



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:09 PM UTC

PDB ID : 3C20 / pdb_00003c20
Title : Crystal Structure of Threonine-sensitive Aspartokinase from *Methanococcus jannaschii* with L-aspartate
Authors : Liu, X.; Pavlovsky, A.G.; Viola, R.E.
Deposited on : 2008-01-24
Resolution : 2.70 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

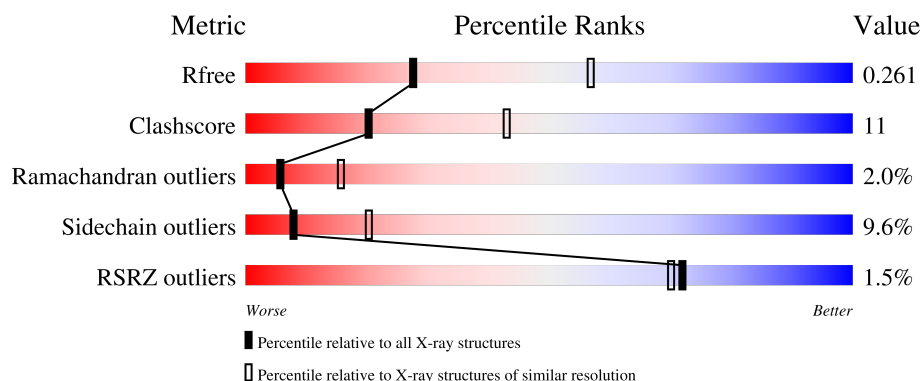
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

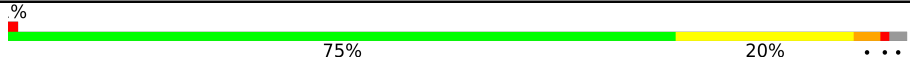
The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	473	
1	B	473	

2 Entry composition [i](#)

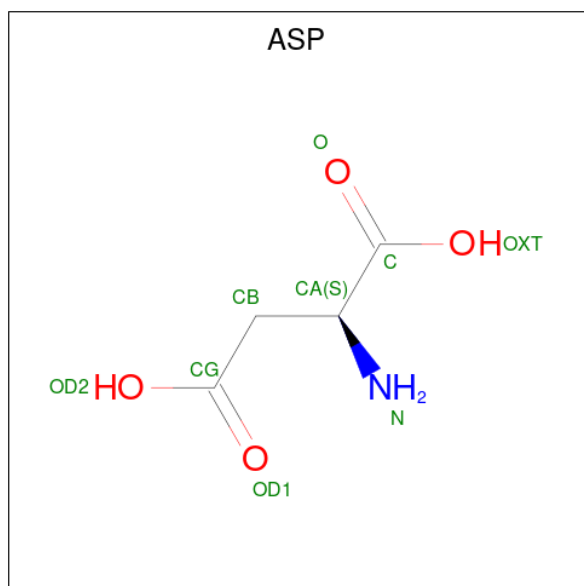
There are 4 unique types of molecules in this entry. The entry contains 7112 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Probable aspartokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3538	2241	593	693	11			
1	B	466	Total	C	N	O	S	0	0	0
			3537	2242	595	690	10			

