



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:59 PM UTC

PDB ID : 1KKR / pdb_00001kkR
Title : CRYSTAL STRUCTURE OF CITROBACTER AMALONATICUS METHYL-
LASPARTATE AMMONIA LYASE CONTAINING (2S,3S)-3-METHYLASP
ARTIC ACID
Authors : Levy, C.W.; Buckley, P.A.; Sedelnikova, S.; Kato, K.; Asano, Y.; Rice, D.W.;
Baker, P.J.
Deposited on : 2001-12-10
Resolution : 2.10 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

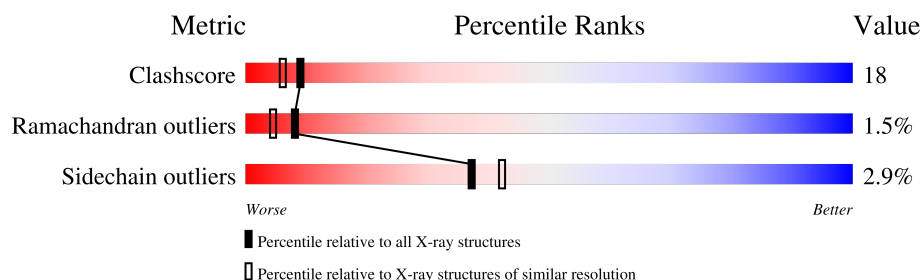
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	413	
1	B	413	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6942 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.

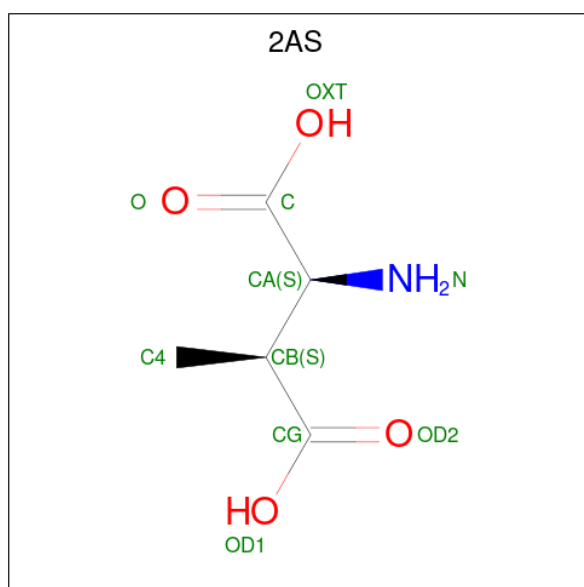
- Molecule 1 is a protein called 3-METHYLASPARTATE AMMONIA-LYASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	Se	0	0	0
			3151	2003	538	590	10	10			
1	B	411	Total	C	N	O	S	Se	0	0	0
			3140	1998	536	586	10	10			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is (2S,3S)-3-methyl-aspartic acid (CCD ID: 2AS) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	338	Total	O	0	0
			338	338		
4	B	291	Total	O	0	0
			291	291		

