OD1	5.12	1.35	1.25
1	C	557	VAL	CA-CB	-5.08	1.48	1.54
1	C	457	ALA	C-N	5.06	1.40	1.33

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	PHE	CA-CB-CG	-11.28	102.53	113.80
1	C	491	PHE	CA-CB-CG	-11.18	102.62	113.80
1	B	250	ARG	C-N-CD	-10.41	82.33	125.00
1	A	91	PHE	CA-CB-CG	-10.29	103.51	113.80
1	C	544	ASN	CB-CA-C	8.96	125.66	109.62
1	A	172	VAL	CB-CA-C	7.97	120.22	110.73
1	C	550	PHE	CA-CB-CG	-7.92	105.88	113.80
1	B	370	LEU	CB-CA-C	7.88	123.64	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ASP	CA-CB-CG	7.52	120.12	112.60
1	C	424	PRO	N-CA-CB	7.50	111.13	103.25
1	A	81	CYS	N-CA-CB	-7.29	98.10	110.50
1	C	481	CYS	N-CA-CB	-6.95	98.69	110.50
1	B	262	HIS	CA-CB-CG	-6.91	106.89	113.80
1	A	14	ARG	CB-CA-C	6.91	122.25	110.79
1	A	62	HIS	CA-CB-CG	-6.89	106.91	113.80
1	A	150	PHE	CA-CB-CG	-6.88	106.92	113.80
1	C	459	CYS	N-CA-C	6.80	118.72	108.46
1	A	46	HIS	CB-CA-C	-6.77	98.73	110.17
1	B	370	LEU	N-CA-CB	6.72	121.63	110.47
1	C	452	ALA	N-CA-C	6.62	119.49	108.96
1	C	422	ASP	N-CA-C	6.58	118.94	110.65
1	A	98	ASP	CA-CB-CG	6.53	119.13	112.60
1	A	36	ASP	CA-CB-CG	6.35	118.95	112.60
1	C	549	HIS	CA-CB-CG	-6.31	107.49	113.80
1	C	491	PHE	N-CA-C	6.29	117.80	111.07
1	A	12	LYS	N-CA-CB	6.27	120.00	110.28
1	C	541	VAL	CB-CA-C	-6.22	100.04	111.36
1	C	412	LYS	N-CA-C	6.13	117.96	111.28
1	B	281	CYS	N-CA-CB	-6.12	100.10	110.50
1	C	544	ASN	CA-CB-CG	6.07	118.67	112.60
1	C	511	ILE	N-CA-CB	-6.04	102.32	110.54
1	A	48	ASP	CA-CB-CG	-5.98	106.62	112.60
1	A	82	ILE	N-CA-C	5.96	116.62	110.36
1	C	536	VAL	CB-CA-C	-5.94	101.55	111.29
1	C	433	GLN	N-CA-C	-5.60	105.08	111.07
1	C	474	ASP	N-CA-C	-5.60	106.61	113.50
1	C	423	ALA	N-CA-C	-5.58	97.05	108.21
1	C	422	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	220	ILE	N-CA-CB	-5.53	104.38	110.51
1	A	65	THR	N-CA-CB	-5.51	101.85	110.44
1	C	544	ASN	N-CA-CB	5.44	118.04	110.04
1	A	119	ILE	CB-CA-C	-5.44	104.89	112.02
1	A	125	CYS	CA-C-N	5.43	125.52	119.87
1	A	125	CYS	C-N-CA	5.43	125.52	119.87
1	B	245	HIS	CA-CB-CG	-5.38	108.42	113.80
1	A	56	THR	N-CA-CB	5.35	119.08	111.05
1	A	65	THR	CA-CB-CG2	5.33	119.56	110.50
1	B	325	CYS	CA-C-N	5.30	126.47	119.84
1	B	325	CYS	C-N-CA	5.30	126.47	119.84
1	C	540	ILE	CB-CA-C	5.25	118.74	111.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	GLY	CA-C-N	-5.23	117.77	122.43
1	B	206	GLY	C-N-CA	-5.23	117.77	122.43
1	A	138	MET	CB-CA-C	-5.22	102.62	111.02
1	B	298	ASP	CB-CA-C	5.19	117.81	109.51
1	A	75	ASP	N-CA-CB	5.18	117.62	110.17
1	B	367	GLU	N-CA-CB	-5.15	101.91	111.13
1	C	453	HIS	CA-CB-CG	-5.15	108.65	113.80
1	C	461	ARG	CB-CA-C	-5.12	100.23	110.42
1	C	451	PRO	CB-CA-C	-5.12	103.12	111.56
1	A	144	ASN	CA-C-N	5.10	127.43	120.54
1	A	144	ASN	C-N-CA	5.10	127.43	120.54
1	A	65	THR	OG1-CB-CG2	5.04	119.37	109.30
1	C	483	THR	N-CA-CB	5.03	117.51	110.12
1	C	482	ILE	N-CA-C	5.02	115.74	110.62