- Molecule 2 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		

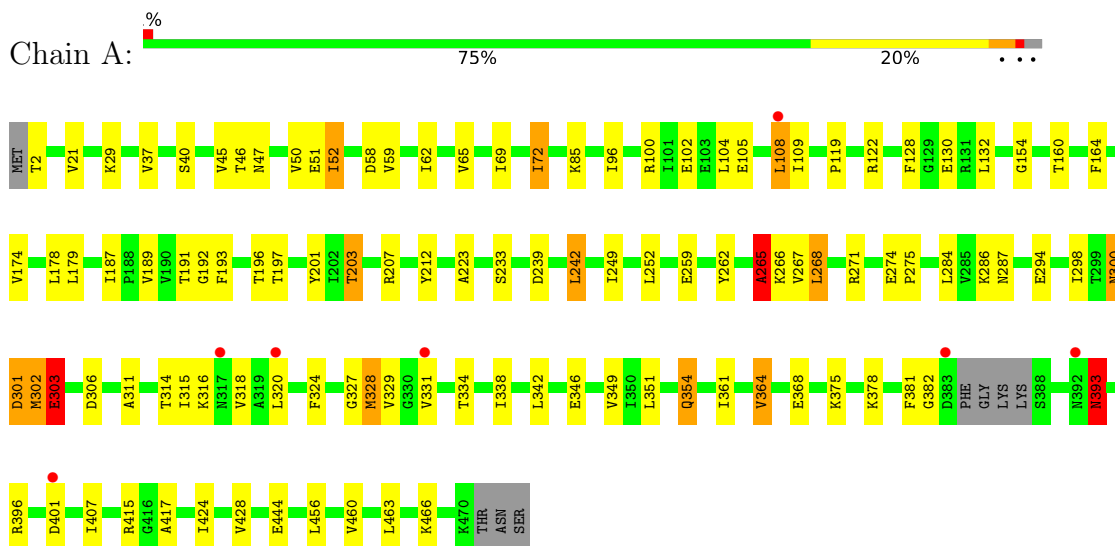
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	9	Total	O	0	0
			9	9		

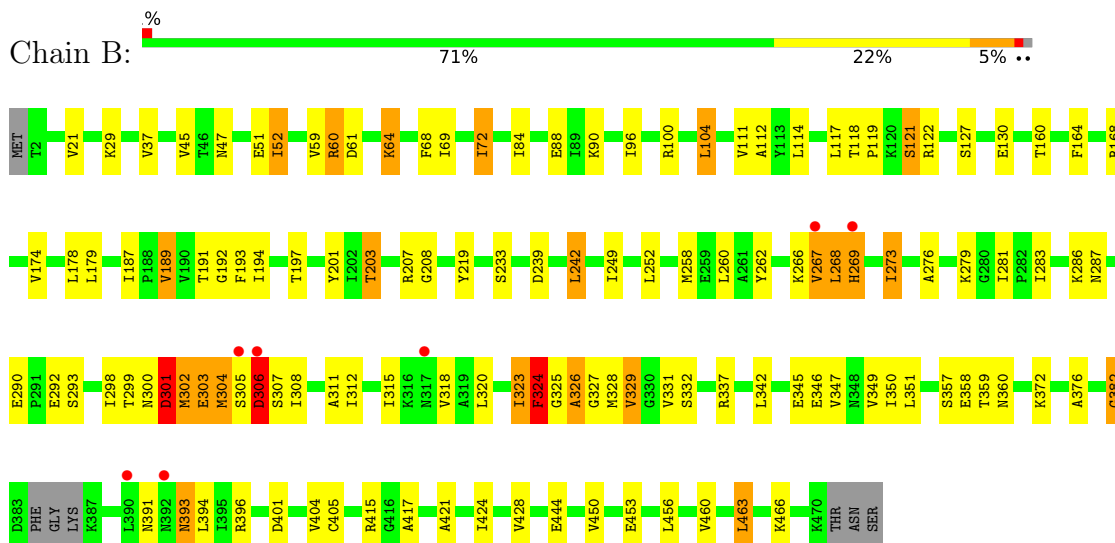
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Probable aspartokinase



- Molecule 1: Probable aspartokinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.97Å 199.07Å 96.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.70) 99.7 (50.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.238 , 0.273 0.226 , 0.261	Depositor DCC
R_{free} test set	1466 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7112	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.50	0/3577	0.90	7/4819 (0.1%)
1	B	0.54	0/3576	0.89	2/4818 (0.0%)
All	All	0.52	0/7153	0.89	9/9637 (0.1%)

