



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:44 PM GMT

PDB ID : 1H0H
Title : Tungsten containing Formate Dehydrogenase from Desulfovibrio Gigas
Authors : Raaijmakers, H.C.A.
Deposited on : 2002-06-19
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

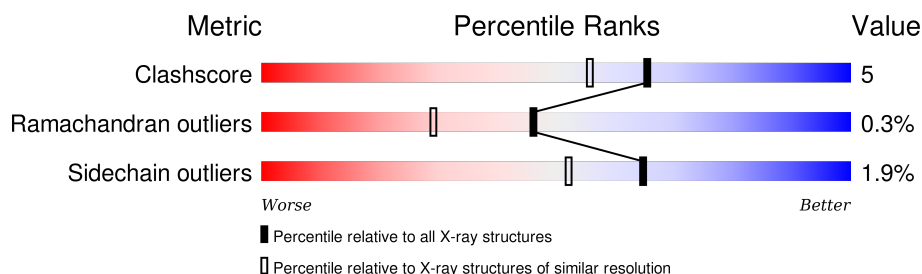
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	977	
1	K	977	
2	B	214	
2	L	214	

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
4	2MD	A	1001	X	-	-	-
4	2MD	K	1001	X	-	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 21055 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 FORMATE DEHYDROGENASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	977	Total	C	N	O	S	Se	4	28	0
			7857	5002	1349	1458	47	1			
1	K	977	Total	C	N	O	S	Se	6	23	0
			7836	4992	1341	1455	47	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	959	ASN	ASP	CONFLICT	UNP Q934F5
K	959	ASN	ASP	CONFLICT	UNP Q934F5

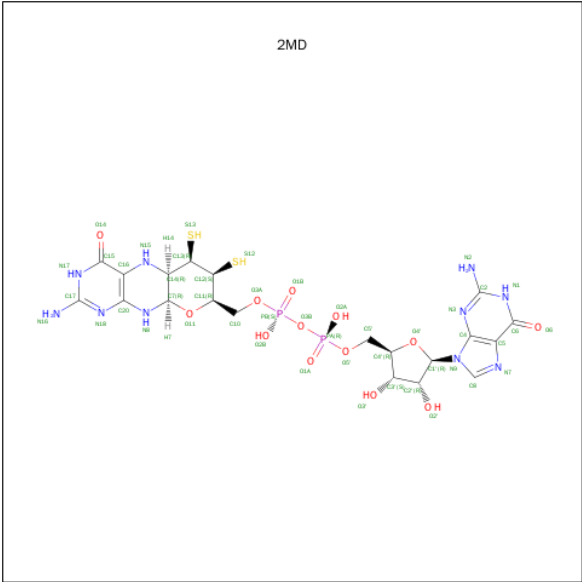
- Molecule 2 is a protein called FORMATE DEHYDROGENASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	8	0
			1697	1051	293	332	21			
2	L	214	Total	C	N	O	S	0	2	0
			1669	1037	287	323	22			

- Molecule 3 is TUNGSTEN ION (three-letter code: W) (formula: W).

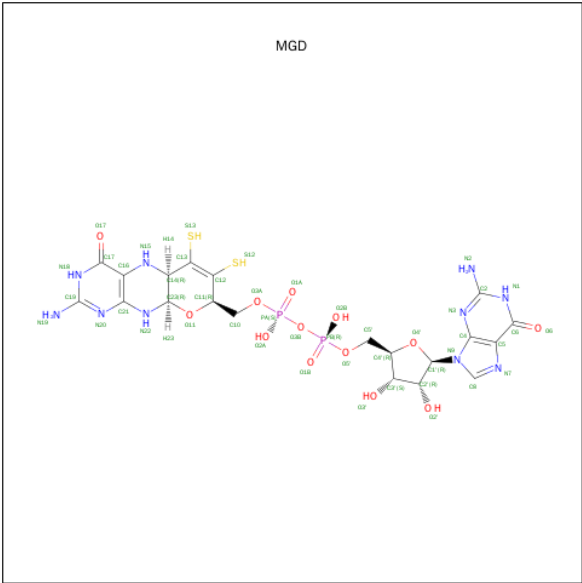
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	W	0	0
			1	1		
3	K	1	Total	W	0	0
			1	1		

- Molecule 4 is GUANYLATE-O'-PHOSPHORIC ACID MONO-(2-AMINO-5,6-DIMERCA PTO-4-OXO-3,5,6,7,8A,9,10,10A-OCTAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTH RACEN-7-YLMETHYL) ESTER (three-letter code: 2MD) (formula: C₂₀H₂₈N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	K	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

Continued on next page...

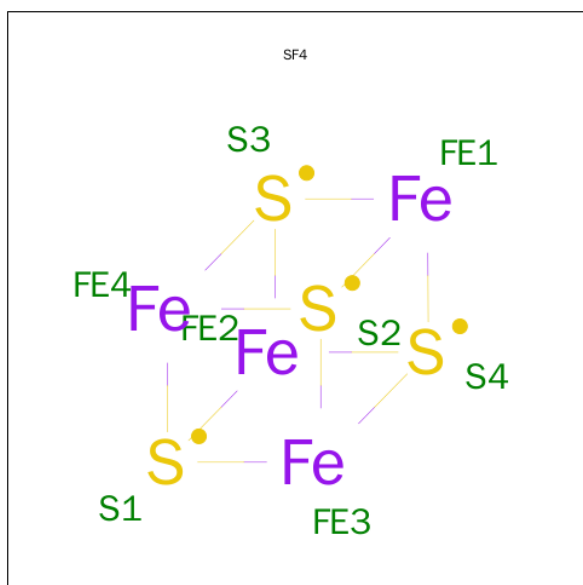
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	K	1	Total	C	N	O	P	S	
			47	20	10	13	2	2	
								0	0

- Molecule 6 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	X	0	0
			1	1		
6	K	1	Total	X	0	0
			1	1		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	K	1	Total	Fe	S	0	0
			8	4	4		
7	L	1	Total	Fe	S	0	0
			8	4	4		

Continued on next page...

