



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 12:24 PM GMT

PDB ID : 3VCY
Title : Structure of MurA (UDP-N-acetylglucosamineenolpyruvyl transferase), from Vibrio fischeri in complex with substrate UDP-N-acetylglucosamineand the drug fosfomycin.
Authors : Bensen, D.C.; Rodriguez, S.; Nix, J.; Cunningham, M.L.; Tari, L.W.
Deposited on : 2012-01-04
Resolution : 1.93 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

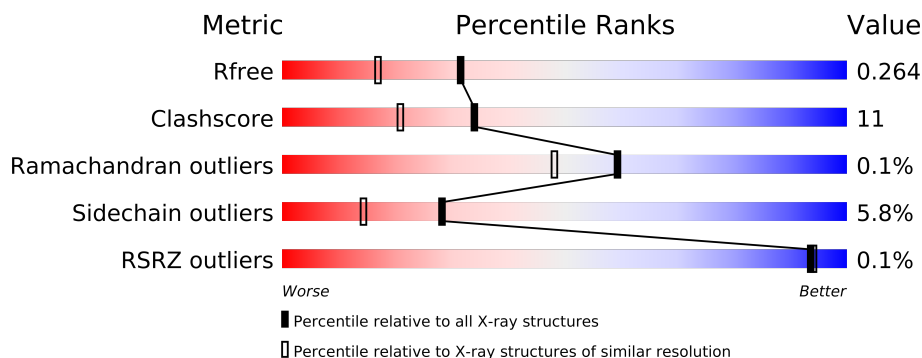
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.93 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}	66092	4387 (1.94-1.90)
Clashscore	79885	5258 (1.94-1.90)
Ramachandran outliers	78287	5193 (1.94-1.90)
Sidechain outliers	78261	5194 (1.94-1.90)
RSRZ outliers	66119	4389 (1.94-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	430	
1	B	430	
1	C	430	
1	D	430	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	FFQ	A	500	-	X
2	FFQ	B	500	-	X
2	FFQ	C	500	-	X
2	FFQ	D	500	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
4	PO4	A	502	-	X
4	PO4	C	502	-	X
4	PO4	D	502	-	X
5	GOL	B	503	-	X
5	GOL	C	503	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13938 atoms, of which 0 are hydrogen and 0 are deuterium.

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 UDP-N-acetylglucosamine1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	5	0
			3123	1958	542	604	19			
1	B	419	Total	C	N	O	S	0	5	0
			3125	1958	544	604	19			
1	C	419	Total	C	N	O	S	0	8	0
			3142	1967	545	611	19			
1	D	419	Total	C	N	O	S	0	9	0
			3145	1973	544	609	19			

There are 36 discrepancies between the modelled and reference sequences:

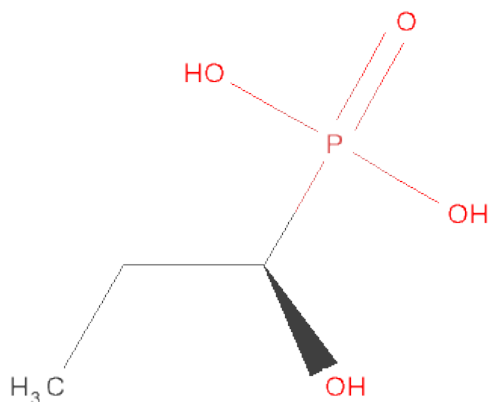
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	TYR	SEE REMARK 999	UNP B5F9P4
A	423	LEU	-	EXPRESSION TAG	UNP B5F9P4
A	424	GLU	-	EXPRESSION TAG	UNP B5F9P4
A	425	HIS	-	EXPRESSION TAG	UNP B5F9P4
A	426	HIS	-	EXPRESSION TAG	UNP B5F9P4
A	427	HIS	-	EXPRESSION TAG	UNP B5F9P4
A	428	HIS	-	EXPRESSION TAG	UNP B5F9P4
A	429	HIS	-	EXPRESSION TAG	UNP B5F9P4
A	430	HIS	-	EXPRESSION TAG	UNP B5F9P4
B	2	ASP	TYR	SEE REMARK 999	UNP B5F9P4
B	423	LEU	-	EXPRESSION TAG	UNP B5F9P4
B	424	GLU	-	EXPRESSION TAG	UNP B5F9P4
B	425	HIS	-	EXPRESSION TAG	UNP B5F9P4
B	426	HIS	-	EXPRESSION TAG	UNP B5F9P4
B	427	HIS	-	EXPRESSION TAG	UNP B5F9P4
B	428	HIS	-	EXPRESSION TAG	UNP B5F9P4
B	429	HIS	-	EXPRESSION TAG	UNP B5F9P4
B	430	HIS	-	EXPRESSION TAG	UNP B5F9P4
C	2	ASP	TYR	SEE REMARK 999	UNP B5F9P4
C	423	LEU	-	EXPRESSION TAG	UNP B5F9P4
C	424	GLU	-	EXPRESSION TAG	UNP B5F9P4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	425	HIS	-	EXPRESSION TAG	UNP B5F9P4
C	426	HIS	-	EXPRESSION TAG	UNP B5F9P4
C	427	HIS	-	EXPRESSION TAG	UNP B5F9P4
C	428	HIS	-	EXPRESSION TAG	UNP B5F9P4
C	429	HIS	-	EXPRESSION TAG	UNP B5F9P4
C	430	HIS	-	EXPRESSION TAG	UNP B5F9P4
D	2	ASP	TYR	SEE REMARK 999	UNP B5F9P4
D	423	LEU	-	EXPRESSION TAG	UNP B5F9P4
D	424	GLU	-	EXPRESSION TAG	UNP B5F9P4
D	425	HIS	-	EXPRESSION TAG	UNP B5F9P4
D	426	HIS	-	EXPRESSION TAG	UNP B5F9P4
D	427	HIS	-	EXPRESSION TAG	UNP B5F9P4
D	428	HIS	-	EXPRESSION TAG	UNP B5F9P4
D	429	HIS	-	EXPRESSION TAG	UNP B5F9P4
D	430	HIS	-	EXPRESSION TAG	UNP B5F9P4

- Molecule 2 is [(1R)-1-HYDROXYPROPYL]PHOSPHONICACID (three-letter code: FFQ) (formula: C₃H₉O₄P).



