



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2017 – 10:38 AM EST

PDB ID : 5SUQ  
Title : Structure of mRNA export factors  
Authors : Ren, Y.; Blobel, G.  
Deposited on : 2016-08-03  
Resolution : 6.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

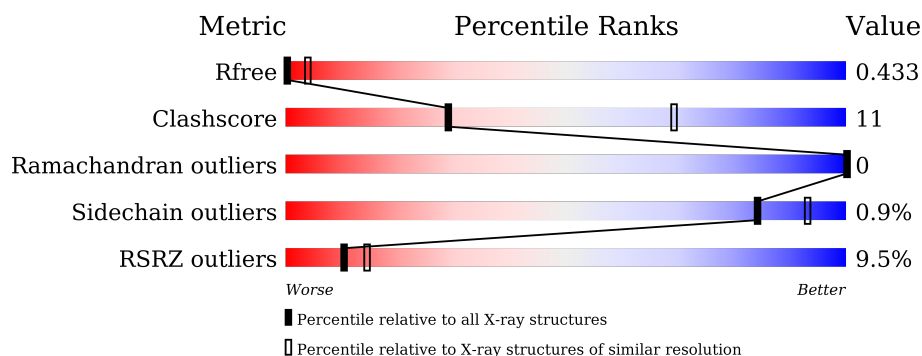
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.00 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))
$R_{free}$	91344	1002 (8.30-3.66)
Clashscore	102246	1050 (8.30-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
Sidechain outliers	100360	1012 (8.30-3.64)
RSRZ outliers	91569	1001 (8.30-3.66)

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. 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	446	<div> <div>9%</div> <div>67%</div> <div>16%</div> <div>•</div> <div>16%</div> </div>
1	C	446	<div> <div>7%</div> <div>66%</div> <div>17%</div> <div>•</div> <div>16%</div> </div>
2	B	400	<div> <div>45%</div> <div>•</div> <div>53%</div> </div>
2	D	400	<div> <div>45%</div> <div>•</div> <div>53%</div> </div>
3	M	2300	<div> <div>93%</div> <div>•</div> <div>•</div> </div>
3	N	2300	<div> <div>93%</div> <div>•</div> <div>•</div> </div>

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	KEG	A	501	-	-	X	-
4	KEG	A	502	-	-	X	-
4	KEG	A	503	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30788 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 ATP-dependent RNA helicase SUB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			3010	1916	523	560	11			
1	C	374	Total	C	N	O	S	0	0	0
			3010	1916	523	560	11			

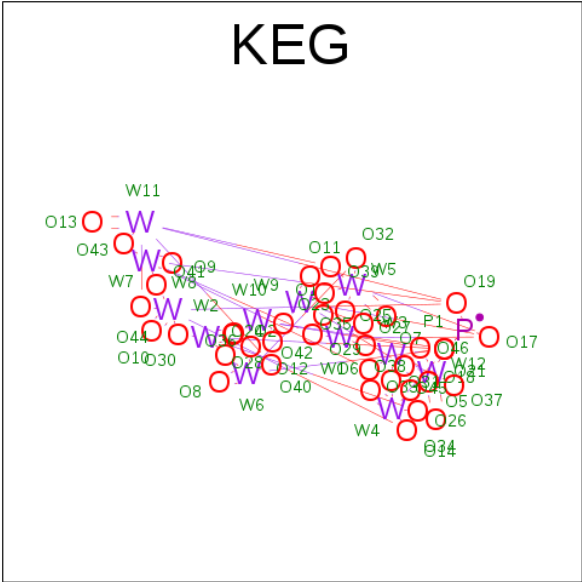
- Molecule 2 is a protein called Tex1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	0	0	0
			940	564	188	188			
2	D	188	Total	C	N	O	0	0	0
			940	564	188	188			

- Molecule 3 is a protein called Tho2, Hpr1, Mft1, and Thp2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	2231	Total	C	N	O	0	0	0
			11155	6693	2231	2231			
3	N	2230	Total	C	N	O	0	0	0
			11150	6690	2230	2230			

- Molecule 4 is 12-TUNGSTOPHOSPHATE (three-letter code: KEG) (formula: O<sub>40</sub>PW<sub>12</sub>).

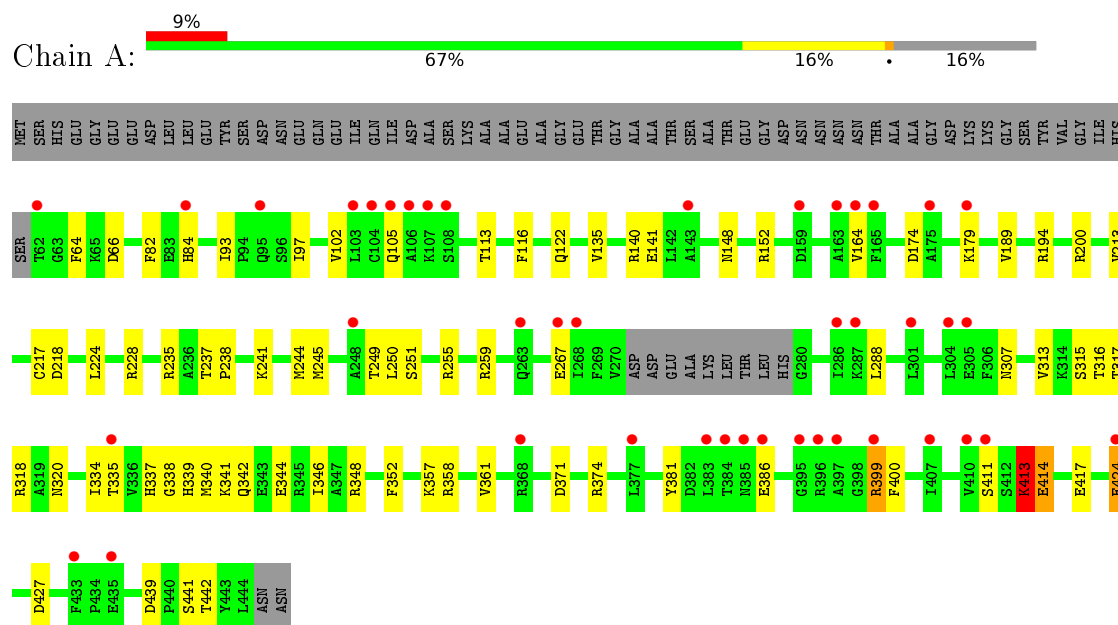


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	O	P	W	0	0
			53	40	1	12		
4	A	1	Total	O	P	W	0	0
			53	40	1	12		
4	A	1	Total	O	P	W	0	0
			53	40	1	12		
4	M	1	Total	O	P	W	0	0
			53	40	1	12		
4	M	1	Total	O	P	W	0	0
			53	40	1	12		
4	M	1	Total	O	P	W	0	0
			53	40	1	12		
4	N	1	Total	O	P	W	0	0
			53	40	1	12		
4	N	1	Total	O	P	W	0	0
			53	40	1	12		
4	N	1	Total	O	P	W	0	0
			53	40	1	12		
4	N	1	Total	O	P	W	0	0
			53	40	1	12		

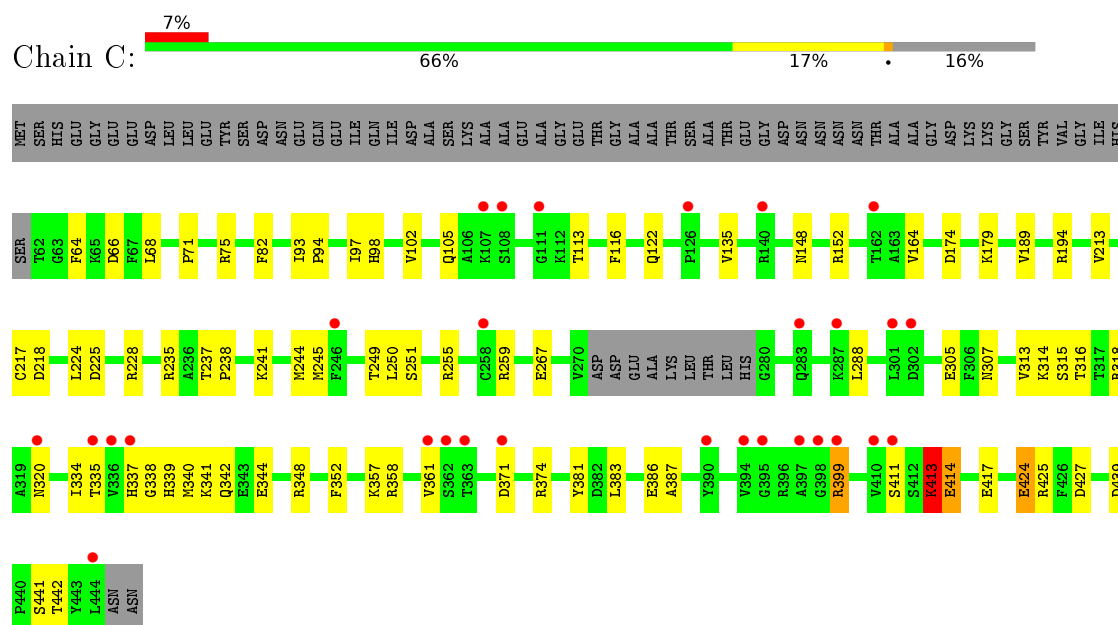
### 3 Residue-property plots

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.

