



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:42 AM UTC

PDB ID : 1NBA / pdb_00001nba
Title : CRYSTAL STRUCTURE ANALYSIS, REFINEMENT AND ENZYMATICAL REACTION MECHANISM OF N-CARBAMOYL-SARCOSINE AMIDOHYDROLASE FROM ARTHROBACTER SP. AT 2.0 ANGSTROMS RESOLUTION
Authors : Romao, M.J.; Turk, D.; Gomis-Ruth, F.-Z.; Huber, R.; Schumacher, G.; Moller, H.; Russmann, L.
Deposited on : 1992-05-18
Resolution : 2.00 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

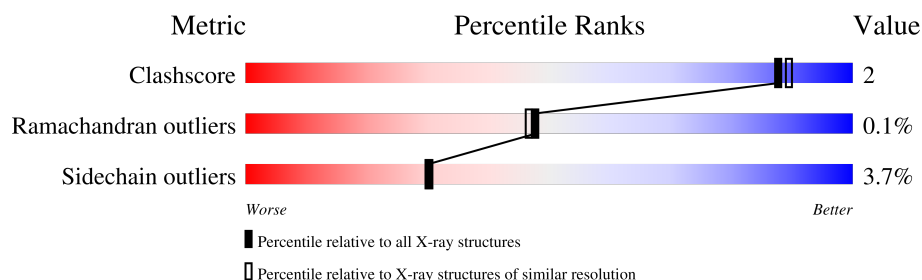
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	264	 79% 15% . .
1	B	264	 77% 16% . 5%
1	C	264	 81% 12% . .
1	D	264	 80% 14% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8304 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 N-CARBAMOYLSARCOSINE AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	12	0	0
			1965	1238	339	384	4			
1	B	252	Total	C	N	O	S	22	0	0
			1958	1234	338	382	4			
1	C	253	Total	C	N	O	S	51	0	0
			1965	1238	339	384	4			
1	D	253	Total	C	N	O	S	22	0	0
			1965	1238	339	384	4			

- 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		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		
3	B	108	Total	O	0	0
			108	108		
3	C	88	Total	O	0	0
			88	88		
3	D	128	Total	O	0	0
			128	128		

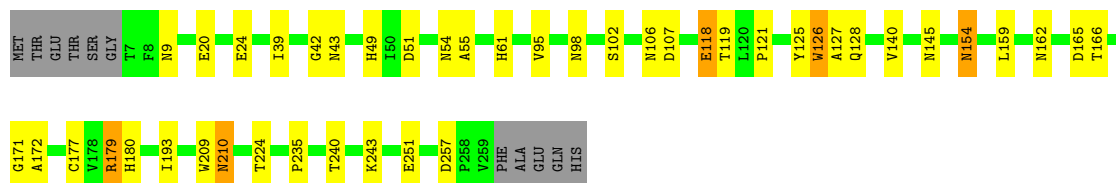
3 Residue-property plots [i](#)

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.

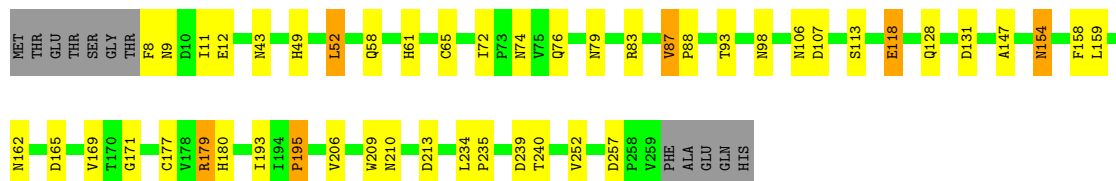
• Molecule 1: N-CARBAMOYLSARCOSINE AMIDOHYDROLASE

Chain A: 