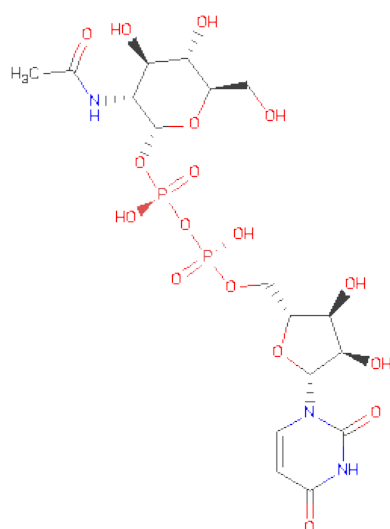
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			8	3	4	1		
2	B	1	Total	C	O	P	0	0
			8	3	4	1		
2	C	1	Total	C	O	P	0	0
			8	3	4	1		

Continued on next page...

Continued from previous page...

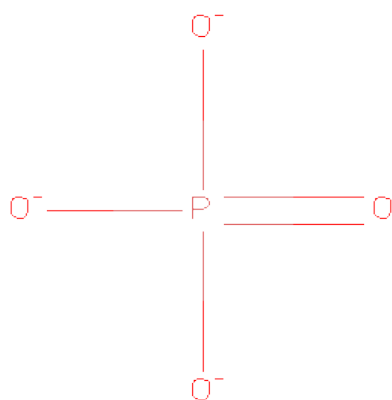
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	O	P	0	0
			8	3	4	1		

- Molecule 3 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



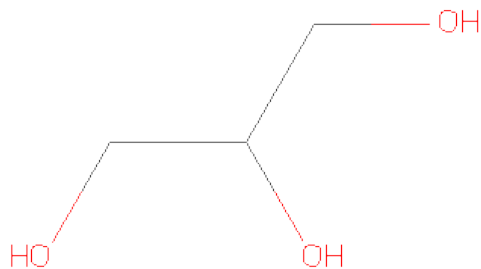
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	D	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

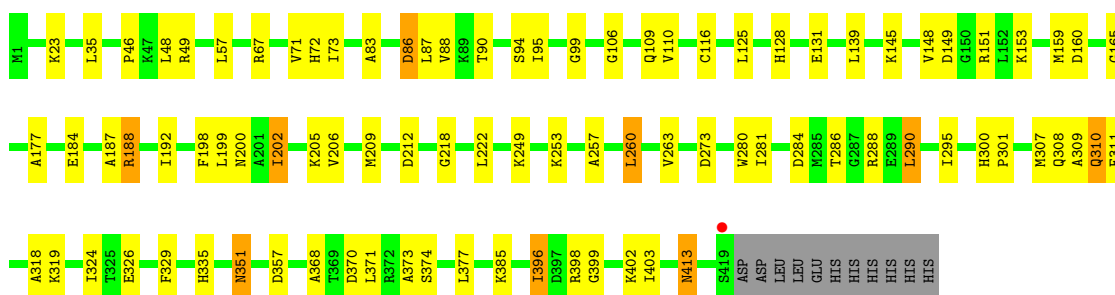
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	281	Total	O	0	0
			281	281		
6	B	258	Total	O	0	0
			258	258		
6	C	304	Total	O	0	0
			304	304		
6	D	328	Total	O	0	0
			328	328		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

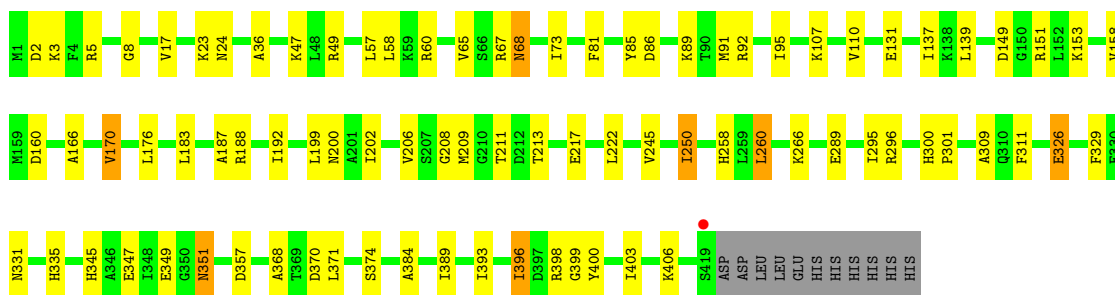
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain A:



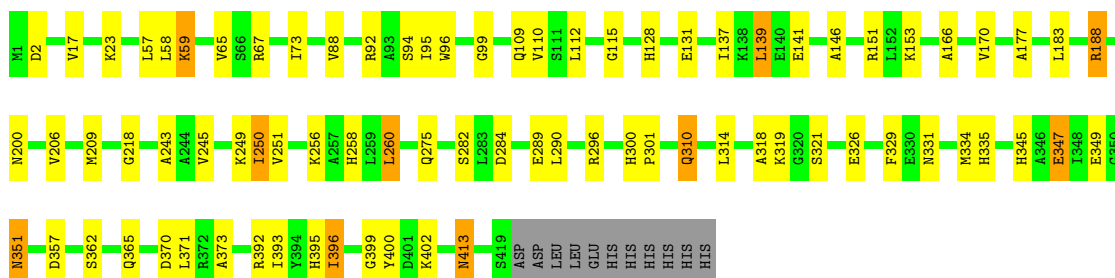
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain B:



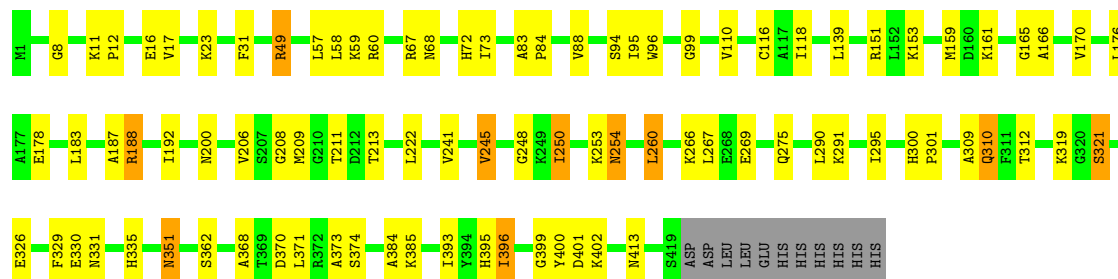
- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain C:



- Molecule 1: UDP-N-acetylglucosamine1-carboxyvinyltransferase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.60Å 118.51Å 92.51Å 90.00° 116.48° 90.00°	Depositor
Resolution (Å)	27.90 – 1.93 27.90 – 1.93	Depositor EDS
% Data completeness (in resolution range)	96.9 (27.90-1.93) 96.9 (27.90-1.93)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.199 , 0.261 0.202 , 0.264	Depositor DCC
R_{free} test set	6151 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 28.8	EDS
Estimated twinning fraction	0.044 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 122356 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13938	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: GOL, PO4, UD1, FFQ

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	0.54	1/3180 (0.0%)	0.70	3/4305 (0.1%)
1	B	0.54	0/3183	0.68	1/4309 (0.0%)
1	C	0.54	1/3208 (0.0%)	0.67	1/4341 (0.0%)
1	D	0.53	1/3215 (0.0%)	0.65	1/4353 (0.0%)
All	All	0.54	3/12786 (0.0%)	0.68	6/17308 (0.0%)

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	C	0	1
1	D	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	96	TRP	CD2-CE2	5.50	1.48	1.41
1	D	96	TRP	CD2-CE2	5.34	1.47	1.41
1	A	280	TRP	CD2-CE2	5.04	1.47	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	LEU	CA-CB-CG	7.61	132.79	115.30
1	B	260	LEU	CA-CB-CG	7.00	131.39	115.30
1	C	260	LEU	CA-CB-CG	6.95	131.28	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	260	LEU	CA-CB-CG	6.86	131.08	115.30
1	A	151	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	151	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	ARG	Peptide
1	C	67	ARG	Peptide
1	D	67	ARG	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3123	0	3185	79	0
1	B	3125	0	3181	62	0
1	C	3142	0	3199	69	0
1	D	3145	0	3209	74	0
2	A	8	0	6	1	0
2	B	8	0	6	1	0
2	C	8	0	6	1	0
2	D	8	0	6	0	0
3	A	39	0	25	0	0
3	B	39	0	25	0	0
3	C	39	0	25	0	0
3	D	39	0	25	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	6	0	8	1	0
6	A	281	0	0	22	0
6	B	258	0	0	8	0
6	C	304	0	0	25	0
6	D	328	0	0	26	0
All	All	13938	0	12930	281	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (281) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:212:ASP:HB3	6:A:832:HOH:O	1.29	1.24
1:A:286:THR:HG22	6:A:801:HOH:O	1.36	1.23
1:A:184:GLU:HG3	6:A:859:HOH:O	1.49	1.13
1:A:202:ILE:HB	6:A:847:HOH:O	1.49	1.11
1:B:199:LEU:O	1:B:202:ILE:HG22	1.55	1.06
1:A:374:SER:HB3	1:A:396[B]:ILE:HG12	1.38	1.05
1:B:208:GLY:O	1:B:211:THR:HG22	1.59	1.00
1:A:310:GLN:HE21	1:A:310:GLN:H	1.03	0.98
1:C:73:ILE:CG1	6:C:738:HOH:O	2.10	0.98
1:D:200:ASN:HD21	1:D:206:VAL:H	1.11	0.98
1:C:310:GLN:HE21	1:C:310:GLN:H	0.99	0.98
1:D:351:ASN:H	1:D:351:ASN:HD22	1.06	0.96
1:C:351:ASN:H	1:C:351:ASN:HD22	1.11	0.96
1:D:310:GLN:HE21	1:D:310:GLN:H	1.05	0.95
1:B:200:ASN:HD21	1:B:206:VAL:H	1.11	0.95
1:A:351:ASN:HD22	1:A:351:ASN:H	1.08	0.94
1:B:368:ALA:HB1	1:B:374:SER:OG	1.69	0.93
1:D:241:VAL:HG23	6:D:924:HOH:O	1.68	0.93
1:C:365:GLN:HB3	6:C:620:HOH:O	1.69	0.91
1:C:73:ILE:HG12	6:C:738:HOH:O	1.66	0.91
1:C:200:ASN:HD21	1:C:206:VAL:H	1.14	0.90
1:D:211[A]:THR:HG21	6:D:848:HOH:O	1.73	0.88
1:D:393:ILE:O	1:D:396:ILE:HG22	1.72	0.88
1:A:200:ASN:HD21	1:A:206:VAL:H	1.24	0.85
1:A:368:ALA:HB1	1:A:374:SER:OG	1.77	0.85
1:C:331:ASN:ND2	6:C:633:HOH:O	2.10	0.83
1:B:211:THR:HG23	1:B:213:THR:H	1.42	0.83
1:C:73:ILE:HG13	6:C:738:HOH:O	1.76	0.82
1:C:151:ARG:HD3	6:C:869:HOH:O	1.80	0.81
1:A:88:VAL:HG22	1:A:94[A]:SER:OG	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:310:GLN:NE2	1:C:310:GLN:H	1.80	0.79
1:C:351:ASN:N	1:C:351:ASN:HD22	1.78	0.79
1:A:374:SER:HB3	1:A:396[B]:ILE:CG1	2.13	0.79
1:A:374:SER:CB	1:A:396[B]:ILE:HG12	2.14	0.77
