



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2021 – 02:09 PM EDT

PDB ID : 7L6G  
Title : MbnP from *Methylosinus trichosporium*  
Authors : Manesis, A.C.; Rosenzweig, A.C.  
Deposited on : 2020-12-23  
Resolution : 2.04 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.18

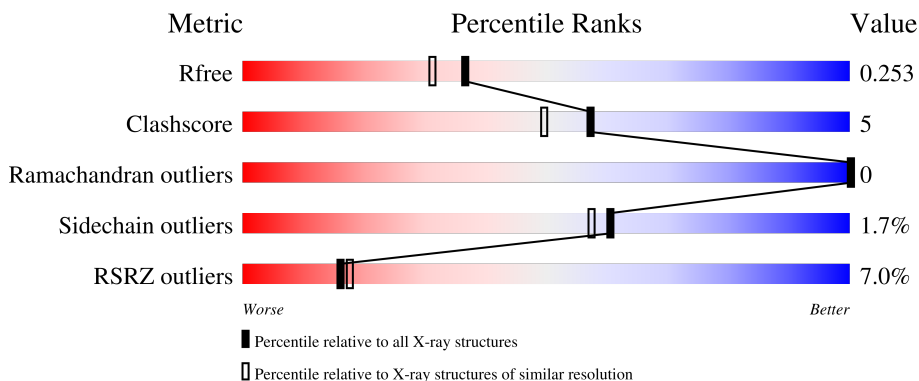
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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.



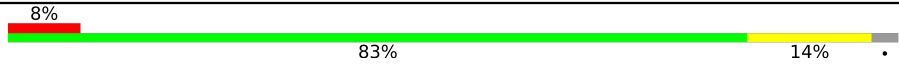
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 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	299	 3% 92% 5% •
1	B	299	 5% 84% 12% ••
1	C	299	 7% 82% 13% ••
1	D	299	 8% 86% 9% ••
1	E	299	 8% 90% 8% ••

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	299	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	409	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13544 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 Metallo-mystery pair system four-Cys motif protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	Total 2133	C 1344	N 376	O 404	S 9	0	0	0
1	B	289	Total 2109	C 1330	N 371	O 399	S 9	0	0	0
1	C	288	Total 2102	C 1325	N 370	O 398	S 9	0	0	0
1	D	287	Total 2097	C 1322	N 369	O 397	S 9	0	0	0
1	E	295	Total 2146	C 1352	N 379	O 406	S 9	0	0	0
1	F	291	Total 2124	C 1339	N 374	O 402	S 9	0	0	0

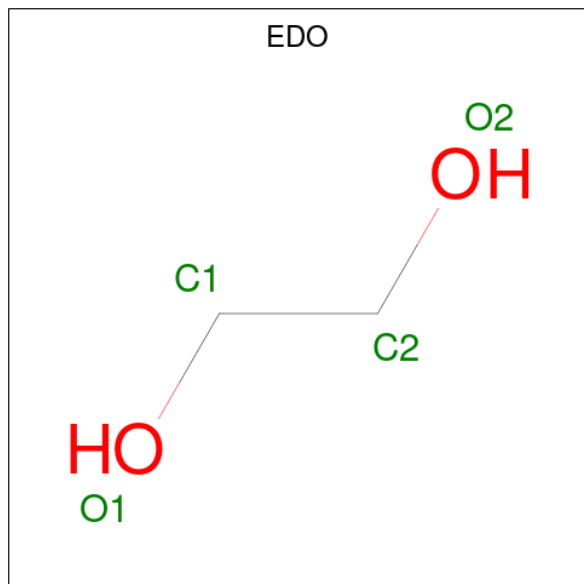
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cu 1	0	0
2	B	1	Total 1	Cu 1	0	0
2	C	1	Total 1	Cu 1	0	0
2	D	1	Total 1	Cu 1	0	0
2	E	1	Total 1	Cu 1	0	0
2	F	1	Total 1	Cu 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: 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
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

*Continued on next page...*

*Continued from previous page...*

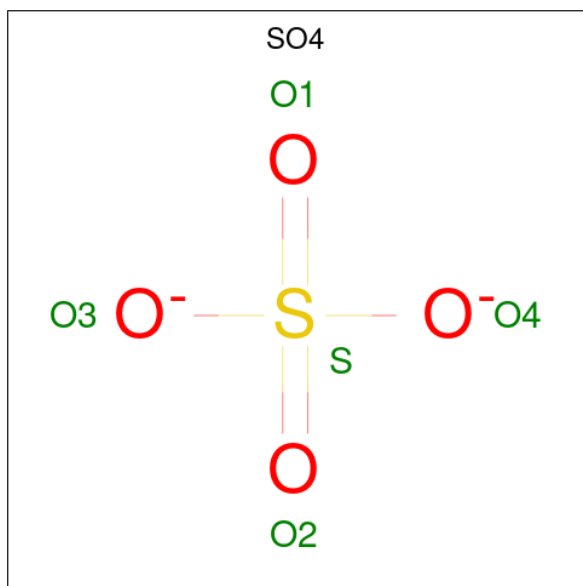
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

Continued on next page...