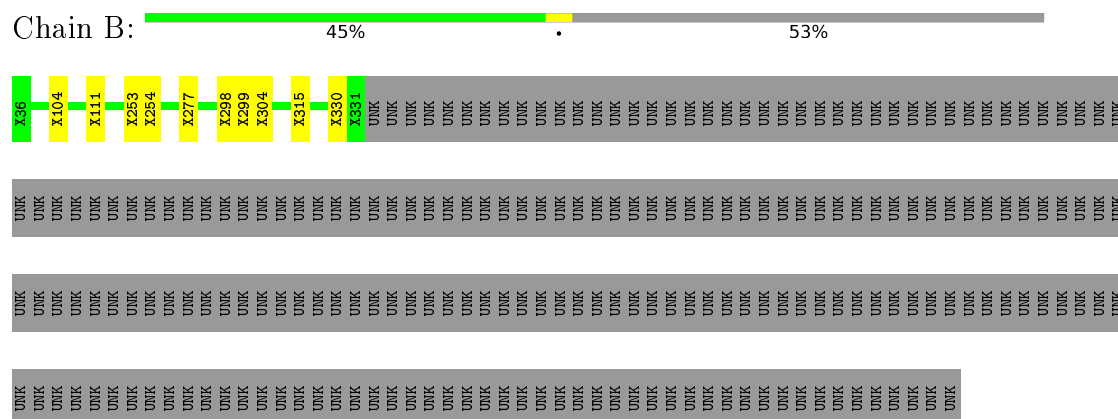
- Molecule 1: ATP-dependent RNA helicase SUB2



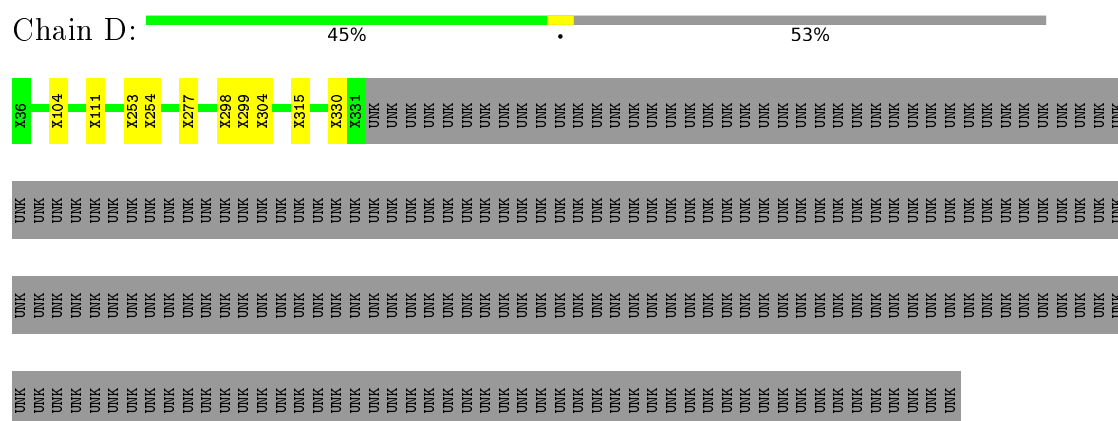
- Molecule 1: ATP-dependent RNA helicase SUB2



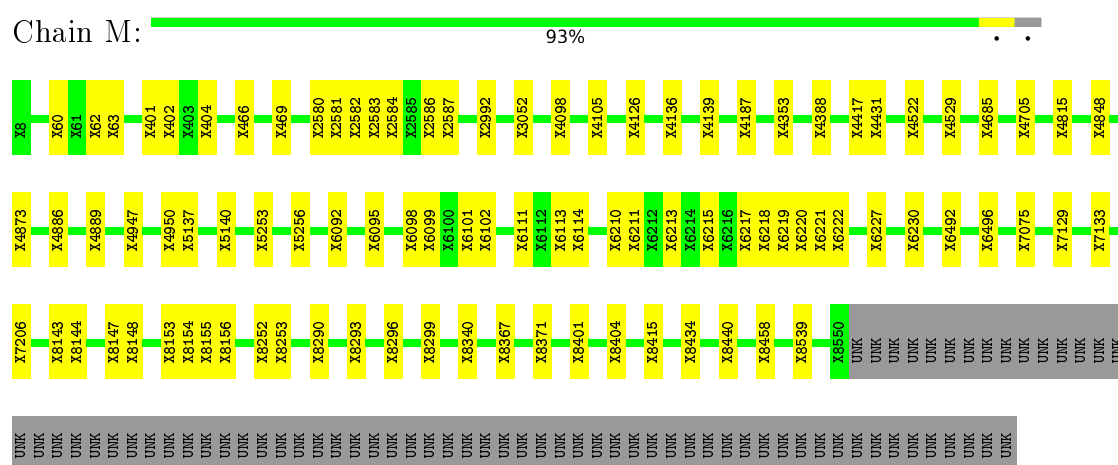
- Molecule 2: Tex1



- Molecule 2: Tex1



- Molecule 3: Tho2, Hpr1, Mft1, and Thp2



- Molecule 3: Tho2, Hpr1, Mft1, and Thp2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.34Å 319.53Å 176.44Å 90.00° 100.96° 90.00°	Depositor
Resolution (Å)	49.57 – 6.00 50.18 – 5.95	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.57-6.00) 96.9 (50.18-5.95)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.71 (at 6.15Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, $R_{free}$	0.436 , 0.434 0.442 , 0.433	Depositor DCC
$R_{free}$ test set	2082 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	293.8	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 316.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.74	EDS
Total number of atoms	30788	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KEG

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	0.41	1/3063 (0.0%)	0.66	9/4131 (0.2%)
1	C	0.41	1/3063 (0.0%)	0.66	9/4131 (0.2%)
All	All	0.41	2/6126 (0.0%)	0.66	18/8262 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	414	GLU	CD-OE1	-5.23	1.19	1.25
1	C	414	GLU	CD-OE1	-5.22	1.20	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	427	ASP	CB-CA-C	-8.73	92.94	110.40
1	A	427	ASP	CB-CA-C	-8.70	93.00	110.40
1	C	427	ASP	CB-CG-OD2	8.41	125.87	118.30
1	A	427	ASP	CB-CG-OD2	8.40	125.86	118.30
1	A	427	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	C	427	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	A	417	GLU	CG-CD-OE2	6.71	131.72	118.30
1	C	417	GLU	CG-CD-OE2	6.69	131.68	118.30
1	C	414	GLU	CB-CA-C	-6.69	97.02	110.40
1	A	414	GLU	CB-CA-C	-6.66	97.07	110.40
1	A	424	GLU	CG-CD-OE1	6.46	131.22	118.30
1	C	424	GLU	CG-CD-OE1	6.44	131.18	118.30
1	C	427	ASP	N-CA-CB	6.07	121.53	110.60
1	A	427	ASP	N-CA-CB	6.04	121.47	110.60
1	C	417	GLU	CA-CB-CG	5.87	126.31	113.40
1	A	417	GLU	CA-CB-CG	5.87	126.30	113.40
1	C	413	LYS	CD-CE-NZ	5.43	124.20	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	LYS	CD-CE-NZ	5.42	124.17	111.70

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	3010	0	3043	158	0
1	C	3010	0	3043	155	0
2	B	940	0	262	6	0
2	D	940	0	262	5	0
3	M	11155	0	2489	100	0
3	N	11150	0	2488	103	0
4	A	159	0	0	53	0
4	M	159	0	0	18	0
4	N	265	0	0	30	0
All	All	30788	0	11587	484	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 11.