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	A	0	1
1	B	0	3
All	All	0	4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	ASP	N-CA-C	-10.73	95.33	110.35
1	A	324	PHE	N-CA-C	7.48	121.55	108.75
1	A	318	VAL	N-CA-C	5.86	118.28	109.20
1	A	265	ALA	CA-C-N	5.81	132.16	121.70
1	A	265	ALA	C-N-CA	5.81	132.16	121.70
1	A	303	GLU	CA-C-N	-5.48	114.45	122.06
1	A	303	GLU	C-N-CA	-5.48	114.45	122.06
1	B	318	VAL	N-CA-C	5.46	117.04	109.29
1	A	328	MET	N-CA-C	5.10	119.60	113.17

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	ALA	Peptide
1	B	306	ASP	Peptide
1	B	323	ILE	Peptide
1	B	324	PHE	Peptide

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	3538	0	3652	64	0
1	B	3537	0	3651	104	0
2	A	9	0	3	3	0
2	B	9	0	3	2	0
3	A	3	0	1	0	0
3	B	3	0	1	1	0
4	A	4	0	0	1	0
4	B	9	0	0	1	0
All	All	7112	0	7311	163	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (163) 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:B:324:PHE:CZ	1:B:328:MET:CB	1.95	1.49
1:B:324:PHE:HD2	1:B:359:THR:C	1.51	1.18
1:B:324:PHE:CE1	1:B:328:MET:CB	2.34	1.09
1:B:345:GLU:HG3	1:B:376:ALA:HB2	1.33	1.07
1:A:351:LEU:HB2	1:A:364:VAL:CG1	1.88	1.03
1:B:324:PHE:HE2	1:B:358:GLU:O	1.45	0.98
1:B:324:PHE:CD2	1:B:359:THR:C	2.42	0.98
1:B:324:PHE:HB3	1:B:325:GLY:HA3	1.45	0.96
1:B:324:PHE:HB3	1:B:359:THR:O	1.65	0.95
1:A:259:GLU:HA	1:B:357:SER:HB3	1.48	0.94
1:B:324:PHE:CB	1:B:325:GLY:HA3	1.99	0.92
1:B:324:PHE:CG	1:B:325:GLY:CA	2.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:PHE:CG	1:B:325:GLY:HA2	2.07	0.89
1:A:351:LEU:HB2	1:A:364:VAL:HG12	1.58	0.84
1:B:324:PHE:CE2	1:B:328:MET:CB	2.60	0.84
1:B:324:PHE:CE2	1:B:358:GLU:O	2.29	0.84
1:B:324:PHE:HD2	1:B:360:ASN:N	1.75	0.83
1:A:327:GLY:HA2	1:B:168:ARG:HH21	1.43	0.83
1:B:324:PHE:CB	1:B:325:GLY:CA	2.56	0.83
1:B:323:ILE:O	1:B:324:PHE:HB2	1.75	0.82
1:B:324:PHE:CG	1:B:325:GLY:HA3	2.16	0.80
1:B:324:PHE:CD1	1:B:325:GLY:HA2	2.17	0.79
1:A:334:THR:O	1:A:338:ILE:HG12	1.82	0.79
1:B:421:ALA:H	3:B:475:FMT:H	1.50	0.77
1:B:305:SER:O	1:B:306:ASP:C	2.30	0.75