*Continued from previous page...*

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	125	Total O 125 125	0	0
6	B	107	Total O 107 107	0	0

*Continued on next page...*



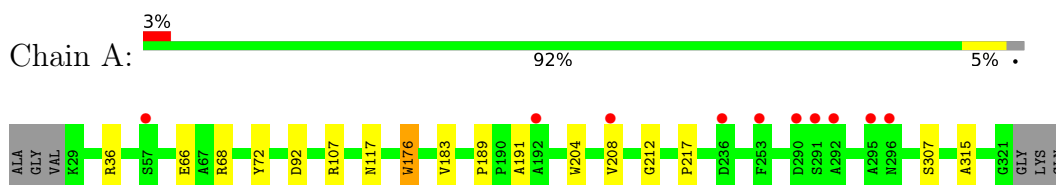
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	C	104	Total 104	O 104	0	0
6	D	83	Total 83	O 83	0	0
6	E	88	Total 88	O 88	0	0
6	F	75	Total 75	O 75	0	0

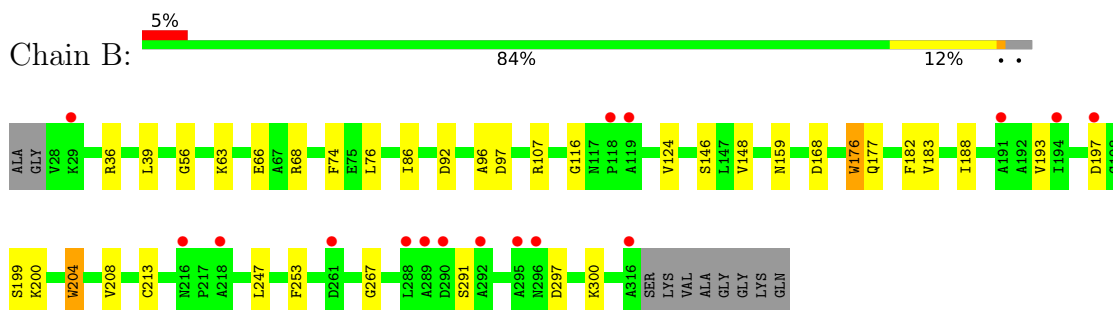
### 3 Residue-property plots [i](#)

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.

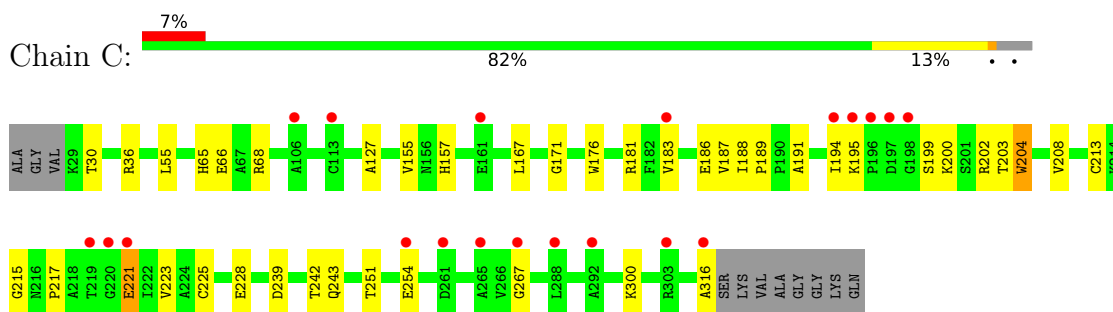
- Molecule 1: Metallo-mystery pair system four-Cys motif protein



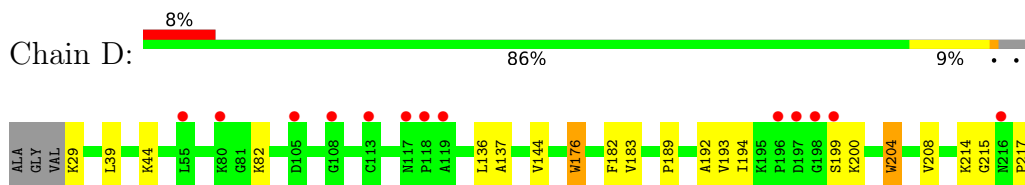
- Molecule 1: Metallo-mystery pair system four-Cys motif protein

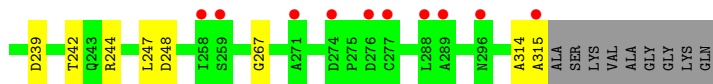


- Molecule 1: Metallo-mystery pair system four-Cys motif protein

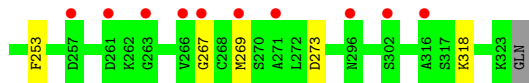
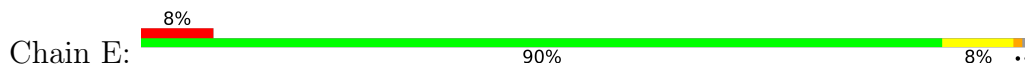


- Molecule 1: Metallo-mystery pair system four-Cys motif protein

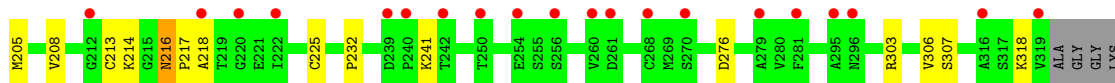
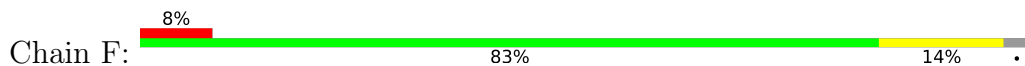