1	B	237	ASP	CB-CA-C	-5.00	101.37	110.63

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	106	1
1	B	1380	0	1379	88	1
1	C	1361	0	1348	117	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	7	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:HG2	1:A:14:ARG:HH11	1.26	1.01
1:B:234:ILE:HD12	1:B:234:ILE:H	1.30	0.95
1:A:145:ARG:HD3	1:A:145:ARG:H	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:401:MET:HE2	1:C:531:LEU:HG	1.59	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:HG3	1:C:560:ARG:HH11	1.45	0.82
1:A:55:ARG:HG3	1:A:55:ARG:HH11	1.45	0.81
1:A:34:ILE:HD13	1:A:34:ILE:H	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:C:530:VAL:C	1:C:531:LEU:HD23	2.08	0.78
1:A:94:GLY:N	1:A:107:MET:HE3	1.99	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
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:B:345:ARG:HG2	1:B:345:ARG:HH11	1.53	0.73
1:B:345:ARG:HG2	1:B:345:ARG:NH1	2.02	0.73
1:A:10:SER:OG	1:A:12:LYS:HG2	1.88	0.73
1:C:460:TRP:HZ3	1:C:489:LEU:HD23	1.52	0.73
1:A:40:ALA:HB1	3:A:776:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:VAL:HG12	1:C:579:ILE:CG1	2.18	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:HG2	1:A:145:ARG:HH11	1.53	0.72
1:C:439:MET:HE2	1:C:439:MET:HA	1.72	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:412:LYS:HE2	1:C:534:ASN:ND2	2.08	0.69
1:C:570:LEU:O	1:C:577:VAL:HG23	1.93	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: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
1:A:97:ASN:N	1:A:97:ASN:OD1	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
3:A:584:HOH:O	1:C:538:MET:HE3	1.96	0.64
1:A:64:ASP:OD1	1:A:64:ASP:N	2.27	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:13:SER:O	1:A:17:GLU:HG3	1.98	0.63
1:C:401:MET:HE2	1:C:531:LEU:CG	2.26	0.63
1:C:477:ILE:HB	1:C:529:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:VAL:HG22	1:A:151:ARG:HH22	1.63	0.63
1:B:213:SER:HB3	1:B:280:GLU:OE2	1.98	0.63
1:C:560:ARG:HH11	1:C:560:ARG:CG	2.11	0.63
1:C:497:ASN:HB2	1:C:502:TRP:HE1	1.63	0.63
1:A:145:ARG:HD3	1:A:145:ARG:N	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:OD1	1:B:264:ASP:N	2.28	0.62
1:A:145:ARG:HH11	1:A:145:ARG:CG	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: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:B:304:TYR:HA	1:B:307:MET:HG3	1.80	0.62
1:C:493:LEU:HD11	1:C:510:ALA:CB	2.29	0.61
1:A:71:LEU:O	1:A:126:PRO:HG2	2.00	0.61
1:A:145:ARG:HA	1:A:148:ARG:NH2	2.14	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:A:1:MET:HE1	1:A:165:ALA:HB2	1.83	0.60
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:C:479:LEU:C	1:C:479:LEU:HD23	2.26	0.59
1:B:235:LEU:O	1:B:238:GLU:HB3	2.02	0.59
1:C:412:LYS:HE2	1:C:533:THR:O	2.03	0.59
1:C:553:ILE:O	1:C:557:VAL:HG23	2.03	0.59
