



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:34 AM GMT

PDB ID : 2F1K  
Title : Crystal structure of Synechocystis arogenate dehydrogenase  
Authors : Legrand, P.; Dumas, R.; Seux, M.; Rippert, P.; Ravelli, R.; Ferrer, J.-L.; Matringe, M.  
Deposited on : 2005-11-14  
Resolution : 1.55 Å(reported)

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

---

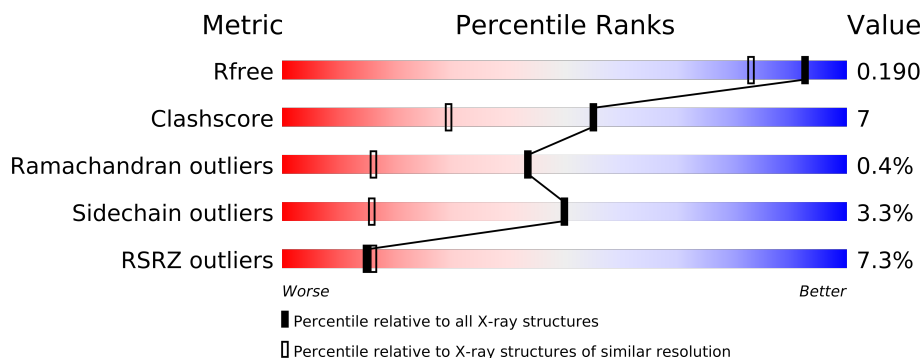
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.55 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	1117 (1.58-1.54)
Clashscore	79885	1249 (1.58-1.54)
Ramachandran outliers	78287	1212 (1.58-1.54)
Sidechain outliers	78261	1210 (1.58-1.54)
RSRZ outliers	66119	1117 (1.58-1.54)

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  $\geq 3$ , 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	279	
1	B	279	
1	C	279	
1	D	279	

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	TRS	C	1001	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9282 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.

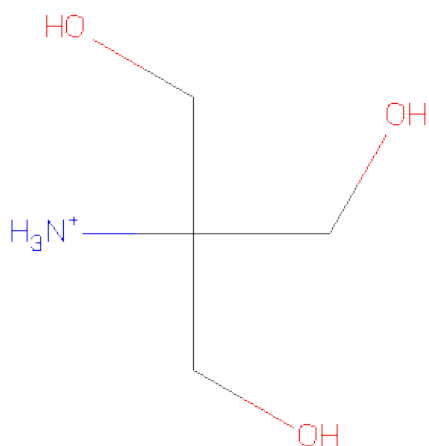
- Molecule 1 is a protein called prephenate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	4	10	0
			2181	1371	381	418	11			
1	B	279	Total	C	N	O	S	0	2	0
			2135	1344	369	410	12			
1	C	278	Total	C	N	O	S	17	4	0
			2133	1341	371	411	10			
1	D	279	Total	C	N	O	S	0	9	0
			2190	1376	381	421	12			

There are 8 discrepancies between the modelled and reference sequences:

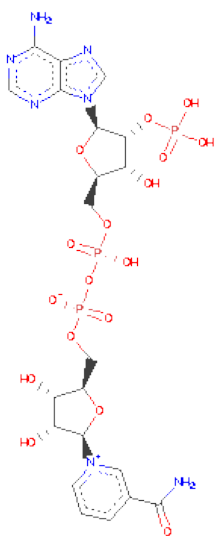
Chain	Residue	Modelled	Actual	Comment	Reference
A	114	OMT	MET	MODIFIED RESIDUE	UNP P73906
A	150	OCS	CYS	MODIFIED RESIDUE	UNP P73906
B	114	OMT	MET	MODIFIED RESIDUE	UNP P73906
B	150	OCS	CYS	MODIFIED RESIDUE	UNP P73906
C	114	OMT	MET	MODIFIED RESIDUE	UNP P73906
C	150	OCS	CYS	MODIFIED RESIDUE	UNP P73906
D	114	OMT	MET	MODIFIED RESIDUE	UNP P73906
D	150	OCS	CYS	MODIFIED RESIDUE	UNP P73906

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula:  $\text{C}_{21}\text{H}_{28}\text{N}_7\text{O}_{17}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			58	22	7	24	5		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

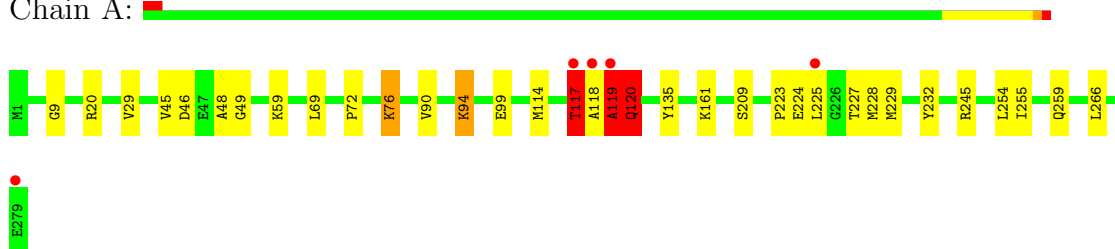
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O	0	0
			127	127		
4	B	129	Total	O	0	0
			129	129		
4	C	43	Total	O	0	0
			43	43		
4	D	125	Total	O	0	1
			126	126		