• Molecule 1: Metallo-mystery pair system four-Cys motif protein



• Molecule 1: Metallo-mystery pair system four-Cys motif protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.28Å 91.28Å 383.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	21.89 – 2.04 79.05 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.0 (21.89-2.04) 85.9 (79.05-1.94)	Depositor EDS
$R_{merge}$	0.35	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 1.94Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.204 , 0.251 0.206 , 0.253	Depositor DCC
$R_{free}$ test set	5541 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.4	Xtrriage
Anisotropy	0.230	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.058 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7483e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, KYN, CA, SO4, CU

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	0.27	0/2167	0.49	0/2953
1	B	0.27	0/2143	0.49	0/2922
1	C	0.29	0/2136	0.49	0/2912
1	D	0.28	0/2131	0.49	0/2905
1	E	0.27	0/2180	0.48	0/2969
1	F	0.27	0/2158	0.48	0/2941
All	All	0.28	0/12915	0.49	0/17602

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2133	0	2100	15	0
1	B	2109	0	2074	22	0
1	C	2102	0	2065	28	0
1	D	2097	0	2060	18	0
1	E	2146	0	2116	20	0
1	F	2124	0	2092	30	0
2	A	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	20	0	30	3	0
4	B	12	0	18	2	0
4	C	12	0	18	2	0
4	D	24	0	36	4	0
4	E	48	0	72	2	0
4	F	28	0	42	2	0
5	A	30	0	0	1	0
5	B	10	0	0	0	0
5	C	15	0	0	0	0
5	D	15	0	0	0	0
5	E	15	0	0	0	0
5	F	10	0	0	0	0
6	A	125	0	0	2	0
6	B	107	0	0	0	0
6	C	104	0	0	0	0
6	D	83	0	0	1	0
6	E	88	0	0	1	0
6	F	75	0	0	2	0
All	All	13544	0	12723	125	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 5.

