



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:38 PM UTC

PDB ID : 6IOR / pdb_00006ior
Title : The ligand binding domain of Mlp24 with asparagine
Authors : Takahashi, Y.; Sumita, K.; Nishiyama, S.; Kawagishi, I.; Imada, K.
Deposited on : 2018-10-31
Resolution : 2.50 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

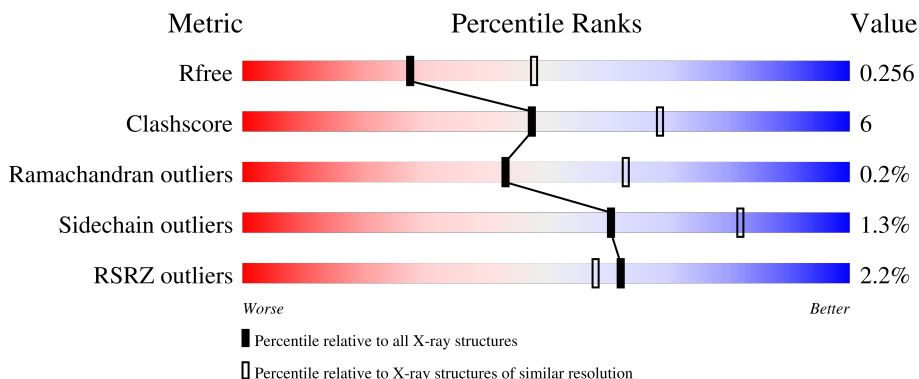
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	256	0% 79% 14% 6%
1	B	256	2% 79% 15% 6%
1	C	256	3% 79% 14% 6%
1	D	256	3% 81% 12% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7707 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 Methyl-accepting chemotaxis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1889	1204	303	378	4			
1	B	241	Total	C	N	O	S	0	0	0
			1889	1204	303	378	4			
1	C	240	Total	C	N	O	S	0	0	0
			1881	1198	302	377	4			
1	D	240	Total	C	N	O	S	0	0	0
			1881	1198	302	377	4			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP A0A0H6VSA0
A	26	PRO	-	expression tag	UNP A0A0H6VSA0
A	27	LEU	-	expression tag	UNP A0A0H6VSA0
A	28	GLY	-	expression tag	UNP A0A0H6VSA0
A	29	SER	-	expression tag	UNP A0A0H6VSA0
A	275	HIS	-	expression tag	UNP A0A0H6VSA0
A	276	HIS	-	expression tag	UNP A0A0H6VSA0
A	277	HIS	-	expression tag	UNP A0A0H6VSA0
A	278	HIS	-	expression tag	UNP A0A0H6VSA0
A	279	HIS	-	expression tag	UNP A0A0H6VSA0
A	280	HIS	-	expression tag	UNP A0A0H6VSA0
B	25	GLY	-	expression tag	UNP A0A0H6VSA0
B	26	PRO	-	expression tag	UNP A0A0H6VSA0
B	27	LEU	-	expression tag	UNP A0A0H6VSA0
B	28	GLY	-	expression tag	UNP A0A0H6VSA0
B	29	SER	-	expression tag	UNP A0A0H6VSA0
B	275	HIS	-	expression tag	UNP A0A0H6VSA0
B	276	HIS	-	expression tag	UNP A0A0H6VSA0
B	277	HIS	-	expression tag	UNP A0A0H6VSA0
B	278	HIS	-	expression tag	UNP A0A0H6VSA0
B	279	HIS	-	expression tag	UNP A0A0H6VSA0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	280	HIS	-	expression tag	UNP A0A0H6VSA0
C	25	GLY	-	expression tag	UNP A0A0H6VSA0
C	26	PRO	-	expression tag	UNP A0A0H6VSA0
C	27	LEU	-	expression tag	UNP A0A0H6VSA0
C	28	GLY	-	expression tag	UNP A0A0H6VSA0
C	29	SER	-	expression tag	UNP A0A0H6VSA0
C	275	HIS	-	expression tag	UNP A0A0H6VSA0
C	276	HIS	-	expression tag	UNP A0A0H6VSA0
C	277	HIS	-	expression tag	UNP A0A0H6VSA0
C	278	HIS	-	expression tag	UNP A0A0H6VSA0
C	279	HIS	-	expression tag	UNP A0A0H6VSA0
C	280	HIS	-	expression tag	UNP A0A0H6VSA0
D	25	GLY	-	expression tag	UNP A0A0H6VSA0
D	26	PRO	-	expression tag	UNP A0A0H6VSA0
D	27	LEU	-	expression tag	UNP A0A0H6VSA0
D	28	GLY	-	expression tag	UNP A0A0H6VSA0
D	29	SER	-	expression tag	UNP A0A0H6VSA0
D	275	HIS	-	expression tag	UNP A0A0H6VSA0
D	276	HIS	-	expression tag	UNP A0A0H6VSA0
D	277	HIS	-	expression tag	UNP A0A0H6VSA0
D	278	HIS	-	expression tag	UNP A0A0H6VSA0
D	279	HIS	-	expression tag	UNP A0A0H6VSA0
D	280	HIS	-	expression tag	UNP A0A0H6VSA0