1:D:211[A]:THR:HG23	1:D:213:THR:H	1.49	0.77
1:B:188:ARG:HH12	1:D:188:ARG:CZ	1.97	0.77
1:D:245:VAL:HB	6:D:923:HOH:O	1.84	0.77
1:A:311:PHE:HD1	6:A:772:HOH:O	1.70	0.75
1:C:351:ASN:ND2	1:C:351:ASN:H	1.86	0.74
1:A:145:LYS:HE2	6:A:881:HOH:O	1.86	0.74
1:D:208:GLY:O	1:D:211[A]:THR:HG22	1.88	0.73
1:B:36:ALA:HB2	1:B:202:ILE:HD11	1.71	0.73
1:A:310:GLN:HB2	6:A:772:HOH:O	1.87	0.73
1:D:310:GLN:HE21	1:D:310:GLN:N	1.83	0.72
1:A:99:GLY:HA3	6:A:880:HOH:O	1.87	0.72
1:D:395:HIS:HD2	6:D:871:HOH:O	1.71	0.72
1:C:112:LEU:HB3	6:C:602:HOH:O	1.88	0.71
1:A:95:ILE:HA	1:A:110[A]:VAL:HG11	1.73	0.71
1:D:368:ALA:HB1	1:D:374:SER:OG	1.92	0.70
1:C:112:LEU:CB	6:C:602:HOH:O	2.39	0.69
1:A:83:ALA:HB3	1:A:110[B]:VAL:HG23	1.74	0.69
1:A:351:ASN:H	1:A:351:ASN:ND2	1.87	0.69
6:C:855:HOH:O	1:D:331:ASN:HB2	1.91	0.69
1:D:151:ARG:HD3	6:D:884:HOH:O	1.93	0.68
1:D:275:GLN:HG2	6:D:881:HOH:O	1.92	0.68
1:C:17:VAL:HG12	1:C:250:ILE:HD11	1.76	0.68
1:D:17:VAL:HG12	1:D:250:ILE:HD11	1.76	0.67
1:B:17:VAL:HG12	1:B:250:ILE:HD11	1.75	0.67
1:D:310:GLN:NE2	1:D:310:GLN:H	1.87	0.67
1:D:351:ASN:H	1:D:351:ASN:ND2	1.86	0.67
1:A:368:ALA:CB	1:A:374:SER:OG	2.43	0.66
1:C:256:LYS:HD3	1:C:258:HIS:CE1	2.30	0.66
1:B:151:ARG:HD2	1:B:176:LEU:O	1.95	0.66
1:A:109:GLN:HG2	1:A:145:LYS:HG2	1.78	0.66
1:A:310:GLN:HE21	1:A:310:GLN:N	1.85	0.66
1:D:319:LYS:NZ	6:D:768:HOH:O	2.11	0.66
1:B:370:ASP:OD1	6:B:825:HOH:O	2.14	0.65
1:C:139:LEU:HD21	6:C:602:HOH:O	1.95	0.65
1:B:351:ASN:HD22	1:B:351:ASN:H	1.42	0.65
1:D:88:VAL:HG22	1:D:94[A]:SER:OG	1.96	0.65
1:D:326:GLU:HG3	1:D:329:PHE:O	1.96	0.64
1:B:326:GLU:HG3	1:B:329:PHE:O	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:95:ILE:HA	1:A:110[B]:VAL:HG21	1.80	0.64
1:D:371:LEU:HD21	1:D:399:GLY:HA3	1.80	0.64
1:D:396:ILE:HD13	1:D:400:TYR:HB2	1.81	0.63
1:B:47:LYS:HE3	6:B:845:HOH:O	1.97	0.63
1:D:16:GLU:OE1	1:D:253:LYS:HE3	1.99	0.62
1:C:310:GLN:N	1:C:310:GLN:HE21	1.84	0.62
1:A:290:LEU:HD13	1:A:318:ALA:HB2	1.81	0.62
1:B:170:VAL:HG21	1:B:183:LEU:HD13	1.81	0.62
1:D:275:GLN:NE2	6:D:881:HOH:O	2.32	0.62
1:C:335:HIS:HB3	1:C:373:ALA:HB1	1.83	0.61
1:D:151:ARG:CD	6:D:884:HOH:O	2.48	0.61
6:A:721:HOH:O	1:B:331:ASN:HB2	1.99	0.61
1:B:200:ASN:ND2	1:B:206:VAL:H	1.92	0.61
1:C:334:MET:HG3	6:C:633:HOH:O	2.01	0.60
1:A:198:PHE:O	1:A:202:ILE:HG22	2.01	0.60
1:A:351:ASN:N	1:A:351:ASN:HD22	1.88	0.60
1:A:357:ASP:OD1	6:A:802:HOH:O	2.16	0.60
1:D:245:VAL:CB	6:D:923:HOH:O	2.47	0.60
1:A:49:ARG:HG3	1:A:398:ARG:HG2	1.83	0.59
1:C:371:LEU:HD21	1:C:399:GLY:HA3	1.83	0.59
1:A:326:GLU:HG3	1:A:329:PHE:O	2.02	0.59
1:D:395:HIS:CD2	6:D:871:HOH:O	2.51	0.58
1:A:273:ASP:HB2	1:A:288:ARG:HH22	1.69	0.57
1:D:241:VAL:CG2	6:D:924:HOH:O	2.40	0.57
1:A:187:ALA:HB3	1:A:192:ILE:CD1	2.34	0.57
6:B:705:HOH:O	1:D:295:ILE:HG12	2.04	0.57
1:C:345:HIS:HD2	1:C:357:ASP:O	1.88	0.57
1:A:165:GLY:HA3	5:A:503:GOL:O1	2.05	0.57
1:A:263:VAL:HG23	6:A:704:HOH:O	2.03	0.57
1:C:88:VAL:HG13	6:C:717:HOH:O	2.04	0.56
1:B:188:ARG:NH1	1:D:188:ARG:CZ	2.68	0.56
1:B:349:GLU:HG3	6:C:605:HOH:O	2.06	0.56
1:D:351:ASN:HD22	1:D:351:ASN:N	1.85	0.55
1:B:345:HIS:HD2	1:B:357:ASP:O	1.88	0.55
1:C:395:HIS:HD2	6:C:899:HOH:O	1.87	0.55
1:C:170:VAL:HG22	1:C:183:LEU:HD22	1.88	0.55
1:B:2:ASP:HB3	1:B:393:ILE:HD11	1.88	0.55
1:A:284:ASP:OD1	1:A:286:THR:HG23	2.07	0.55
1:C:58:LEU:HD13	1:C:73:ILE:HD12	1.90	0.54
1:A:187:ALA:HB3	1:A:192:ILE:HD13	1.89	0.54
1:B:170:VAL:HG22	1:B:183:LEU:HD22	1.88	0.54
1:A:202:ILE:HG12	1:A:222:LEU:HB3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:371:LEU:CD1	1:A:399:GLY:HA3	2.37	0.54
1:C:413:ASN:HD22	1:C:413:ASN:C	2.11	0.54
1:C:88:VAL:HG22	1:C:94[A]:SER:OG	2.07	0.54
1:C:396:ILE:HD13	1:C:400:TYR:CD1	2.42	0.54