All (125) 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:C:215:GLY:CA	1:C:221:GLU:OE2	2.29	0.80
1:D:225:CYS:H	4:D:407:EDO:H22	1.46	0.79
1:C:228:GLU:H	1:C:300:LYS:HZ1	1.33	0.77
1:C:215:GLY:HA2	1:C:221:GLU:OE2	1.87	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:LYS:HD3	1:D:215:GLY:H	1.58	0.68
1:B:183:VAL:HB	1:B:208:VAL:HB	1.76	0.67
1:D:194:ILE:HD12	1:D:199:SER:O	1.93	0.67
1:C:155:VAL:HG13	1:C:167:LEU:HD21	1.76	0.66
1:D:248:ASP:HB2	4:D:406:EDO:H11	1.77	0.65
1:B:297:ASP:HA	1:B:300:LYS:HE2	1.79	0.65
1:A:176:TRP:H	1:A:176:TRP:HD1	1.45	0.64
1:D:214:LYS:HD3	1:D:215:GLY:N	2.13	0.63
1:A:117:ASN:ND2	1:E:92:ASP:OD2	2.26	0.62
1:D:183:VAL:HB	1:D:208:VAL:HB	1.80	0.62
1:F:303:ARG:HD3	1:F:306:VAL:HG11	1.80	0.62
1:F:183:VAL:HB	1:F:208:VAL:HB	1.82	0.60
1:B:168:ASP:OD1	1:F:107:ARG:NH2	2.35	0.60
1:E:186:GLU:HG2	1:E:205:MET:HG2	1.82	0.60
1:D:82:LYS:NZ	6:D:502:HOH:O	2.34	0.59
1:F:116:GLY:H	4:F:406:EDO:H12	1.67	0.59
1:B:107:ARG:HD3	1:F:92:ASP:HB3	1.83	0.59
1:C:183:VAL:HB	1:C:208:VAL:HB	1.84	0.58
1:F:216:ASN:ND2	1:F:218:ALA:H	2.01	0.57
1:C:228:GLU:H	1:C:300:LYS:NZ	2.00	0.57
1:C:228:GLU:HG3	1:C:300:LYS:HZ1	1.69	0.57
1:B:63:LYS:NZ	1:F:170:SER:OG	2.37	0.57
1:A:66:GLU:OE1	1:A:68:ARG:NH2	2.39	0.56
1:E:183:VAL:HB	1:E:208:VAL:HB	1.87	0.56
1:F:303:ARG:O	1:F:306:VAL:HG12	2.05	0.56
1:A:183:VAL:HB	1:A:208:VAL:HB	1.88	0.55
1:C:242:THR:HG23	1:C:243:GLN:HG3	1.88	0.55
1:E:207:HIS:HB2	1:E:269:MET:HG2	1.89	0.55
1:F:241:LYS:HG2	1:F:318:LYS:HB2	1.87	0.55
1:E:36:ARG:HD3	4:E:409:EDO:H11	1.89	0.55
1:F:192:ALA:HB3	1:F:200:LYS:HD3	1.89	0.55
1:A:176:TRP:N	1:A:176:TRP:CD1	2.75	0.54
1:B:56:GLY:HA2	1:B:253:PHE:O	2.07	0.54
1:A:68:ARG:HH12	4:A:407:EDO:H12	1.71	0.53
1:F:74:PHE:HB3	1:F:86:ILE:HD12	1.90	0.53
1:D:314:ALA:HB1	1:F:214:LYS:HG2	1.90	0.53
1:C:36:ARG:HD2	4:C:404:EDO:H22	1.91	0.53
1:C:215:GLY:HA3	1:C:221:GLU:OE2	2.08	0.53
1:E:160:VAL:HG21	1:E:170:SER:HA	1.91	0.52
1:C:171:GLY:O	1:C:181:ARG:NH1	2.43	0.52
1:A:176:TRP:HB2	1:A:217:PRO:HG2	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:HE	1:A:315:ALA:HB1	1.76	0.50
1:A:212:GLY:N	5:A:411:SO4:O4	2.30	0.50
1:B:36:ARG:HH12	4:B:403:EDO:H22	1.75	0.50
1:E:318:LYS:HZ1	4:E:409:EDO:H21	1.77	0.50
1:D:39:LEU:HD12	1:D:247:LEU:HB3	1.94	0.50
1:C:66:GLU:OE2	1:C:68:ARG:NE	2.45	0.50
1:C:251:THR:O	1:C:254:GLU:HG2	2.11	0.50
1:B:197:ASP:HB2	1:B:199:SER:H	1.77	0.50
1:F:303:ARG:HB3	1:F:306:VAL:CG1	2.42	0.49
1:C:316:ALA:N	4:C:404:EDO:O1	2.40	0.49
1:E:204:TRP:CE2	1:E:267:GLY:HA2	2.47	0.49
1:C:157:HIS:CE1	1:C:223:VAL:HG11	2.47	0.49
1:B:193:VAL:O	1:B:200:LYS:HA	2.13	0.48
1:C:30:THR:HB	1:C:127:ALA:HB1	1.96	0.48
1:C:195:LYS:HD2	1:C:199:SER:HB2	1.94	0.48
1:E:56:GLY:HA2	1:E:253:PHE:O	2.14	0.48
1:F:68:ARG:NH1	6:F:504:HOH:O	2.38	0.47
1:B:96:ALA:HB2	1:B:148:VAL:HG13	1.96	0.47
1:E:195:LYS:HB3	1:E:196:PRO:HD2	1.96	0.47
1:F:186:GLU:HG2	1:F:205:MET:HG2	1.95	0.47
1:B:66:GLU:OE2	1:B:68:ARG:NH2	2.46	0.47
1:D:189:PRO:HG3	1:D:193:VAL:HG22	1.97	0.47
1:C:217:PRO:HG3	1:C:223:VAL:CG2	2.45	0.47
1:A:72:TYR:OH	4:A:405:EDO:H22	2.15	0.47
1:D:192:ALA:HB3	1:D:200:LYS:HE2	1.97	0.47