All (484) 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:339:HIS:CB	1:C:341:LYS:CA	1.85	1.53
1:A:339:HIS:CB	1:C:341:LYS:HA	1.36	1.51
1:C:98:HIS:CG	3:N:4695:UNK:CB	1.99	1.45
1:A:316:THR:C	1:C:341:LYS:HZ2	1.14	1.43
1:A:316:THR:C	1:C:341:LYS:NZ	1.70	1.42
3:N:4815:UNK:CB	3:N:4873:UNK:CB	2.03	1.36
1:A:339:HIS:HB3	1:C:341:LYS:CA	1.43	1.36
3:M:4815:UNK:CB	3:M:4873:UNK:CB	2.02	1.34
4:A:501:KEG:O45	1:C:341:LYS:HG2	1.19	1.32
1:C:98:HIS:ND1	3:N:4695:UNK:CB	1.85	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:401:UNK:O	3:M:404:UNK:CB	1.83	1.27
3:N:401:UNK:O	3:N:404:UNK:CB	1.83	1.25
3:M:4098:UNK:CB	3:M:4126:UNK:HA	1.69	1.23
3:N:4098:UNK:CB	3:N:4126:UNK:HA	1.69	1.23
3:M:466:UNK:HA	3:M:5253:UNK:CB	1.69	1.23
4:A:503:KEG:O10	1:C:314:LYS:O	1.54	1.22
1:A:200:ARG:NH1	4:A:502:KEG:O2	1.72	1.21
1:A:141:GLU:OE2	1:A:342:GLN:HG2	1.42	1.20
4:A:501:KEG:O5	1:C:344:GLU:HG2	1.42	1.20
2:D:277:UNK:CB	2:D:304:UNK:O	1.90	1.20
1:A:340:MET:HA	4:A:501:KEG:O35	1.27	1.19
2:B:277:UNK:CB	2:B:304:UNK:O	1.90	1.18
1:A:340:MET:O	1:C:339:HIS:HA	1.40	1.17
1:A:339:HIS:CG	1:C:341:LYS:CA	1.92	1.17
1:C:71:PRO:HG2	3:N:4895:UNK:O	1.43	1.16
4:A:501:KEG:O27	1:C:341:LYS:N	1.70	1.16
4:A:502:KEG:O5	1:C:387:ALA:HB3	1.44	1.16
1:A:339:HIS:CB	1:C:341:LYS:N	1.86	1.16
1:A:141:GLU:HG2	1:A:342:GLN:HE21	1.11	1.13
1:A:339:HIS:HB3	1:C:341:LYS:N	1.01	1.11
1:A:342:GLN:HB2	1:C:339:HIS:CE1	1.85	1.10
4:A:501:KEG:O5	1:C:344:GLU:CG	2.00	1.10
4:A:503:KEG:O10	1:C:315:SER:CA	2.00	1.10
1:A:339:HIS:HB2	1:C:341:LYS:HA	1.28	1.09
1:A:342:GLN:CB	1:C:339:HIS:CE1	2.36	1.09
3:M:6098:UNK:O	3:M:6101:UNK:CB	2.02	1.08
3:N:6098:UNK:O	3:N:6101:UNK:CB	2.02	1.08
3:N:4886:UNK:HA	3:N:4950:UNK:C	1.84	1.07
4:A:501:KEG:O45	1:C:341:LYS:CG	2.01	1.07
1:A:340:MET:CA	4:A:501:KEG:O35	2.01	1.07
3:M:4886:UNK:HA	3:M:4950:UNK:C	1.84	1.07
3:N:2992:UNK:O	3:N:3052:UNK:O	1.72	1.06
1:C:413:LYS:HD2	1:C:414:GLU:H	1.19	1.06
1:A:339:HIS:CG	1:C:341:LYS:HA	1.70	1.06
3:M:2992:UNK:O	3:M:3052:UNK:O	1.72	1.05
3:N:4886:UNK:CB	3:N:4950:UNK:O	2.05	1.05
1:A:413:LYS:HD2	1:A:414:GLU:H	1.19	1.04
1:A:358:ARG:NH1	3:M:4353:UNK:HA	1.73	1.04
3:M:4886:UNK:CB	3:M:4950:UNK:O	2.05	1.03
1:C:98:HIS:CD2	3:N:4695:UNK:CB	2.41	1.03
3:N:6219:UNK:O	3:N:6222:UNK:N	1.93	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ARG:NH1	3:M:4353:UNK:CA	2.21	1.01
1:A:141:GLU:CG	1:A:342:GLN:HE21	1.73	1.01
3:M:6219:UNK:O	3:M:6222:UNK:N	1.93	1.01
4:A:503:KEG:O10	1:C:315:SER:HA	1.55	1.00
3:N:8143:UNK:O	3:N:8147:UNK:N	1.94	1.00
3:M:8143:UNK:O	3:M:8147:UNK:N	1.94	0.99
1:A:340:MET:C	1:C:339:HIS:HA	1.83	0.98
1:A:342:GLN:HB2	1:C:339:HIS:HE1	1.23	0.98
3:N:7129:UNK:O	3:N:7133:UNK:N	1.98	0.96
1:A:339:HIS:O	1:C:340:MET:CA	2.13	0.96
1:C:75:ARG:HH12	3:N:4943:UNK:CB	1.79	0.95
3:M:7129:UNK:O	3:M:7133:UNK:N	1.98	0.94
3:M:4388:UNK:CB	3:M:4417:UNK:CB	2.46	0.94
3:N:4388:UNK:CB	3:N:4417:UNK:CB	2.46	0.93
3:M:466:UNK:CA	3:M:5253:UNK:CB	2.47	0.93
1:A:358:ARG:HH11	3:M:4353:UNK:CA	1.82	0.93
3:N:4886:UNK:CA	3:N:4950:UNK:C	2.46	0.93
1:A:374:ARG:NE	3:M:4431:UNK:H2	1.67	0.92
3:M:4886:UNK:CA	3:M:4950:UNK:C	2.46	0.92
1:A:317:THR:N	1:C:341:LYS:NZ	2.17	0.92
1:A:341:LYS:N	1:C:339:HIS:HB3	1.85	0.91
3:N:466:UNK:HA	3:N:5253:UNK:CB	2.01	0.91
3:M:8153:UNK:O	3:M:8156:UNK:CB	2.19	0.90
4:A:503:KEG:O10	1:C:315:SER:CB	2.20	0.90
1:A:337:HIS:CE1	1:C:341:LYS:HD3	2.06	0.90
1:A:339:HIS:O	1:C:340:MET:HA	1.72	0.90
3:N:8153:UNK:O	3:N:8156:UNK:CB	2.19	0.90
1:A:340:MET:C	1:C:339:HIS:CA	2.39	0.90
1:A:339:HIS:C	1:C:340:MET:N	2.27	0.88
3:M:2583:UNK:O	3:M:2587:UNK:N	2.07	0.88
3:M:4105:UNK:C	3:M:4187:UNK:O	2.22	0.88
3:N:2583:UNK:O	3:N:2587:UNK:N	2.07	0.87
3:N:4105:UNK:C	3:N:4187:UNK:O	2.22	0.87
3:M:401:UNK:O	3:M:404:UNK:N	2.07	0.87
1:A:316:THR:CB	1:C:341:LYS:NZ	2.37	0.87
1:C:413:LYS:HD2	1:C:414:GLU:N	1.91	0.86
1:A:316:THR:HB	1:C:341:LYS:CE	2.06	0.85
1:A:340:MET:O	1:C:339:HIS:CA	2.24	0.85
2:B:253:UNK:O	2:B:254:UNK:CB	2.25	0.85
3:N:401:UNK:O	3:N:404:UNK:N	2.08	0.85
1:A:141:GLU:CD	1:A:342:GLN:HG2	1.96	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:HIS:HE1	4:A:501:KEG:O11	1.59	0.84
1:A:235:ARG:HH12	3:M:6215:UNK:CB	1.89	0.84
3:M:4889:UNK:CB	3:M:4950:UNK:CB	2.54	0.84
3:N:4889:UNK:CB	3:N:4950:UNK:CB	2.55	0.84
1:A:141:GLU:OE2	1:A:342:GLN:CG	2.23	0.84
2:D:253:UNK:O	2:D:254:UNK:CB	2.25	0.84
1:A:140:ARG:HD2	4:A:503:KEG:O36	1.76	0.84
1:A:337:HIS:CE1	4:A:501:KEG:O11	2.31	0.83
1:A:413:LYS:HD2	1:A:414:GLU:N	1.91	0.83
1:A:339:HIS:HE1	1:C:342:GLN:OE1	1.61	0.82
3:N:4886:UNK:HA	3:N:4950:UNK:CB	2.09	0.82
3:M:8415:UNK:CB	3:M:8440:UNK:CB	2.57	0.82
3:M:4886:UNK:HA	3:M:4950:UNK:CB	2.10	0.81
3:M:6210:UNK:O	3:M:6213:UNK:N	2.13	0.81
3:N:8415:UNK:CB	3:N:8440:UNK:CB	2.57	0.81
3:M:4522:UNK:CB	3:M:4529:UNK:N	2.43	0.81
3:N:4522:UNK:CB	3:N:4529:UNK:N	2.43	0.81
4:A:501:KEG:O11	1:C:341:LYS:HD3	1.81	0.81
3:M:4886:UNK:CA	3:M:4950:UNK:O	2.29	0.81
3:M:6111:UNK:O	3:M:6114:UNK:HA	1.81	0.80
3:N:6210:UNK:O	3:N:6213:UNK:N	2.13	0.80
1:A:374:ARG:HE	3:M:4431:UNK:H2	1.29	0.80
3:N:6111:UNK:O	3:N:6114:UNK:HA	1.82	0.79
3:N:8252:UNK:O	3:N:8253:UNK:C	2.30	0.79
3:N:2580:UNK:O	3:N:2584:UNK:N	2.16	0.79
1:A:84:HIS:HB2	1:A:400:PHE:HZ	1.47	0.78
4:A:503:KEG:O10	1:C:314:LYS:C	2.20	0.78
3:M:8252:UNK:O	3:M:8253:UNK:C	2.31	0.78
3:N:4886:UNK:CA	3:N:4950:UNK:O	2.28	0.78
1:A:316:THR:CA	1:C:341:LYS:NZ	2.47	0.78
3:N:4889:UNK:CB	3:N:4947:UNK:HA	2.14	0.78