### 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.

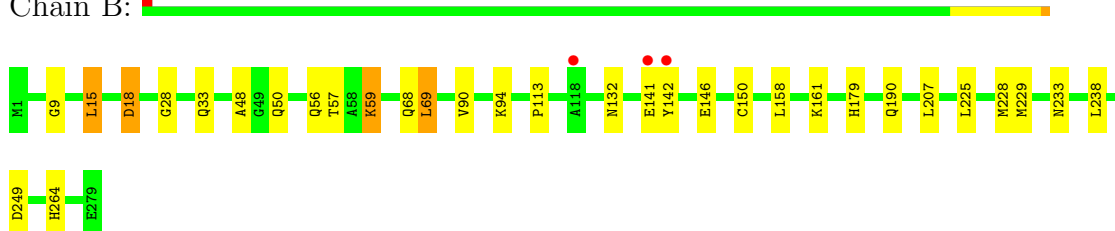
- Molecule 1: prephenate dehydrogenase

Chain A:



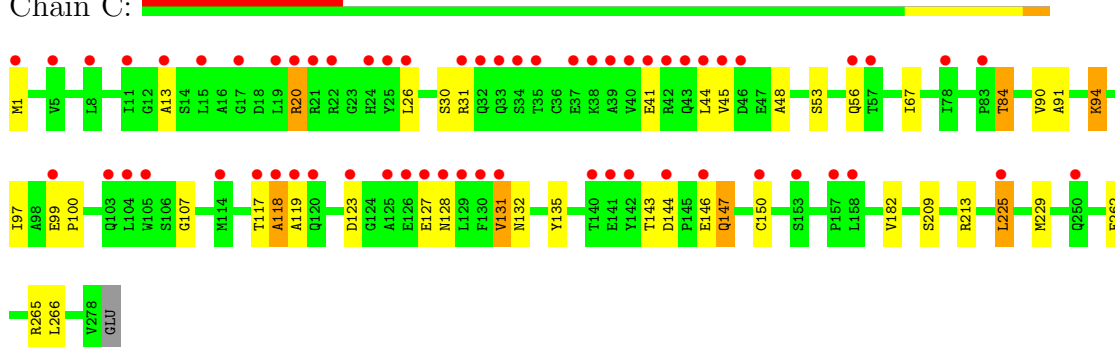
- Molecule 1: prephenate dehydrogenase

Chain B:



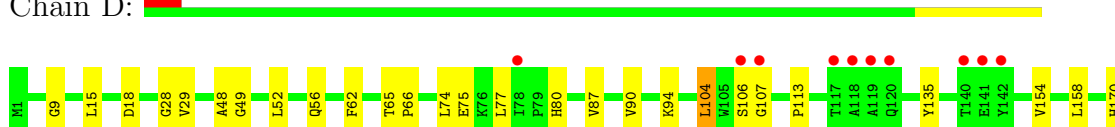
- Molecule 1: prephenate dehydrogenase

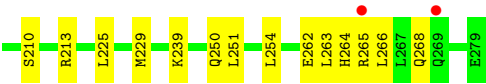
Chain C:



- Molecule 1: prephenate dehydrogenase

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.15Å 70.85Å 104.49Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	20.00 – 1.55 29.94 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-1.55) 99.0 (29.94-1.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.189 , 0.222 0.190 , 0.190	Depositor DCC
$R_{free}$ test set	6964 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.6	EDS
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 138618 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OCS, TRS, NAP, OMT