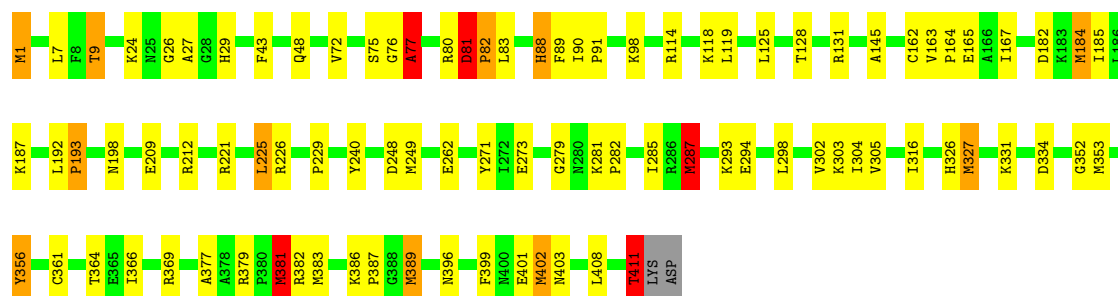
3 Residue-property plots

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

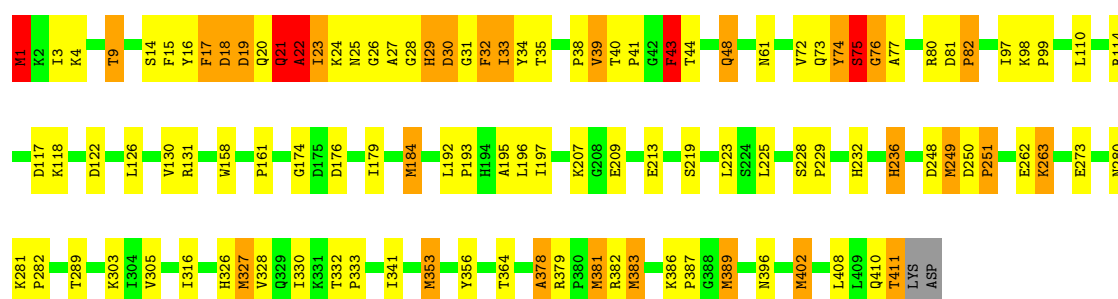
• Molecule 1: 3-METHYLASPARTATE AMMONIA-LYASE

Chain A: 



• Molecule 1: 3-METHYLASPARTATE AMMONIA-LYASE

Chain B: 



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 2	Depositor
Cell constants a, b, c, α , β , γ	129.54Å 238.93Å 66.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.10	Depositor
% Data completeness (in resolution range)	93.2 (18.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6942	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: 2AS, MG

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	1.58	14/3208 (0.4%)	1.31	17/4341 (0.4%)
1	B	1.60	18/3197 (0.6%)	1.36	24/4327 (0.6%)
All	All	1.59	32/6405 (0.5%)	1.33	41/8668 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	MSE	SE-CE	-32.93	0.96	1.95
1	A	383	MSE	SE-CE	-29.58	1.06	1.95
1	A	184	MSE	SE-CE	-26.74	1.15	1.95
1	A	327	MSE	SE-CE	-22.99	1.26	1.95
1	B	389	MSE	SE-CE	-22.82	1.26	1.95
1	B	402	MSE	SE-CE	-22.01	1.29	1.95
1	A	1	MSE	SE-CE	-21.96	1.29	1.95
1	B	383	MSE	SE-CE	-21.56	1.30	1.95
1	A	389	MSE	SE-CE	-20.37	1.34	1.95
1	B	353	MSE	SE-CE	-19.88	1.35	1.95
1	A	402	MSE	SE-CE	-18.80	1.39	1.95
1	B	327	MSE	SE-CE	-14.01	1.53	1.95
1	B	1	MSE	SE-CE	-10.12	1.65	1.95
1	B	249	MSE	SE-CE	-9.63	1.66	1.95
1	B	381	MSE	SE-CE	-8.93	1.68	1.95
1	A	77	ALA	CA-C	7.45	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	MSE	CB-CG	7.44	1.74	1.52
1	A	381	MSE	SE-CE	-7.10	1.74	1.95
1	B	74	TYR	CA-C	-7.01	1.46	1.53
1	A	353	MSE	SE-CE	-6.83	1.75	1.95
1	A	185	ILE	CA-CB	-6.52	1.46	1.54
1	A	285	ILE	CA-CB	-6.39	1.47	1.54
1	B	19	ASP	C-N	6.23	1.42	1.33
1	B	232	HIS	CA-CB	6.00	1.60	1.53
1	A	1	MSE	CG-SE	-5.85	1.77	1.95
1	B	30	ASP	CA-C	5.55	1.59	1.53
1	B	33	ILE	CA-C	-5.54	1.45	1.52
1	B	33	ILE	CA-CB	-5.48	1.47	1.54