1:B:324:PHE:HB2	1:B:360:ASN:HA	1.66	0.74
1:A:301:ASP:O	1:A:301:ASP:CG	2.30	0.74
1:B:302:MET:O	1:B:303:GLU:CB	2.34	0.73
1:B:324:PHE:CD2	1:B:360:ASN:N	2.56	0.73
1:A:207:ARG:NH1	2:A:474:ASP:O	2.22	0.71
1:B:207:ARG:HH11	2:B:474:ASP:N	1.90	0.70
1:B:324:PHE:CB	1:B:359:THR:O	2.37	0.70
1:A:267:VAL:O	1:A:268:LEU:HB2	1.92	0.69
1:B:324:PHE:HZ	1:B:328:MET:CB	1.98	0.69
1:A:50:VAL:HG13	1:A:122:ARG:HH22	1.57	0.69
1:A:301:ASP:C	1:A:302:MET:O	2.36	0.68
1:A:300:ASN:O	1:A:302:MET:N	2.24	0.68
1:B:197:THR:HG22	1:B:201:TYR:H	1.58	0.67
1:A:197:THR:HG22	1:A:201:TYR:H	1.59	0.67
1:B:267:VAL:O	1:B:268:LEU:HB2	1.94	0.67
1:A:239:ASP:HB3	1:A:242:LEU:HD22	1.77	0.67
1:B:305:SER:C	1:B:306:ASP:O	2.30	0.66
1:A:46:THR:HG1	2:A:474:ASP:N	1.94	0.66
1:A:105:GLU:O	1:A:109:ILE:HG12	1.97	0.65
1:A:327:GLY:HA2	1:B:168:ARG:NH2	2.13	0.64
1:B:269:HIS:CD2	1:B:269:HIS:H	2.14	0.64
1:B:405:CYS:SG	1:B:453:GLU:HG3	2.38	0.64
1:B:302:MET:HE3	1:B:302:MET:CA	2.29	0.63
1:A:351:LEU:HB2	1:A:364:VAL:HG13	1.78	0.61
1:A:40:SER:HB3	2:A:474:ASP:HB2	1.81	0.61
1:B:302:MET:HA	1:B:302:MET:CE	2.32	0.59
1:A:29:LYS:HG3	1:A:187:ILE:HD11	1.84	0.59
1:B:29:LYS:HG3	1:B:187:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASN:C	1:A:302:MET:H	2.11	0.58
1:A:259:GLU:HA	1:B:357:SER:CB	2.28	0.58
1:B:117:LEU:HD12	1:B:121:SER:HB3	1.86	0.58
1:B:326:ALA:O	1:B:329:VAL:CG1	2.52	0.57
1:B:208:GLY:H	2:B:474:ASP:N	2.02	0.57
1:B:262:TYR:CD2	1:B:315:ILE:HG12	2.41	0.56
1:A:456:LEU:O	1:A:460:VAL:HG23	2.06	0.55
1:B:59:VAL:O	1:B:59:VAL:HG12	2.07	0.55
1:B:239:ASP:HB3	1:B:242:LEU:HD22	1.88	0.55
1:B:323:ILE:O	1:B:324:PHE:CB	2.47	0.54
1:B:405:CYS:SG	1:B:456:LEU:HD22	2.48	0.54
1:A:301:ASP:O	1:A:302:MET:C	2.50	0.54
1:A:160:THR:OG1	1:A:203:THR:HG21	2.09	0.53
1:B:130:GLU:HG2	1:B:192:GLY:O	2.08	0.53
1:B:160:THR:OG1	1:B:203:THR:HG21	2.08	0.53
1:B:300:ASN:O	1:B:302:MET:HE3	2.09	0.53
1:B:345:GLU:HG3	1:B:376:ALA:CB	2.23	0.53
1:B:301:ASP:O	1:B:302:MET:CB	2.55	0.52
1:A:122:ARG:HD2	4:A:476:HOH:O	2.09	0.52
1:B:292:GLU:HA	1:B:292:GLU:OE1	2.09	0.52