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	0.61	0/2225	0.75	1/3017 (0.0%)
1	B	0.56	0/2159	0.67	2/2931 (0.1%)
1	C	0.99	8/2161 (0.4%)	1.12	5/2936 (0.2%)
1	D	0.56	0/2218	0.71	0/3008
All	All	0.70	8/8763 (0.1%)	0.83	8/11892 (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	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147	GLN	CD-NE2	21.12	1.85	1.32
1	C	1	MET	CA-CB	18.64	1.95	1.53
1	C	147	GLN	CG-CD	13.93	1.83	1.51
1	C	84	THR	CB-OG1	11.10	1.65	1.43
1	C	123	ASP	CG-OD1	9.53	1.47	1.25
1	C	132	ASN	CG-OD1	7.20	1.39	1.24
1	C	132	ASN	CG-ND2	5.90	1.47	1.32
1	C	84	THR	CB-CG2	5.83	1.71	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	MET	N-CA-CB	-48.15	23.92	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLN	CB-CG-CD	8.71	134.25	111.60
1	C	1	MET	CB-CA-C	-8.49	93.41	110.40
1	C	147	GLN	CG-CD-NE2	-7.18	99.48	116.70
1	C	147	GLN	CG-CD-OE1	6.06	133.72	121.60
1	C	20	ARG	CB-CA-C	5.52	121.43	110.40
1	B	18	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	15	LEU	CA-CB-CG	5.31	127.51	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	THR	Peptide
1	A	119	ALA	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	2181	0	2210	31	0
1	B	2135	0	2160	38	0
1	C	2133	0	2154	33	1
1	D	2190	0	2211	30	1
2	C	8	0	12	0	0
2	D	8	0	12	0	0
3	A	58	0	10	2	0
3	B	48	0	25	4	0
3	C	48	0	25	2	0
3	D	48	0	25	3	0
4	A	127	0	0	3	0
4	B	129	0	0	3	0
4	C	43	0	0	0	0
4	D	126	0	0	3	0
All	All	9282	0	8844	119	1

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 7.