1	A	125	LEU	CA-C	-5.23	1.46	1.52
1	B	289	THR	CA-CB	-5.18	1.45	1.53
1	B	17	PHE	C-N	-5.06	1.26	1.33
1	B	263	LYS	CA-CB	5.03	1.61	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	PHE	O-C-N	-13.24	107.70	123.19
1	A	1	MSE	CG-SE-CE	8.27	117.12	98.92
1	A	81	ASP	CA-C-N	7.48	129.19	119.84
1	A	81	ASP	C-N-CA	7.48	129.19	119.84
1	A	287	MSE	CG-SE-CE	-7.42	82.59	98.92
1	A	366	ILE	N-CA-C	7.32	117.45	110.42
1	A	381	MSE	CB-CG-SE	-7.32	90.74	112.70
1	B	250	ASP	CA-C-O	7.24	123.99	119.29
1	B	74	TYR	N-CA-C	-7.15	98.96	109.11
1	B	341	ILE	N-CA-C	-7.02	103.93	110.53
1	B	75	SER	N-CA-C	-6.83	96.25	110.80
1	B	22	ALA	N-CA-C	-6.77	96.38	110.80
1	A	377	ALA	N-CA-C	6.51	118.17	111.14
1	B	18	ASP	O-C-N	-6.42	115.80	123.31
1	B	77	ALA	N-CA-C	6.40	118.27	109.18
1	A	77	ALA	N-CA-C	6.35	124.32	110.80
1	A	279	GLY	N-CA-C	6.09	124.02	115.43
1	A	411	THR	N-CA-CB	-5.88	101.51	111.50
1	B	32	PHE	CA-C-N	-5.78	111.56	121.97
1	B	32	PHE	C-N-CA	-5.78	111.56	121.97
1	B	378	ALA	N-CA-C	5.65	118.38	111.82
1	B	3	ILE	N-CA-C	-5.61	100.35	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	VAL	N-CA-C	-5.59	104.90	111.00
1	B	9	THR	OG1-CB-CG2	-5.50	98.30	109.30
1	B	43	PHE	N-CA-C	5.48	122.47	110.80
1	A	225	LEU	N-CA-C	5.30	119.01	112.54
1	B	251	PRO	N-CA-C	5.29	120.50	113.57
1	B	21	GLN	O-C-N	5.25	129.57	122.59
1	A	119	LEU	N-CA-C	5.24	117.91	110.10
1	A	316	ILE	N-CA-C	-5.24	105.43	110.72
1	A	352	GLY	N-CA-C	5.23	122.01	115.21
1	B	4	LYS	N-CA-C	-5.21	106.61	113.12
1	B	161	PRO	N-CA-C	5.21	120.37	113.86
1	B	21	GLN	N-CA-C	-5.20	99.73	110.80
1	A	353	MSE	CG-SE-CE	-5.17	87.54	98.92
1	A	9	THR	OG1-CB-CG2	-5.14	99.02	109.30
1	A	192	LEU	N-CA-C	5.13	112.84	108.22
1	B	225	LEU	N-CA-C	5.13	119.25	112.89
1	B	17	PHE	N-CA-C	-5.11	101.38	109.76
1	B	76	GLY	N-CA-C	5.08	120.86	114.25
1	B	383	MSE	CG-SE-CE	-5.05	87.80	98.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	17	PHE	Mainchain