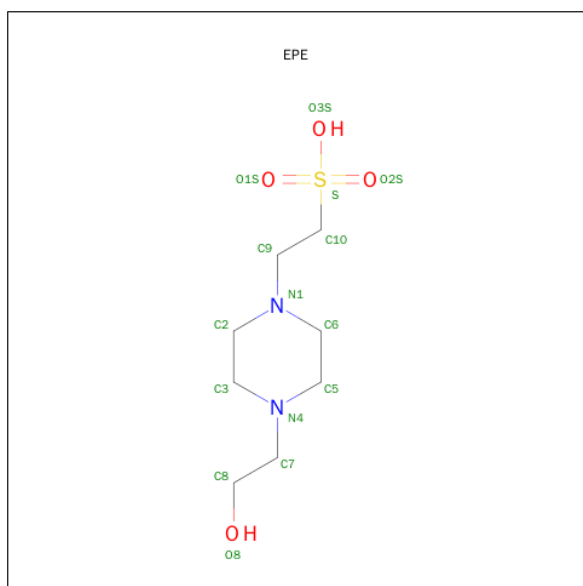
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	Fe	S	0	0
			8	4	4		
7	L	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		
8	K	1	Total	Ca	0	0
			1	1		

- Molecule 9 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
9	K	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 10 is water.

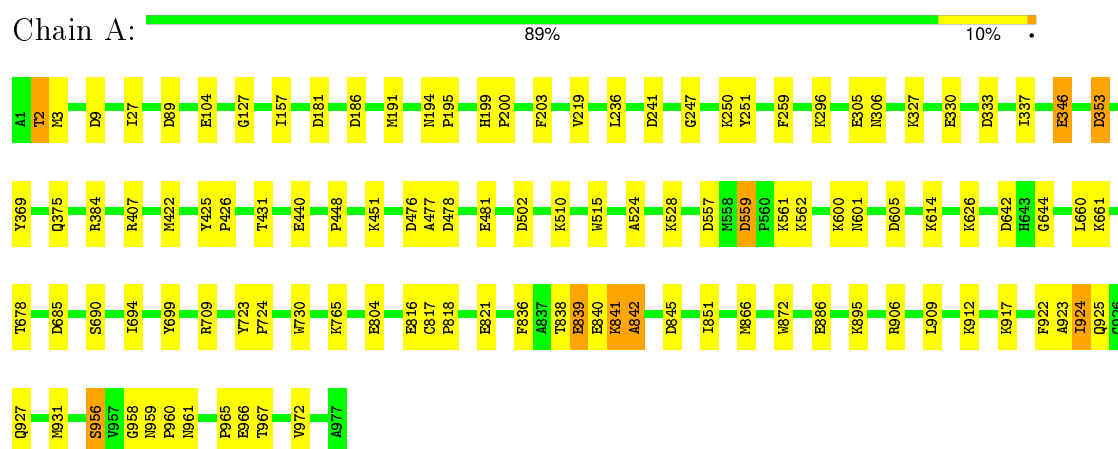
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	704	Total 704	O 704	0	0
10	B	188	Total 188	O 188	0	0
10	K	623	Total 623	O 623	0	0
10	L	193	Total 193	O 193	0	0

3 Residue-property plots

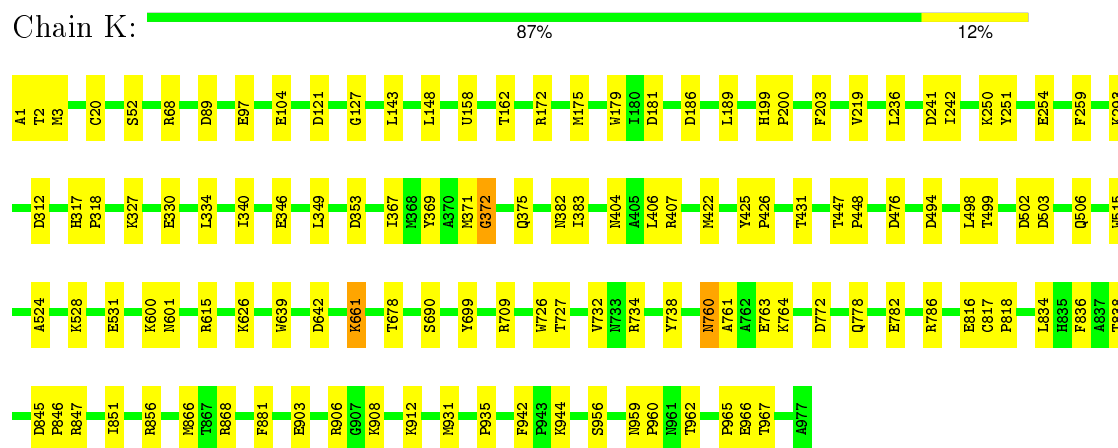
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