- ASN
-
- The diagram shows the chemical structure of Asparagine (ASN) with atoms color-coded by type: Carbon (grey), Oxygen (red), Nitrogen (blue), and Hydrogen (white). The structure includes a carboxylate group (COO-) on the right, an amide group (CONH2) on the left, and a side chain with an amine group (NH2) on a wedge bond. Atoms are labeled with green text: O, C, OH, OXT, CB, CA(S), CG, ND2, H2N, OD1, and N. The amine group is represented by a blue arrow pointing to the nitrogen atom.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 9 4 2 3	0	0
2	B	1	Total C N O 9 4 2 3	0	0
2	C	1	Total C N O 9 4 2 3	0	0
2	D	1	Total C N O 9 4 2 3	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

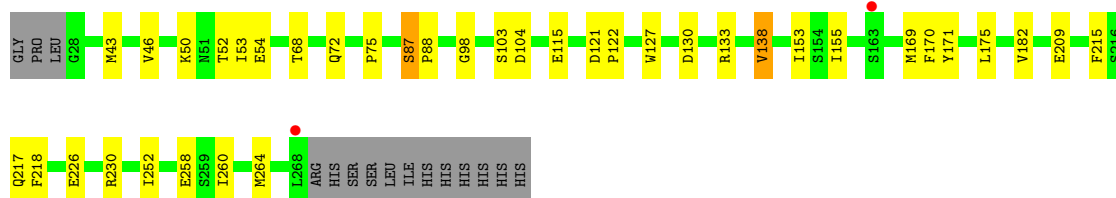
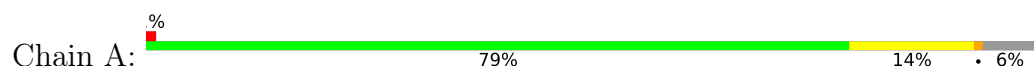
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0
4	B	31	Total O 31 31	0	0
4	C	21	Total O 21 21	0	0
4	D	29	Total O 29 29	0	0

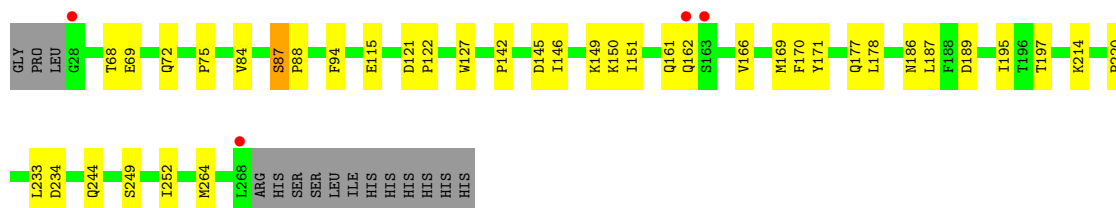
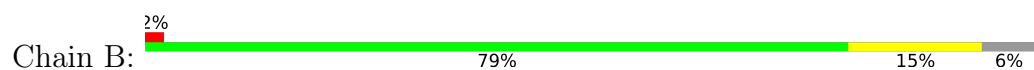
3 Residue-property plots [i](#)

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 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.