1:B:302:MET:HE3	1:B:302:MET:HA	1.91	0.52
1:A:65:VAL:HG13	1:A:108:LEU:HD23	1.90	0.52
1:B:415:ARG:O	1:B:444:GLU:OE1	2.28	0.52
1:B:122:ARG:HD2	4:B:477:HOH:O	2.10	0.52
1:B:252:LEU:O	1:B:298:ILE:HA	2.10	0.52
1:B:260:LEU:HD21	1:B:311:ALA:HB3	1.92	0.52
1:A:252:LEU:O	1:A:298:ILE:HA	2.10	0.51
1:B:324:PHE:CD2	1:B:359:THR:O	2.63	0.51
1:A:212:TYR:CE1	1:A:271:ARG:HG2	2.46	0.51
1:A:197:THR:HG22	1:A:201:TYR:N	2.25	0.51
1:A:47:ASN:OD1	1:A:207:ARG:NH2	2.43	0.51
1:A:351:LEU:CB	1:A:364:VAL:HG12	2.37	0.51
1:B:456:LEU:O	1:B:460:VAL:HG23	2.11	0.51
1:A:262:TYR:CD2	1:A:315:ILE:HG12	2.47	0.50
1:A:274:GLU:HB3	1:A:275:PRO:HD3	1.93	0.50
1:A:265:ALA:HA	1:A:266:LYS:HG2	1.94	0.49
1:A:301:ASP:O	1:A:301:ASP:OD1	2.29	0.49
1:B:197:THR:HG22	1:B:201:TYR:N	2.24	0.49
1:B:325:GLY:O	1:B:326:ALA:C	2.55	0.49
1:A:302:MET:C	1:A:303:GLU:HG3	2.38	0.49
1:A:424:ILE:O	1:A:428:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:HB3	1:B:191:THR:HB	1.94	0.49
1:B:192:GLY:O	1:B:193:PHE:HB3	2.12	0.49
1:A:267:VAL:O	1:A:268:LEU:CB	2.61	0.49
1:A:301:ASP:O	1:A:302:MET:O	2.29	0.49
1:B:47:ASN:OD1	1:B:207:ARG:NH2	2.45	0.48
1:B:174:VAL:CG1	1:B:178:LEU:HD12	2.43	0.48
1:B:302:MET:CA	1:B:302:MET:CE	2.90	0.48
1:A:300:ASN:C	1:A:302:MET:N	2.67	0.48
1:B:269:HIS:H	1:B:269:HIS:HD2	1.59	0.48
1:B:307:SER:OG	1:B:308:ILE:N	2.47	0.48
1:B:405:CYS:SG	1:B:453:GLU:HA	2.53	0.48
1:B:424:ILE:O	1:B:428:VAL:HG23	2.14	0.48
1:A:174:VAL:CG1	1:A:178:LEU:HD12	2.43	0.48
1:B:283:ILE:HB	1:B:298:ILE:HB	1.95	0.47
1:A:174:VAL:HG13	1:A:178:LEU:HD12	1.96	0.47
1:A:415:ARG:O	1:A:444:GLU:OE1	2.32	0.47
1:B:233:SER:HA	1:B:287:ASN:HB2	1.97	0.47
1:A:62:ILE:HG23	1:A:109:ILE:HD12	1.96	0.47
1:B:84:ILE:O	1:B:90:LYS:HD2	2.14	0.47
1:B:60:ARG:HG2	1:B:112:ALA:O	2.15	0.46
1:A:128:PHE:O	1:A:132:LEU:HG	2.15	0.46
1:B:249:ILE:HG21	1:B:252:LEU:HD13	1.96	0.46
1:B:305:SER:O	1:B:305:SER:OG	2.30	0.46
1:B:61:ASP:HB3	1:B:64:LYS:HG2	1.97	0.46
1:A:192:GLY:O	1:A:193:PHE:HB3	2.15	0.45
1:A:96:ILE:O	1:A:100:ARG:HG2	2.17	0.45
1:B:189:VAL:CG2	1:B:189:VAL:O	2.64	0.45