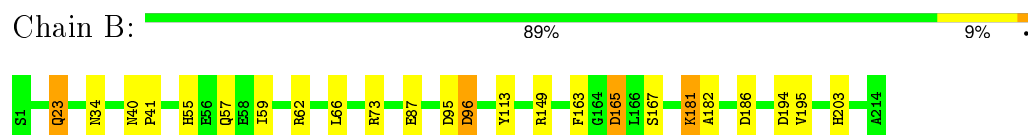
• Molecule 1: FORMATE DEHYDROGENASE SUBUNIT ALPHA



• Molecule 1: FORMATE DEHYDROGENASE SUBUNIT ALPHA



• Molecule 2: FORMATE DEHYDROGENASE SUBUNIT BETA



- Molecule 2: FORMATE DEHYDROGENASE SUBUNIT BETA

Chain L: 90% 9% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.41 Å 110.40 Å 156.19 Å 90.00° 93.53° 90.00°	Depositor
Resolution (Å)	35.00 – 1.80	Depositor
% Data completeness (in resolution range)	95.7 (35.00-1.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.167 , 0.201	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21055	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MD, MGD, UNX, SF4, SEC, W, EPE, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/8171	0.83	18/11073 (0.2%)
1	K	0.55	0/8120	0.82	8/11010 (0.1%)
2	B	0.55	0/1771	0.87	7/2404 (0.3%)
2	L	0.57	0/1720	0.88	6/2334 (0.3%)
All	All	0.57	0/19782	0.83	39/26821 (0.1%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ASP	CB-CG-OD2	7.17	124.75	118.30
1	A	685	ASP	CB-CG-OD2	6.85	124.47	118.30
1	K	121	ASP	CB-CG-OD2	6.46	124.11	118.30
2	B	194	ASP	CB-CG-OD2	6.34	124.01	118.30
1	K	89	ASP	CB-CG-OD2	6.29	123.96	118.30
2	L	123	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	605	ASP	CB-CG-OD2	6.14	123.82	118.30
2	B	95	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	241	ASP	CB-CG-OD2	6.10	123.79	118.30
2	B	186	ASP	CB-CG-OD2	6.05	123.74	118.30
1	K	476	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	181	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	353[A]	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	353[B]	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	476	ASP	CB-CG-OD2	5.88	123.59	118.30
2	L	95	ASP	CB-CG-OD2	5.84	123.56	118.30
2	B	96[A]	ASP	CB-CG-OD2	5.76	123.49	118.30
2	B	96[B]	ASP	CB-CG-OD2	5.76	123.49	118.30
2	L	191	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	502	ASP	CB-CG-OD2	5.65	123.39	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	845	ASP	CB-CG-OD2	5.60	123.34	118.30
1	K	186	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	89	ASP	CB-CG-OD2	5.53	123.27	118.30
1	K	181	ASP	CB-CG-OD2	5.51	123.26	118.30
2	B	165[A]	ASP	CB-CG-OD2	5.50	123.25	118.30
2	B	165[B]	ASP	CB-CG-OD2	5.50	123.25	118.30
2	L	165	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	972	VAL	CB-CA-C	-5.35	101.24	111.40
1	A	557	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	333	ASP	CB-CG-OD2	5.25	123.03	118.30
1	K	312	ASP	CB-CG-OD2	5.24	123.02	118.30
2	L	7	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	384	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	559	ASP	CB-CG-OD2	5.10	122.89	118.30
1	K	503	ASP	CB-CG-OD2	5.06	122.85	118.30
1	K	642	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	642	ASP	CB-CG-OD2	5.04	122.84	118.30
2	L	193	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	9	ASP	CB-CG-OD2	5.02	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7857	0	7657	78	0
1	K	7836	0	7633	80	1
2	B	1697	0	1575	19	1
2	L	1669	0	1570	16	0
3	A	1	0	0	0	0
3	K	1	0	0	0	0
4	A	47	0	23	2	0
4	K	47	0	22	2	0
5	A	47	0	22	0	0
5	K	47	0	22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
6	K	1	0	0	0	0
7	A	8	0	0	0	0
7	B	24	0	0	0	0
7	K	8	0	0	0	0
7	L	24	0	0	0	0
8	A	1	0	0	0	0
8	K	1	0	0	0	0
9	A	15	0	17	1	0
9	K	15	0	17	1	0
10	A	704	0	0	6	0
10	B	188	0	0	5	0
10	K	623	0	0	12	0
10	L	193	0	0	5	0
All	All	21055	0	18558	189	1