All (119) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:147:GLN:CG	1:C:147:GLN:CD	1.83	1.45
1:C:84:THR:CB	1:C:84:THR:OG1	1.65	1.39
1:C:147:GLN:CD	1:C:147:GLN:NE2	1.85	1.28
1:A:266:LEU:HD11	1:B:190:GLN:NE2	1.78	0.97
1:A:255:ILE:HG22	1:B:238:LEU:CD2	2.11	0.81
1:A:266:LEU:HD11	1:B:190:GLN:HE21	1.52	0.74
1:B:68:GLN:HG2	1:B:69:LEU:HD13	1.72	0.71
1:A:72:PRO:O	1:A:76:LYS:HD2	1.91	0.70
1:A:117:THR:C	1:A:119:ALA:H	1.95	0.70
1:B:179:HIS:HD2	1:B:233:ASN:HD22	1.38	0.70
1:A:255:ILE:HG22	1:B:238:LEU:HD21	1.74	0.69
1:A:223:PRO:O	1:A:227[A]:THR:HG23	1.94	0.67
1:D:75:GLU:HG2	1:D:104:LEU:HD21	1.77	0.66
1:D:94[A]:LYS:HG2	1:D:170:HIS:ND1	2.10	0.65
1:A:117:THR:C	1:A:119:ALA:N	2.50	0.65
1:C:67:ILE:HG23	1:C:97:ILE:HD11	1.79	0.65
1:B:179:HIS:CE1	1:B:229[A]:MET:CE	2.81	0.64
1:A:209[A]:SER:OG	4:A:1408:HOH:O	2.15	0.64
1:A:255:ILE:CG2	1:B:238:LEU:CD2	2.77	0.62
1:B:179:HIS:CE1	1:B:229[A]:MET:HE3	2.34	0.62
1:D:94[B]:LYS:HA	1:D:94[B]:LYS:HE3	1.82	0.62
1:D:107[B]:GLY:CA	4:D:4471:HOH:O	2.48	0.62
1:C:147:GLN:CB	1:C:147:GLN:CD	2.66	0.61
1:D:251:LEU:HD23	1:D:266:LEU:HD13	1.83	0.60
1:D:250:GLN:O	1:D:254:LEU:HD13	2.01	0.60
1:C:84:THR:CB	1:C:84:THR:HG1	2.09	0.60
1:C:53:SER:O	1:C:56:GLN:HG3	2.02	0.59
1:C:209[B]:SER:OG	4:D:4375[B]:HOH:O	2.16	0.59
1:A:228:MET:HB2	1:A:229[A]:MET:HE2	1.85	0.59
1:C:182:VAL:HG21	1:C:229:MET:HE1	1.86	0.58
1:D:94[A]:LYS:HG2	1:D:170:HIS:CE1	2.39	0.57
1:A:9:GLY:HA3	3:A:1350[A]:NAP:O5B	2.04	0.56
1:B:132:ASN:HA	1:B:161:LYS:HE3	1.86	0.56
1:B:179:HIS:HE1	1:B:229[A]:MET:HE2	1.71	0.55
1:D:251:LEU:CD2	1:D:266:LEU:HD13	2.37	0.54
1:C:225:LEU:O	1:C:229:MET:HG3	2.08	0.54
1:A:227[A]:THR:HG21	1:B:264:HIS:HB2	1.90	0.53
1:B:161:LYS:HD2	4:B:2413:HOH:O	2.08	0.53
1:B:229[B]:MET:SD	4:B:2388:HOH:O	2.59	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:179:HIS:CE1	1:B:229[A]:MET:HE2	2.44	0.52
1:B:68:GLN:OE1	1:B:228[B]:MET:SD	2.68	0.52
1:B:33:GLN:NE2	1:B:50:GLN:OE1	2.44	0.51
1:A:94:LYS:HE3	1:A:94:LYS:HA	1.91	0.51
1:C:146:GLU:O	1:C:150:OCS:HB3	2.11	0.51
1:C:84:THR:CA	1:C:84:THR:OG1	2.55	0.50
3:B:2350:NAP:N7N	3:B:2350:NAP:O1N	2.40	0.50
1:C:94:LYS:HA	1:C:94:LYS:HE3	1.93	0.50
1:A:117:THR:HG22	1:A:119:ALA:HA	1.94	0.49
1:C:144:ASP:HB3	1:C:147:GLN:HB2	1.95	0.49
1:A:245[B]:ARG:HD3	1:B:249:ASP:OD1	2.12	0.49
1:D:254:LEU:HD21	1:D:262:GLU:HG3	1.95	0.49
1:A:255:ILE:HG22	1:B:238:LEU:HD23	1.91	0.48
1:C:99:GLU:HB3	1:C:100:PRO:HD3	1.96	0.48
1:C:107[B]:GLY:HA2	1:C:143:THR:HA	1.95	0.48
1:B:18:ASP:HB3	1:B:158:LEU:HD22	1.97	0.47
1:D:15[A]:LEU:HD21	1:D:62:PHE:CD1	2.50	0.47
1:C:128:ASN:O	1:C:131:VAL:HG12	2.15	0.47
1:C:91:ALA:HB3	1:C:97:ILE:HD12	1.96	0.46
1:D:251:LEU:HD21	1:D:266:LEU:CD2	2.45	0.46
1:C:262:GLU:HG3	1:C:265:ARG:HH12	1.80	0.46
1:D:254:LEU:HD23	1:D:263:LEU:HA	1.98	0.46
1:B:90:VAL:O	3:B:2350:NAP:H6N	2.16	0.46
1:D:264:HIS:CE1	1:D:268:GLN:NE2	2.84	0.46
1:B:229[B]:MET:CE	4:B:2388:HOH:O	2.63	0.46
1:B:59:LYS:HA	1:B:59:LYS:CE	2.46	0.46
1:A:266:LEU:HD11	1:B:190:GLN:HE22	1.70	0.45
1:B:161:LYS:HE2	1:C:213:ARG:NH2	2.31	0.45
1:C:90:VAL:O	3:C:3350:NAP:H6N	2.16	0.45
1:A:266:LEU:HD12	4:A:1446:HOH:O	2.17	0.45
1:A:20:ARG:HE	1:A:46:ASP:CG	2.20	0.45
1:B:28:GLY:O	1:B:48:ALA:HA	2.17	0.45
1:D:74:LEU:HD13	1:D:87:VAL:HG11	1.99	0.45
1:D:29:VAL:HA	1:D:49:GLY:O	2.17	0.45
1:D:229[B]:MET:HB2	1:D:229[B]:MET:HE2	1.79	0.45
1:A:114:OMT:HE1	1:B:207:LEU:HD13	1.97	0.45
1:D:52:LEU:HD22	1:D:77:LEU:HD13	1.98	0.45
1:B:113:PRO:O	3:B:2350:NAP:H5N	2.16	0.44
1:D:210:SER:HB3	1:D:213[A]:ARG:NH2	2.32	0.44
1:B:9:GLY:HA3	3:B:2350:NAP:O5B	2.17	0.44
1:D:9:GLY:HA3	3:D:4350:NAP:O5B	2.18	0.44
1:A:45:VAL:HG21	1:A:48:ALA:HB2	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:29:VAL:HA	1:A:49:GLY:O	2.17	0.44
1:B:56:GLN:HG3	1:B:57:THR:HG23	1.99	0.44
1:D:113:PRO:O	3:D:4350:NAP:H5N	2.17	0.44
1:B:141:GLU:HG2	1:B:141:GLU:H	1.63	0.44
1:D:251:LEU:CD2	1:D:266:LEU:CD1	2.95	0.44
1:C:117:THR:C	1:C:119:ALA:H	2.20	0.44
1:A:254:LEU:HD23	1:A:259[B]:GLN:NE2	2.31	0.44
1:C:67:ILE:HG12	1:C:91:ALA:HB1	2.00	0.43
1:A:114:OMT:OD1	4:A:1473:HOH:O	2.20	0.43
1:C:147:GLN:CG	1:C:147:GLN:NE2	2.81	0.43
1:D:107[B]:GLY:HA2	4:D:4471:HOH:O	2.14	0.43
1:C:53:SER:HB2	1:C:56:GLN:HE21	1.83	0.43
1:B:179:HIS:NE2	1:B:229[A]:MET:HE3	2.33	0.43
1:A:225:LEU:O	1:A:229[A]:MET:HG2	2.19	0.43
1:D:56:GLN:HA	1:D:80:HIS:O	2.19	0.42
1:D:65:THR:HB	1:D:66:PRO:HD2	2.00	0.42
1:C:13:ALA:HB1	1:C:44:LEU:HD13	2.01	0.42
1:C:182:VAL:CG2	1:C:229:MET:HE1	2.49	0.42
1:C:31:ARG:HH21	3:C:3350:NAP:H2B	1.84	0.42
1:D:90:VAL:O	3:D:4350:NAP:H6N	2.20	0.42
1:B:150:OCS:OD3	1:C:118:ALA:HB1	2.20	0.42
1:B:225:LEU:O	1:B:229[A]:MET:HG2	2.19	0.41
1:B:179:HIS:CD2	1:B:233:ASN:HD22	2.28	0.41
1:A:255:ILE:CG2	1:B:238:LEU:HD21	2.43	0.41
1:D:251:LEU:HD21	1:D:266:LEU:CD1	2.50	0.41
1:B:161:LYS:HD3	1:C:213:ARG:HH22	1.86	0.41
1:D:18:ASP:HB3	1:D:158:LEU:HD22	2.03	0.41
1:C:182:VAL:HG21	1:C:229:MET:CE	2.50	0.41
1:D:28:GLY:O	1:D:48:ALA:HA	2.21	0.41
1:C:45:VAL:HG21	1:C:48:ALA:HB2	2.02	0.41
1:D:251:LEU:HD21	1:D:266:LEU:HD22	2.03	0.41
1:A:228:MET:HE2	1:A:232:TYR:HE2	1.86	0.41
1:B:161:LYS:HE2	1:C:213:ARG:HH21	1.84	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	Distance(Å)	Clash(Å)
1:C:41:GLU:OE2	1:D:265:ARG:NH2[2_656]	2.19	0.01