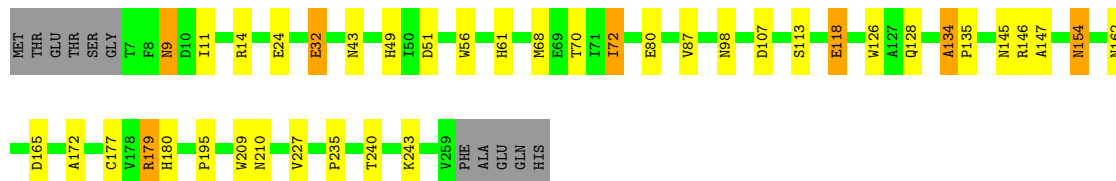
• Molecule 1: N-CARBAMOYLSARCOSINE AMIDOHYDROLASE

Chain B: 



• Molecule 1: N-CARBAMOYLSARCOSINE AMIDOHYDROLASE

Chain C: 



• Molecule 1: N-CARBAMOYLSARCOSINE AMIDOHYDROLASE

Chain D: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.22Å 122.29Å 70.87Å 90.00° 91.82° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8304	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.82	3/2012 (0.1%)	1.59	26/2751 (0.9%)
1	B	0.82	3/2005 (0.1%)	1.63	35/2741 (1.3%)
1	C	0.81	3/2012 (0.1%)	1.63	33/2751 (1.2%)
1	D	0.81	3/2012 (0.1%)	1.63	32/2751 (1.2%)
All	All	0.82	12/8041 (0.1%)	1.62	126/10994 (1.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	HIS	CD2-NE2	-6.74	1.30	1.37
1	B	49	HIS	CD2-NE2	-6.68	1.30	1.37
1	B	180	HIS	CD2-NE2	-6.67	1.30	1.37
1	C	180	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	180	HIS	CD2-NE2	-6.65	1.30	1.37
1	D	180	HIS	CD2-NE2	-6.52	1.30	1.37
1	C	61	HIS	CD2-NE2	-6.51	1.30	1.37
1	D	49	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	49	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	61	HIS	CD2-NE2	-6.16	1.31	1.37
1	D	61	HIS	CD2-NE2	-6.08	1.31	1.37
1	C	49	HIS	CD2-NE2	-5.86	1.31	1.37