1:B:76:LEU:HG	1:B:86:ILE:HD11	1.97	0.46
1:F:74:PHE:CZ	1:F:124:VAL:HG21	2.50	0.46
1:C:194:ILE:HD13	1:C:200:LYS:HG2	1.97	0.46
1:D:176:TRP:HB3	1:D:217:PRO:HG2	1.96	0.46
1:B:97:ASP:OD1	1:B:146:SER:OG	2.30	0.46
1:F:64:LEU:HD11	1:F:67:ALA:HB2	1.97	0.46
1:E:176:TRP:CB	1:E:217:PRO:HG2	2.45	0.46
1:B:92:ASP:HB3	1:F:107:ARG:HD2	1.97	0.46
1:C:186:GLU:HB3	1:C:203:THR:HG21	1.97	0.46
1:C:194:ILE:HD11	1:C:200:LYS:HE3	1.98	0.46
1:F:216:ASN:HD22	1:F:217:PRO:HD2	1.80	0.45
1:D:44:LYS:HA	4:D:404:EDO:H11	1.97	0.45
1:F:303:ARG:HB3	1:F:306:VAL:HG12	1.99	0.45
1:C:189:PRO:HG2	1:C:191:ALA:O	2.17	0.44
1:C:213:CYS:HA	1:C:225:CYS:HA	1.99	0.44
1:C:217:PRO:HG3	1:C:223:VAL:HG21	1.98	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:TRP:CE2	1:D:267:GLY:HA2	2.52	0.44
1:E:273:ASP:OD1	1:E:273:ASP:N	2.45	0.44
1:B:39:LEU:HD12	1:B:247:LEU:HB3	1.99	0.44
1:F:174:KYN:HBA	4:F:408:EDO:H12	2.00	0.44
1:B:74:PHE:CZ	1:B:124:VAL:HG21	2.53	0.44
1:A:189:PRO:HG2	1:A:191:ALA:O	2.18	0.43
1:B:159:ASN:HB2	1:B:176:TRP:CH2	2.53	0.43
1:E:74:PHE:CZ	1:E:124:VAL:HG21	2.54	0.43
1:B:63:LYS:HB2	1:B:188:ILE:HB	1.99	0.43
1:F:29:LYS:HE3	1:F:29:LYS:HB3	1.72	0.43
6:A:518:HOH:O	1:E:107:ARG:HD2	2.18	0.43
1:F:146:SER:OG	1:F:147:LEU:N	2.52	0.43
1:D:244:ARG:HB3	1:D:315:ALA:HB2	2.01	0.43
1:C:239:ASP:HB3	1:C:242:THR:HG22	2.00	0.43
1:B:204:TRP:CE2	1:B:267:GLY:HA2	2.54	0.43
1:B:116:GLY:H	4:B:405:EDO:H12	1.83	0.42
1:C:204:TRP:CE2	1:C:267:GLY:HA2	2.54	0.42
1:E:176:TRP:H	1:E:176:TRP:HD1	1.68	0.42
1:E:176:TRP:HB3	1:E:217:PRO:HG2	2.00	0.42
1:F:139:SER:HA	1:F:232:PRO:HA	2.02	0.42
1:B:197:ASP:HB2	1:B:199:SER:OG	2.19	0.42
1:E:74:PHE:HB3	1:E:86:ILE:HD12	2.02	0.42
1:E:216:ASN:O	1:E:221:GLU:HG2	2.19	0.42
1:E:115:PRO:HG2	1:F:196:PRO:HB3	2.01	0.42
1:A:107:ARG:HD3	1:E:92:ASP:HB3	2.00	0.42
1:F:213:CYS:HA	1:F:225:CYS:HA	2.00	0.41
1:F:52:LEU:HD11	1:F:64:LEU:HB2	2.01	0.41
1:A:36:ARG:NH1	6:A:516:HOH:O	2.53	0.41
1:B:177:GLN:NE2	1:B:213:CYS:O	2.51	0.41
1:D:144:VAL:HG21	4:D:407:EDO:H11	2.03	0.41
1:F:276:ASP:O	6:F:501:HOH:O	2.22	0.41
1:D:136:LEU:HG	1:D:137:ALA:N	2.36	0.41
1:D:239:ASP:HB3	1:D:242:THR:HB	2.03	0.41
1:C:65:HIS:HB2	1:C:188:ILE:HD11	2.03	0.41
1:F:54:ASN:HB3	1:F:59:ARG:HB3	2.03	0.41
1:F:171:GLY:O	1:F:181:ARG:NH1	2.54	0.40
1:A:92:ASP:OD1	4:A:404:EDO:O1	2.33	0.40
1:A:107:ARG:HD2	6:E:528:HOH:O	2.22	0.40
1:C:55:LEU:HD21	1:C:187:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	290/299 (97%)	280 (97%)	10 (3%)	0	100	100
1	B	286/299 (96%)	275 (96%)	11 (4%)	0	100	100
1	C	285/299 (95%)	276 (97%)	9 (3%)	0	100	100
1	D	284/299 (95%)	271 (95%)	13 (5%)	0	100	100
1	E	292/299 (98%)	282 (97%)	10 (3%)	0	100	100
1	F	288/299 (96%)	274 (95%)	14 (5%)	0	100	100
All	All	1725/1794 (96%)	1658 (96%)	67 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	219/222 (99%)	216 (99%)	3 (1%)	67	65
1	B	217/222 (98%)	213 (98%)	4 (2%)	59	55
1	C	216/222 (97%)	212 (98%)	4 (2%)	57	53
1	D	216/222 (97%)	212 (98%)	4 (2%)	57	53
1	E	220/222 (99%)	218 (99%)	2 (1%)	78	79
1	F	219/222 (99%)	214 (98%)	5 (2%)	50	44
All	All	1307/1332 (98%)	1285 (98%)	22 (2%)	60	57