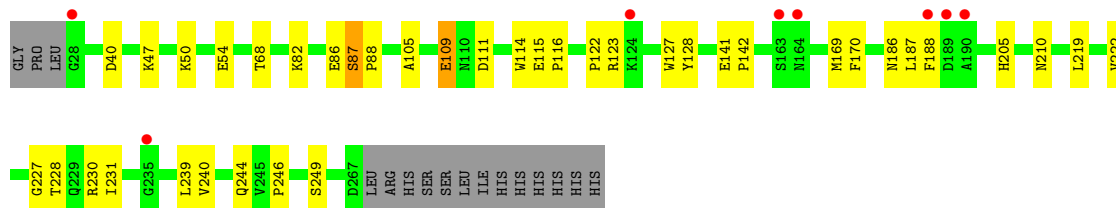
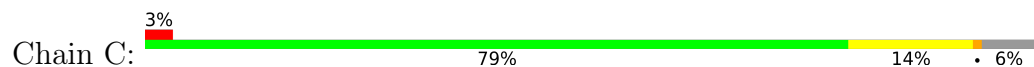
- Molecule 1: Methyl-accepting chemotaxis protein



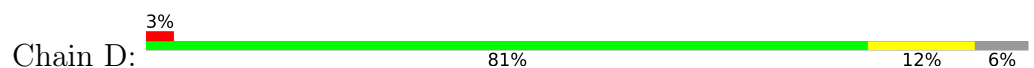
- Molecule 1: Methyl-accepting chemotaxis protein

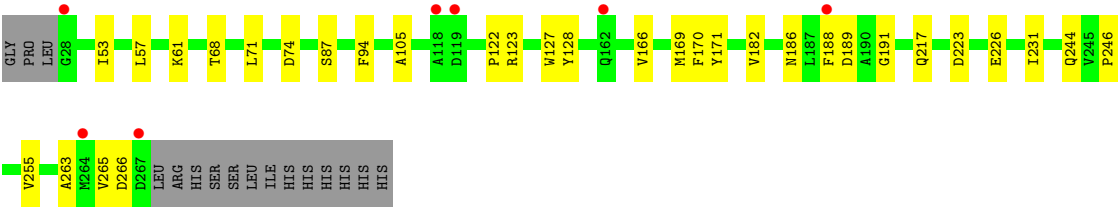


- Molecule 1: Methyl-accepting chemotaxis protein



- Molecule 1: Methyl-accepting chemotaxis protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.88Å 101.35Å 128.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.07 – 2.50 68.07 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.07-2.50) 100.0 (68.07-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.199 , 0.256 0.199 , 0.256	Depositor DCC
R_{free} test set	2050 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7707	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.73% 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: CA

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	0.58	0/1925	0.83	2/2613 (0.1%)
1	B	0.53	0/1925	0.85	2/2613 (0.1%)
1	C	0.55	0/1917	0.84	2/2602 (0.1%)
1	D	0.56	0/1917	0.87	5/2602 (0.2%)
All	All	0.55	0/7684	0.85	11/10430 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	87	SER	CA-C-N	6.84	126.08	118.97
1	D	87	SER	C-N-CA	6.84	126.08	118.97
1	D	74	ASP	CA-C-N	6.69	126.48	119.05
1	D	74	ASP	C-N-CA	6.69	126.48	119.05
1	A	87	SER	CA-C-N	6.39	125.89	119.24
1	A	87	SER	C-N-CA	6.39	125.89	119.24
1	C	87	SER	CA-C-N	5.96	127.29	119.84
1	C	87	SER	C-N-CA	5.96	127.29	119.84
1	D	53	ILE	N-CA-C	5.59	116.23	110.36
1	B	87	SER	CA-C-N	5.43	126.63	119.84
1	B	87	SER	C-N-CA	5.43	126.63	119.84

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	1889	0	1862	24	0
1	B	1889	0	1862	22	0
1	C	1881	0	1851	24	0
1	D	1881	0	1851	17	0
2	A	9	0	5	0	0
2	B	9	0	5	1	0
2	C	9	0	5	1	0
2	D	9	0	5	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	46	0	0	3	0
4	B	31	0	0	2	0
4	C	21	0	0	1	0
4	D	29	0	0	2	0
All	All	7707	0	7446	84	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 6.