4:A:501:KEG:O1	1:C:341:LYS:N	2.15	0.78
3:M:4889:UNK:CB	3:M:4947:UNK:HA	2.14	0.78
3:M:2580:UNK:O	3:M:2584:UNK:N	2.16	0.78
1:C:358:ARG:NH1	3:N:4352:UNK:O	2.16	0.77
1:A:200:ARG:NH1	4:A:502:KEG:O30	2.18	0.76
1:A:341:LYS:N	1:C:339:HIS:CB	2.43	0.76
1:A:141:GLU:HG2	1:A:342:GLN:NE2	1.96	0.76
3:M:4886:UNK:CB	3:M:4950:UNK:C	2.64	0.75
3:N:4098:UNK:CB	3:N:4126:UNK:CA	2.59	0.75
3:N:4886:UNK:CB	3:N:4950:UNK:C	2.64	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:HIS:CE1	1:C:342:GLN:OE1	2.39	0.75
3:N:4522:UNK:CB	3:N:4529:UNK:H2	2.00	0.75
4:A:501:KEG:O5	1:C:344:GLU:CD	2.24	0.75
3:M:4522:UNK:CB	3:M:4529:UNK:H2	2.00	0.75
3:N:401:UNK:O	3:N:404:UNK:CA	2.35	0.75
1:A:316:THR:HB	1:C:341:LYS:NZ	2.02	0.74
3:M:401:UNK:O	3:M:404:UNK:CA	2.35	0.74
3:M:466:UNK:CB	3:M:5253:UNK:CB	2.66	0.74
3:N:8144:UNK:HA	3:N:8147:UNK:CB	2.18	0.74
3:M:8144:UNK:HA	3:M:8147:UNK:CB	2.18	0.74
3:N:62:UNK:O	3:N:63:UNK:C	2.34	0.74
1:A:358:ARG:HH12	3:M:4353:UNK:HA	1.49	0.74
3:M:62:UNK:O	3:M:63:UNK:C	2.34	0.74
3:M:2582:UNK:O	3:M:2586:UNK:N	2.21	0.73
1:C:71:PRO:HG2	3:N:4895:UNK:C	2.18	0.73
1:A:339:HIS:C	1:C:340:MET:CA	2.53	0.73
1:A:340:MET:O	1:C:339:HIS:CG	2.42	0.72
3:N:6219:UNK:O	3:N:6220:UNK:C	2.36	0.72
1:A:337:HIS:CE1	1:C:341:LYS:HE2	2.24	0.72
3:N:2582:UNK:O	3:N:2586:UNK:N	2.21	0.72
3:N:6219:UNK:C	3:N:6221:UNK:N	2.51	0.71
3:M:4098:UNK:CB	3:M:4126:UNK:CA	2.59	0.71
1:C:66:ASP:OD1	3:N:4705:UNK:CB	2.38	0.71
1:A:339:HIS:CG	1:C:341:LYS:N	2.43	0.71
1:A:339:HIS:O	1:C:340:MET:C	2.29	0.71
1:A:84:HIS:HB2	1:A:400:PHE:CZ	2.26	0.71
3:M:6219:UNK:O	3:M:6220:UNK:C	2.36	0.71
1:A:340:MET:C	1:C:339:HIS:CB	2.59	0.71
1:A:339:HIS:C	1:C:339:HIS:C	2.49	0.71
1:A:337:HIS:HE1	1:C:341:LYS:HD3	1.53	0.70
4:A:502:KEG:O5	1:C:387:ALA:CB	2.33	0.70
4:A:503:KEG:O41	1:C:314:LYS:O	2.10	0.69
3:N:8340:UNK:CB	3:N:8539:UNK:HA	2.22	0.69
1:A:316:THR:O	1:C:341:LYS:NZ	1.92	0.69
3:M:8340:UNK:CB	3:M:8539:UNK:HA	2.22	0.68
1:A:374:ARG:CZ	3:M:4431:UNK:H2	2.05	0.68
1:A:141:GLU:CD	1:A:342:GLN:CG	2.63	0.68
1:C:94:PRO:HB3	3:N:4699:UNK:HA	1.76	0.68
3:N:6492:UNK:O	3:N:6496:UNK:CB	2.42	0.67
1:A:337:HIS:CE1	1:C:341:LYS:CD	2.79	0.66
3:M:6219:UNK:C	3:M:6221:UNK:N	2.51	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:6492:UNK:O	3:M:6496:UNK:CB	2.42	0.66
1:A:317:THR:N	1:C:341:LYS:HZ2	1.80	0.66
1:C:75:ARG:NH1	3:N:4943:UNK:CB	2.56	0.66
1:A:342:GLN:CA	1:C:339:HIS:CE1	2.55	0.66
1:A:337:HIS:ND1	1:A:338:GLY:O	2.29	0.66
1:A:341:LYS:HE2	1:C:316:THR:HB	1.77	0.65
1:C:337:HIS:ND1	1:C:338:GLY:O	2.29	0.65
1:A:340:MET:N	1:C:339:HIS:C	2.50	0.65
1:C:439:ASP:OD2	1:C:441:SER:OG	2.15	0.65
1:C:174:ASP:OD1	1:C:194:ARG:NH1	2.30	0.64
1:A:358:ARG:HH11	3:M:4353:UNK:C	2.10	0.64
1:A:174:ASP:OD1	1:A:194:ARG:NH1	2.30	0.64
1:C:235:ARG:HH12	3:N:6215:UNK:CB	2.10	0.64
1:A:341:LYS:HE2	1:C:316:THR:CB	2.28	0.64
1:A:358:ARG:NH1	3:M:4353:UNK:N	2.17	0.64
2:B:298:UNK:O	2:B:299:UNK:CB	2.46	0.64
1:A:141:GLU:CG	1:A:342:GLN:NE2	2.56	0.63
3:N:7129:UNK:O	3:N:7133:UNK:CB	2.47	0.63
1:A:224:LEU:O	1:A:228:ARG:HG3	1.99	0.63
3:M:7129:UNK:O	3:M:7133:UNK:CB	2.47	0.63
1:A:316:THR:HB	1:C:341:LYS:CD	2.28	0.62
1:A:339:HIS:HA	1:C:340:MET:N	2.14	0.62
1:A:439:ASP:OD2	1:A:441:SER:OG	2.15	0.62
1:C:237:THR:OG1	1:C:241:LYS:NZ	2.29	0.62
4:A:502:KEG:O31	1:C:386:GLU:HG3	2.00	0.62
1:C:224:LEU:O	1:C:228:ARG:HG3	1.99	0.62
1:C:318:ARG:NH2	1:C:381:TYR:HE2	1.99	0.61
3:N:8434:UNK:CB	3:N:8458:UNK:CB	2.79	0.61
1:A:318:ARG:NH2	1:A:381:TYR:HE2	1.99	0.60
3:N:8155:UNK:C	3:N:8156:UNK:O	2.49	0.60
1:A:339:HIS:CA	1:C:340:MET:N	2.64	0.60
3:M:8434:UNK:CB	3:M:8458:UNK:CB	2.79	0.60
1:A:341:LYS:NZ	1:C:316:THR:OG1	2.34	0.60
1:C:68:LEU:HD21	3:N:4868:UNK:CB	2.31	0.60
3:M:2580:UNK:O	3:M:2584:UNK:CB	2.50	0.60
1:A:337:HIS:CE1	1:C:341:LYS:CE	2.85	0.60
2:D:298:UNK:O	2:D:299:UNK:CB	2.46	0.60
3:M:8155:UNK:O	3:M:8156:UNK:C	2.49	0.60
3:N:2580:UNK:O	3:N:2584:UNK:CB	2.50	0.60
1:A:141:GLU:CD	1:A:342:GLN:HE21	2.05	0.60
3:N:8155:UNK:O	3:N:8156:UNK:C	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:MET:HA	1:C:339:HIS:O	2.01	0.59
1:A:341:LYS:CD	1:C:339:HIS:CB	2.81	0.58
3:M:6218:UNK:O	3:M:6221:UNK:CB	2.51	0.58
3:N:6218:UNK:O	3:N:6221:UNK:CB	2.52	0.58
3:M:8155:UNK:C	3:M:8156:UNK:O	2.49	0.58
3:N:4685:UNK:CB	3:N:4848:UNK:HA	2.35	0.57
3:N:8367:UNK:CB	3:N:8404:UNK:O	2.53	0.57
1:A:313:VAL:HG12	1:A:315:SER:H	1.70	0.56
1:A:316:THR:HB	1:C:341:LYS:HD2	1.86	0.56
1:A:340:MET:CA	1:C:339:HIS:O	2.53	0.56
3:M:4685:UNK:CB	3:M:4848:UNK:HA	2.35	0.56
1:A:141:GLU:CD	1:A:342:GLN:NE2	2.59	0.56
1:C:334:ILE:HG23	1:C:357:LYS:HD2	1.87	0.56
1:A:339:HIS:HB3	4:A:501:KEG:O27	2.04	0.56
1:C:313:VAL:HG12	1:C:315:SER:H	1.70	0.56
3:M:6210:UNK:H	3:M:6213:UNK:CB	2.19	0.56
3:M:8367:UNK:CB	3:M:8404:UNK:O	2.53	0.56
1:A:334:ILE:HG23	1:A:357:LYS:HD2	1.87	0.56
3:N:4886:UNK:HA	3:N:4950:UNK:CA	2.36	0.56
3:N:6210:UNK:H	3:N:6213:UNK:CB	2.19	0.55
2:B:104:UNK:O	2:B:111:UNK:HA	2.06	0.55
1:A:337:HIS:NE2	1:C:341:LYS:HE2	2.22	0.55
1:A:341:LYS:CE	1:C:316:THR:OG1	2.55	0.55
3:M:4886:UNK:HA	3:M:4950:UNK:CA	2.36	0.54
1:A:374:ARG:NE	3:M:4431:UNK:N	2.44	0.54
2:D:104:UNK:O	2:D:111:UNK:HA	2.06	0.54
3:N:6227:UNK:O	3:N:6230:UNK:CB	2.56	0.54
3:M:6227:UNK:O	3:M:6230:UNK:CB	2.56	0.53
4:A:502:KEG:O25	1:C:425:ARG:NE	2.35	0.53
4:A:503:KEG:O10	1:C:315:SER:N	2.39	0.53
3:M:60:UNK:O	3:M:63:UNK:CB	2.57	0.53
3:M:6099:UNK:O	3:M:6102:UNK:N	2.42	0.53
3:M:6210:UNK:O	3:M:6211:UNK:C	2.57	0.53