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	TRP
1	A	204	TRP
1	A	307	SER
1	B	176	TRP
1	B	182	PHE
1	B	204	TRP
1	B	291	SER
1	C	176	TRP
1	C	202	ARG
1	C	204	TRP
1	C	221	GLU
1	D	29	LYS
1	D	176	TRP
1	D	182	PHE
1	D	204	TRP
1	E	176	TRP
1	E	204	TRP
1	F	69	LEU
1	F	176	TRP
1	F	204	TRP
1	F	216	ASN
1	F	307	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	216	ASN
1	F	296	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 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	KYN	D	174	1	13,14,15	0.79	0	13,18,20	0.50	0
1	KYN	C	174	1	13,14,15	0.75	0	13,18,20	0.57	0
1	KYN	A	174	1	13,14,15	0.79	0	13,18,20	0.59	0
1	KYN	E	174	1	13,14,15	0.77	0	13,18,20	0.60	0
1	KYN	F	174	1	13,14,15	0.79	0	13,18,20	0.67	0
1	KYN	B	174	1	13,14,15	0.77	0	13,18,20	0.52	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
1	KYN	D	174	1	-	1/9/10/12	0/1/1/1
1	KYN	C	174	1	-	1/9/10/12	0/1/1/1
1	KYN	A	174	1	-	1/9/10/12	0/1/1/1
1	KYN	E	174	1	-	1/9/10/12	0/1/1/1
1	KYN	F	174	1	-	1/9/10/12	0/1/1/1
1	KYN	B	174	1	-	2/9/10/12	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	174	KYN	O2-C1-CD2-CE2
1	A	174	KYN	CB-C1-CD2-CE2
1	B	174	KYN	CB-C1-CD2-CE2
1	C	174	KYN	CB-C1-CD2-CE2
1	D	174	KYN	CB-C1-CD2-CE2
1	E	174	KYN	CB-C1-CD2-CE2
1	F	174	KYN	CB-C1-CD2-CE2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	174	KYN	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 67 ligands modelled in this entry, 12 are monoatomic - leaving 55 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	$\# Z  > 2$
4	EDO	F	405	-	3,3,3	0.46	0	2,2,2	0.35	0
5	SO4	D	411	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	C	408	-	4,4,4	0.14	0	6,6,6	0.06	0
4	EDO	D	405	-	3,3,3	0.46	0	2,2,2	0.34	0
5	SO4	B	406	-	4,4,4	0.16	0	6,6,6	0.16	0
4	EDO	E	414	-	3,3,3	0.47	0	2,2,2	0.31	0
4	EDO	F	407	-	3,3,3	0.46	0	2,2,2	0.33	0
5	SO4	B	407	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	D	408	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	B	404	-	3,3,3	0.45	0	2,2,2	0.37	0
5	SO4	A	408	-	4,4,4	0.14	0	6,6,6	0.06	0
4	EDO	E	408	-	3,3,3	0.46	0	2,2,2	0.33	0
5	SO4	A	412	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	E	413	-	3,3,3	0.47	0	2,2,2	0.31	0
5	SO4	E	416	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	B	405	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	E	411	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	F	408	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	B	403	-	3,3,3	0.45	0	2,2,2	0.33	0
5	SO4	F	410	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	A	403	-	3,3,3	0.45	0	2,2,2	0.32	0
4	EDO	E	401	-	3,3,3	0.45	0	2,2,2	0.38	0
4	EDO	D	403	-	3,3,3	0.45	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	407	-	3,3,3	0.46	0	2,2,2	0.30	0
4	EDO	E	412	-	3,3,3	0.47	0	2,2,2	0.32	0
5	SO4	D	410	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	F	411	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	409	-	4,4,4	0.15	0	6,6,6	0.04	0
5	SO4	E	417	-	4,4,4	0.14	0	6,6,6	0.06	0
4	EDO	A	406	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	E	404	-	3,3,3	0.45	0	2,2,2	0.32	0
5	SO4	D	409	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	F	403	-	3,3,3	0.47	0	2,2,2	0.32	0
4	EDO	C	403	-	3,3,3	0.45	0	2,2,2	0.31	0
5	SO4	A	413	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	F	409	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	A	404	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	C	405	-	3,3,3	0.44	0	2,2,2	0.25	0
4	EDO	E	410	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	D	404	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	E	409	-	3,3,3	0.46	0	2,2,2	0.29	0
4	EDO	F	406	-	3,3,3	0.46	0	2,2,2	0.30	0
5	SO4	C	407	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	E	406	-	3,3,3	0.46	0	2,2,2	0.35	0
5	SO4	E	415	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	411	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	C	406	-	4,4,4	0.14	0	6,6,6	0.04	0
4	EDO	E	407	-	3,3,3	0.45	0	2,2,2	0.35	0