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	3151	0	3105	105	0
1	B	3140	0	3091	136	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	20	0	14	0	0
4	A	338	0	0	15	1
4	B	291	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6942	0	6210	230	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 18.

All (230) 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:381:MSE:CG	1:A:381:MSE:CB	1.74	1.57
1:A:389:MSE:CE	1:A:389:MSE:SE	1.34	1.53
1:B:383:MSE:SE	1:B:383:MSE:CE	1.30	1.49
1:B:402:MSE:SE	1:B:402:MSE:CE	1.29	1.48
1:A:1:MSE:CE	1:A:1:MSE:SE	1.29	1.47
1:B:389:MSE:CE	1:B:389:MSE:SE	1.27	1.46
1:A:327:MSE:SE	1:A:327:MSE:CE	1.26	1.46
1:A:184:MSE:SE	1:A:184:MSE:CE	1.15	1.34
1:B:21:GLN:O	1:B:39:VAL:HG21	1.12	1.26
1:B:9:THR:HG22	4:B:747:HOH:O	1.41	1.18
1:A:1:MSE:SE	1:A:1:MSE:HE1	1.86	1.16
1:B:21:GLN:O	1:B:39:VAL:CG2	1.92	1.15
1:A:1:MSE:SE	1:A:1:MSE:HE3	1.86	1.15
1:A:327:MSE:SE	1:A:327:MSE:HE2	1.83	1.14
1:B:402:MSE:SE	1:B:402:MSE:HE2	1.85	1.14
1:B:389:MSE:SE	1:B:389:MSE:HE2	1.83	1.14
1:A:389:MSE:SE	1:A:389:MSE:HE3	1.90	1.12
1:B:383:MSE:SE	1:B:383:MSE:HE2	1.87	1.12
1:B:383:MSE:SE	1:B:383:MSE:HE3	1.87	1.12
1:B:402:MSE:SE	1:B:402:MSE:HE3	1.85	1.12
1:B:389:MSE:SE	1:B:389:MSE:HE3	1.83	1.11
1:A:184:MSE:CE	1:A:184:MSE:CG	2.27	1.11
1:A:327:MSE:SE	1:A:327:MSE:HE3	1.83	1.10
1:A:389:MSE:SE	1:A:389:MSE:HE2	1.90	1.09
1:A:1:MSE:SE	1:A:1:MSE:HE2	1.86	1.09
1:A:389:MSE:SE	1:A:389:MSE:HE1	1.90	1.09
1:B:19:ASP:OD1	1:B:39:VAL:HG23	1.53	1.08
1:A:327:MSE:SE	1:A:327:MSE:HE1	1.83	1.07
1:B:389:MSE:CE	1:B:389:MSE:CG	2.30	1.07
1:B:402:MSE:SE	1:B:402:MSE:HE1	1.85	1.07
1:B:383:MSE:CE	1:B:383:MSE:CG	2.32	1.07
1:B:383:MSE:SE	1:B:383:MSE:HE1	1.87	1.06
1:B:389:MSE:SE	1:B:389:MSE:HE1	1.83	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MSE:SE	1:A:184:MSE:HE2	1.73	1.05
1:A:184:MSE:SE	1:A:184:MSE:HE1	1.73	1.04
1:A:381:MSE:HG3	4:A:907:HOH:O	1.54	1.04
1:B:122:ASP:HB3	4:B:722:HOH:O	1.55	1.04
1:A:184:MSE:SE	1:A:184:MSE:HE3	1.73	1.03
1:B:18:ASP:OD2	1:B:73:GLN:NE2	1.94	1.00
1:A:80:ARG:HB2	4:A:1092:HOH:O	1.60	0.99
1:A:88:HIS:C	1:A:88:HIS:CD2	2.40	0.99
1:A:331:LYS:HD3	4:A:1069:HOH:O	1.63	0.99
1:B:72:VAL:HG21	1:B:80:ARG:HD3	1.45	0.99
1:A:72:VAL:HG21	1:A:80:ARG:HD2	1.44	0.98
1:A:327:MSE:CE	1:A:327:MSE:CG	2.41	0.97
1:A:381:MSE:CB	1:A:381:MSE:SE	2.62	0.97
1:A:114:ARG:O	1:A:118:LYS:HD3	1.63	0.96
1:B:81:ASP:HB3	1:B:82:PRO:HD2	1.47	0.95
1:B:402:MSE:CE	1:B:402:MSE:CG	2.45	0.94
1:B:383:MSE:HE2	4:B:638:HOH:O	1.69	0.92
1:B:75:SER:HB2	4:B:690:HOH:O	1.70	0.91