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 (189) 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:A:839[B]:GLU:HG2	1:A:840[B]:GLU:OE1	1.01	1.17
1:K:531:GLU:HG3	10:K:2066:HOH:O	1.41	1.16
1:A:839[B]:GLU:CG	1:A:840[B]:GLU:OE1	1.96	1.12
2:L:168:GLU:OE1	10:L:2152:HOH:O	1.78	1.01
2:L:62:ARG:HH11	2:L:62:ARG:HG3	1.27	0.97
1:K:966:GLU:HG2	10:K:2613:HOH:O	1.65	0.94
1:K:965:PRO:HB2	1:K:967:THR:HG22	1.51	0.91
1:A:346:GLU:HG3	10:A:2301:HOH:O	1.71	0.91
1:A:965:PRO:HB2	1:A:967:THR:HG22	1.54	0.88
1:A:296:LYS:HD3	1:A:804[A]:GLU:OE1	1.73	0.88
1:A:528:LYS:NZ	1:A:961[A]:ASN:HD22	1.78	0.81
1:A:959:ASN:N	1:A:960:PRO:CD	2.44	0.80
1:A:958:GLY:C	1:A:960:PRO:HD2	2.03	0.78
1:K:709:ARG:HD2	10:K:2468:HOH:O	1.84	0.78
1:K:761:ALA:O	1:K:764:LYS:HD3	1.86	0.74
2:B:113:TYR:OH	1:K:763:GLU:OE2	2.04	0.74
1:A:959:ASN:N	1:A:960:PRO:HD2	2.03	0.73
2:B:87:GLU:HG2	10:B:2102:HOH:O	1.88	0.73
2:L:55:HIS:HD2	10:L:2066:HOH:O	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LYS:O	1:A:330:GLU:HG2	1.91	0.71
1:A:528:LYS:HZ3	1:A:961[A]:ASN:HB2	1.54	0.70
1:K:371[B]:MET:O	10:K:2276:HOH:O	2.09	0.70
2:L:62:ARG:NH1	2:L:62:ARG:HG3	2.04	0.69
1:K:760:ASN:ND2	1:K:763:GLU:OE1	2.25	0.69
2:L:55:HIS:CD2	10:L:2066:HOH:O	2.45	0.69
1:A:528:LYS:NZ	1:A:961[A]:ASN:ND2	2.41	0.69
1:K:965:PRO:HB2	1:K:967:THR:CG2	2.23	0.68
1:K:293:LYS:HE3	10:K:2232:HOH:O	1.93	0.68
1:K:1:ALA:H3	1:K:3:MET:CE	2.09	0.66
9:A:1200:EPE:O8	9:A:1200:EPE:H31	1.95	0.66
1:K:524:ALA:HB2	1:K:965:PRO:HA	1.78	0.66
1:K:502[B]:ASP:OD2	1:K:506[B]:GLN:NE2	2.29	0.64
2:B:62:ARG:HG2	2:B:62:ARG:HH11	1.62	0.64
1:K:760:ASN:ND2	1:K:763:GLU:H	1.95	0.64
1:K:327:LYS:O	1:K:330:GLU:HG2	1.99	0.63
1:A:840[A]:GLU:HG2	10:A:2638:HOH:O	1.99	0.63
2:B:62:ARG:CG	2:B:62:ARG:HH11	2.12	0.62
1:K:1:ALA:N	1:K:3:MET:CE	2.61	0.62
1:A:528:LYS:HZ3	1:A:961[B]:ASN:HB3	1.65	0.62
1:K:959[A]:ASN:N	1:K:960:PRO:CD	2.63	0.62
1:A:247:GLY:HA3	1:A:337:ILE:CD1	2.30	0.61
1:K:317:HIS:ND1	1:K:318:PRO:HD2	2.16	0.60
1:A:528:LYS:HZ3	1:A:961[A]:ASN:HD22	1.49	0.60
1:K:250:LYS:HE3	1:K:330:GLU:O	2.01	0.60
1:A:250:LYS:HE3	1:A:330:GLU:O	2.02	0.60
1:A:922:PHE:CE2	10:A:2210:HOH:O	2.52	0.60
2:L:87:GLU:OE2	2:L:111:GLU:HG2	2.03	0.59
1:K:944:LYS:HG2	10:K:2604:HOH:O	2.02	0.59
1:K:1:ALA:H3	1:K:3:MET:HE3	1.69	0.58
1:K:760:ASN:C	1:K:760:ASN:HD22	2.07	0.58
1:K:912:LYS:HE2	2:L:34:ASN:O	2.03	0.58
1:A:559:ASP:OD1	1:A:561[B]:LYS:HG2	2.03	0.58
2:B:55:HIS:HD2	10:B:2069:HOH:O	1.88	0.57
1:A:528:LYS:NZ	1:A:961[A]:ASN:HB2	2.20	0.57
1:K:104:GLU:OE2	1:K:626:LYS:HG3	2.04	0.57
1:K:241:ASP:HB2	1:K:382[B]:ASN:HD21	1.70	0.56
1:A:375[B]:GLN:NE2	1:A:966:GLU:HG2	2.19	0.56
1:K:494[B]:ASP:OD2	1:K:499:THR:HG23	2.04	0.56
1:A:956:SER:OG	1:A:960:PRO:O	2.22	0.56
1:K:189:LEU:O	1:K:367:ILE:HD12	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:LYS:NZ	1:A:644:GLY:O	2.36	0.56