All (84) 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:145:ASP:OD1	2:B:501:ASN:N	2.18	0.76
1:B:161:GLN:HG2	1:B:162:GLN:HG2	1.68	0.75
1:A:115:GLU:OE1	4:A:601:HOH:O	2.06	0.73
1:D:223:ASP:OD2	4:D:601:HOH:O	2.05	0.73
1:B:195:ILE:HG12	1:B:252:ILE:HD12	1.69	0.72
1:B:234:ASP:OD1	4:B:601:HOH:O	2.07	0.72
1:A:209:GLU:OE1	4:A:602:HOH:O	2.08	0.71
1:C:115:GLU:OE2	4:C:601:HOH:O	2.09	0.70
1:A:153:ILE:HG12	1:A:175:LEU:HD21	1.74	0.69
1:A:50:LYS:HA	1:A:54:GLU:HB3	1.74	0.69
1:B:177:GLN:H	1:B:177:GLN:CD	2.01	0.68
1:B:84:VAL:O	1:B:87:SER:OG	2.09	0.68
1:B:115:GLU:OE2	4:B:602:HOH:O	2.12	0.68
1:A:217:GLN:NE2	4:A:603:HOH:O	2.27	0.67
1:A:53:ILE:HD12	1:A:53:ILE:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LYS:HD2	1:B:151:ILE:H	1.58	0.67
1:D:68:THR:HG23	1:D:169:MET:HE3	1.79	0.64
1:B:68:THR:HA	1:B:169:MET:HE1	1.78	0.64
1:B:75:PRO:HG2	1:B:161:GLN:HB2	1.78	0.64
1:A:52:THR:OG1	1:A:53:ILE:HD12	1.99	0.63
1:C:244:GLN:HE21	1:C:249:SER:HA	1.68	0.58
1:A:72:GLN:HA	1:A:75:PRO:HG3	1.86	0.57
1:A:68:THR:HG23	1:A:169:MET:HE3	1.86	0.57
1:C:105:ALA:HB1	1:C:122:PRO:HD2	1.88	0.55
1:D:127:TRP:CD2	1:D:170:PHE:HB3	2.42	0.55
1:C:219:LEU:HD21	1:C:240:VAL:HG21	1.90	0.53
1:A:130:ASP:HB3	1:A:138:VAL:HG11	1.90	0.53
1:A:46:VAL:HG22	1:A:252:ILE:HD12	1.91	0.53
1:C:68:THR:HA	1:C:169:MET:HE1	1.91	0.53
1:B:244:GLN:HE21	1:B:249:SER:HA	1.75	0.52
1:D:123:ARG:HG2	1:D:128:TYR:CZ	2.44	0.52
1:D:123:ARG:HA	1:D:128:TYR:CG	2.44	0.52
1:C:127:TRP:CD2	1:C:170:PHE:HB3	2.45	0.52
1:B:69:GLU:HA	1:B:72:GLN:HG3	1.92	0.51
1:D:170:PHE:CE2	2:D:501:ASN:HB3	2.47	0.50
1:A:230:ARG:NH1	1:A:258:GLU:OE2	2.44	0.50
1:C:82:LYS:NZ	1:C:86:GLU:OE2	2.45	0.50
1:C:123:ARG:HG2	1:C:128:TYR:CZ	2.47	0.49
1:C:50:LYS:HA	1:C:54:GLU:HB3	1.95	0.49
1:A:50:LYS:NZ	1:C:40:ASP:OD1	2.44	0.48
1:B:94:PHE:CD1	1:B:171:TYR:HB3	2.48	0.48