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	128	GLN	OE1-CD-NE2	-12.08	110.52	122.60
1	D	128	GLN	CG-CD-NE2	9.46	130.60	116.40
1	D	162	ASN	OD1-CG-ND2	-9.06	113.54	122.60
1	A	98	ASN	OD1-CG-ND2	-8.85	113.75	122.60
1	A	171	GLY	N-CA-C	8.13	119.77	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ASN	OD1-CG-ND2	-8.05	114.55	122.60
1	C	43	ASN	CA-CB-CG	8.02	120.62	112.60
1	D	98	ASN	OD1-CG-ND2	-8.00	114.60	122.60
1	A	172	ALA	O-C-N	-7.89	113.64	123.27
1	C	9	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	A	98	ASN	CB-CG-ND2	7.80	128.10	116.40
1	D	128	GLN	CB-CG-CD	7.45	125.26	112.60
1	D	171	GLY	N-CA-C	7.35	118.98	111.56
1	D	107	ASP	CA-CB-CG	7.30	119.90	112.60
1	B	98	ASN	OD1-CG-ND2	-7.24	115.36	122.60
1	D	154	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	C	162	ASN	OD1-CG-ND2	-7.12	115.47	122.60
1	A	177	CYS	N-CA-C	7.11	119.89	111.71
1	B	11	ILE	N-CA-C	7.04	118.67	111.00
1	C	98	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	D	177	CYS	N-CA-C	6.97	120.67	111.75
1	A	118	GLU	CA-CB-CG	6.95	127.99	114.10
1	D	162	ASN	CB-CG-ND2	6.91	126.77	116.40
1	B	12	GLU	N-CA-C	6.90	118.80	111.28
1	B	162	ASN	OD1-CG-ND2	-6.79	115.81	122.60
1	B	72	ILE	N-CA-CB	-6.78	105.16	110.45
1	C	165	ASP	CA-CB-CG	6.74	119.34	112.60
1	C	9	ASN	CB-CG-ND2	6.74	126.51	116.40
1	A	107	ASP	CA-CB-CG	6.73	119.33	112.60
1	C	32	GLU	CA-CB-CG	6.66	127.42	114.10
1	B	158	PHE	CA-CB-CG	6.62	120.42	113.80
1	B	43	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	C	154	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	A	162	ASN	OD1-CG-ND2	-6.52	116.08	122.60
1	C	107	ASP	CA-CB-CG	6.52	119.12	112.60
1	B	177	CYS	N-CA-C	6.51	118.37	111.28
1	A	43	ASN	OD1-CG-ND2	-6.45	116.15	122.60
1	B	239	ASP	CA-CB-CG	6.31	118.91	112.60
1	C	147	ALA	N-CA-C	6.27	118.67	111.02
1	D	145	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	C	118	GLU	CA-CB-CG	6.20	126.49	114.10
1	C	177	CYS	N-CA-C	6.16	118.79	111.71
1	A	224	THR	N-CA-C	-6.16	104.65	111.36
1	B	209	TRP	CA-CB-CG	6.15	125.29	113.60
1	D	209	TRP	CA-CB-CG	6.14	125.27	113.60
1	C	209	TRP	CA-CB-CG	6.13	125.24	113.60
1	B	147	ALA	N-CA-C	6.04	117.53	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ARG	CA-CB-CG	-6.02	102.06	114.10
1	D	61	HIS	CB-CG-CD2	-5.98	123.42	131.20
1	D	147	ALA	N-CA-C	5.97	118.28	111.11
1	A	154	ASN	CB-CG-ND2	5.97	125.36	116.40
1	A	209	TRP	CA-CB-CG	5.94	124.88	113.60
1	D	145	ASN	CA-CB-CG	5.91	118.51	112.60
1	B	107	ASP	CA-CB-CG	5.91	118.50	112.60
1	B	165	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	172	ALA	O-C-N	-5.86	116.12	123.27
1	B	162	ASN	CB-CG-ND2	5.85	125.18	116.40
1	C	134	ALA	N-CA-C	5.84	116.31	109.60
1	D	100	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	93	THR	N-CA-C	-5.82	98.93	108.76
1	C	172	ALA	O-C-N	-5.80	116.19	123.27
1	B	118	GLU	CA-CB-CG	5.79	125.69	114.10
1	A	251	GLU	N-CA-C	5.76	118.91	109.76