1:B:320:LEU:HB3	1:B:401:ASP:HB3	1.98	0.45
1:B:96:ILE:O	1:B:100:ARG:HG2	2.17	0.45
1:A:328:MET:HG2	1:A:334:THR:HG21	1.98	0.45
1:A:130:GLU:HB3	1:A:191:THR:HB	1.99	0.45
1:B:325:GLY:HA3	1:B:359:THR:O	2.17	0.45
1:A:354:GLN:HG3	1:A:361:ILE:HG12	2.00	0.44
1:B:68:PHE:HE2	1:B:104:LEU:HD11	1.81	0.44
1:B:219:TYR:CE1	1:B:279:LYS:HG3	2.52	0.44
1:B:320:LEU:HD22	1:B:450:VAL:HG11	1.99	0.44
1:B:127:SER:HB2	1:B:194:ILE:HG21	1.98	0.44
1:A:320:LEU:HB3	1:A:401:ASP:HB3	2.00	0.44
1:A:119:PRO:HB2	1:A:164:PHE:HB2	2.00	0.44
1:B:325:GLY:O	1:B:327:GLY:N	2.51	0.44
1:A:381:PHE:HB3	1:A:393:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:GLY:N	1:B:393:ASN:HD21	2.16	0.43
1:B:324:PHE:CB	1:B:360:ASN:HA	2.42	0.43
1:B:276:ALA:HB2	1:B:283:ILE:HD11	2.00	0.43
1:B:189:VAL:O	1:B:189:VAL:HG23	2.19	0.43
1:B:303:GLU:O	1:B:304:MET:O	2.37	0.43
1:B:174:VAL:HG13	1:B:178:LEU:HD12	2.01	0.42
1:B:312:ILE:HD13	1:B:463:LEU:HB3	2.00	0.42
1:A:249:ILE:HD11	1:A:311:ALA:HB2	2.02	0.42
1:A:284:LEU:HG	1:A:286:LYS:HG3	2.00	0.42
1:A:301:ASP:C	1:A:301:ASP:OD1	2.62	0.42
1:A:354:GLN:NE2	1:B:350:ILE:O	2.45	0.42
1:B:290:GLU:OE2	1:B:293:SER:HB2	2.19	0.42
1:B:52:ILE:HG13	1:B:68:PHE:CG	2.54	0.42
1:B:119:PRO:HB2	1:B:164:PHE:HB2	2.01	0.42
1:A:45:VAL:HG13	1:A:72:ILE:HD11	2.02	0.41
1:B:258:MET:HE2	1:B:273:ILE:HB	2.02	0.41
1:A:154:GLY:HA3	1:A:196:THR:HB	2.01	0.41
1:A:314:THR:HG22	1:A:407:ILE:HG12	2.02	0.41
1:A:2:THR:O	1:A:223:ALA:HB1	2.21	0.41
1:B:328:MET:C	1:B:332:SER:HG	2.29	0.41
1:B:45:VAL:HG13	1:B:72:ILE:HD11	2.02	0.41
1:B:302:MET:HE3	1:B:302:MET:N	2.35	0.41
1:B:326:ALA:O	1:B:329:VAL:HG12	2.21	0.41
1:B:405:CYS:SG	1:B:456:LEU:HB2	2.61	0.41
1:A:233:SER:HA	1:A:287:ASN:HB2	2.03	0.41
1:A:130:GLU:HG2	1:A:192:GLY:O	2.20	0.40
1:B:328:MET:O	1:B:332:SER:OG	2.39	0.40
1:A:52:ILE:CG2	1:A:108:LEU:HD21	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	461/473 (98%)	431 (94%)	21 (5%)	9 (2%)	6	16
1	B	462/473 (98%)	429 (93%)	24 (5%)	9 (2%)	6	17
All	All	923/946 (98%)	860 (93%)	45 (5%)	18 (2%)	6	16