1:A:98:GLY:HA3	1:A:170:PHE:CE2	2.48	0.48
1:C:228:THR:HG23	1:C:239:LEU:HD11	1.96	0.48
1:B:186:ASN:HD21	1:B:189:ASP:HA	1.79	0.47
1:D:226:GLU:HG3	4:D:615:HOH:O	2.14	0.47
1:A:43:MET:HE3	1:C:47:LYS:HE2	1.96	0.47
1:C:205:HIS:CE1	1:C:210:ASN:HD22	2.33	0.47
1:B:127:TRP:CD2	1:B:170:PHE:HB3	2.50	0.46
1:B:142:PRO:HG2	1:B:197:THR:HG22	1.97	0.46
1:A:87:SER:HA	1:A:88:PRO:HD3	1.79	0.46
1:C:141:GLU:HG3	1:C:142:PRO:HD2	1.96	0.46
1:D:57:LEU:O	1:D:61:LYS:HG3	2.15	0.46
1:D:244:GLN:O	1:D:246:PRO:HD3	2.17	0.45
1:C:228:THR:CG2	1:C:239:LEU:HD11	2.47	0.44
1:C:244:GLN:O	1:C:246:PRO:HD3	2.18	0.44
1:C:186:ASN:O	1:C:188:PHE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ARG:HG2	1:C:239:LEU:HD13	1.99	0.44
1:D:68:THR:HA	1:D:169:MET:HE1	1.99	0.43
1:A:103:SER:OG	1:A:104:ASP:N	2.51	0.43
1:B:214:LYS:HE2	1:B:214:LYS:HB3	1.83	0.43
1:B:264:MET:HE2	1:B:264:MET:HB3	1.86	0.43
1:A:155:ILE:HB	1:A:171:TYR:HB2	2.01	0.43
1:D:94:PHE:CD1	1:D:171:TYR:HB3	2.54	0.43
1:D:263:ALA:O	1:D:266:ASP:HB3	2.18	0.43
1:C:114:TRP:CH2	1:C:116:PRO:HG3	2.54	0.42
1:D:105:ALA:HB1	1:D:122:PRO:HD2	2.02	0.42
1:A:130:ASP:HA	1:A:133:ARG:NH1	2.35	0.42
1:D:186:ASN:HD21	1:D:189:ASP:HA	1.85	0.42
1:B:87:SER:HA	1:B:88:PRO:HD3	1.79	0.41
1:D:71:LEU:HD12	1:D:169:MET:CE	2.50	0.41
1:A:121:ASP:HA	1:A:122:PRO:HD2	1.82	0.41
1:A:127:TRP:CD2	1:A:170:PHE:HB3	2.55	0.41
1:C:222:VAL:HG23	1:C:231:ILE:HD13	2.02	0.41
1:B:220:PRO:HD2	1:B:233:LEU:HD22	2.02	0.41
1:B:121:ASP:HA	1:B:122:PRO:HD2	1.85	0.41
1:C:109:GLU:HG2	1:C:111:ASP:H	1.85	0.41
1:A:260:ILE:O	1:A:264:MET:HG3	2.21	0.41
1:D:188:PHE:N	1:D:188:PHE:CD1	2.87	0.41
1:A:215:PHE:HA	1:A:218:PHE:CE2	2.56	0.41
1:C:87:SER:HA	1:C:88:PRO:HD3	1.76	0.40
1:C:170:PHE:CE1	2:C:501:ASN:HB3	2.56	0.40
1:A:226:GLU:CD	1:C:227:GLY:HA2	2.46	0.40
1:D:191:GLY:HA3	1:D:255:VAL:O	2.21	0.40
1:B:149:LYS:HA	1:B:149:LYS:HD3	1.92	0.40