1:B:19:ASP:OD1	1:B:39:VAL:CG2	2.18	0.91
1:B:22:ALA:HB2	1:B:39:VAL:HG22	1.48	0.91
1:A:389:MSE:CE	1:A:389:MSE:CG	2.52	0.88
1:B:184:MSE:HE1	1:B:192:LEU:HB2	1.55	0.86
1:A:88:HIS:HD2	1:A:89:PHE:N	1.74	0.85
1:B:389:MSE:HE3	1:B:389:MSE:CB	2.08	0.84
1:B:74:TYR:C	1:B:75:SER:O	2.18	0.84
1:A:249:MSE:HE3	1:A:287:MSE:HE1	1.58	0.83
1:A:182:ASP:OD2	1:B:32:PHE:N	2.11	0.82
1:B:19:ASP:OD2	1:B:39:VAL:N	2.11	0.82
1:A:80:ARG:CB	4:A:1092:HOH:O	2.23	0.81
1:A:88:HIS:CD2	1:A:89:PHE:N	2.52	0.77
1:B:184:MSE:CE	1:B:192:LEU:HB2	2.15	0.77
1:A:88:HIS:C	1:A:88:HIS:HD2	1.88	0.76
1:A:182:ASP:CB	1:B:32:PHE:HB3	2.16	0.76
1:B:381:MSE:HE2	4:B:699:HOH:O	1.86	0.75
1:A:381:MSE:SE	1:A:381:MSE:HB3	2.37	0.74
1:A:1:MSE:HE3	1:A:145:ALA:HB1	1.67	0.74
1:A:1:MSE:HE1	1:A:145:ALA:HA	1.69	0.74
1:A:408:LEU:O	1:A:411:THR:HB	1.88	0.73
1:A:1:MSE:HE3	1:A:145:ALA:CB	2.18	0.73
1:A:88:HIS:HD2	1:A:89:PHE:CA	2.02	0.72
1:B:389:MSE:CE	1:B:389:MSE:CB	2.66	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MSE:CE	1:A:1:MSE:CG	2.63	0.71
1:B:29:HIS:NE2	4:B:727:HOH:O	2.24	0.70
1:B:22:ALA:O	1:B:27:ALA:HB2	1.91	0.70
1:A:381:MSE:CG	4:A:907:HOH:O	2.22	0.70
1:B:213:GLU:CD	4:B:666:HOH:O	2.36	0.69
1:B:408:LEU:O	1:B:411:THR:HB	1.93	0.68
1:B:72:VAL:CG2	1:B:80:ARG:HD3	2.23	0.68
1:B:81:ASP:HB3	1:B:82:PRO:CD	2.23	0.67
1:B:236:HIS:HD2	1:B:382:ARG:HH11	1.41	0.67
1:B:43:PHE:HA	1:B:48:GLN:HE22	1.59	0.67
1:A:88:HIS:HD2	1:A:89:PHE:HA	1.59	0.66
1:B:184:MSE:HE1	1:B:192:LEU:CB	2.26	0.66
1:B:23:ILE:O	1:B:25:ASN:N	2.30	0.65
1:A:304:ILE:H	1:A:326:HIS:HD2	1.44	0.65
1:A:128:THR:HG22	1:A:131:ARG:NH2	2.11	0.65
1:B:389:MSE:HE3	1:B:389:MSE:CA	2.26	0.65
1:A:209:GLU:OE1	1:A:212:ARG:NE	2.30	0.63
1:B:43:PHE:HA	1:B:48:GLN:NE2	2.13	0.63
1:B:281:LYS:HB3	1:B:282:PRO:HD3	1.80	0.62
1:A:81:ASP:CB	1:A:82:PRO:HD2	2.31	0.61
1:A:381:MSE:HG2	4:A:1023:HOH:O	2.01	0.61
1:B:184:MSE:CE	1:B:192:LEU:CB	2.78	0.60
1:B:389:MSE:HE3	1:B:389:MSE:HA	1.83	0.60
1:A:1:MSE:CE	1:A:145:ALA:HA	2.31	0.60
1:B:19:ASP:OD2	1:B:38:PRO:CA	2.50	0.60
1:B:29:HIS:CE1	4:B:727:HOH:O	2.54	0.60
1:B:389:MSE:HE3	1:B:389:MSE:HB3	1.84	0.59
1:A:182:ASP:HB3	1:B:32:PHE:HB3	1.83	0.59
1:B:236:HIS:CD2	1:B:382:ARG:HH11	2.20	0.59
1:A:184:MSE:CE	1:A:184:MSE:HG3	2.32	0.57
1:B:23:ILE:C	1:B:25:ASN:N	2.62	0.57
1:A:72:VAL:HG21	1:A:80:ARG:CD	2.26	0.57
1:B:23:ILE:C	1:B:25:ASN:H	2.14	0.56
1:B:114:ARG:O	1:B:118:LYS:HD3	2.05	0.56
1:A:221:ARG:NH2	1:B:30:ASP:O	2.37	0.56
1:B:18:ASP:HB2	1:B:74:TYR:CE2	2.40	0.56
1:B:328:VAL:HG13	1:B:353:MSE:HE3	1.88	0.56
1:A:386:LYS:HB2	1:A:387:PRO:HA	1.87	0.55