1:A:115:ILE:C	1:A:119:ILE:HD12	2.28	0.58
1:A:140:ILE:CD1	1:B:351:ARG:HG3	2.33	0.58
1:B:279:LEU:C	1:B:279:LEU:HD23	2.27	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:141:VAL:HG22	1:A:151:ARG:NH2	2.18	0.58
1:A:175:ILE:HD13	1:C:580:LYS:HB2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:296:GLU:O	1:B:296:GLU:HG2	2.03	0.56
1:C:472:ALA:HB3	1:C:475:ASP:OD2	2.05	0.56
1:A:3:LEU:HD11	1:A:133:THR:CG2	2.35	0.56
1:A:79:LEU:C	1:A:79:LEU:HD23	2.31	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:A:27:LEU:HD12	1:A:28:TYR:N	2.20	0.55
1:C:425:GLN:HE21	1:C:453:HIS:HB3	1.71	0.55
1:A:98:ASP:O	1:A:101:GLN:HG2	2.05	0.55
1:C:405:THR:HB	1:C:533:THR:HG22	1.88	0.55
1:B:261:ARG:HH11	1:B:261:ARG:HB2	1.71	0.55
1:B:261:ARG:HH11	1:B:261:ARG:HB3	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:401:MET:CE	1:C:531:LEU:HG	2.36	0.54
1:C:515:ILE:O	1:C:519:ILE:HG13	2.07	0.54
1:B:324:ARG:O	1:B:326:PRO:HD3	2.07	0.54
1:B:342:PRO:HG2	1:B:348:ARG:HA	1.88	0.54
1:C:434:ILE:H	1:C:434:ILE:CD1	2.16	0.54
1:C:565:ALA:O	1:C:580:LYS:NZ	2.27	0.54
1:B:210:SER:OG	1:B:212:LYS:HG2	2.08	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:B:212:LYS:HG3	2:B:802:SO4:O1	2.07	0.53
1:C:426:VAL:HG12	1:C:454:TRP:HA	1.90	0.53
1:B:201:MET:HE2	1:B:365:ALA:HA	1.91	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:B:272:ALA:O	1:B:275:ASP:HB2	2.09	0.52
1:C:568:VAL:CG1	1:C:579:ILE:HG13	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:CD	1:A:178:LYS:HZ2	2.18	0.52
1:C:439:MET:C	1:C:441:ALA:H	2.18	0.52
1:B:301:GLN:HG2	3:B:771:HOH:O	2.09	0.51
1:C:401:MET:HG2	1:C:402:ILE:N	2.24	0.51
1:C:503:ASP:O	1:C:507:MET:HG3	2.10	0.51
1:A:34:ILE:HD13	1:A:34:ILE:N	2.20	0.51
1:C:463:LEU:O	1:C:467:ILE:HG13	2.09	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: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:402:ILE:HG23	1:C:567:GLU:O	2.11	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:HH11	1:A:14:ARG:CG	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:B:279:LEU:HD23	1:B:280:GLU:N	2.27	0.49
1:C:405:THR:HB	1:C:533:THR:CG2	2.43	0.49
1:A:63:LEU:C	1:A:65:THR:H	2.20	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:B:313:ASP:HB3	3:B:718:HOH:O	2.14	0.48
1:C:426:VAL:HG12	1:C:454:TRP:CG	2.49	0.48
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: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: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:C:479:LEU:HD23	1:C:480:GLU:N	2.30	0.47
1:A:1:MET:HE2	1:A:165:ALA:CB	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ILE:HG23	1:C:567:GLU:C	2.40	0.46
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: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:B:223:ALA:O	1:B:252:ALA:HB1	2.16	0.46
1:B:282:ILE:HD12	1:B:361:LEU:HD11	1.97	0.46
1:B:287:THR:CG2	1:B:350:PHE:CE1	2.97	0.46