1:A:339:HIS:CG	1:C:340:MET:C	2.30	0.53
3:N:6210:UNK:O	3:N:6211:UNK:C	2.57	0.53
4:A:501:KEG:O13	1:C:320:ASN:ND2	2.42	0.52
1:A:342:GLN:CB	1:C:339:HIS:HE1	1.95	0.52
1:A:386:GLU:OE2	1:C:225:ASP:OD2	2.27	0.52
3:N:6219:UNK:O	3:N:6221:UNK:N	2.43	0.52
1:A:340:MET:HA	4:A:501:KEG:O32	2.10	0.52
1:A:316:THR:O	1:C:341:LYS:CE	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:6455:UNK:CB	3:N:8119:UNK:CB	2.87	0.52
3:M:5137:UNK:N	3:M:5140:UNK:CB	2.73	0.52
3:M:6219:UNK:O	3:M:6221:UNK:N	2.43	0.52
3:N:6092:UNK:N	3:N:6095:UNK:CB	2.73	0.52
3:N:6099:UNK:O	3:N:6102:UNK:N	2.42	0.52
1:A:413:LYS:CD	1:A:414:GLU:N	2.69	0.52
1:C:344:GLU:O	1:C:348:ARG:HG3	2.10	0.52
3:N:60:UNK:O	3:N:63:UNK:CB	2.57	0.52
3:N:5137:UNK:N	3:N:5140:UNK:CB	2.73	0.52
3:N:469:UNK:CB	3:N:5253:UNK:HA	2.40	0.52
1:A:237:THR:OG1	1:A:241:LYS:NZ	2.29	0.51
1:A:141:GLU:HG2	1:A:346:ILE:CG1	2.40	0.51
1:A:344:GLU:O	1:A:348:ARG:HG3	2.10	0.51
1:A:341:LYS:HD2	1:C:339:HIS:CG	2.44	0.51
1:A:340:MET:CA	1:C:339:HIS:C	2.78	0.51
3:M:469:UNK:CB	3:M:5256:UNK:CB	2.88	0.51
3:M:6092:UNK:N	3:M:6095:UNK:CB	2.73	0.51
1:A:255:ARG:O	1:A:259:ARG:HG3	2.10	0.51
4:A:503:KEG:O10	1:C:315:SER:HB3	2.09	0.51
1:C:255:ARG:O	1:C:259:ARG:HG3	2.10	0.51
3:N:6099:UNK:C	3:N:6101:UNK:N	2.73	0.50
1:C:413:LYS:CD	1:C:414:GLU:N	2.69	0.50
3:M:62:UNK:O	3:M:63:UNK:O	2.30	0.50
3:M:8290:UNK:O	3:M:8293:UNK:CB	2.60	0.50
3:M:8296:UNK:O	3:M:8299:UNK:O	2.30	0.50
3:N:8340:UNK:CB	3:N:8539:UNK:CA	2.90	0.50
3:M:8252:UNK:O	3:M:8253:UNK:O	2.30	0.50
1:A:288:LEU:O	1:A:411:SER:HA	2.12	0.50
3:N:8155:UNK:O	3:N:8156:UNK:O	2.30	0.50
3:N:8371:UNK:CB	3:N:8401:UNK:HA	2.42	0.50
3:M:8155:UNK:O	3:M:8156:UNK:O	2.30	0.49
1:C:71:PRO:CG	3:N:4895:UNK:O	2.37	0.49
4:A:503:KEG:O34	1:C:315:SER:HA	2.11	0.49
1:A:340:MET:C	1:C:339:HIS:CG	2.81	0.49
1:C:288:LEU:O	1:C:411:SER:HA	2.12	0.49
3:M:8154:UNK:O	3:M:8156:UNK:O	2.30	0.49
3:M:8371:UNK:CB	3:M:8401:UNK:HA	2.42	0.49
1:C:305:GLU:OE1	3:N:4407:UNK:CB	2.60	0.49
3:N:62:UNK:O	3:N:63:UNK:O	2.30	0.49
3:N:8252:UNK:O	3:N:8253:UNK:O	2.30	0.49
3:N:8290:UNK:O	3:N:8293:UNK:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:8296:UNK:O	3:N:8299:UNK:O	2.30	0.49
1:A:340:MET:O	1:C:339:HIS:CB	2.61	0.49
3:N:8154:UNK:O	3:N:8156:UNK:O	2.30	0.49
1:A:339:HIS:CD2	1:C:340:MET:C	2.78	0.49
1:A:93:ILE:O	1:A:97:ILE:HG12	2.12	0.49
3:M:469:UNK:CB	3:M:5253:UNK:HA	2.43	0.49
3:N:4886:UNK:N	3:N:4950:UNK:O	2.46	0.49
1:C:93:ILE:O	1:C:97:ILE:HG12	2.12	0.48
1:A:358:ARG:HH11	3:M:4353:UNK:HA	1.50	0.48
1:A:341:LYS:HD3	1:C:339:HIS:CB	2.43	0.48
3:N:401:UNK:C	3:N:404:UNK:CB	2.83	0.48
1:A:358:ARG:HH12	3:M:4353:UNK:CA	2.12	0.48
1:A:316:THR:HB	1:C:341:LYS:HE2	1.95	0.48
3:M:4136:UNK:O	3:M:4139:UNK:N	2.47	0.48
3:N:7075:UNK:CB	3:N:7206:UNK:CB	2.92	0.48
4:A:503:KEG:O19	4:A:503:KEG:O41	2.32	0.48
4:N:8705:KEG:O19	4:N:8705:KEG:O41	2.32	0.48
3:M:4886:UNK:N	3:M:4950:UNK:O	2.47	0.47
1:C:164:VAL:HA	1:C:189:VAL:O	2.14	0.47
4:M:8701:KEG:O41	4:M:8701:KEG:O19	2.32	0.47
4:N:8701:KEG:O41	4:N:8701:KEG:O19	2.32	0.47
4:A:501:KEG:O41	4:A:501:KEG:O19	2.32	0.47
3:N:4136:UNK:O	3:N:4139:UNK:N	2.47	0.47
4:N:8702:KEG:O41	4:N:8702:KEG:O19	2.32	0.47
3:M:6098:UNK:O	3:M:6101:UNK:N	2.48	0.47
3:M:7075:UNK:CB	3:M:7206:UNK:CB	2.92	0.47
1:C:305:GLU:OE2	3:N:4407:UNK:CB	2.62	0.47
1:A:341:LYS:HD3	1:C:339:HIS:HB2	1.96	0.47
1:A:164:VAL:HA	1:A:189:VAL:O	2.14	0.47
3:M:8340:UNK:CB	3:M:8539:UNK:CA	2.90	0.47
4:N:8703:KEG:O41	4:N:8703:KEG:O19	2.33	0.47
1:A:371:ASP:OD2	1:A:399:ARG:HD3	2.15	0.47
1:C:439:ASP:HB3	1:C:442:THR:HG23	1.97	0.47
4:M:8703:KEG:O17	4:M:8703:KEG:O35	2.33	0.47
4:N:8704:KEG:O41	4:N:8704:KEG:O19	2.32	0.47
4:A:501:KEG:O35	4:A:501:KEG:O17	2.33	0.47
1:C:307:ASN:HB3	1:C:374:ARG:O	2.15	0.47
4:M:8702:KEG:O19	4:M:8702:KEG:O41	2.32	0.47
3:N:6098:UNK:O	3:N:6101:UNK:N	2.48	0.47
4:M:8703:KEG:O19	4:M:8703:KEG:O41	2.32	0.47
4:A:502:KEG:O19	4:A:502:KEG:O43	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:6112:UNK:HA	3:N:6113:UNK:HA	1.71	0.46
1:A:307:ASN:HB3	1:A:374:ARG:O	2.16	0.46
4:M:8701:KEG:O35	4:M:8701:KEG:O17	2.33	0.46
4:N:8702:KEG:O43	4:N:8702:KEG:O19	2.34	0.46
1:C:238:PRO:O	1:C:241:LYS:HD3	2.16	0.46
4:A:501:KEG:O38	4:A:501:KEG:O21	2.34	0.46
3:M:6099:UNK:C	3:M:6101:UNK:N	2.73	0.46
4:M:8702:KEG:O35	4:M:8702:KEG:O17	2.33	0.46
4:N:8702:KEG:O35	4:N:8702:KEG:O17	2.33	0.46
4:A:501:KEG:O43	4:A:501:KEG:O19	2.34	0.46
4:A:502:KEG:O19	4:A:502:KEG:O41	2.32	0.46
3:M:8340:UNK:CB	3:M:8539:UNK:N	2.79	0.46
4:M:8702:KEG:O43	4:M:8702:KEG:O19	2.33	0.46
4:N:8701:KEG:O21	4:N:8701:KEG:O38	2.34	0.46
4:M:8703:KEG:O19	4:M:8703:KEG:O43	2.33	0.46
4:M:8703:KEG:O38	4:M:8703:KEG:O21	2.34	0.46
4:N:8701:KEG:O43	4:N:8701:KEG:O19	2.34	0.46
4:N:8702:KEG:O38	4:N:8702:KEG:O21	2.34	0.46
4:M:8701:KEG:O21	4:M:8701:KEG:O38	2.34	0.46
4:M:8702:KEG:O38	4:M:8702:KEG:O21	2.34	0.46
3:N:8340:UNK:CB	3:N:8539:UNK:N	2.79	0.46
1:A:341:LYS:CD	1:C:339:HIS:HB3	2.45	0.46
4:N:8705:KEG:O19	4:N:8705:KEG:O43	2.34	0.46
1:A:179:LYS:HE3	1:A:179:LYS:HB2	1.57	0.46
3:M:402:UNK:C	3:M:404:UNK:N	2.76	0.46
4:N:8703:KEG:O35	4:N:8703:KEG:O17	2.33	0.46
4:N:8705:KEG:O21	4:N:8705:KEG:O38	2.34	0.46
1:A:339:HIS:HA	1:C:340:MET:H	1.81	0.46
4:A:502:KEG:O17	4:A:502:KEG:O35	2.33	0.46
4:N:8704:KEG:O43	4:N:8704:KEG:O19	2.33	0.46
1:C:371:ASP:OD2	1:C:399:ARG:HD3	2.15	0.45
1:A:374:ARG:NH2	3:M:4431:UNK:H2	2.14	0.45
4:N:8704:KEG:O35	4:N:8704:KEG:O17	2.33	0.45