4	EDO	D	407	-	3,3,3	0.46	0	2,2,2	0.32	0
5	SO4	A	410	-	4,4,4	0.14	0	6,6,6	0.04	0
4	EDO	E	405	-	3,3,3	0.47	0	2,2,2	0.28	0
4	EDO	F	404	-	3,3,3	0.47	0	2,2,2	0.28	0
4	EDO	C	404	-	3,3,3	0.44	0	2,2,2	0.42	0
4	EDO	D	406	-	3,3,3	0.47	0	2,2,2	0.24	0
4	EDO	A	405	-	3,3,3	0.44	0	2,2,2	0.34	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
4	EDO	F	405	-	-	0/1/1/1	-
4	EDO	D	405	-	-	0/1/1/1	-
4	EDO	E	414	-	-	0/1/1/1	-
4	EDO	F	407	-	-	0/1/1/1	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	408	-	-	1/1/1/1	-
4	EDO	B	404	-	-	0/1/1/1	-
4	EDO	E	408	-	-	0/1/1/1	-
4	EDO	E	413	-	-	0/1/1/1	-
4	EDO	B	405	-	-	0/1/1/1	-
4	EDO	E	411	-	-	0/1/1/1	-
4	EDO	F	408	-	-	0/1/1/1	-
4	EDO	B	403	-	-	0/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	E	401	-	-	1/1/1/1	-
4	EDO	D	403	-	-	0/1/1/1	-
4	EDO	A	407	-	-	0/1/1/1	-
4	EDO	E	412	-	-	1/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-
4	EDO	E	404	-	-	1/1/1/1	-
4	EDO	F	403	-	-	1/1/1/1	-
4	EDO	C	403	-	-	0/1/1/1	-
4	EDO	F	409	-	-	1/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	C	405	-	-	1/1/1/1	-
4	EDO	E	410	-	-	0/1/1/1	-
4	EDO	D	404	-	-	0/1/1/1	-
4	EDO	E	409	-	-	0/1/1/1	-
4	EDO	F	406	-	-	0/1/1/1	-
4	EDO	E	406	-	-	0/1/1/1	-
4	EDO	E	407	-	-	0/1/1/1	-
4	EDO	D	407	-	-	0/1/1/1	-
4	EDO	E	405	-	-	1/1/1/1	-
4	EDO	F	404	-	-	1/1/1/1	-
4	EDO	C	404	-	-	0/1/1/1	-
4	EDO	D	406	-	-	1/1/1/1	-
4	EDO	A	405	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	405	EDO	O1-C1-C2-O2
4	D	406	EDO	O1-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	E	404	EDO	O1-C1-C2-O2
4	F	409	EDO	O1-C1-C2-O2
4	E	405	EDO	O1-C1-C2-O2
4	E	412	EDO	O1-C1-C2-O2
4	F	403	EDO	O1-C1-C2-O2
4	A	405	EDO	O1-C1-C2-O2
4	A	406	EDO	O1-C1-C2-O2
4	E	401	EDO	O1-C1-C2-O2
4	F	404	EDO	O1-C1-C2-O2
4	D	408	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	405	EDO	1	0
4	F	408	EDO	1	0
4	B	403	EDO	1	0
4	A	407	EDO	1	0
4	A	404	EDO	1	0
4	D	404	EDO	1	0
4	E	409	EDO	2	0
4	F	406	EDO	1	0
5	A	411	SO4	1	0
4	D	407	EDO	2	0
4	C	404	EDO	2	0
4	D	406	EDO	1	0
4	A	405	EDO	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, 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	292/299 (97%)	0.44	10 (3%) 45 49	26, 39, 64, 94	0
1	B	288/299 (96%)	0.49	16 (5%) 24 26	31, 44, 73, 98	0
1	C	287/299 (95%)	0.57	20 (6%) 16 18	30, 42, 70, 96	0
1	D	286/299 (95%)	0.59	25 (8%) 10 10	28, 48, 82, 126	0
1	E	294/299 (98%)	0.66	25 (8%) 10 11	33, 47, 74, 85	0
1	F	290/299 (96%)	0.72	25 (8%) 10 11	32, 52, 79, 90	0
All	All	1737/1794 (96%)	0.58	121 (6%) 16 18	26, 45, 74, 126	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	196	PRO	8.5
1	D	196	PRO	7.8
1	D	197	ASP	6.4
1	C	197	ASP	5.7
1	B	218	ALA	5.5
1	E	119	ALA	5.5
1	F	222	ILE	5.3
1	D	296	ASN	5.3
1	D	198	GLY	5.2
1	E	296	ASN	5.0
1	C	220	GLY	4.9
1	E	218	ALA	4.9
1	B	292	ALA	4.9
1	F	268	CYS	4.5
1	B	261	ASP	4.5
1	B	316	ALA	4.4
1	D	315	ALA	4.1
1	F	261	ASP	4.1
1	E	257	ASP	4.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	216	ASN	4.0
1	F	270	SER	3.9
1	E	267	GLY	3.8
1	C	316	ALA	3.8
1	F	319	VAL	3.7
1	C	292	ALA	3.6
1	F	279	ALA	3.6
1	F	254	GLU	3.6
1	E	271	ALA	3.6
1	E	302	SER	3.5
1	E	191	ALA	3.5
1	B	29	LYS	3.5
1	C	198	GLY	3.5
1	B	295	ALA	3.4
1	E	261	ASP	3.4
1	F	218	ALA	3.3
1	D	113	CYS	3.3
1	E	198	GLY	3.3
1	B	216	ASN	3.3
1	B	118	PRO	3.2
1	B	289	ALA	3.2
1	E	195	LYS	3.2
1	F	239	ASP	3.1
1	B	296	ASN	3.1
1	B	290	ASP	3.1
1	C	221	GLU	3.1
1	B	194	ILE	3.1
1	C	195	LYS	3.0
1	B	119	ALA	3.0
1	C	254	GLU	3.0
1	F	175	ASN	3.0
1	D	218	ALA	2.9
1	F	316	ALA	2.9
1	B	197	ASP	2.9
1	E	153	VAL	2.9
1	F	59	ARG	2.9
1	C	194	ILE	2.9
1	C	265	ALA	2.9
1	B	288	LEU	2.9
1	E	160	VAL	2.8
1	A	236	ASP	2.8
1	E	225	CYS	2.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	263	GLY	2.8
1	A	57	SER	2.8
1	D	117	ASN	2.8
1	A	290	ASP	2.8
1	F	134	VAL	2.8
1	D	221	GLU	2.8
1	D	118	PRO	2.7
1	E	199	SER	2.7
1	C	106	ALA	2.7
1	D	80	LYS	2.7
1	A	296	ASN	2.7
1	A	192	ALA	2.7
1	F	113	CYS	2.6
1	F	260	VAL	2.6
1	E	219	THR	2.5
1	A	291	SER	2.5
1	B	191	ALA	2.5
1	E	239	ASP	2.5
1	C	267	GLY	2.5