1	B	179	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	B	49	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	D	154	ASN	CB-CG-ND2	5.73	124.99	116.40
1	D	49	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	D	87	VAL	CA-C-N	5.70	125.99	119.83
1	D	87	VAL	C-N-CA	5.70	125.99	119.83
1	B	87	VAL	CA-C-N	5.69	125.98	119.83
1	B	87	VAL	C-N-CA	5.69	125.98	119.83
1	C	179	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	A	179	ARG	NE-CZ-NH1	5.61	127.11	121.50
1	C	61	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	C	51	ASP	N-CA-C	5.58	119.09	111.39
1	B	128	GLN	CA-CB-CG	5.54	125.18	114.10
1	C	72	ILE	CA-C-O	-5.54	114.98	118.69
1	C	87	VAL	CA-C-N	5.49	125.76	119.83
1	C	87	VAL	C-N-CA	5.49	125.76	119.83
1	A	145	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	A	106	ASN	CA-CB-CG	5.46	118.06	112.60
1	B	61	HIS	CB-CG-CD2	-5.45	124.11	131.20
1	D	206	VAL	N-CA-C	5.43	116.81	110.62
1	C	11	ILE	N-CA-C	-5.42	105.44	110.53
1	B	179	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	D	43	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	49	HIS	CB-CG-CD2	-5.37	124.21	131.20
1	B	58	GLN	OE1-CD-NE2	-5.37	117.23	122.60
1	A	145	ASN	CB-CG-ND2	5.35	124.43	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	206	VAL	N-CA-C	5.34	116.71	110.62
1	D	58	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	C	179	ARG	CA-CB-CG	-5.33	103.43	114.10
1	A	54	ASN	N-CA-C	5.33	117.83	111.71
1	C	179	ARG	CB-CG-CD	5.32	123.54	111.30
1	A	257	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	145	ASN	CB-CG-ND2	5.28	124.31	116.40
1	C	49	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	B	257	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	56	TRP	CG-CD2-CE3	5.25	139.15	133.90
1	B	76	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	A	51	ASP	N-CA-C	5.25	118.63	111.39
1	D	179	ARG	CA-CB-CG	-5.25	103.61	114.10
1	B	154	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	A	165	ASP	CA-CB-CG	5.23	117.83	112.60
1	C	243	LYS	N-CA-C	-5.20	101.30	109.25
1	D	8	PHE	N-CA-C	-5.20	99.73	110.80
1	B	195	PRO	CB-CA-C	5.19	116.23	111.87
1	A	126	TRP	CG-CD2-CE3	5.18	139.08	133.90
1	C	98	ASN	CB-CG-ND2	5.18	124.17	116.40
1	C	179	ARG	NE-CZ-NH1	5.18	126.68	121.50
1	A	210	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	D	158	PHE	CA-CB-CG	5.12	118.92	113.80
1	D	106	ASN	CA-CB-CG	5.11	117.71	112.60
1	B	74	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	D	247	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	203	VAL	O-C-N	-5.11	118.14	121.72
1	B	98	ASN	CB-CG-ND2	5.10	124.04	116.40
1	C	32	GLU	CB-CG-CD	5.09	121.25	112.60
1	B	65	CYS	CA-CB-SG	-5.09	102.70	114.40
1	D	43	ASN	CB-CG-ND2	5.08	124.03	116.40
1	B	131	ASP	N-CA-C	5.07	117.46	111.33
1	C	145	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	B	106	ASN	CA-CB-CG	5.03	117.63	112.60
1	C	145	ASN	CB-CG-ND2	5.02	123.93	116.40
1	C	126	TRP	CE2-CD2-CG	-5.00	101.20	107.20