1:D:170:VAL:HG22	1:D:183:LEU:HD22	1.90	0.54
1:A:368:ALA:HB1	1:A:374:SER:HG	1.71	0.54
1:B:187:ALA:HB3	1:B:192:ILE:CD1	2.38	0.54
1:A:371:LEU:HD11	1:A:399:GLY:HA3	1.90	0.53
1:C:141:GLU:HG2	6:D:912:HOH:O	2.07	0.53
1:A:413:ASN:C	1:A:413:ASN:HD22	2.10	0.53
1:D:267:LEU:HD21	6:D:924:HOH:O	2.07	0.53
1:B:5:ARG:HG3	1:B:389:ILE:CD1	2.39	0.53
1:D:11:LYS:HE3	6:D:897:HOH:O	2.08	0.53
1:D:187:ALA:HB3	1:D:192:ILE:CD1	2.39	0.53
1:D:72:HIS:HE1	6:D:779:HOH:O	1.92	0.52
1:B:95:ILE:HA	1:B:110:VAL:HG11	1.91	0.52
1:D:321:SER:OG	6:D:833:HOH:O	2.18	0.52
1:D:335:HIS:HB3	1:D:373:ALA:HB1	1.90	0.52
1:D:99:GLY:HA3	6:D:841:HOH:O	2.07	0.52
1:C:128:HIS:HD2	1:C:131:GLU:OE1	1.93	0.52
1:C:170:VAL:HG21	1:C:183:LEU:HD13	1.92	0.52
1:A:273:ASP:HB2	1:A:288:ARG:NH2	2.24	0.52
1:A:35:LEU:HB3	1:A:222:LEU:HD12	1.91	0.51
1:D:153:LYS:NZ	1:D:178:GLU:OE1	2.43	0.51
1:C:95:ILE:HA	1:C:110:VAL:HG11	1.92	0.51
1:B:17:VAL:CG2	1:B:406:LYS:HD3	2.40	0.51
6:B:705:HOH:O	1:D:266:LYS:HG3	2.09	0.51
1:B:67:ARG:O	1:B:68:ASN:HB2	2.10	0.51
1:B:158:VAL:HG12	6:B:607:HOH:O	2.10	0.51
1:B:188:ARG:HH12	1:D:188:ARG:NH2	2.08	0.51
1:D:326:GLU:CG	1:D:329:PHE:O	2.58	0.51
1:D:401:ASP:OD1	1:D:402:LYS:HD2	2.10	0.51
1:B:166:ALA:O	1:B:170:VAL:HG13	2.11	0.50
1:D:58:LEU:HD13	1:D:73:ILE:HD12	1.93	0.50
1:B:258:HIS:CE1	6:B:832:HOH:O	2.64	0.50
1:C:393:ILE:O	1:C:396:ILE:HG22	2.11	0.50
1:A:128:HIS:HD2	1:A:131:GLU:OE1	1.94	0.50
1:B:58:LEU:HD13	1:B:73:ILE:HD12	1.94	0.50
1:B:85:TYR:CE2	1:B:89:LYS:HE3	2.46	0.50
1:A:300:HIS:CG	1:A:301:PRO:HA	2.46	0.50
1:B:309:ALA:HA	1:B:335:HIS:CE1	2.46	0.50
1:D:373:ALA:HB2	6:D:714:HOH:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:205:LYS:HE2	6:A:837:HOH:O	2.11	0.50
1:B:295:ILE:HD11	1:B:311:PHE:CD2	2.47	0.50
1:A:253:LYS:HD2	6:A:653:HOH:O	2.10	0.49
1:A:335:HIS:CD2	1:A:335:HIS:H	2.29	0.49
1:A:373:ALA:O	1:A:377:LEU:HG	2.11	0.49
1:A:307:MET:HE3	6:A:772:HOH:O	2.12	0.49
1:C:256:LYS:HD3	1:C:258:HIS:HE1	1.76	0.49
1:A:71:VAL:HG12	1:A:73:ILE:HD11	1.95	0.49
1:A:86:ASP:O	1:A:90:THR:HG23	2.12	0.49
1:C:326:GLU:HG3	1:C:329:PHE:O	2.12	0.49
1:A:199:LEU:HA	1:A:202:ILE:CG2	2.43	0.48
1:D:396:ILE:CD1	1:D:400:TYR:HB2	2.42	0.48
1:A:310:GLN:NE2	1:A:310:GLN:H	1.88	0.48
1:C:166:ALA:O	1:C:170:VAL:HG13	2.13	0.48
1:A:177:ALA:O	1:A:218:GLY:HA3	2.13	0.48
1:A:188:ARG:NH1	6:A:656:HOH:O	2.44	0.48
1:D:396:ILE:HB	6:D:921:HOH:O	2.13	0.48
1:B:368:ALA:CB	1:B:374:SER:OG	2.53	0.48
1:A:23:LYS:HB2	1:A:48:LEU:HD11	1.95	0.48
1:C:112:LEU:HB2	6:C:602:HOH:O	2.09	0.48
1:A:295:ILE:HD11	1:A:311:PHE:CD2	2.49	0.47
1:D:159:MET:HG2	1:D:183:LEU:HD11	1.96	0.47
1:C:290:LEU:HG	1:C:318:ALA:HB2	1.96	0.47
1:D:245:VAL:CG2	6:D:923:HOH:O	2.63	0.47
1:C:92:ARG:O	1:C:95:ILE:HG22	2.14	0.47
1:B:396:ILE:HD12	1:B:403:ILE:HG21	1.95	0.47
1:B:86:ASP:HA	1:B:89:LYS:NZ	2.30	0.47
1:B:371:LEU:HD21	1:B:399:GLY:HA3	1.96	0.47
1:B:3:LYS:NZ	6:B:734:HOH:O	2.41	0.46
1:D:8:GLY:HA3	1:D:384:ALA:O	2.15	0.46
1:C:392:ARG:HD2	6:C:778:HOH:O	2.15	0.46
1:B:200:ASN:HD21	1:B:206:VAL:N	1.94	0.46
1:C:59:LYS:HD2	1:C:65:VAL:HB	1.98	0.46
1:D:166:ALA:O	1:D:170:VAL:HG13	2.15	0.46
1:A:307:MET:CE	6:A:772:HOH:O	2.63	0.46
1:D:83:ALA:HB3	1:D:110[A]:VAL:HG12	1.96	0.46
1:B:8:GLY:HA3	1:B:384:ALA:O	2.15	0.46
1:B:92:ARG:HG2	6:B:831:HOH:O	2.16	0.46
1:B:326:GLU:CG	1:B:329:PHE:O	2.64	0.45
1:B:345:HIS:CD2	1:B:357:ASP:O	2.69	0.45
1:B:65:VAL:HG13	1:B:73:ILE:HD13	1.99	0.45
1:C:115:GLY:HA3	6:D:820:HOH:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:335:HIS:CD2	1:C:335:HIS:H	2.35	0.45
1:A:257:ALA:HA	1:A:281:ILE:HD11	1.97	0.45
1:C:23:LYS:HE2	6:C:895:HOH:O	2.15	0.45
1:C:275:GLN:NE2	6:C:795:HOH:O	2.50	0.45
1:C:88:VAL:CG1	6:C:717:HOH:O	2.62	0.45
1:A:249:LYS:HD2	6:A:798:HOH:O	2.17	0.45