1	D	271	ALA	2.5
1	C	261	ASP	2.4
1	F	256	SER	2.4
1	F	240	PRO	2.4
1	A	208	VAL	2.4
1	F	295	ALA	2.4
1	D	274	ASP	2.4
1	D	199	SER	2.4
1	C	161	GLU	2.4
1	E	220	GLY	2.4
1	E	266	VAL	2.3
1	A	295	ALA	2.3
1	D	108	GLY	2.3
1	D	288	LEU	2.3
1	C	113	CYS	2.3
1	E	316	ALA	2.3
1	A	253	PHE	2.2
1	F	250	THR	2.2
1	F	281	PHE	2.2
1	D	259	SER	2.2
1	E	196	PRO	2.2
1	F	220	GLY	2.2
1	D	258	ILE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	242	THR	2.2
1	D	55	LEU	2.1
1	E	197	ASP	2.1
1	F	42	ASP	2.1
1	C	219	THR	2.1
1	A	292	ALA	2.1
1	E	108	GLY	2.1
1	C	303	ARG	2.1
1	D	277	CYS	2.1
1	C	288	LEU	2.1
1	D	289	ALA	2.1
1	D	105	ASP	2.0
1	E	269	MET	2.0
1	C	183	VAL	2.0
1	F	296	ASN	2.0
1	D	276	ASP	2.0
1	D	119	ALA	2.0
1	F	212	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	KYN	F	174	14/15	0.84	0.19	27,40,48,48	0
1	KYN	C	174	14/15	0.87	0.20	30,40,51,58	0
1	KYN	A	174	14/15	0.87	0.19	28,30,44,47	0
1	KYN	B	174	14/15	0.89	0.18	32,41,52,63	0
1	KYN	E	174	14/15	0.90	0.21	32,45,50,51	0
1	KYN	D	174	14/15	0.90	0.16	39,44,59,59	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	E	413	4/4	0.38	0.21	62,65,68,70	0
4	EDO	E	411	4/4	0.45	0.35	115,116,118,118	0
4	EDO	B	403	4/4	0.54	0.22	87,87,90,91	0
4	EDO	E	410	4/4	0.54	0.19	66,69,69,70	0
4	EDO	F	404	4/4	0.55	0.18	68,68,71,74	0
4	EDO	D	405	4/4	0.61	0.16	74,77,78,79	0
4	EDO	E	414	4/4	0.62	0.21	51,51,52,53	0
4	EDO	A	404	4/4	0.63	0.22	80,80,81,82	0
5	SO4	A	409	5/5	0.64	0.47	131,135,137,138	0
5	SO4	C	406	5/5	0.64	0.20	123,125,129,130	0
4	EDO	F	406	4/4	0.65	0.18	68,70,74,80	0
4	EDO	E	407	4/4	0.65	0.23	71,72,77,79	0
4	EDO	E	406	4/4	0.65	0.20	56,58,62,71	0
4	EDO	A	406	4/4	0.66	0.23	85,86,86,87	0
4	EDO	C	405	4/4	0.67	0.20	58,59,59,59	0
4	EDO	E	409	4/4	0.67	0.26	81,84,86,87	0
5	SO4	A	412	5/5	0.68	0.36	125,128,129,133	0
4	EDO	F	409	4/4	0.69	0.25	61,64,65,69	0
4	EDO	E	405	4/4	0.71	0.20	53,54,54,55	0
4	EDO	E	412	4/4	0.73	0.26	62,65,69,77	0
4	EDO	E	404	4/4	0.74	0.20	69,69,70,73	0
4	EDO	A	403	4/4	0.74	0.24	79,86,89,90	0
5	SO4	E	417	5/5	0.74	0.32	111,112,114,119	0
5	SO4	E	416	5/5	0.76	0.24	124,130,131,135	0
4	EDO	F	403	4/4	0.77	0.20	49,53,54,56	0
4	EDO	A	407	4/4	0.80	0.13	58,60,60,62	0
4	EDO	F	407	4/4	0.80	0.14	62,65,69,70	0
5	SO4	D	410	5/5	0.80	0.25	118,122,126,131	0
4	EDO	D	404	4/4	0.80	0.19	76,77,79,79	0
4	EDO	A	405	4/4	0.80	0.19	62,63,67,73	0
5	SO4	C	408	5/5	0.81	0.62	133,133,137,140	0
4	EDO	E	401	4/4	0.82	0.14	53,63,64,64	0
5	SO4	C	407	5/5	0.82	0.20	130,131,132,134	0
4	EDO	D	403	4/4	0.82	0.34	85,86,87,87	0
5	SO4	A	411	5/5	0.83	0.28	101,105,110,112	0
4	EDO	F	408	4/4	0.83	0.18	64,65,68,72	0
5	SO4	A	413	5/5	0.83	0.31	143,146,148,149	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	D	406	4/4	0.84	0.28	57,65,68,77	0
4	EDO	B	405	4/4	0.84	0.19	61,66,70,71	0
5	SO4	D	411	5/5	0.85	0.56	132,136,137,141	0
5	SO4	D	409	5/5	0.85	0.44	135,136,137,139	0
5	SO4	A	410	5/5	0.85	0.34	129,131,134,135	0
5	SO4	F	410	5/5	0.85	0.23	112,113,118,120	0
4	EDO	D	407	4/4	0.86	0.23	59,63,66,69	0
4	EDO	D	408	4/4	0.86	0.25	49,50,64,81	0
4	EDO	C	403	4/4	0.86	0.21	74,75,75,75	0
5	SO4	B	406	5/5	0.88	0.27	74,75,77,82	0
5	SO4	F	411	5/5	0.89	0.16	111,113,117,117	0
4	EDO	E	408	4/4	0.90	0.16	60,66,69,73	0
4	EDO	C	404	4/4	0.91	0.17	63,70,71,72	0
5	SO4	E	415	5/5	0.91	0.16	103,108,112,114	0
4	EDO	B	404	4/4	0.92	0.17	55,56,57,57	0
3	CA	B	402	1/1	0.92	0.08	54,54,54,54	0
2	CU	A	401	1/1	0.93	0.09	44,44,44,44	0
5	SO4	B	407	5/5	0.94	0.24	97,98,102,103	0
3	CA	D	402	1/1	0.94	0.06	52,52,52,52	0
2	CU	B	401	1/1	0.95	0.07	49,49,49,49	0
4	EDO	F	405	4/4	0.95	0.11	54,64,73,80	0
2	CU	E	402	1/1	0.95	0.07	54,54,54,54	0
3	CA	F	402	1/1	0.95	0.11	51,51,51,51	0
2	CU	D	401	1/1	0.96	0.04	52,52,52,52	0
5	SO4	A	408	5/5	0.96	0.16	80,83,84,86	0
2	CU	F	401	1/1	0.96	0.07	54,54,54,54	0
3	CA	E	403	1/1	0.96	0.14	58,58,58,58	0
2	CU	C	401	1/1	0.97	0.06	49,49,49,49	0
3	CA	C	402	1/1	0.97	0.07	43,43,43,43	0
3	CA	A	402	1/1	0.99	0.07	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.