1:A:364:THR:HA	1:B:396:ASN:HD21	1.71	0.55
1:B:81:ASP:CB	1:B:82:PRO:HD2	2.30	0.55
1:B:236:HIS:HE1	1:B:273:GLU:OE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:PHE:CZ	1:A:403:ASN:ND2	2.75	0.55
1:A:1:MSE:CE	1:A:1:MSE:CB	2.84	0.55
1:A:81:ASP:CB	1:A:82:PRO:CD	2.84	0.55
1:A:293:LYS:HD3	4:A:1047:HOH:O	2.05	0.55
1:A:182:ASP:HB2	1:B:32:PHE:HB3	1.87	0.54
1:A:327:MSE:HE2	1:A:356:TYR:HB2	1.91	0.53
1:B:305:VAL:CG2	1:B:327:MSE:HE2	2.38	0.53
1:A:88:HIS:CD2	1:A:88:HIS:O	2.61	0.53
1:B:19:ASP:OD2	1:B:38:PRO:CB	2.57	0.53
1:B:184:MSE:CE	1:B:184:MSE:CB	2.73	0.53
1:B:195:ALA:O	1:B:196:LEU:C	2.52	0.53
1:B:303:LYS:HA	1:B:326:HIS:CE1	2.43	0.52
1:A:361:CYS:HB3	1:A:389:MSE:HE2	1.93	0.51
1:A:327:MSE:HE1	1:A:382:ARG:CZ	2.40	0.51
1:B:174:GLY:N	1:B:389:MSE:HE1	2.25	0.51
1:A:81:ASP:CG	1:A:82:PRO:HD2	2.35	0.51
1:A:9:THR:HG23	4:A:830:HOH:O	2.11	0.51
1:A:90:ILE:HB	1:A:91:PRO:HD3	1.93	0.50
1:B:383:MSE:CE	1:B:383:MSE:HG3	2.34	0.50
4:A:1032:HOH:O	1:B:73:GLN:HB3	2.11	0.49
1:A:182:ASP:HB2	1:B:32:PHE:CB	2.42	0.49
1:A:88:HIS:CD2	1:A:89:PHE:HA	2.45	0.49
1:B:20:GLN:O	1:B:21:GLN:CB	2.61	0.49
1:B:174:GLY:HA3	1:B:389:MSE:HE2	1.94	0.49
1:A:72:VAL:CG2	1:A:80:ARG:HD2	2.29	0.48
1:B:383:MSE:HE2	1:B:383:MSE:CG	2.31	0.48
1:A:76:GLY:O	1:A:77:ALA:HB2	2.13	0.48
1:B:28:GLY:O	1:B:34:TYR:HA	2.14	0.48
1:B:19:ASP:O	1:B:22:ALA:HB3	2.13	0.48
1:B:98:LYS:HB3	1:B:99:PRO:HD3	1.96	0.48
1:B:327:MSE:HE3	1:B:356:TYR:CB	2.43	0.47
1:B:248:ASP:C	1:B:249:MSE:HG2	2.38	0.47
1:B:18:ASP:CB	1:B:74:TYR:CE2	2.97	0.47
1:B:228:SER:HB2	1:B:229:PRO:CD	2.44	0.47
1:B:74:TYR:O	1:B:75:SER:C	2.54	0.47
1:B:209:GLU:O	1:B:213:GLU:HG3	2.14	0.47
1:A:294:GLU:O	1:A:298:LEU:HG	2.15	0.47
1:A:198:ASN:HB2	1:A:240:TYR:CD1	2.50	0.47
1:B:19:ASP:OD2	1:B:38:PRO:HB2	2.15	0.47
1:B:316:ILE:HD13	1:B:330:ILE:HG12	1.95	0.46
1:B:383:MSE:HE3	1:B:383:MSE:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASP:HB3	1:A:82:PRO:HD2	1.97	0.46
1:A:262:GLU:HB2	1:A:302:VAL:HG23	1.97	0.46
1:A:369:ARG:HG3	1:A:401:GLU:HG2	1.97	0.46
1:B:80:ARG:N	4:B:550:HOH:O	2.49	0.46
1:B:249:MSE:HB3	1:B:249:MSE:HE3	1.62	0.46
1:B:305:VAL:CG1	1:B:327:MSE:HE2	2.45	0.46
1:A:43:PHE:HA	1:A:48:GLN:OE1	2.16	0.46
1:B:29:HIS:ND1	1:B:33:ILE:O	2.43	0.46
1:B:174:GLY:HA3	1:B:389:MSE:CE	2.46	0.46
1:B:19:ASP:OD2	1:B:38:PRO:C	2.58	0.46
1:A:226:ARG:CZ	1:A:229:PRO:HA	2.46	0.45
1:B:389:MSE:CE	1:B:389:MSE:HB3	2.42	0.45
1:A:167:ILE:H	1:A:402:MSE:SE	2.49	0.45
1:A:281:LYS:HB3	1:A:282:PRO:HD3	1.99	0.45
1:A:381:MSE:CG	1:A:381:MSE:CA	2.82	0.45
1:B:40:THR:CG2	1:B:41:PRO:HD2	2.46	0.45