1:A:159:MET:HE3	6:A:633:HOH:O	2.17	0.45
1:B:81:PHE:CE2	1:B:107:LYS:HE3	2.51	0.45
1:B:396:ILE:HD13	1:B:400:TYR:HB2	1.99	0.45
1:B:393:ILE:O	1:B:396:ILE:HG22	2.17	0.44
1:A:309:ALA:HA	1:A:335:HIS:CE1	2.52	0.44
1:D:385:LYS:HA	1:D:385:LYS:HD2	1.81	0.44
1:B:371:LEU:CD2	1:B:399:GLY:HA3	2.47	0.44
1:C:243:ALA:HB2	1:C:250:ILE:CG2	2.48	0.44
1:A:23:LYS:HB2	1:A:48:LEU:CD1	2.47	0.44
1:B:23:LYS:NZ	1:B:24:ASN:OD1	2.46	0.44
1:D:330:GLU:HG3	6:D:628:HOH:O	2.17	0.44
1:D:254:ASN:HD22	1:D:254:ASN:N	2.14	0.44
1:C:249:LYS:HD2	1:C:284:ASP:CG	2.38	0.44
1:D:213:THR:HG23	6:D:766:HOH:O	2.17	0.44
2:B:500:FFQ:O4	2:B:500:FFQ:H3	2.17	0.44
1:C:296[A]:ARG:NH1	6:C:824:HOH:O	2.50	0.44
1:C:99:GLY:HA3	6:C:799:HOH:O	2.16	0.44
1:D:165:GLY:HA3	5:D:503:GOL:O1	2.17	0.44
1:C:319:LYS:HD3	1:C:319:LYS:HA	1.82	0.44
1:A:319:LYS:HE2	6:A:843:HOH:O	2.17	0.44
1:A:308:GLN:HG2	1:A:324:ILE:HG21	2.00	0.44
1:C:177:ALA:O	1:C:218:GLY:HA3	2.18	0.44
1:A:72:HIS:HD2	6:A:661:HOH:O	2.00	0.44
1:C:300:HIS:CG	1:C:301:PRO:HA	2.53	0.44
1:C:335:HIS:HD2	6:C:762:HOH:O	2.00	0.43
1:C:58:LEU:CD1	1:C:73:ILE:HD12	2.49	0.43
1:D:49:ARG:HB2	6:D:604:HOH:O	2.18	0.43
1:D:245:VAL:HG23	6:D:923:HOH:O	2.17	0.43
1:D:266:LYS:HD3	1:D:266:LYS:HA	1.76	0.43
1:A:188:ARG:HH12	1:C:188:ARG:NH2	2.16	0.43
1:C:137:ILE:HG12	1:C:146:ALA:HB2	2.01	0.43
1:C:396:ILE:CD1	1:C:400:TYR:CD1	3.02	0.43
1:A:125:LEU:HD21	1:A:160:ASP:HB2	2.01	0.43
1:C:335:HIS:HB3	1:C:373:ALA:CB	2.49	0.43
1:A:188:ARG:CZ	6:A:656:HOH:O	2.67	0.43
1:D:23:LYS:HD2	1:D:399:GLY:HA2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:266:LYS:HD3	1:B:266:LYS:HA	1.83	0.42
2:C:500:FFQ:H3	6:C:859:HOH:O	2.18	0.42
1:B:202:ILE:HD13	1:B:202:ILE:HG21	1.81	0.42
1:B:202:ILE:HG23	1:B:222:LEU:HD22	2.00	0.42
1:B:131:GLU:HG3	1:B:137:ILE:HD12	2.02	0.42
1:A:202:ILE:HD13	1:A:202:ILE:HG21	1.66	0.42
1:A:109:GLN:CG	1:A:145:LYS:HG2	2.47	0.42
1:B:351:ASN:HD22	1:B:351:ASN:N	2.14	0.42
1:D:300:HIS:CG	1:D:301:PRO:HA	2.54	0.42
1:A:396[A]:ILE:HD12	1:A:403:ILE:HG21	2.01	0.42
1:D:12:PRO:HB3	1:D:248:GLY:HA2	2.01	0.42
1:A:295:ILE:HD11	1:A:311:PHE:HD2	1.85	0.42
1:D:335:HIS:CD2	1:D:335:HIS:H	2.36	0.42
1:C:128:HIS:CE1	6:C:888:HOH:O	2.72	0.42
1:B:86:ASP:HA	1:B:89:LYS:HZ1	1.85	0.42
1:C:251:VAL:HG22	1:C:282:SER:HB3	2.02	0.42
1:B:335:HIS:CD2	1:B:335:HIS:H	2.38	0.41
1:B:91:MET:HG3	1:B:91:MET:O	2.20	0.41
1:C:314:LEU:HD23	1:C:314:LEU:C	2.40	0.41
1:A:311:PHE:CD1	6:A:772:HOH:O	2.55	0.41
1:C:326:GLU:CG	1:C:329:PHE:O	2.69	0.41
1:A:49:ARG:HG2	1:A:398:ARG:HA	2.01	0.41
1:D:49:ARG:HG2	1:D:49:ARG:H	1.77	0.41
1:A:116:CYS:HB2	2:A:500:FFQ:H20	1.90	0.41
1:D:60:ARG:NH2	1:D:84:PRO:HG2	2.36	0.41
1:D:309:ALA:O	1:D:312:THR:HB	2.19	0.41
1:C:243:ALA:CB	1:C:250:ILE:HG22	2.50	0.41
1:C:345:HIS:CD2	1:C:357:ASP:O	2.70	0.41
1:B:49:ARG:HG2	1:B:398:ARG:HA	2.02	0.41
1:C:243:ALA:HB2	1:C:250:ILE:HG22	2.02	0.41
1:A:106:GLY:HA2	1:A:148:VAL:HG12	2.03	0.41
1:D:116:CYS:SG	1:D:118:ILE:HG12	2.61	0.41
1:B:296:ARG:HD2	1:D:161:LYS:HE3	2.03	0.41
1:C:2:ASP:HB3	1:C:393:ILE:HD11	2.03	0.41
1:C:347:GLU:HG3	6:C:637:HOH:O	2.20	0.41
1:A:46:PRO:HB2	1:A:48:LEU:HG	2.03	0.40
1:D:31:PHE:HE1	1:D:57:LEU:HD12	1.86	0.40
1:A:87:LEU:HA	1:A:87:LEU:HD23	1.74	0.40
1:B:17:VAL:HG23	1:B:406:LYS:HD3	2.03	0.40
1:B:300:HIS:CG	1:B:301:PRO:HA	2.56	0.40
1:D:176:LEU:HD21	1:D:222:LEU:HG	2.03	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	422/430 (98%)	415 (98%)	7 (2%)	0	100	100
1	B	422/430 (98%)	412 (98%)	9 (2%)	1 (0%)	56	44
1	C	425/430 (99%)	415 (98%)	10 (2%)	0	100	100
1	D	426/430 (99%)	417 (98%)	8 (2%)	1 (0%)	56	44
All	All	1695/1720 (98%)	1659 (98%)	34 (2%)	2 (0%)	59	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	ASN
1	D	68	ASN