1:C:383:LEU:HA	1:C:383:LEU:HD12	1.85	0.45
4:N:8703:KEG:O21	4:N:8703:KEG:O38	2.34	0.45
4:N:8705:KEG:O17	4:N:8705:KEG:O35	2.33	0.45
1:A:238:PRO:O	1:A:241:LYS:HD3	2.15	0.45
4:A:502:KEG:O21	4:A:502:KEG:O38	2.34	0.45
3:N:466:UNK:CA	3:N:5253:UNK:CB	2.86	0.45
4:A:503:KEG:O17	4:A:503:KEG:O35	2.33	0.45
4:M:8701:KEG:O43	4:M:8701:KEG:O19	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:401:UNK:C	3:N:404:UNK:N	2.79	0.45
4:N:8701:KEG:O17	4:N:8701:KEG:O35	2.33	0.45
4:N:8703:KEG:O43	4:N:8703:KEG:O19	2.33	0.45
1:A:439:ASP:HB3	1:A:442:THR:HG23	1.97	0.45
4:A:503:KEG:O21	4:A:503:KEG:O38	2.34	0.45
1:A:64:PHE:CE2	1:A:82:PHE:HB3	2.51	0.45
1:C:64:PHE:CE2	1:C:82:PHE:HB3	2.51	0.45
3:N:402:UNK:C	3:N:404:UNK:N	2.75	0.45
4:A:503:KEG:O19	4:A:503:KEG:O43	2.34	0.45
1:C:251:SER:O	1:C:255:ARG:HG3	2.16	0.45
4:N:8704:KEG:O21	4:N:8704:KEG:O38	2.34	0.45
3:M:401:UNK:C	3:M:404:UNK:N	2.78	0.45
3:M:6113:UNK:CB	3:M:6114:UNK:CB	2.95	0.45
1:A:141:GLU:HB3	1:A:346:ILE:HD11	1.98	0.45
1:A:251:SER:O	1:A:255:ARG:HG3	2.16	0.45
1:A:339:HIS:O	1:C:341:LYS:N	2.48	0.45
3:N:6113:UNK:CB	3:N:6114:UNK:CB	2.95	0.45
1:A:340:MET:C	4:A:501:KEG:O7	2.56	0.44
1:A:66:ASP:HB3	3:M:4705:UNK:CB	2.47	0.44
1:C:179:LYS:HB2	1:C:179:LYS:HE3	1.57	0.44
3:M:6217:UNK:O	3:M:6220:UNK:CB	2.66	0.44
3:N:4886:UNK:CA	3:N:4950:UNK:CB	2.91	0.44
1:A:342:GLN:CB	1:C:339:HIS:NE2	2.39	0.44
1:C:97:ILE:HD12	1:C:122:GLN:HG2	1.99	0.44
1:A:341:LYS:HE2	1:C:316:THR:OG1	2.18	0.44
1:A:341:LYS:HD2	1:C:339:HIS:CB	2.47	0.44
3:N:2582:UNK:O	3:N:2586:UNK:CB	2.65	0.44
1:A:97:ILE:HD12	1:A:122:GLN:HG2	1.99	0.44
3:M:2582:UNK:O	3:M:2586:UNK:CB	2.65	0.44
3:M:401:UNK:C	3:M:404:UNK:CB	2.83	0.44
3:M:6492:UNK:O	3:M:6496:UNK:N	2.51	0.44
4:N:8702:KEG:O37	4:N:8702:KEG:O21	2.36	0.44
1:C:334:ILE:HD11	1:C:352:PHE:HB2	2.00	0.44
3:N:6492:UNK:O	3:N:6496:UNK:N	2.51	0.44
4:A:502:KEG:O19	4:A:502:KEG:O44	2.37	0.43
4:N:8701:KEG:O37	4:N:8701:KEG:O21	2.37	0.43
1:A:320:ASN:ND2	1:C:341:LYS:HE3	2.34	0.43
4:N:8704:KEG:O44	4:N:8704:KEG:O19	2.37	0.43
4:A:501:KEG:O37	4:A:501:KEG:O21	2.36	0.43
4:M:8703:KEG:O37	4:M:8703:KEG:O21	2.36	0.43
3:N:8144:UNK:O	3:N:8148:UNK:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:8701:KEG:O19	4:N:8701:KEG:O44	2.37	0.43
1:A:102:VAL:HB	1:A:244:MET:HG2	2.00	0.43
4:M:8702:KEG:O37	4:M:8702:KEG:O21	2.36	0.43
4:N:8704:KEG:O21	4:N:8704:KEG:O37	2.36	0.43
4:N:8705:KEG:O44	4:N:8705:KEG:O19	2.37	0.43
4:A:501:KEG:O44	4:A:501:KEG:O19	2.37	0.43
4:N:8705:KEG:O21	4:N:8705:KEG:O37	2.36	0.43
1:A:135:VAL:HG22	1:A:213:VAL:HB	2.01	0.43
4:A:502:KEG:O21	4:A:502:KEG:O37	2.37	0.43
3:N:6217:UNK:O	3:N:6220:UNK:CB	2.66	0.43
3:N:7129:UNK:O	3:N:7133:UNK:CA	2.66	0.43
3:M:7129:UNK:O	3:M:7133:UNK:CA	2.66	0.42
3:M:8144:UNK:O	3:M:8148:UNK:N	2.52	0.42
1:A:113:THR:HA	1:A:116:PHE:CE2	2.53	0.42
4:A:503:KEG:O21	4:A:503:KEG:O37	2.37	0.42
1:A:341:LYS:HD2	1:C:339:HIS:CD2	2.54	0.42
4:N:8703:KEG:O37	4:N:8703:KEG:O21	2.36	0.42
4:M:8701:KEG:O37	4:M:8701:KEG:O21	2.37	0.42
4:M:8701:KEG:O44	4:M:8701:KEG:O19	2.37	0.42
4:M:8702:KEG:O44	4:M:8702:KEG:O19	2.37	0.42
4:M:8703:KEG:O19	4:M:8703:KEG:O44	2.36	0.42
2:B:277:UNK:CB	2:B:304:UNK:C	2.86	0.42
1:C:113:THR:HA	1:C:116:PHE:CE2	2.54	0.42
1:A:141:GLU:CG	1:A:346:ILE:HG13	2.49	0.42
4:N:8702:KEG:O44	4:N:8702:KEG:O19	2.37	0.42
1:A:341:LYS:N	4:A:501:KEG:O32	2.47	0.42
4:A:503:KEG:O19	4:A:503:KEG:O44	2.37	0.42
4:N:8703:KEG:O19	4:N:8703:KEG:O44	2.37	0.42
1:A:141:GLU:HG3	1:A:346:ILE:HG13	2.01	0.42
1:A:334:ILE:HD11	1:A:352:PHE:HB2	2.00	0.42
1:C:135:VAL:HG22	1:C:213:VAL:HB	2.01	0.42
1:C:102:VAL:HB	1:C:244:MET:HG2	2.00	0.42
3:N:2581:UNK:HA	3:N:2584:UNK:CB	2.50	0.42
1:A:313:VAL:HG11	1:A:318:ARG:HB2	2.02	0.42
4:A:502:KEG:O6	1:C:386:GLU:HA	2.19	0.42
1:C:105:GLN:HB2	1:C:250:LEU:HD12	2.02	0.41
3:N:62:UNK:C	3:N:63:UNK:O	2.65	0.41
1:A:235:ARG:NH1	3:M:6215:UNK:CB	2.70	0.41
1:C:218:ASP:OD2	1:C:249:THR:OG1	2.38	0.41
3:M:2581:UNK:HA	3:M:2584:UNK:CB	2.50	0.41
1:A:105:GLN:HB2	1:A:250:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ARG:NH1	1:A:267:GLU:OE1	2.53	0.41
1:C:148:ASN:O	1:C:152:ARG:HG3	2.20	0.41
3:N:6098:UNK:O	3:N:6101:UNK:CA	2.67	0.41
1:A:313:VAL:CG1	1:A:318:ARG:HB2	2.51	0.41
1:C:313:VAL:HG11	1:C:318:ARG:HB2	2.02	0.41
1:A:341:LYS:CD	1:C:339:HIS:HB2	2.49	0.41
1:A:148:ASN:O	1:A:152:ARG:HG3	2.20	0.41
1:C:316:THR:HG22	1:C:337:HIS:HB2	2.02	0.41
4:A:501:KEG:O27	1:C:341:LYS:HG2	2.20	0.41
1:A:316:THR:HG22	1:A:337:HIS:HB2	2.02	0.41
1:A:335:THR:HA	1:A:361:VAL:O	2.21	0.41
1:C:259:ARG:NH1	1:C:267:GLU:OE1	2.53	0.41
1:A:316:THR:OG1	1:C:341:LYS:NZ	2.54	0.41
3:N:6092:UNK:N	3:N:6095:UNK:N	2.60	0.41
1:C:313:VAL:CG1	1:C:318:ARG:HB2	2.51	0.41
1:A:218:ASP:OD2	1:A:249:THR:OG1	2.38	0.40
2:B:315:UNK:HA	2:B:330:UNK:O	2.22	0.40
1:C:335:THR:HA	1:C:361:VAL:O	2.21	0.40
2:D:315:UNK:HA	2:D:330:UNK:O	2.22	0.40
1:C:217:CYS:SG	1:C:245:MET:HB3	2.62	0.40
3:N:6099:UNK:O	3:N:6102:UNK:CB	2.69	0.40
1:A:217:CYS:SG	1:A:245:MET:HB3	2.61	0.40
3:M:6099:UNK:O	3:M:6102:UNK:CB	2.69	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	370/446 (83%)	362 (98%)	8 (2%)	0	100	100
1	C	370/446 (83%)	362 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	740/892 (83%)	724 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	331/386 (86%)	328 (99%)	3 (1%)	84	93
1	C	331/386 (86%)	328 (99%)	3 (1%)	84	93
All	All	662/772 (86%)	656 (99%)	6 (1%)	84	93