1:K:425:TYR:CE2	1:K:431:THR:HA	2.41	0.56
1:A:247:GLY:HA3	1:A:337:ILE:HD11	1.87	0.55
1:K:524:ALA:HB2	1:K:965:PRO:CA	2.36	0.55
1:A:524:ALA:HB2	1:A:965:PRO:HA	1.89	0.55
1:K:219:VAL:HG12	1:K:236:LEU:HD22	1.89	0.55
2:B:182:ALA:HB3	10:B:2161:HOH:O	2.07	0.54
1:A:528:LYS:NZ	1:A:961[B]:ASN:HB3	2.21	0.54
1:K:172:ARG:HB2	1:K:738:TYR:OH	2.08	0.54
1:K:528:LYS:HG2	1:K:962:THR:CG2	2.37	0.54
1:K:866:MET:SD	4:K:1001:2MD:H2'	2.48	0.54
1:A:528:LYS:NZ	1:A:961[A]:ASN:CB	2.71	0.54
1:K:856:ARG:HH22	4:K:1001:2MD:HNF	1.56	0.54
1:K:498:LEU:HD12	10:K:2610:HOH:O	2.09	0.53
1:A:104:GLU:OE2	1:A:626:LYS:HG3	2.08	0.53
1:A:816:GLU:HG2	1:A:836:PHE:CD1	2.43	0.53
1:A:528:LYS:NZ	1:A:961[B]:ASN:CB	2.71	0.52
1:A:841[B]:LYS:O	1:A:842[B]:ALA:O	2.28	0.52
1:A:425:TYR:HB3	1:A:426:PRO:HD2	1.92	0.52
1:A:199:HIS:N	1:A:200:PRO:HD3	2.24	0.52
1:A:912:LYS:HE2	2:B:34:ASN:O	2.10	0.52
2:B:149[B]:ARG:HH21	2:B:163:PHE:H	1.57	0.51
1:K:734:ARG:HD3	1:K:772:ASP:HA	1.94	0.50
1:A:296:LYS:CD	1:A:804[A]:GLU:OE1	2.54	0.50
1:A:866:MET:SD	4:A:1001:2MD:H2'	2.52	0.50
1:K:1:ALA:H3	1:K:3:MET:HE2	1.77	0.50
2:L:40:ASN:HA	2:L:41:PRO:C	2.32	0.50
1:A:886:GLU:OE2	1:A:917[B]:LYS:NZ	2.35	0.49
1:A:425:TYR:CE2	1:A:431:THR:HA	2.48	0.49
1:K:334:LEU:HD11	1:K:349:LEU:HD13	1.93	0.49
1:A:851:ILE:O	1:A:931:MET:HA	2.13	0.49
1:K:903:GLU:HG2	1:K:908:LYS:HE3	1.95	0.49
1:K:956:SER:OG	1:K:960:PRO:O	2.30	0.48
1:K:199:HIS:N	1:K:200:PRO:HD3	2.28	0.48
1:K:845:ASP:OD1	1:K:846:PRO:HD2	2.13	0.48
1:A:895[B]:LYS:HB2	1:A:895[B]:LYS:NZ	2.29	0.48
2:B:59:ILE:HD13	2:B:203:HIS:CE1	2.49	0.48
9:K:1200:EPE:H72	2:L:123:ASP:OD1	2.13	0.48
1:A:836:PHE:HB2	10:A:2637:HOH:O	2.12	0.48
1:K:1:ALA:N	1:K:3:MET:HE3	2.25	0.47
1:K:179:TRP:CH2	1:K:406:LEU:HD22	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:GLU:HG2	1:A:836:PHE:HD1	1.79	0.47
1:K:251:TYR:OH	1:K:353:ASP:OD1	2.20	0.47
1:K:816:GLU:HG2	1:K:836:PHE:HD1	1.78	0.47
2:L:62:ARG:HH11	2:L:62:ARG:CG	2.08	0.47
1:K:760:ASN:O	1:K:764:LYS:N	2.47	0.47
1:A:251:TYR:OH	1:A:353[A]:ASP:OD1	2.23	0.47
1:K:1:ALA:N	1:K:3:MET:HE2	2.29	0.47
1:K:661:LYS:HB3	1:K:661:LYS:HE3	1.57	0.47
1:A:818:PRO:HB2	1:A:927:GLN:HE22	1.80	0.46
2:L:149:ARG:CD	10:L:2146:HOH:O	2.64	0.46
1:A:958:GLY:CA	1:A:960:PRO:HD2	2.45	0.46
1:A:127:GLY:HA3	1:A:515:TRP:O	2.16	0.46
1:K:371[B]:MET:O	1:K:372[B]:GLY:O	2.34	0.45
1:A:247:GLY:HA3	1:A:337:ILE:HD13	1.99	0.45
1:A:194:ASN:N	1:A:195:PRO:HD3	2.32	0.45
1:A:2:THR:HG23	1:A:3:MET:H	1.81	0.45
1:K:425:TYR:HB3	1:K:426:PRO:HD2	1.99	0.45
1:K:340:ILE:HD12	1:K:340:ILE:HA	1.78	0.45
2:B:149[B]:ARG:NH2	2:B:163:PHE:H	2.15	0.45
1:A:524:ALA:HB2	1:A:965:PRO:CA	2.48	0.44
1:A:965:PRO:HB2	1:A:967:THR:CG2	2.37	0.44
1:A:840[B]:GLU:N	1:A:840[B]:GLU:OE1	2.50	0.44
1:K:966:GLU:HG3	10:K:2279:HOH:O	2.16	0.44