1:A:164:PRO:HA	4:A:1051:HOH:O	2.17	0.45
1:B:40:THR:HA	1:B:41:PRO:HD3	1.88	0.45
1:A:327:MSE:CE	1:A:327:MSE:HG3	2.42	0.45
1:A:88:HIS:CE1	4:A:886:HOH:O	2.68	0.45
1:B:327:MSE:HE3	1:B:356:TYR:HB2	1.99	0.45
1:B:378:ALA:C	1:B:379:ARG:HG2	2.42	0.45
1:B:381:MSE:O	1:B:381:MSE:HG3	2.17	0.45
1:A:248:ASP:HA	4:A:1039:HOH:O	2.15	0.44
1:B:174:GLY:CA	1:B:389:MSE:HE1	2.47	0.44
1:B:1:MSE:HE1	1:B:61:ASN:CG	2.43	0.44
1:B:197:ILE:O	1:B:197:ILE:HG22	2.18	0.44
1:A:1:MSE:CE	1:A:145:ALA:CA	2.96	0.44
1:A:273:GLU:HA	1:A:305:VAL:HB	2.00	0.44
1:B:15:PHE:C	1:B:16:TYR:CD1	2.95	0.44
1:B:76:GLY:N	4:B:690:HOH:O	2.51	0.44
1:B:176:ASP:OD1	1:B:179:ILE:HB	2.18	0.44
1:A:184:MSE:CG	1:A:184:MSE:HE3	2.26	0.44
1:B:19:ASP:CG	1:B:40:THR:H	2.26	0.43
1:B:21:GLN:C	1:B:39:VAL:HG21	2.18	0.43
1:B:117:ASP:OD1	1:B:131:ARG:HD2	2.18	0.43
1:A:29:HIS:HD2	4:A:937:HOH:O	2.01	0.43
1:B:40:THR:HG22	1:B:41:PRO:HD2	1.99	0.43
1:A:248:ASP:CA	4:A:1039:HOH:O	2.67	0.43
1:B:228:SER:HB2	1:B:229:PRO:HD2	2.01	0.43
1:A:163:VAL:HA	1:A:164:PRO:HD3	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:GLN:NE2	4:B:776:HOH:O	2.51	0.42
1:A:26:GLY:O	1:A:27:ALA:C	2.62	0.42
1:B:1:MSE:N	4:B:656:HOH:O	2.52	0.42
1:A:7:LEU:HD12	1:A:7:LEU:N	2.34	0.42
1:A:221:ARG:NH2	1:B:31:GLY:HA3	2.34	0.42
1:B:19:ASP:OD1	1:B:39:VAL:HG22	2.14	0.42
1:B:110:LEU:HD13	1:B:158:TRP:CH2	2.55	0.42
1:B:280:ASN:OD1	1:B:282:PRO:HD2	2.19	0.42
1:B:32:PHE:C	1:B:33:ILE:CG2	2.92	0.42
1:B:262:GLU:O	1:B:263:LYS:C	2.63	0.42
1:B:386:LYS:HB2	1:B:387:PRO:HA	2.02	0.42
1:B:19:ASP:CG	1:B:39:VAL:H	2.24	0.42
1:A:118:LYS:HE2	4:A:977:HOH:O	2.19	0.42
1:B:32:PHE:CG	1:B:32:PHE:O	2.71	0.42
1:A:80:ARG:HD3	1:A:334:ASP:OD2	2.20	0.41
1:B:44:THR:H	1:B:48:GLN:NE2	2.18	0.41
1:B:327:MSE:HE3	1:B:356:TYR:CD2	2.55	0.41
1:B:389:MSE:HE2	1:B:389:MSE:CG	2.29	0.41
1:A:165:GLU:HB3	1:A:379:ARG:NH2	2.35	0.41
1:A:184:MSE:CG	1:A:184:MSE:HE2	2.26	0.41
1:B:249:MSE:O	1:B:251:PRO:HD3	2.20	0.41
1:A:221:ARG:HH22	1:B:30:ASP:C	2.27	0.41
1:A:396:ASN:HD21	1:B:364:THR:HA	1.85	0.41
1:B:219:SER:O	1:B:223:LEU:HG	2.21	0.41
1:A:221:ARG:HD2	1:A:225:LEU:HD13	2.03	0.41
1:B:21:GLN:O	1:B:39:VAL:HG11	2.21	0.41
1:A:187:LYS:HE3	1:B:16:TYR:CE2	2.56	0.40
1:A:271:TYR:CZ	1:A:303:LYS:HD2	2.56	0.40
1:B:97:ILE:HD11	1:B:126:LEU:HD21	2.02	0.40
1:B:332:THR:OG1	1:B:333:PRO:HD3	2.22	0.40
1:A:75:SER:OG	1:A:83:LEU:HA	2.21	0.40
1:A:399:PHE:CE2	1:A:403:ASN:ND2	2.90	0.40
1:B:14:SER:HB2	1:B:387:PRO:HB2	2.04	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)
4:A:982:HOH:O	4:A:982:HOH:O[3_453]	2.19	0.01