1:B:266:LEU:HD12	1:B:266:LEU:HA	1.60	0.46
1:C:460:TRP:CE3	1:C:489:LEU:CD2	2.99	0.46
1:A:27:LEU:HD12	1:A:27:LEU:C	2.41	0.45
1:B:267:ILE:HG22	1:B:321:ALA:O	2.16	0.45
1:C:466:LEU:C	1:C:468:THR:HG23	2.41	0.45
1:A:94:GLY:CA	1:A:107:MET:HE3	2.46	0.45
1:A:32:SER:OG	1:A:35:LEU:HG	2.17	0.45
1:C:420:ILE:H	1:C:420:ILE:HG12	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:B:299:PRO:HA	1:B:302:TRP:CE2	2.52	0.45
1:C:507:MET:O	1:C:511:ILE:HG13	2.16	0.45
1:B:201:MET:HE3	1:B:203:LEU:HB2	2.00	0.44
1:A:138:MET:HB3	1:B:338:MET:HB2	1.98	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:424:PRO:O	1:C:453:HIS:N	2.48	0.44
1:B:234:ILE:H	1:B:234:ILE:CD1	2.04	0.44
1:C:480:GLU:HB2	1:C:532:VAL:HB	1.99	0.44
1:A:43:ILE:O	1:A:47:LYS:N	2.50	0.44
1:B:202:ILE:HG12	1:B:367:GLU:HB3	1.99	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:94:GLY:N	1:A:107:MET:CE	2.78	0.44
1:C:557:VAL:O	1:C:561:LEU:HG	2.17	0.43
1:A:145:ARG:CG	1:A:145:ARG:NH1	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:B:201:MET:HE2	1:B:365:ALA:CA	2.48	0.43
1:B:209:ARG:N	1:B:209:ARG:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:LEU:C	1:B:265:THR:N	2.77	0.43
1:C:412:LYS:CE	1:C:534:ASN:ND2	2.79	0.43
1:A:145:ARG:HA	1:A:148:ARG:CZ	2.47	0.43
1:A:1:MET:HE3	1:A:3:LEU:HB2	2.00	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:A:35:LEU:HA	1:A:35:LEU:HD23	1.73	0.42
1:A:120:ALA:O	1:A:124:ARG:HG3	2.19	0.42
1:B:336:VAL:O	1:B:336:VAL:HG23	2.17	0.42
1:C:480:GLU:HA	1:C:481:CYS:HA	1.79	0.42
1:B:298:ASP:O	1:B:300:GLU:N	2.52	0.42
1:B:307:MET:HE2	1:B:307:MET:HB3	1.87	0.42
1:C:422:ASP:OD1	1:C:422:ASP:O	2.37	0.42
1:A:170:LEU:O	1:A:177:VAL:N	2.51	0.42
1:B:262:HIS:N	1:B:314:GLU:OE2	2.44	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:B:290:LEU:HD12	1:B:290:LEU:HA	1.87	0.42
1:C:511:ILE:O	1:C:515:ILE:HG12	2.19	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:498:ASP:C	1:C:500:GLU:N	2.76	0.41
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:460:TRP:CZ3	1:C:489:LEU:CD2	2.97	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:B:271:LEU:HD11	1:B:277:ILE:HD11	2.02	0.41
1:C:439:MET:HE3	3:C:752:HOH:O	2.19	0.41
1:C:460:TRP:CD1	1:C:460:TRP:N	2.89	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:A:30:ALA:HB3	1:A:36:ASP:HB2	2.03	0.41
1:A:63:LEU:C	1:A:65:THR:N	2.78	0.41
1:A:79:LEU:HD23	1:A:79:LEU:O	2.21	0.41
1:B:271:LEU:HD13	1:B:327:ALA:CB	2.51	0.41
1:B:333:THR:OG1	1:B:334:ASN:N	2.54	0.41
1:C:469:ALA:HA	1:C:526:PRO:HD3	2.03	0.41
1:C:478:LEU:CD1	1:C:530:VAL:HG12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ALA:HA	1:A:24:PRO:HD3	1.96	0.40
1:A:94:GLY:HA3	1:A:102:TRP:CE2	2.56	0.40
1:C:479:LEU:HB3	1:C:531:LEU:CD2	2.39	0.40
1:B:230:ALA:HA	1:B:280:GLU:O	2.22	0.40
1:B:261:ARG:HB2	1:B:261:ARG:NH1	2.33	0.40
1:B:208:ALA:O	1:B:209:ARG:HB2	2.21	0.40