There are no symmetry-related clashes.

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	239/256 (93%)	235 (98%)	4 (2%)	0	100	100
1	B	239/256 (93%)	222 (93%)	16 (7%)	1 (0%)	30	49
1	C	238/256 (93%)	232 (98%)	5 (2%)	1 (0%)	30	49
1	D	238/256 (93%)	228 (96%)	10 (4%)	0	100	100
All	All	954/1024 (93%)	917 (96%)	35 (4%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	LEU
1	C	187	LEU

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	209/223 (94%)	207 (99%)	2 (1%)	68	86
1	B	209/223 (94%)	206 (99%)	3 (1%)	59	81
1	C	208/223 (93%)	207 (100%)	1 (0%)	81	92
1	D	208/223 (93%)	203 (98%)	5 (2%)	43	70
All	All	834/892 (94%)	823 (99%)	11 (1%)	61	82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	VAL
1	A	182	VAL
1	B	146	ILE
1	B	166	VAL
1	B	178	LEU
1	C	109	GLU
1	D	166	VAL
1	D	182	VAL
1	D	217	GLN

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Mol	Chain	Res	Type
1	D	231	ILE
1	D	265	VAL

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	89	ASN
1	A	161	GLN
1	A	210	ASN
1	A	211	ASN
1	B	210	ASN
1	B	244	GLN
1	C	72	GLN
1	C	210	ASN
1	C	244	GLN
1	D	65	GLN
1	D	72	GLN
1	D	183	ASN
1	D	244	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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
2	ASN	C	501	-	7,8,8	0.88	1 (14%)	6,10,10	0.99	1 (16%)
2	ASN	A	501	-	7,8,8	0.87	1 (14%)	6,10,10	1.01	1 (16%)
2	ASN	D	501	-	7,8,8	0.96	1 (14%)	6,10,10	1.24	1 (16%)
2	ASN	B	501	-	7,8,8	0.91	1 (14%)	6,10,10	0.90	1 (16%)

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	ASN	C	501	-	-	0/8/8/8	-
2	ASN	A	501	-	-	0/8/8/8	-
2	ASN	D	501	-	-	0/8/8/8	-
2	ASN	B	501	-	-	2/8/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	ASN	OXT-C	-2.22	1.23	1.30
2	C	501	ASN	OXT-C	-2.17	1.23	1.30
2	B	501	ASN	OXT-C	-2.14	1.23	1.30
2	A	501	ASN	OXT-C	-2.02	1.24	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	ASN	OXT-C-O	-2.94	117.42	124.08
2	A	501	ASN	OXT-C-O	-2.38	118.68	124.08
2	C	501	ASN	OXT-C-O	-2.32	118.82	124.08
2	B	501	ASN	OXT-C-O	-2.13	119.25	124.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	ASN	OXT-C-CA-CB
2	B	501	ASN	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	ASN	1	0
2	D	501	ASN	1	0
2	B	501	ASN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	241/256 (94%)	-0.23	2 (0%) 82 80	21, 32, 46, 64	0
1	B	241/256 (94%)	0.07	4 (1%) 69 65	24, 38, 57, 78	0
1	C	240/256 (93%)	0.07	8 (3%) 49 45	26, 37, 58, 71	0
1	D	240/256 (93%)	-0.01	7 (2%) 53 49	24, 36, 57, 94	0
All	All	962/1024 (93%)	-0.02	21 (2%) 62 58	21, 36, 57, 94	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	267	ASP	4.2
1	B	268	LEU	4.2
1	D	118	ALA	3.4
1	D	188	PHE	3.3
1	A	268	LEU	2.9
1	C	190	ALA	2.8
1	D	264	MET	2.7
1	B	162	GLN	2.6
1	D	28	GLY	2.5
1	C	28	GLY	2.5
1	C	124	LYS	2.4
1	C	163	SER	2.4
1	B	28	GLY	2.3
1	D	119	ASP	2.2
1	C	188	PHE	2.2
1	C	164	ASN	2.2
1	D	162	GLN	2.2
1	C	235	GLY	2.1
1	A	163	SER	2.1
1	B	163	SER	2.1
1	C	189	ASP	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($\text{\AA}^2$)	Q<0.9
2	ASN	B	501	9/9	0.86	0.14	47,50,55,55	0
2	ASN	C	501	9/9	0.91	0.12	39,45,56,58	0
2	ASN	A	501	9/9	0.93	0.10	25,31,40,48	0
2	ASN	D	501	9/9	0.93	0.10	36,38,47,50	0
3	CA	D	502	1/1	0.97	0.04	46,46,46,46	0
3	CA	C	502	1/1	0.98	0.03	46,46,46,46	0
3	CA	B	502	1/1	0.98	0.04	46,46,46,46	0
3	CA	A	502	1/1	0.99	0.04	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.