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	330/336 (98%)	312 (94%)	18 (6%)	30	16
1	B	330/336 (98%)	313 (95%)	17 (5%)	32	18
1	C	333/336 (99%)	311 (93%)	22 (7%)	24	11
1	D	334/336 (99%)	314 (94%)	20 (6%)	27	13
All	All	1327/1344 (99%)	1250 (94%)	77 (6%)	28	14

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	86	ASP
1	A	139	LEU
1	A	149	ASP
1	A	153	LYS
1	A	188	ARG
1	A	202	ILE
1	A	209	MET
1	A	260	LEU
1	A	290	LEU
1	A	310	GLN
1	A	351	ASN
1	A	370	ASP
1	A	385	LYS
1	A	396[A]	ILE
1	A	396[B]	ILE
1	A	402	LYS
1	A	413	ASN
1	B	57	LEU
1	B	60	ARG
1	B	139	LEU
1	B	149	ASP
1	B	153	LYS
1	B	160	ASP
1	B	170	VAL
1	B	209	MET
1	B	217	GLU
1	B	245	VAL
1	B	250	ILE
1	B	260	LEU
1	B	289	GLU
1	B	326	GLU
1	B	347	GLU
1	B	351	ASN
1	B	396	ILE
1	C	57	LEU
1	C	59	LYS
1	C	109	GLN
1	C	139	LEU
1	C	153	LYS
1	C	188	ARG
1	C	209	MET
1	C	245	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	250	ILE
1	C	260	LEU
1	C	289	GLU
1	C	310	GLN
1	C	321	SER
1	C	347	GLU
1	C	349[A]	GLU
1	C	349[B]	GLU
1	C	351	ASN
1	C	362	SER
1	C	370	ASP
1	C	396	ILE
1	C	402	LYS
1	C	413	ASN
1	D	49	ARG
1	D	59	LYS
1	D	95	ILE
1	D	139	LEU
1	D	188	ARG
1	D	209	MET
1	D	245	VAL
1	D	250	ILE
1	D	254	ASN
1	D	260	LEU
1	D	269	GLU
1	D	290	LEU
1	D	291	LYS
1	D	310	GLN
1	D	321	SER
1	D	351	ASN
1	D	362	SER
1	D	370	ASP
1	D	396	ILE
1	D	413	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	200	ASN
1	A	254	ASN
1	A	308	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	310	GLN
1	A	335	HIS
1	A	345	HIS
1	A	351	ASN
1	A	395	HIS
1	A	413	ASN
1	B	109	GLN
1	B	132	GLN
1	B	200	ASN
1	B	254	ASN
1	B	308	GLN
1	B	335	HIS
1	B	345	HIS
1	B	351	ASN
1	B	365	GLN
1	C	72	HIS
1	C	128	HIS
1	C	200	ASN
1	C	254	ASN
1	C	275	GLN
1	C	308	GLN
1	C	310	GLN
1	C	331	ASN
1	C	335	HIS
1	C	345	HIS
1	C	351	ASN
1	C	413	ASN
1	D	72	HIS
1	D	200	ASN
1	D	254	ASN
1	D	308	GLN
1	D	310	GLN
1	D	335	HIS
1	D	345	HIS
1	D	351	ASN
1	D	395	HIS
1	D	413	ASN
1	D	418	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 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	FFQ	A	500	1	7,7,7	2.72	3 (42%)	10,10,10	1.35	1 (10%)
3	UD1	A	501	-	41,41,41	0.88	2 (4%)	58,62,62	1.09	2 (3%)
4	PO4	A	502	-	4,4,4	0.51	0	6,6,6	0.30	0
5	GOL	A	503	-	5,5,5	0.22	0	5,5,5	0.85	0
2	FFQ	B	500	1	7,7,7	2.46	3 (42%)	10,10,10	1.46	3 (30%)
3	UD1	B	501	-	41,41,41	0.95	2 (4%)	58,62,62	1.24	4 (6%)
4	PO4	B	502	-	4,4,4	0.57	0	6,6,6	0.31	0
5	GOL	B	503	-	5,5,5	0.24	0	5,5,5	0.75	0
2	FFQ	C	500	1	7,7,7	2.42	2 (28%)	10,10,10	1.80	2 (20%)
3	UD1	C	501	-	41,41,41	0.94	2 (4%)	58,62,62	1.14	4 (6%)
4	PO4	C	502	-	4,4,4	0.54	0	6,6,6	0.31	0
5	GOL	C	503	-	5,5,5	0.37	0	5,5,5	0.85	0
2	FFQ	D	500	1	7,7,7	2.35	2 (28%)	10,10,10	1.60	2 (20%)
3	UD1	D	501	-	41,41,41	1.01	2 (4%)	58,62,62	1.23	3 (5%)
4	PO4	D	502	-	4,4,4	0.56	0	6,6,6	0.32	0
5	GOL	D	503	-	5,5,5	0.29	0	5,5,5	0.73	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	FFQ	A	500	1	-	0/8/8/8	0/0/0/0
3	UD1	A	501	-	-	0/25/63/63	0/3/3/3
4	PO4	A	502	-	-	0/0/0/0	0/0/0/0
5	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	FFQ	B	500	1	-	0/8/8/8	0/0/0/0
3	UD1	B	501	-	-	0/25/63/63	0/3/3/3
4	PO4	B	502	-	-	0/0/0/0	0/0/0/0
5	GOL	B	503	-	-	0/4/4/4	0/0/0/0
2	FFQ	C	500	1	-	1/8/8/8	0/0/0/0
3	UD1	C	501	-	-	0/25/63/63	0/3/3/3
4	PO4	C	502	-	-	0/0/0/0	0/0/0/0
5	GOL	C	503	-	-	0/4/4/4	0/0/0/0
2	FFQ	D	500	1	-	0/8/8/8	0/0/0/0
3	UD1	D	501	-	-	0/25/63/63	0/3/3/3
4	PO4	D	502	-	-	0/0/0/0	0/0/0/0
5	GOL	D	503	-	-	0/4/4/4	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FFQ	P1-O2	4.30	1.62	1.54
2	C	500	FFQ	P1-O2	4.28	1.62	1.54
2	D	500	FFQ	P1-O4	4.22	1.62	1.54
2	C	500	FFQ	P1-O4	4.21	1.62	1.54
3	D	501	UD1	C2-N1	4.19	1.43	1.38
2	D	500	FFQ	P1-O2	4.15	1.62	1.54
2	B	500	FFQ	P1-O4	4.10	1.61	1.54
2	B	500	FFQ	P1-O2	3.94	1.61	1.54
3	B	501	UD1	C2-N1	3.89	1.42	1.38
2	A	500	FFQ	P1-O4	3.72	1.61	1.54
2	A	500	FFQ	C1-C2	3.46	1.54	1.52
3	C	501	UD1	C2-N1	3.24	1.41	1.38
3	A	501	UD1	C2-N1	2.80	1.41	1.38
3	C	501	UD1	PA-O3A	2.72	1.64	1.59
3	A	501	UD1	C6-C5	2.45	1.40	1.36
3	B	501	UD1	C6-C5	2.26	1.39	1.36
2	B	500	FFQ	O1-C2	2.20	1.44	1.41
3	D	501	UD1	C6-C5	2.05	1.39	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	UD1	N3-C2-N1	5.70	120.73	115.97
3	B	501	UD1	N3-C2-N1	5.34	120.43	115.97
3	A	501	UD1	N3-C2-N1	4.55	119.77	115.97
3	C	501	UD1	N3-C2-N1	4.53	119.75	115.97
3	B	501	UD1	C2-N1-C1B	3.83	120.61	118.21
3	D	501	UD1	C2-N1-C1B	3.43	120.36	118.21
2	C	500	FFQ	O3-P1-C2	-3.29	105.50	112.68
2	D	500	FFQ	O3-P1-C2	-3.29	105.52	112.68
3	C	501	UD1	PB-O3A-PA	-3.17	122.39	131.68
2	D	500	FFQ	O4-P1-C2	2.97	113.74	106.06
2	A	500	FFQ	P1-C2-C1	2.80	117.95	113.31
2	C	500	FFQ	O4-P1-C2	2.63	112.86	106.06
2	B	500	FFQ	O3-P1-C2	-2.59	107.03	112.68
3	C	501	UD1	C4B-O4B-C1B	2.48	112.44	109.75
3	A	501	UD1	C5-C4-N3	2.38	121.19	116.70
3	C	501	UD1	C4'-C3'-C2'	-2.38	107.06	110.44
3	D	501	UD1	O4B-C1B-C2B	-2.36	103.16	106.77
3	B	501	UD1	C5-C4-N3	2.22	120.89	116.70
2	B	500	FFQ	O4-P1-C2	2.10	111.50	106.06
2	B	500	FFQ	O4-P1-O3	-2.06	108.32	113.60
3	B	501	UD1	C3B-C2B-C1B	2.01	104.06	100.91