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	399	ARG
1	A	413	LYS
1	A	424	GLU
1	C	399	ARG
1	C	413	LYS
1	C	424	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	GLN
1	A	342	GLN
1	C	98	HIS
1	C	299	GLN
1	C	339	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 ⓘ

11 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	$\# Z  > 2$
4	KEG	A	501	-	76,76,76	3.19	43 (56%)	6,234,234	2.32	2 (33%)
4	KEG	A	502	-	76,76,76	3.19	43 (56%)	6,234,234	2.32	2 (33%)
4	KEG	A	503	-	76,76,76	3.19	43 (56%)	6,234,234	2.30	2 (33%)
4	KEG	M	8701	-	76,76,76	3.19	43 (56%)	6,234,234	2.36	2 (33%)
4	KEG	M	8702	-	76,76,76	3.19	43 (56%)	6,234,234	2.31	2 (33%)
4	KEG	M	8703	-	76,76,76	3.19	43 (56%)	6,234,234	2.34	2 (33%)
4	KEG	N	8701	-	76,76,76	3.19	43 (56%)	6,234,234	2.31	2 (33%)
4	KEG	N	8702	-	76,76,76	3.19	43 (56%)	6,234,234	2.34	2 (33%)
4	KEG	N	8703	-	76,76,76	3.19	43 (56%)	6,234,234	2.32	2 (33%)
4	KEG	N	8704	-	76,76,76	3.19	43 (56%)	6,234,234	2.33	2 (33%)
4	KEG	N	8705	-	76,76,76	3.19	43 (56%)	6,234,234	2.35	2 (33%)