## 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	285/279 (102%)	275 (96%)	7 (2%)	3 (1%)	21	3
1	B	277/279 (99%)	273 (99%)	4 (1%)	0	100	100
1	C	278/279 (100%)	271 (98%)	6 (2%)	1 (0%)	43	16
1	D	284/279 (102%)	275 (97%)	9 (3%)	0	100	100
All	All	1124/1116 (101%)	1094 (97%)	26 (2%)	4 (0%)	43	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ALA
1	A	118	ALA
1	C	118	ALA
1	A	120	GLN

### 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	237/227 (104%)	227 (96%)	10 (4%)	40	9
1	B	229/227 (101%)	223 (97%)	6 (3%)	59	23
1	C	229/227 (101%)	220 (96%)	9 (4%)	43	11
1	D	235/227 (104%)	228 (97%)	7 (3%)	53	18
All	All	930/908 (102%)	898 (97%)	32 (3%)	50	15

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59[A]	LYS
1	A	59[B]	LYS
1	A	69	LEU
1	A	76	LYS
1	A	94	LYS
1	A	99	GLU
1	A	117	THR
1	A	120	GLN
1	A	135	TYR
1	A	224	GLU
1	B	15	LEU
1	B	59	LYS
1	B	69	LEU
1	B	94	LYS
1	B	142	TYR
1	B	146	GLU
1	C	20	ARG
1	C	26	LEU
1	C	30	SER
1	C	94	LYS
1	C	127	GLU
1	C	131	VAL
1	C	135	TYR
1	C	225	LEU
1	C	266	LEU
1	D	104	LEU
1	D	106[A]	SER
1	D	106[B]	SER
1	D	135	TYR
1	D	154	VAL
1	D	225	LEU
1	D	239	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	172	GLN
1	B	33	GLN
1	B	50	GLN
1	B	56	GLN
1	B	120	GLN
1	B	179	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	190	GLN
1	B	205	GLN
1	B	257	ASN
1	C	56	GLN
1	C	120	GLN
1	C	172	GLN
1	C	250	GLN
1	C	258	GLN
1	C	268	GLN
1	D	120	GLN
1	D	268	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

8 non-standard protein/DNA/RNA residues 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
1	OMT	A	114	1	9,9,10	7.01	3 (33%)	10,12,14	3.74	4 (40%)
1	OCS	A	150	1	8,8,9	6.47	2 (25%)	9,11,13	1.58	2 (22%)
1	OMT	B	114	1	9,9,10	6.91	3 (33%)	10,12,14	16.69	6 (60%)
1	OCS	B	150	1	8,8,9	6.85	2 (25%)	9,11,13	1.41	1 (11%)
1	OMT	C	114	1	9,9,10	6.54	3 (33%)	10,12,14	18.24	7 (70%)
1	OCS	C	150	1	8,8,9	9.61	6 (75%)	9,11,13	2.45	4 (44%)
1	OMT	D	114	1	9,9,10	7.10	3 (33%)	10,12,14	17.47	6 (60%)
1	OCS	D	150	1	8,8,9	6.32	2 (25%)	9,11,13	1.49	1 (11%)