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	409/413 (99%)	389 (95%)	17 (4%)	3 (1%)	18	15
1	B	409/413 (99%)	382 (93%)	18 (4%)	9 (2%)	5	2
All	All	818/826 (99%)	771 (94%)	35 (4%)	12 (2%)	8	4

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	GLN
1	B	22	ALA
1	B	24	LYS
1	B	26	GLY
1	A	77	ALA
1	B	43	PHE
1	B	75	SER
1	A	82	PRO
1	B	82	PRO
1	B	23	ILE
1	A	193	PRO
1	B	193	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	333/331 (101%)	323 (97%)	10 (3%)	36	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	330/331 (100%)	321 (97%)	9 (3%)	39	45
All	All	663/662 (100%)	644 (97%)	19 (3%)	37	42

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	81	ASP
1	A	88	HIS
1	A	98	LYS
1	A	162	CYS
1	A	193	PRO
1	A	287	MSE
1	A	356	TYR
1	A	381	MSE
1	A	411	THR
1	B	1	MSE
1	B	29	HIS
1	B	35	THR
1	B	39	VAL
1	B	48	GLN
1	B	75	SER
1	B	207	LYS
1	B	236	HIS
1	B	411	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	88	HIS
1	A	232	HIS
1	A	326	HIS
1	A	357	GLN
1	A	410	GLN
1	B	25	ASN
1	B	48	GLN
1	B	96	HIS
1	B	236	HIS
1	B	351	HIS
1	B	357	GLN

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Mol	Chain	Res	Type
1	B	396	ASN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
3	2AS	A	801	2	9,9,9	1.17	2 (22%)	10,12,12	2.10	3 (30%)
3	2AS	A	800	2	9,9,9	1.37	3 (33%)	10,12,12	1.40	1 (10%)

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
3	2AS	A	801	2	-	0/12/12/12	-
3	2AS	A	800	2	-	0/12/12/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	2AS	OXT-C	-2.53	1.22	1.30
3	A	800	2AS	OD1-CG	-2.40	1.23	1.30
3	A	801	2AS	OD1-CG	-2.27	1.23	1.30
3	A	801	2AS	OXT-C	-2.13	1.23	1.30
3	A	800	2AS	CB-CA	-2.13	1.52	1.55

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	2AS	C4-CB-CA	4.18	117.50	111.12
3	A	801	2AS	OXT-C-O	-2.57	118.24	124.08
3	A	801	2AS	OD1-CG-CB	2.36	122.72	114.46
3	A	800	2AS	OXT-C-CA	2.03	121.14	114.15

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.