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	MET
1	A	417	ALA
1	B	304	MET
1	B	266	LYS
1	B	301	ASP
1	B	303	GLU
1	B	417	ALA
1	A	268	LEU
1	A	382	GLY
1	B	268	LEU
1	B	326	ALA
1	B	382	GLY
1	A	301	ASP
1	A	393	ASN
1	A	59	VAL
1	A	306	ASP
1	B	331	VAL
1	A	331	VAL

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	387/397 (98%)	355 (92%)	32 (8%)	10	26
1	B	385/397 (97%)	343 (89%)	42 (11%)	6	16
All	All	772/794 (97%)	698 (90%)	74 (10%)	8	20

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	37	VAL
1	A	51	GLU
1	A	52	ILE
1	A	58	ASP
1	A	69	ILE
1	A	72	ILE
1	A	85	LYS
1	A	102	GLU
1	A	104	LEU
1	A	108	LEU
1	A	179	LEU
1	A	189	VAL
1	A	203	THR
1	A	242	LEU
1	A	294	GLU
1	A	300	ASN
1	A	303	GLU
1	A	316	LYS
1	A	329	VAL
1	A	342	LEU
1	A	346	GLU
1	A	349	VAL
1	A	354	GLN
1	A	364	VAL
1	A	368	GLU
1	A	375	LYS
1	A	378	LYS
1	A	393	ASN
1	A	396	ARG
1	A	463	LEU
1	A	466	LYS
1	B	21	VAL
1	B	37	VAL
1	B	51	GLU
1	B	52	ILE
1	B	60	ARG
1	B	64	LYS
1	B	69	ILE
1	B	72	ILE
1	B	88	GLU
1	B	104	LEU
1	B	111	VAL

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Mol	Chain	Res	Type
1	B	114	LEU
1	B	118	THR
1	B	121	SER
1	B	179	LEU
1	B	189	VAL
1	B	203	THR
1	B	242	LEU
1	B	267	VAL
1	B	269	HIS
1	B	273	ILE
1	B	281	ILE
1	B	286	LYS
1	B	299	THR
1	B	301	ASP
1	B	302	MET
1	B	324	PHE
1	B	329	VAL
1	B	337	ARG
1	B	342	LEU
1	B	346	GLU
1	B	347	VAL
1	B	349	VAL
1	B	351	LEU
1	B	372	LYS
1	B	391	ASN
1	B	393	ASN
1	B	394	LEU
1	B	396	ARG
1	B	404	VAL
1	B	463	LEU
1	B	466	LYS

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	163	ASN
1	A	322	ASN
1	A	348	ASN
1	A	354	GLN
1	A	434	ASN
1	A	440	GLN
1	B	163	ASN

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Mol	Chain	Res	Type
1	B	269	HIS
1	B	300	ASN
1	B	391	ASN
1	B	393	ASN
1	B	434	ASN
1	B	440	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	ASP	B	474	-	7,8,8	1.20	1 (14%)	6,10,10	1.14	0
3	FMT	B	475	-	2,2,2	0.69	0	1,1,1	0.10	0
2	ASP	A	474	-	7,8,8	1.17	1 (14%)	6,10,10	1.44	1 (16%)
3	FMT	A	475	-	2,2,2	0.67	0	1,1,1	0.15	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	ASP	B	474	-	-	6/8/8/8	-
2	ASP	A	474	-	-	0/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	474	ASP	OXT-C	-2.41	1.23	1.30
2	A	474	ASP	OXT-C	-2.29	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	474	ASP	OXT-C-O	-2.42	118.60	124.08

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	474	ASP	O-C-CA-N
2	B	474	ASP	C-CA-CB-CG
2	B	474	ASP	OXT-C-CA-N
2	B	474	ASP	N-CA-CB-CG
2	B	474	ASP	O-C-CA-CB
2	B	474	ASP	OXT-C-CA-CB

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	474	ASP	2	0
3	B	475	FMT	1	0
2	A	474	ASP	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	465/473 (98%)	0.03	7 (1%) 72 70	23, 32, 46, 55	0
1	B	466/473 (98%)	-0.10	7 (1%) 72 70	23, 32, 46, 55	0
All	All	931/946 (98%)	-0.03	14 (1%) 72 70	23, 32, 46, 55	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	ASP	3.6
1	B	305	SER	2.7
1	A	320	LEU	2.6
1	B	317	ASN	2.5
1	B	390	LEU	2.3
1	A	317	ASN	2.2
1	B	392	ASN	2.2
1	A	401	ASP	2.2
1	B	267	VAL	2.1
1	B	269	HIS	2.1
1	A	392	ASN	2.1
1	A	108	LEU	2.1
1	A	383	ASP	2.1
1	A	331	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FMT	A	475	3/3	0.68	0.19	65,65,65,65	0
3	FMT	B	475	3/3	0.71	0.18	57,57,57,58	0
2	ASP	B	474	9/9	0.86	0.13	55,55,56,56	0
2	ASP	A	474	9/9	0.87	0.13	62,63,63,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.