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
1	OMT	A	114	1	-	0/6/8/10	0/0/0/0
1	OCS	A	150	1	-	0/5/7/9	0/0/0/0
1	OMT	B	114	1	-	0/6/8/10	0/0/0/0
1	OCS	B	150	1	-	0/5/7/9	0/0/0/0
1	OMT	C	114	1	-	0/6/8/10	0/0/0/0
1	OCS	C	150	1	-	0/5/7/9	0/0/0/0
1	OMT	D	114	1	-	0/6/8/10	0/0/0/0
1	OCS	D	150	1	-	0/5/7/9	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	OCS	O-C	19.49	1.24	1.11
1	B	150	OCS	O-C	18.98	1.24	1.11
1	D	114	OMT	O-C	18.82	1.24	1.11
1	A	114	OMT	O-C	18.54	1.24	1.11
1	B	114	OMT	O-C	18.24	1.24	1.11
1	A	150	OCS	O-C	17.79	1.23	1.11
1	C	114	OMT	O-C	17.35	1.23	1.11
1	D	150	OCS	O-C	17.34	1.23	1.11
1	C	150	OCS	CB-SG	11.18	1.90	1.77
1	C	150	OCS	OD2-SG	11.12	1.73	1.46
1	C	150	OCS	OD3-SG	9.10	1.75	1.45
1	B	114	OMT	CG-SD	-7.85	1.68	1.78
1	D	114	OMT	CG-SD	-7.54	1.68	1.78
1	A	114	OMT	CE-SD	-7.09	1.65	1.75
1	C	114	OMT	CG-SD	-7.01	1.69	1.78
1	A	114	OMT	CG-SD	-6.66	1.69	1.78
1	D	114	OMT	CE-SD	-6.13	1.67	1.75
1	B	114	OMT	CE-SD	-5.48	1.68	1.75
1	C	114	OMT	CE-SD	-5.22	1.68	1.75
1	C	150	OCS	OD1-SG	4.20	1.59	1.45
1	D	150	OCS	CA-C	3.63	1.55	1.48
1	B	150	OCS	CA-C	3.28	1.54	1.48
1	A	150	OCS	CA-C	3.25	1.54	1.48
1	C	150	OCS	CA-C	3.06	1.54	1.48

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	OMT	OD2-SD-CG	-37.35	83.95	108.27
1	C	114	OMT	OD2-SD-CE	-36.56	82.95	108.80
1	D	114	OMT	OD2-SD-CG	-30.00	88.74	108.27
1	D	114	OMT	OD2-SD-CE	-29.41	88.00	108.80
1	B	114	OMT	OD1-SD-CE	28.70	129.09	108.80
1	B	114	OMT	OD1-SD-CG	28.28	126.69	108.27
1	D	114	OMT	OD1-SD-CG	26.36	125.44	108.27
1	B	114	OMT	OD2-SD-CG	-22.13	93.86	108.27
1	B	114	OMT	OD2-SD-CE	-21.95	93.28	108.80
1	D	114	OMT	OD1-SD-CE	20.18	123.07	108.80
1	C	114	OMT	OD1-SD-CG	14.94	118.00	108.27
1	C	114	OMT	OD2-SD-OD1	-13.33	81.95	116.95
1	C	114	OMT	OD1-SD-CE	13.30	118.20	108.80
1	D	114	OMT	OD2-SD-OD1	-12.83	83.28	116.95
1	B	114	OMT	OD2-SD-OD1	-12.37	84.48	116.95
1	A	114	OMT	C-CA-N	-9.55	104.29	113.83
1	B	114	OMT	C-CA-N	-5.90	107.93	113.83
1	A	114	OMT	OD1-SD-CG	5.46	111.83	108.27
1	C	150	OCS	OD2-SG-CB	-3.89	100.62	105.64
1	D	114	OMT	C-CA-N	-3.85	109.98	113.83
1	A	150	OCS	C-CA-N	-3.79	110.05	113.83
1	C	150	OCS	OD1-SG-CB	3.70	113.51	107.03
1	C	150	OCS	C-CA-N	-3.70	110.14	113.83
1	D	150	OCS	C-CA-N	-3.68	110.16	113.83
1	C	114	OMT	CE-SD-CG	3.21	119.35	105.64
1	A	114	OMT	OD2-SD-OD1	-3.10	108.82	116.95
1	B	150	OCS	C-CA-N	-2.84	111.00	113.83
1	C	150	OCS	OD3-SG-CB	-2.83	102.07	107.03
1	A	114	OMT	OD2-SD-CE	2.28	110.41	108.80
1	C	114	OMT	C-CA-N	-2.24	111.59	113.83
1	A	150	OCS	OD2-SG-CB	2.08	108.32	105.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 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$
3	NAP	A	1350[A]	-	8,9,52	2.40	2 (25%)	13,14,80	1.62	4 (30%)
3	NAP	A	1350[B]	-	8,9,52	2.46	1 (12%)	13,14,80	1.49	2 (15%)
3	NAP	B	2350	-	52,52,52	1.37	4 (7%)	80,80,80	1.85	7 (8%)
2	TRS	C	1001	-	7,7,7	1.00	1 (14%)	9,9,9	0.91	0
3	NAP	C	3350	-	52,52,52	1.37	3 (5%)	80,80,80	1.69	7 (8%)
2	TRS	D	1002	-	7,7,7	1.14	1 (14%)	9,9,9	0.77	0
3	NAP	D	4350	-	52,52,52	1.44	4 (7%)	80,80,80	1.99	12 (15%)