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	FFQ	O2-P1-C2-O1

There are no ring outliers.

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

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	419/430 (97%)	-0.41	1 (0%) 93 94	15, 23, 35, 59	0
1	B	419/430 (97%)	-0.38	1 (0%) 93 94	15, 25, 37, 58	0
1	C	419/430 (97%)	-0.40	0 100 100	15, 24, 35, 52	0
1	D	419/430 (97%)	-0.41	0 100 100	14, 23, 34, 47	0
All	All	1676/1720 (97%)	-0.40	2 (0%) 93 94	14, 24, 35, 59	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	SER	2.6
1	B	419	SER	2.4

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	PO4	A	502	5/5	0.12	5.65	30,33,37,37	0
2	FFQ	D	500	8/8	0.14	5.09	34,39,47,50	0
2	FFQ	A	500	8/8	0.22	4.29	40,51,53,55	0
2	FFQ	B	500	8/8	0.16	4.09	35,46,51,52	0
4	PO4	D	502	5/5	0.13	4.05	28,30,32,34	0
2	FFQ	C	500	8/8	0.14	2.93	37,47,51,52	0
4	PO4	C	502	5/5	0.12	2.43	29,29,32,32	0
5	GOL	C	503	6/6	0.10	2.25	23,24,25,25	0
5	GOL	B	503	6/6	0.10	2.02	22,24,26,28	0
5	GOL	D	503	6/6	0.09	1.78	21,22,22,22	0
5	GOL	A	503	6/6	0.11	1.69	22,23,24,25	0
4	PO4	B	502	5/5	0.10	0.99	27,31,33,35	0
3	UD1	C	501	39/39	0.07	-0.27	19,20,22,23	0
3	UD1	A	501	39/39	0.08	-0.34	15,19,21,24	0
3	UD1	D	501	39/39	0.07	-0.73	16,19,22,24	0
3	UD1	B	501	39/39	0.07	-1.00	17,19,24,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.