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	1965	0	1901	11	0
1	B	1958	0	1894	8	0
1	C	1965	0	1901	7	0
1	D	1965	0	1901	8	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	107	0	0	1	1
3	B	108	0	0	0	0
3	C	88	0	0	0	1
3	D	128	0	0	2	0
All	All	8304	0	7597	31	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 2.

All (31) 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:235:PRO:HG2	1:C:240:THR:HG22	1.72	0.71
1:A:39:ILE:HA	1:B:113:SER:HB3	1.80	0.64
1:B:79:ASN:O	1:B:83:ARG:HG2	2.00	0.62
1:D:79:ASN:O	1:D:83:ARG:HG2	2.00	0.62
1:A:179:ARG:HE	1:A:210:ASN:HD22	1.52	0.57
1:D:179:ARG:HE	1:D:210:ASN:HD22	1.53	0.57
1:B:179:ARG:HE	1:B:210:ASN:HD22	1.53	0.56
1:D:226:SER:HB3	3:D:454:HOH:O	2.06	0.56
1:D:44:ARG:HD3	1:D:242:PRO:HD3	1.91	0.53
1:C:195:PRO:HG3	1:C:227:VAL:HG21	1.89	0.52
1:A:235:PRO:HG2	1:A:240:THR:HG22	1.90	0.52
1:B:235:PRO:HG2	1:B:240:THR:HG22	1.94	0.50
1:A:125:TYR:HA	1:A:128:GLN:OE1	2.14	0.47
1:C:68:MET:HB3	1:C:72:ILE:HD12	1.96	0.46
1:A:166:THR:HG23	1:A:193:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:HG11	1:A:127:ALA:CB	2.47	0.45
1:B:169:VAL:O	1:B:195:PRO:HD2	2.16	0.45
1:C:179:ARG:HE	1:C:210:ASN:HD22	1.65	0.44
1:C:179:ARG:HB3	3:D:406:HOH:O	2.18	0.44
1:D:95:VAL:HG11	1:D:127:ALA:CB	2.48	0.43
1:A:55:ALA:HB2	1:A:126:TRP:HB3	2.02	0.42
1:C:146:ARG:HD2	1:D:187:ALA:HA	2.02	0.42
1:A:119:THR:CG2	1:B:252:VAL:HG23	2.50	0.42
1:B:87:VAL:HA	1:B:88:PRO:HD3	1.94	0.41
1:B:52:LEU:HD13	1:B:171:GLY:HA2	2.03	0.41
1:A:42:GLY:HA2	1:A:243:LYS:HD2	2.03	0.41
1:D:37:ARG:HB3	1:D:249:GLN:NE2	2.36	0.41
1:A:140:VAL:HG13	3:A:467:HOH:O	2.21	0.41
1:D:16:ALA:HA	1:D:208:GLN:HE22	1.86	0.40
1:A:119:THR:O	1:A:121:PRO:HD3	2.21	0.40
1:C:134:ALA:HA	1:C:135:PRO:HD3	1.93	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)
3:A:501:HOH:O	3:C:487:HOH:O[4_546]	1.72	0.48

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	251/264 (95%)	240 (96%)	11 (4%)	0	100	100
1	B	250/264 (95%)	238 (95%)	12 (5%)	0	100	100
1	C	251/264 (95%)	241 (96%)	10 (4%)	0	100	100
1	D	251/264 (95%)	238 (95%)	12 (5%)	1 (0%)	30	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1003/1056 (95%)	957 (95%)	45 (4%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	8	PHE

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	210/219 (96%)	203 (97%)	7 (3%)	33	34
1	B	209/219 (95%)	201 (96%)	8 (4%)	29	29
1	C	210/219 (96%)	200 (95%)	10 (5%)	23	21
1	D	210/219 (96%)	204 (97%)	6 (3%)	37	40
All	All	839/876 (96%)	808 (96%)	31 (4%)	30	30

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	20	GLU
1	A	24	GLU
1	A	102	SER
1	A	118	GLU
1	A	154	ASN
1	A	159	LEU
1	B	8	PHE
1	B	9	ASN
1	B	52	LEU
1	B	118	GLU
1	B	154	ASN
1	B	159	LEU
1	B	193	ILE

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Mol	Chain	Res	Type
1	B	234	LEU
1	C	9	ASN
1	C	14	ARG
1	C	24	GLU
1	C	32	GLU
1	C	70	THR
1	C	80	GLU
1	C	113	SER
1	C	118	GLU
1	C	128	GLN
1	C	154	ASN
1	D	24	GLU
1	D	83	ARG
1	D	113	SER
1	D	128	GLN
1	D	154	ASN
1	D	193	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	74	ASN
1	A	98	ASN
1	A	154	ASN
1	A	210	ASN
1	B	43	ASN
1	B	54	ASN
1	B	128	GLN
1	B	210	ASN
1	C	54	ASN
1	C	154	ASN
1	C	210	ASN
1	C	249	GLN
1	D	43	ASN
1	D	74	ASN
1	D	154	ASN
1	D	208	GLN
1	D	210	ASN
1	D	249	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	400	-	4,4,4	0.65	0	6,6,6	0.44	0
2	SO4	B	400	-	4,4,4	0.66	0	6,6,6	0.23	0
2	SO4	C	400	-	4,4,4	0.62	0	6,6,6	0.26	0
2	SO4	D	400	-	4,4,4	0.64	0	6,6,6	0.20	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.