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	NAP	A	1350[A]	-	-	0/9/9/67	0/0/0/5
3	NAP	A	1350[B]	-	-	0/9/9/67	0/0/0/5
3	NAP	B	2350	-	-	0/35/67/67	0/3/5/5
2	TRS	C	1001	-	-	0/9/9/9	0/0/0/0
3	NAP	C	3350	-	-	0/35/67/67	0/3/5/5
2	TRS	D	1002	-	-	0/9/9/9	0/0/0/0
3	NAP	D	4350	-	-	0/35/67/67	0/3/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2350	NAP	O7N-C7N	7.44	1.41	1.24
3	D	4350	NAP	O7N-C7N	7.40	1.41	1.24
3	C	3350	NAP	O7N-C7N	7.16	1.40	1.24
3	A	1350[B]	NAP	PN-O5D	6.15	1.62	1.51
3	A	1350[A]	NAP	PN-O5D	4.79	1.60	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1350[A]	NAP	PN-O2N	-4.05	1.45	1.51
3	C	3350	NAP	C2A-N3A	3.55	1.39	1.32
3	D	4350	NAP	C2A-N3A	3.38	1.38	1.32
3	B	2350	NAP	C2A-N3A	3.05	1.38	1.32
2	D	1002	TRS	C-N	-2.97	1.46	1.50
3	D	4350	NAP	C2N-N1N	2.96	1.39	1.35
3	D	4350	NAP	C2A-N1A	2.81	1.39	1.33
3	C	3350	NAP	C2A-N1A	2.58	1.39	1.33
2	C	1001	TRS	C-N	-2.56	1.47	1.50
3	B	2350	NAP	C2N-N1N	2.35	1.38	1.35
3	B	2350	NAP	C2A-N1A	2.23	1.38	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2350	NAP	N3A-C2A-N1A	-12.82	117.99	128.71
3	D	4350	NAP	N3A-C2A-N1A	-11.28	119.28	128.71
3	C	3350	NAP	N3A-C2A-N1A	-10.96	119.55	128.71
3	D	4350	NAP	C8A-N9A-C4A	5.74	111.28	106.90
3	C	3350	NAP	O4D-C1D-N1N	5.12	113.19	107.95
3	D	4350	NAP	C4B-O4B-C1B	-4.99	104.33	109.75
3	D	4350	NAP	O4B-C1B-N9A	-4.37	104.38	108.44
3	C	3350	NAP	N3A-C4A-N9A	4.04	132.73	125.43
3	D	4350	NAP	N3A-C4A-N9A	3.82	132.33	125.43
3	B	2350	NAP	N3A-C4A-N9A	3.33	131.45	125.43
3	A	1350[B]	NAP	O5D-PN-O2N	-3.20	105.94	112.88
3	A	1350[A]	NAP	PN-O3-PA	-3.09	122.18	133.31
3	D	4350	NAP	O4D-C1D-N1N	3.02	111.04	107.95
3	D	4350	NAP	N7A-C8A-N9A	-2.81	106.41	114.36
3	B	2350	NAP	C1B-N9A-C4A	-2.79	121.81	126.64
3	D	4350	NAP	C1B-N9A-C4A	-2.79	121.82	126.64
3	A	1350[B]	NAP	O2N-PN-O1N	2.70	118.94	112.73
3	B	2350	NAP	C8A-N9A-C4A	2.64	108.92	106.90
3	D	4350	NAP	O4B-C1B-C2B	2.58	109.36	106.95
3	A	1350[A]	NAP	O5D-PN-O1N	-2.50	106.98	112.73
3	C	3350	NAP	C5A-C4A-N3A	-2.41	120.45	125.70
3	C	3350	NAP	C2A-N3A-C4A	2.40	120.84	114.01
3	B	2350	NAP	N7A-C8A-N9A	-2.39	107.59	114.36
3	D	4350	NAP	O5B-C5B-C4B	-2.34	100.34	108.94
3	C	3350	NAP	N7A-C8A-N9A	-2.30	107.87	114.36
3	A	1350[A]	NAP	O2N-PN-O1N	2.25	117.91	112.73
3	B	2350	NAP	C2A-N3A-C4A	2.25	120.41	114.01

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2350	NAP	C4B-O4B-C1B	-2.16	107.40	109.75
3	C	3350	NAP	C3N-C7N-N7N	2.16	120.22	117.77
3	A	1350[A]	NAP	O2N-PN-O3	2.14	112.83	105.27
3	D	4350	NAP	PN-O5D-C5D	2.10	127.49	120.24
3	D	4350	NAP	C5A-C4A-N9A	-2.07	104.18	107.16

There are no chirality outliers.