1:A:872:TRP:CH2	2:B:23:GLN:HA	2.52	0.44
2:B:55:HIS:CD2	10:B:2069:HOH:O	2.67	0.44
1:K:175:MET:HG3	1:K:404:ASN:HA	2.00	0.44
2:L:62:ARG:NH1	2:L:62:ARG:CG	2.72	0.44
2:B:165[B]:ASP:OD2	2:B:167:SER:HB2	2.18	0.44
1:A:191:MET:HG3	1:A:219:VAL:HB	1.99	0.44
2:B:73:ARG:HB3	2:B:195:VAL:HB	1.99	0.44
1:K:851:ILE:O	1:K:931:MET:HA	2.18	0.44
1:K:143:LEU:HD22	1:K:148:LEU:HD22	2.00	0.44
1:K:371[B]:MET:C	10:K:2276:HOH:O	2.51	0.43
2:B:181:LYS:CE	2:B:181:LYS:HA	2.48	0.43
1:K:375:GLN:HE21	1:K:966:GLU:CD	2.22	0.43
1:A:600:LYS:HA	1:A:601:ASN:HA	1.84	0.43
1:A:305[B]:GLU:HG3	10:A:2278:HOH:O	2.19	0.43
1:A:27:ILE:HD13	1:A:27:ILE:HA	1.86	0.43
1:A:528:LYS:HZ3	1:A:961[A]:ASN:CB	2.25	0.43
1:K:242:ILE:HG13	10:K:2193:HOH:O	2.18	0.43
1:K:868:ARG:HD2	1:K:942:PHE:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASN:O	1:A:451:LYS:HE2	2.17	0.43
1:K:817:CYS:HA	1:K:818:PRO:C	2.38	0.43
1:A:821:GLU:O	1:A:925:GLN:NE2	2.43	0.43
1:K:959[B]:ASN:N	1:K:960:PRO:CD	2.82	0.43
1:A:909:LEU:C	1:A:909:LEU:HD12	2.39	0.43
2:L:55:HIS:HE1	10:L:2185:HOH:O	2.02	0.43
1:K:68:ARG:HD2	10:K:2070:HOH:O	2.19	0.42
1:K:162:THR:HA	1:K:383:ILE:HD13	1.99	0.42
1:K:158:SEC:CB	1:K:371[B]:MET:HG3	2.48	0.42
1:A:528:LYS:HZ3	1:A:961[B]:ASN:CB	2.26	0.42
1:A:660:LEU:HA	1:A:660:LEU:HD23	1.90	0.42
1:A:477:ALA:HB1	1:A:481[A]:GLU:HG3	2.02	0.42
1:A:965:PRO:O	1:A:967:THR:HG23	2.19	0.42
1:K:615:ARG:HD3	1:K:615:ARG:HH11	1.65	0.42
2:B:57:GLN:HG3	2:B:66:LEU:HD12	2.01	0.42
1:K:447:THR:HA	1:K:448:PRO:HD3	1.88	0.42
1:A:723:TYR:N	1:A:724:PRO:HD3	2.35	0.42
1:K:600:LYS:HA	1:K:601:ASN:HA	1.83	0.42
1:K:369[A]:TYR:CD1	1:K:369[A]:TYR:C	2.93	0.42
1:K:317:HIS:CG	1:K:318:PRO:HD2	2.55	0.42
1:K:127:GLY:HA3	1:K:515:TRP:O	2.19	0.42
1:A:923:ALA:C	1:A:924:ILE:HG12	2.37	0.42
1:K:732:VAL:HG12	10:K:2442:HOH:O	2.19	0.42
1:A:559:ASP:HB3	1:A:562:LYS:HE2	2.01	0.41
1:K:639:TRP:N	1:K:639:TRP:CD1	2.86	0.41
1:K:881:PHE:CE2	1:K:935:PRO:HG3	2.55	0.41
2:B:87:GLU:CG	10:B:2102:HOH:O	2.59	0.41
1:A:709:ARG:HD2	10:A:2012:HOH:O	2.20	0.41
1:K:778:GLN:OE1	1:K:786:ARG:HA	2.20	0.41
1:K:726:TRP:CD1	1:K:727:THR:HG23	2.56	0.41
2:L:181:LYS:NZ	2:L:187:ALA:O	2.38	0.41
1:A:817:CYS:HA	1:A:818:PRO:C	2.40	0.41
1:A:219:VAL:HG12	1:A:236:LEU:HD22	2.03	0.41
2:B:40:ASN:HA	2:B:41:PRO:C	2.41	0.41
1:K:250:LYS:NZ	1:K:254:GLU:OE1	2.49	0.41
1:K:52[B]:SER:HB3	2:L:155:SER:O	2.20	0.41
2:B:62:ARG:CG	2:B:62:ARG:NH1	2.75	0.40
1:A:157:ILE:HG21	4:A:1001:2MD:H14	2.03	0.40
1:A:478:ASP:O	1:A:481[A]:GLU:HG2	2.21	0.40
1:A:694:ILE:HD12	1:A:730:TRP:CE2	2.56	0.40
1:A:369:TYR:CD1	1:A:369:TYR:C	2.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:103:PHE:CD1	2:L:136:LYS:HE3	2.57	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	Interatomic distance (Å)	Clash overlap (Å)
2:B:96[A]:ASP:OD2	1:K:847:ARG:NH1[1_545]	2.18	0.02