1:B:369:TRP:CZ2	1:B:378:LYS:HG3	2.56	0.40
1:C:517:ILE:O	1:C:520:ALA:HB3	2.22	0.40
1:A:150:PHE:HD2	1:C:540:ILE:HD11	1.80	0.40
1:A:167:GLU:CD	1:A:178:LYS:NZ	2.80	0.40
1:B:267:ILE:HD12	1:B:318:LEU:CD1	2.51	0.40
1:C:518:LEU:C	1:C:518:LEU:HD12	2.47	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 [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	178/180 (99%)	171 (96%)	7 (4%)	0	100	100
1	B	178/180 (99%)	169 (95%)	6 (3%)	3 (2%)	7	7
1	C	175/180 (97%)	157 (90%)	15 (9%)	3 (2%)	7	7
All	All	531/540 (98%)	497 (94%)	28 (5%)	6 (1%)	11	13

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%)	102 (72%)	39 (28%)	0	0
1	B	142/143 (99%)	105 (74%)	37 (26%)	0	0
1	C	139/143 (97%)	91 (66%)	48 (34%)	0	0
All	All	422/429 (98%)	298 (71%)	124 (29%)	0	0

All (124) 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	19	LEU
1	A	20	ILE
1	A	22	ASP
1	A	25	GLN
1	A	34	ILE
1	A	36	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

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Mol	Chain	Res	Type
1	A	61	ARG
1	A	65	THR
1	A	77	ILE
1	A	78	LEU
1	A	82	ILE
1	A	87	THR
1	A	97	ASN
1	A	111	ILE
1	A	116	GLN
1	A	118	LEU
1	A	119	ILE
1	A	123	GLN
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	170	LEU
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	220	ILE
1	B	222	ASP
1	B	227	LEU
1	B	234	ILE
1	B	239	MET
1	B	244	GLN
1	B	247	LYS
1	B	248	ASP
1	B	261	ARG
1	B	265	THR
1	B	266	LEU
1	B	270	ASP
1	B	278	LEU
1	B	282	ILE
1	B	290	LEU

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Mol	Chain	Res	Type
1	B	296	GLU
1	B	298	ASP
1	B	301	GLN
1	B	307	MET
1	B	318	LEU
1	B	319	ILE
1	B	323	GLN
1	B	328	LYS
1	B	336	VAL
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	413	SER
1	C	414	ARG
1	C	419	LEU
1	C	422	ASP
1	C	426	VAL
1	C	427	LEU
1	C	429	ILE
1	C	432	SER
1	C	433	GLN
1	C	439	MET
1	C	442	ARG
1	C	443	ILE
1	C	446	HIS
1	C	455	ARG
1	C	456	THR
1	C	459	CYS
1	C	463	LEU
1	C	466	LEU
1	C	467	ILE
1	C	471	LEU
1	C	474	ASP
1	C	480	GLU
1	C	483	THR
1	C	484	THR

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Mol	Chain	Res	Type
1	C	485	MET
1	C	487	THR
1	C	493	LEU
1	C	496	GLU
1	C	501	GLN
1	C	508	GLU
1	C	514	GLU
1	C	516	GLN
1	C	518	LEU
1	C	523	GLN
1	C	524	ARG
1	C	528	LYS
1	C	530	VAL
1	C	531	LEU
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	567	GLU
1	C	572	VAL
1	C	577	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) 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	B	245	HIS
1	C	425	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	802	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	A	801	-	4,4,4	0.36	0	6,6,6	0.15	0
2	SO4	C	803	-	4,4,4	0.27	0	6,6,6	0.08	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	B	802	SO4	3	0
2	A	801	SO4	2	0

5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.