There are no torsion outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	279/279 (100%)	-0.00	5 (1%) 65 71	11, 16, 24, 39	3 (1%)
1	B	279/279 (100%)	0.01	3 (1%) 77 82	11, 16, 24, 33	1 (0%)
1	C	278/279 (99%)	1.15	61 (21%) 1 1	10, 16, 24, 29	4 (1%)
1	D	279/279 (100%)	0.20	12 (4%) 34 35	11, 16, 24, 35	0
All	All	1115/1116 (99%)	0.34	81 (7%) 15 16	10, 16, 24, 39	8 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	118	ALA	24.7
1	C	119	ALA	12.2
1	B	142	TYR	9.6
1	D	118	ALA	8.3
1	A	117	THR	7.2
1	C	41	GLU	6.5
1	C	117	THR	6.4
1	C	40	VAL	6.0
1	C	104	LEU	5.7
1	D	142	TYR	5.7
1	C	44	LEU	5.5
1	C	25	TYR	5.2
1	D	119	ALA	5.1
1	C	142	TYR	5.1
1	A	118	ALA	5.0
1	C	120	GLN	4.6
1	C	21	ARG	4.5
1	C	26	LEU	4.4
1	D	265	ARG	4.0
1	C	158	LEU	4.0
1	C	141	GLU	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	57	THR	3.8
1	A	119	ALA	3.8
1	C	153	SER	3.6
1	C	78	ILE	3.5
1	C	225	LEU	3.5
1	C	130	PHE	3.5
1	D	117	THR	3.4
1	C	43	GLN	3.4
1	C	17	GLY	3.4
1	C	144	ASP	3.3
1	C	20	ARG	3.2
1	C	140	THR	3.2
1	C	39	ALA	3.0
1	C	150	OCS	3.0
1	C	127	GLU	2.9
1	C	56	GLN	2.8
1	C	22	ARG	2.8
1	C	1	MET	2.8
1	C	131	VAL	2.8
1	C	128	ASN	2.8
1	C	103	GLN	2.7
1	C	83	PRO	2.7
1	C	34	SER	2.7
1	C	13	ALA	2.7
1	C	45	VAL	2.7
1	C	46	ASP	2.7
1	B	118	ALA	2.6
1	C	250	GLN	2.6
1	C	105	TRP	2.6
1	C	123	ASP	2.5
1	C	19	LEU	2.5
1	D	269	GLN	2.5
1	C	146	GLU	2.5
1	C	38	LYS	2.5
1	C	125	ALA	2.4
1	C	8	LEU	2.4
1	C	126	GLU	2.4
1	A	225	LEU	2.4
1	C	11	ILE	2.4
1	C	37	GLU	2.4
1	D	106[A]	SER	2.3
1	C	129	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	279	GLU	2.3
1	B	141	GLU	2.3
1	C	24	HIS	2.3
1	D	141	GLU	2.3
1	C	32	GLN	2.3
1	C	42	ARG	2.2
1	C	15	LEU	2.2
1	D	107[A]	GLY	2.2
1	C	5	VAL	2.1
1	C	157	PRO	2.1
1	C	99	GLU	2.1
1	D	120	GLN	2.1
1	C	35	THR	2.1
1	C	31	ARG	2.1
1	D	140	THR	2.0
1	C	33	GLN	2.0
1	C	114	OMT	2.0
1	D	78	ILE	2.0

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

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
1	OMT	A	114	10/11	0.16	2.42	20,25,36,37	2
1	OMT	C	114	10/11	0.16	1.37	18,21,29,30	2
1	OMT	B	114	10/11	0.12	1.36	14,16,20,21	2
1	OCS	C	150	9/10	0.17	0.08	21,22,24,25	0
1	OCS	B	150	9/10	0.08	-0.43	19,20,23,26	0
1	OCS	A	150	9/10	0.07	-0.52	15,16,24,25	0
1	OCS	D	150	9/10	0.06	-0.70	17,17,21,24	0
1	OMT	D	114	10/11	0.07	-0.96	14,15,24,24	2

## 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	TRS	C	1001	8/8	0.17	2.27	25,26,26,27	0
2	TRS	D	1002	8/8	0.12	1.47	25,25,26,26	0
3	NAP	C	3350	48/48	0.28	1.11	21,26,35,36	0
3	NAP	A	1350[B]	10/48	0.12	0.81	16,17,18,18	10
3	NAP	B	2350	48/48	0.11	0.28	16,19,27,30	0
3	NAP	A	1350[A]	10/48	0.12	0.08	14,20,23,23	10
3	NAP	D	4350	48/48	0.10	0.05	15,22,26,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.