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	1002/977 (103%)	968 (97%)	29 (3%)	5 (0%)	34	17
1	K	997/977 (102%)	965 (97%)	28 (3%)	4 (0%)	39	23
2	B	220/214 (103%)	213 (97%)	7 (3%)	0	100	100
2	L	214/214 (100%)	207 (97%)	7 (3%)	0	100	100
All	All	2433/2382 (102%)	2353 (97%)	71 (3%)	9 (0%)	46	23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	841[A]	LYS
1	A	841[B]	LYS
1	A	842[A]	ALA
1	A	842[B]	ALA
1	K	838	THR
1	K	372[A]	GLY
1	K	372[B]	GLY
1	K	690	SER
1	A	690	SER

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	836/809 (103%)	817 (98%)	19 (2%)	58	42
1	K	829/809 (102%)	814 (98%)	15 (2%)	66	54
2	B	190/182 (104%)	188 (99%)	2 (1%)	80	74
2	L	184/182 (101%)	180 (98%)	4 (2%)	60	45
All	All	2039/1982 (103%)	1999 (98%)	40 (2%)	65	49

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	203	PHE
1	A	259	PHE
1	A	346	GLU
1	A	407	ARG
1	A	422	MET
1	A	440	GLU
1	A	448	PRO
1	A	661	LYS
1	A	678	THR
1	A	699	TYR
1	A	765	LYS
1	A	838[A]	THR
1	A	838[B]	THR
1	A	839[A]	GLU
1	A	839[B]	GLU
1	A	906	ARG
1	A	924	ILE
1	A	956	SER
2	B	23	GLN
2	B	181	LYS
1	K	2	THR
1	K	20	CYS
1	K	97[A]	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	97[B]	GLU
1	K	203	PHE
1	K	259	PHE
1	K	346	GLU
1	K	407	ARG
1	K	422	MET
1	K	661	LYS
1	K	678	THR
1	K	699	TYR
1	K	760	ASN
1	K	782	GLU
1	K	906	ARG
2	L	23	GLN
2	L	62	ARG
2	L	181	LYS
2	L	185	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	480	ASN
1	A	927	GLN
2	B	55	HIS
1	K	12	GLN
1	K	760	ASN
2	L	55	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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

Of 20 ligands modelled in this entry, 2 are unknown and 4 are monoatomic - leaving 14 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	2MD	A	1001	3	40,52,52	1.48	7 (17%)	50,81,81	2.00	15 (30%)
5	MGD	A	1002	3	38,52,52	1.42	6 (15%)	43,81,81	2.26	12 (27%)
7	SF4	A	1010	1	0,12,12	0.00	-	0,24,24	0.00	-
9	EPE	A	1200	-	14,15,15	0.44	0	18,20,20	2.05	7 (38%)
7	SF4	B	1011	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	1012	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	1013	2	0,12,12	0.00	-	0,24,24	0.00	-
4	2MD	K	1001	3	40,52,52	1.41	7 (17%)	50,81,81	2.08	13 (26%)
5	MGD	K	1002	3	38,52,52	1.42	6 (15%)	43,81,81	2.16	16 (37%)
7	SF4	K	1010	1	0,12,12	0.00	-	0,24,24	0.00	-
9	EPE	K	1200	-	14,15,15	0.41	0	18,20,20	2.01	4 (22%)
7	SF4	L	1011	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	L	1012	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	L	1013	2	0,12,12	0.00	-	0,24,24	0.00	-

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	2MD	A	1001	3	1/1/11/13	0/18/66/66	0/6/6/6
5	MGD	A	1002	3	-	0/18/66/66	0/6/6/6
7	SF4	A	1010	1	-	0/0/48/48	0/6/5/5
9	EPE	A	1200	-	-	0/9/19/19	0/1/1/1
7	SF4	B	1011	2	-	0/0/48/48	0/6/5/5
7	SF4	B	1012	2	-	0/0/48/48	0/6/5/5
7	SF4	B	1013	2	-	0/0/48/48	0/6/5/5
4	2MD	K	1001	3	2/2/11/13	0/18/66/66	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MGD	K	1002	3	-	0/18/66/66	0/6/6/6
7	SF4	K	1010	1	-	0/0/48/48	2/6/5/5
9	EPE	K	1200	-	-	0/9/19/19	0/1/1/1
7	SF4	L	1011	2	-	0/0/48/48	0/6/5/5
7	SF4	L	1012	2	-	0/0/48/48	0/6/5/5
7	SF4	L	1013	2	-	0/0/48/48	0/6/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	2MD	C16-C20	-3.38	1.35	1.41
5	K	1002	MGD	C16-C21	-3.08	1.35	1.41
5	A	1002	MGD	PB-O2B	-2.67	1.43	1.54
4	K	1001	2MD	C16-C20	-2.50	1.36	1.41
4	A	1001	2MD	C4-N3	-2.50	1.31	1.35
4	K	1001	2MD	PB-O2B	-2.20	1.45	1.54
5	K	1002	MGD	PB-O2B	-2.09	1.46	1.54
5	A	1002	MGD	PA-O2A	-2.02	1.46	1.54
5	K	1002	MGD	C5-C4	2.04	1.45	1.40
4	K	1001	2MD	C17-N16	2.21	1.38	1.34
4	A	1001	2MD	C17-N16	2.43	1.39	1.34
4	A	1001	2MD	C2-N2	2.49	1.39	1.34
5	A	1002	MGD	C6-C5	2.52	1.46	1.41
4	K	1001	2MD	C5-C4	2.57	1.46	1.40
5	K	1002	MGD	C6-C5	2.76	1.46	1.41
4	A	1001	2MD	C14-N15	2.77	1.48	1.45
5	A	1002	MGD	C5-C4	2.83	1.46	1.40
4	K	1001	2MD	C14-N15	2.88	1.48	1.45
4	K	1001	2MD	C2-N2	2.99	1.40	1.34
4	A	1001	2MD	C5-C4	3.10	1.47	1.40
5	A	1002	MGD	C2-N2	3.35	1.40	1.34
5	K	1002	MGD	C2-N2	3.38	1.40	1.34
4	K	1001	2MD	C6-C5	3.62	1.48	1.41
4	A	1001	2MD	C6-C5	3.75	1.48	1.41
5	K	1002	MGD	C19-N19	3.94	1.42	1.34
5	A	1002	MGD	C19-N19	4.13	1.42	1.34

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1001	2MD	C5-C6-N1	-4.68	117.19	123.59
5	A	1002	MGD	C6-C5-C4	-4.55	115.46	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	2MD	C13-C14-N15	-4.38	106.79	109.73
5	A	1002	MGD	C1'-N9-C4	-4.36	120.36	126.94
4	A	1001	2MD	C5-C6-N1	-4.30	117.71	123.59
4	K	1001	2MD	O11-C7-C14	-4.23	106.00	108.97
4	A	1001	2MD	C6-C5-C4	-4.01	116.10	120.90
5	A	1002	MGD	C5-C6-N1	-3.94	118.20	123.59
4	K	1001	2MD	C1'-N9-C4	-3.87	121.11	126.94
5	K	1002	MGD	C5-C6-N1	-3.78	118.43	123.59
5	K	1002	MGD	C6-C5-C4	-3.74	116.42	120.90
5	K	1002	MGD	C1'-N9-C4	-3.73	121.32	126.94
4	K	1001	2MD	C13-C14-N15	-3.70	107.25	109.73
4	K	1001	2MD	C4-C5-N7	-3.59	106.17	109.48
4	K	1001	2MD	C6-C5-C4	-3.56	116.65	120.90
5	K	1002	MGD	N3-C2-N1	-3.50	122.11	127.44
5	K	1002	MGD	C4-C5-N7	-3.46	106.30	109.48
5	A	1002	MGD	N3-C2-N1	-3.32	122.38	127.44
5	K	1002	MGD	O11-C23-C14	-3.32	106.69	108.96
4	A	1001	2MD	C1'-N9-C4	-3.12	122.23	126.94
4	A	1001	2MD	C4-C5-N7	-2.74	106.95	109.48
4	K	1001	2MD	N3-C2-N1	-2.70	123.34	127.44
5	K	1002	MGD	N18-C19-N20	-2.29	121.77	125.53
4	K	1001	2MD	C10-C11-C12	-2.24	106.98	112.09
4	A	1001	2MD	N3-C2-N1	-2.03	124.36	127.44
5	K	1002	MGD	C21-C16-N15	2.02	121.40	118.85
9	A	1200	EPE	C7-N4-C5	2.04	116.49	111.27
4	K	1001	2MD	C17-N18-C20	2.08	119.22	114.54
4	A	1001	2MD	C17-N18-C20	2.10	119.27	114.54
9	A	1200	EPE	O2S-S-C10	2.18	108.77	106.91
4	A	1001	2MD	N8-C20-N18	2.23	120.18	116.62
5	K	1002	MGD	O3B-PB-O5'	2.24	108.88	102.94
9	A	1200	EPE	C2-C3-N4	2.28	114.71	110.63
4	A	1001	2MD	O3B-PA-O5'	2.29	109.01	102.94
4	A	1001	2MD	O11-C7-C14	2.35	110.61	108.97
5	K	1002	MGD	N22-C21-N20	2.41	120.46	116.62
9	A	1200	EPE	C3-C2-N1	2.53	115.16	110.63
9	A	1200	EPE	C7-N4-C3	2.54	117.78	111.27
4	K	1001	2MD	C16-C20-N8	2.57	121.03	118.34
5	K	1002	MGD	C2'-C1'-N9	2.60	118.26	114.29
5	A	1002	MGD	C19-N20-C21	2.61	120.40	114.54
9	K	1200	EPE	C7-N4-C5	2.62	118.00	111.27
5	A	1002	MGD	C16-C21-N22	2.64	121.10	118.34
5	K	1002	MGD	C19-N20-C21	2.73	120.69	114.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	1002	MGD	N19-C19-N18	2.84	121.90	117.20
5	A	1002	MGD	C2'-C1'-N9	3.02	118.91	114.29
5	A	1002	MGD	O11-C23-C14	3.05	111.05	108.96
4	A	1001	2MD	C2'-C1'-N9	3.24	119.23	114.29
9	K	1200	EPE	C7-N4-C3	3.46	120.15	111.27
5	K	1002	MGD	C17-N18-C19	3.49	120.78	115.94
4	A	1001	2MD	C15-N17-C17	3.51	120.81	115.94
4	A	1001	2MD	C11-O11-C7	3.63	117.77	112.49
9	A	1200	EPE	C5-N4-C3	3.74	117.00	108.90
5	A	1002	MGD	PA-O3B-PB	3.83	143.50	132.73
5	A	1002	MGD	C17-N18-C19	3.89	121.34	115.94
4	A	1001	2MD	C6-N1-C2	3.92	121.38	115.94
9	K	1200	EPE	O1S-S-C10	4.02	110.34	106.91
5	K	1002	MGD	C6-N1-C2	4.26	121.86	115.94
4	K	1001	2MD	C15-N17-C17	4.37	122.00	115.94
4	A	1001	2MD	C15-C16-C20	4.55	118.68	114.56
4	K	1001	2MD	C6-N1-C2	4.55	122.26	115.94
5	K	1002	MGD	C17-C16-C21	4.65	118.77	114.56
9	A	1200	EPE	O1S-S-C10	4.96	111.14	106.91
5	A	1002	MGD	C17-C16-C21	5.15	119.23	114.56
9	K	1200	EPE	C5-N4-C3	5.18	120.12	108.90
4	K	1001	2MD	C15-C16-C20	5.34	119.39	114.56
5	A	1002	MGD	C6-N1-C2	5.36	123.38	115.94

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1001	2MD	C12
4	K	1001	2MD	C12
4	K	1001	2MD	C13

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	K	1010	SF4	FE1-FE3-S2-S4
7	K	1010	SF4	FE2-FE4-S1-S3

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	2MD	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1200	EPE	1	0
4	K	1001	2MD	2	0
9	K	1200	EPE	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.