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	KEG	A	501	-	-	0/0/456/456	0/0/24/24
4	KEG	A	502	-	-	0/0/456/456	0/0/24/24
4	KEG	A	503	-	-	0/0/456/456	0/0/24/24
4	KEG	M	8701	-	-	0/0/456/456	0/0/24/24
4	KEG	M	8702	-	-	0/0/456/456	0/0/24/24
4	KEG	M	8703	-	-	0/0/456/456	0/0/24/24
4	KEG	N	8701	-	-	0/0/456/456	0/0/24/24
4	KEG	N	8702	-	-	0/0/456/456	0/0/24/24
4	KEG	N	8703	-	-	0/0/456/456	0/0/24/24
4	KEG	N	8704	-	-	0/0/456/456	0/0/24/24
4	KEG	N	8705	-	-	0/0/456/456	0/0/24/24

All (473) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	8702	KEG	W2-O28	-8.07	1.55	1.93
4	N	8704	KEG	W2-O28	-8.04	1.55	1.93
4	A	503	KEG	W2-O28	-8.04	1.55	1.93
4	M	8703	KEG	W2-O28	-8.04	1.55	1.93
4	M	8701	KEG	W2-O28	-8.03	1.55	1.93
4	N	8705	KEG	W2-O28	-8.03	1.55	1.93
4	A	501	KEG	W2-O28	-8.03	1.55	1.93
4	N	8701	KEG	W2-O28	-8.03	1.55	1.93
4	N	8702	KEG	W2-O28	-8.03	1.55	1.93
4	A	502	KEG	W2-O28	-8.02	1.55	1.93
4	N	8703	KEG	W2-O28	-8.02	1.55	1.93
4	N	8704	KEG	P1-O18	-7.80	1.27	1.54
4	A	503	KEG	P1-O18	-7.79	1.27	1.54
4	M	8701	KEG	P1-O18	-7.79	1.27	1.54
4	N	8701	KEG	P1-O18	-7.79	1.27	1.54
4	A	501	KEG	P1-O18	-7.78	1.27	1.54
4	M	8702	KEG	P1-O18	-7.78	1.27	1.54
4	A	502	KEG	P1-O18	-7.78	1.27	1.54
4	N	8705	KEG	P1-O18	-7.77	1.27	1.54
4	N	8703	KEG	P1-O18	-7.77	1.27	1.54
4	M	8703	KEG	P1-O18	-7.76	1.27	1.54
4	N	8702	KEG	P1-O18	-7.75	1.27	1.54
4	A	501	KEG	W6-O36	-7.53	1.58	1.93
4	M	8701	KEG	W6-O36	-7.52	1.58	1.93
4	M	8702	KEG	W6-O36	-7.52	1.58	1.93
4	A	503	KEG	W6-O36	-7.51	1.58	1.93
4	N	8705	KEG	W6-O36	-7.51	1.58	1.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8701	KEG	W6-O36	-7.51	1.58	1.93
4	M	8703	KEG	W6-O36	-7.50	1.58	1.93
4	N	8703	KEG	W6-O36	-7.50	1.58	1.93
4	A	502	KEG	W6-O36	-7.50	1.58	1.93
4	N	8704	KEG	W6-O36	-7.50	1.58	1.93
4	N	8702	KEG	W6-O36	-7.49	1.58	1.93
4	N	8704	KEG	W1-O29	-7.07	1.60	1.91
4	A	502	KEG	W1-O29	-7.07	1.60	1.91
4	N	8702	KEG	W1-O29	-7.06	1.60	1.91
4	N	8701	KEG	W1-O29	-7.06	1.60	1.91
4	M	8703	KEG	W1-O29	-7.06	1.60	1.91
4	M	8702	KEG	W1-O29	-7.06	1.60	1.91
4	M	8701	KEG	W1-O29	-7.06	1.60	1.91
4	A	503	KEG	W1-O29	-7.06	1.60	1.91
4	A	501	KEG	W1-O29	-7.06	1.60	1.91
4	N	8703	KEG	W1-O29	-7.04	1.60	1.91
4	N	8705	KEG	W1-O29	-7.04	1.60	1.91
4	A	502	KEG	W3-O33	-6.96	1.61	1.91
4	M	8702	KEG	W3-O33	-6.95	1.61	1.91
4	A	501	KEG	W3-O33	-6.94	1.61	1.91
4	M	8701	KEG	W3-O33	-6.94	1.61	1.91
4	N	8703	KEG	W3-O33	-6.93	1.61	1.91
4	A	503	KEG	W3-O33	-6.92	1.61	1.91
4	N	8701	KEG	W3-O33	-6.92	1.61	1.91
4	M	8703	KEG	W3-O33	-6.91	1.61	1.91
4	N	8705	KEG	W3-O33	-6.91	1.61	1.91
4	N	8704	KEG	W3-O33	-6.91	1.61	1.91
4	N	8702	KEG	W3-O33	-6.90	1.61	1.91
4	N	8703	KEG	W10-O28	-5.84	1.66	1.93
4	A	501	KEG	W10-O28	-5.83	1.66	1.93
4	A	502	KEG	W10-O28	-5.83	1.66	1.93
4	N	8701	KEG	W10-O28	-5.83	1.66	1.93
4	M	8703	KEG	W10-O28	-5.83	1.66	1.93
4	M	8702	KEG	W10-O28	-5.83	1.66	1.93
4	N	8702	KEG	W10-O28	-5.82	1.66	1.93
4	M	8701	KEG	W10-O28	-5.82	1.66	1.93
4	N	8705	KEG	W10-O28	-5.82	1.66	1.93
4	A	503	KEG	W10-O28	-5.82	1.66	1.93
4	N	8704	KEG	W10-O28	-5.81	1.66	1.93
4	A	502	KEG	W5-O23	-5.40	1.68	1.93
4	M	8703	KEG	W5-O23	-5.39	1.68	1.93
4	A	503	KEG	W5-O23	-5.38	1.68	1.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	KEG	W5-O23	-5.38	1.68	1.93
4	M	8701	KEG	W5-O23	-5.38	1.68	1.93
4	M	8702	KEG	W5-O23	-5.38	1.68	1.93
4	N	8703	KEG	W5-O23	-5.37	1.68	1.93
4	N	8701	KEG	W5-O23	-5.37	1.68	1.93
4	N	8705	KEG	W5-O23	-5.37	1.68	1.93
4	N	8702	KEG	W5-O23	-5.37	1.68	1.93
4	N	8704	KEG	W5-O23	-5.35	1.68	1.93
4	M	8702	KEG	W7-O29	-4.72	1.70	1.91
4	N	8705	KEG	W7-O29	-4.72	1.70	1.91
4	A	503	KEG	W7-O29	-4.72	1.70	1.91
4	M	8701	KEG	W7-O29	-4.72	1.70	1.91
4	N	8704	KEG	W7-O29	-4.72	1.70	1.91
4	A	501	KEG	W7-O29	-4.72	1.70	1.91
4	A	502	KEG	W7-O29	-4.72	1.70	1.91
4	N	8701	KEG	W7-O29	-4.71	1.70	1.91
4	A	503	KEG	W2-O2	-4.71	1.58	1.71
4	N	8703	KEG	W7-O29	-4.70	1.70	1.91
4	N	8703	KEG	P1-O19	-4.69	1.38	1.54
4	M	8703	KEG	W7-O29	-4.69	1.70	1.91
4	N	8702	KEG	W7-O29	-4.69	1.70	1.91
4	N	8702	KEG	W2-O2	-4.69	1.58	1.71
4	A	502	KEG	W2-O2	-4.68	1.58	1.71
4	N	8704	KEG	W2-O2	-4.68	1.58	1.71
4	A	503	KEG	P1-O19	-4.67	1.38	1.54
4	A	501	KEG	P1-O19	-4.67	1.38	1.54
4	N	8702	KEG	P1-O19	-4.66	1.38	1.54
4	N	8701	KEG	W2-O2	-4.66	1.58	1.71
4	M	8701	KEG	W2-O2	-4.66	1.58	1.71
4	N	8701	KEG	P1-O19	-4.65	1.38	1.54
4	M	8702	KEG	W2-O2	-4.65	1.58	1.71
4	N	8703	KEG	W2-O2	-4.65	1.58	1.71
4	M	8701	KEG	P1-O19	-4.65	1.38	1.54
4	M	8703	KEG	P1-O19	-4.65	1.38	1.54
4	N	8705	KEG	P1-O19	-4.65	1.38	1.54
4	N	8705	KEG	W2-O2	-4.65	1.58	1.71
4	M	8702	KEG	P1-O19	-4.64	1.38	1.54
4	A	501	KEG	W2-O2	-4.64	1.58	1.71
4	A	502	KEG	W1-O23	-4.64	1.71	1.93
4	N	8704	KEG	P1-O19	-4.64	1.38	1.54
4	A	503	KEG	W1-O23	-4.63	1.71	1.93
4	M	8701	KEG	W1-O23	-4.63	1.71	1.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8701	KEG	W1-O23	-4.63	1.71	1.93
4	N	8704	KEG	W1-O23	-4.63	1.71	1.93
4	A	501	KEG	W1-O23	-4.63	1.71	1.93
4	M	8703	KEG	W2-O2	-4.62	1.58	1.71
4	M	8703	KEG	W1-O23	-4.62	1.71	1.93
4	A	502	KEG	P1-O19	-4.62	1.38	1.54
4	N	8702	KEG	W1-O23	-4.61	1.71	1.93
4	N	8705	KEG	W1-O23	-4.61	1.71	1.93
4	N	8703	KEG	W1-O23	-4.60	1.71	1.93
4	M	8702	KEG	W1-O23	-4.60	1.71	1.93
4	A	502	KEG	W10-O18	-4.47	2.19	2.43
4	A	501	KEG	W10-O18	-4.45	2.19	2.43
4	M	8702	KEG	W10-O18	-4.44	2.19	2.43
4	M	8703	KEG	W10-O18	-4.44	2.19	2.43
4	A	503	KEG	W10-O18	-4.44	2.19	2.43
4	N	8703	KEG	W10-O18	-4.44	2.19	2.43
4	N	8704	KEG	W10-O18	-4.43	2.19	2.43
4	M	8701	KEG	W10-O18	-4.42	2.19	2.43
4	N	8701	KEG	W10-O18	-4.42	2.19	2.43
4	N	8705	KEG	W10-O18	-4.42	2.19	2.43
4	N	8702	KEG	W10-O18	-4.41	2.19	2.43
4	N	8701	KEG	W2-O18	-4.35	2.19	2.43
4	M	8702	KEG	W2-O18	-4.35	2.19	2.43
4	N	8705	KEG	W2-O18	-4.35	2.19	2.43
4	M	8703	KEG	W2-O18	-4.34	2.19	2.43
4	N	8702	KEG	W2-O18	-4.34	2.19	2.43
4	A	502	KEG	W2-O18	-4.34	2.19	2.43
4	N	8703	KEG	W2-O18	-4.33	2.19	2.43
4	A	501	KEG	W2-O18	-4.33	2.19	2.43
4	A	503	KEG	W2-O18	-4.33	2.19	2.43
4	N	8704	KEG	W2-O18	-4.32	2.19	2.43
4	M	8701	KEG	W2-O18	-4.32	2.19	2.43
4	A	503	KEG	W11-O13	-4.15	1.60	1.71
4	A	501	KEG	W11-O13	-4.14	1.60	1.71
4	N	8705	KEG	W11-O13	-4.14	1.60	1.71
4	N	8704	KEG	W11-O13	-4.14	1.60	1.71
4	N	8703	KEG	W11-O13	-4.14	1.60	1.71
4	M	8703	KEG	W11-O13	-4.13	1.60	1.71
4	N	8701	KEG	W11-O13	-4.13	1.60	1.71
4	M	8701	KEG	W11-O13	-4.12	1.60	1.71
4	N	8702	KEG	W11-O13	-4.12	1.60	1.71
4	M	8702	KEG	W11-O13	-4.12	1.60	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	KEG	W11-O13	-4.11	1.60	1.71
4	A	502	KEG	W12-O14	-4.02	1.60	1.71
4	M	8702	KEG	W9-O42	-4.01	1.73	1.91
4	A	503	KEG	W9-O42	-4.01	1.73	1.91
4	N	8705	KEG	W9-O42	-4.01	1.73	1.91
4	N	8701	KEG	W9-O42	-4.01	1.73	1.91
4	M	8701	KEG	W9-O42	-4.00	1.73	1.91
4	N	8702	KEG	W9-O42	-4.00	1.73	1.91
4	A	501	KEG	W9-O42	-4.00	1.73	1.91
4	N	8704	KEG	W9-O42	-3.99	1.73	1.91
4	A	502	KEG	W9-O42	-3.99	1.73	1.91
4	A	501	KEG	W12-O14	-3.99	1.60	1.71
4	N	8703	KEG	W9-O42	-3.99	1.73	1.91
4	M	8701	KEG	W12-O14	-3.99	1.60	1.71
4	N	8702	KEG	W12-O14	-3.99	1.60	1.71
4	A	502	KEG	W10-O36	-3.99	1.74	1.93
4	N	8702	KEG	W10-O36	-3.98	1.74	1.93
4	A	503	KEG	W12-O14	-3.98	1.60	1.71
4	M	8702	KEG	W12-O14	-3.98	1.60	1.71
4	M	8701	KEG	W10-O36	-3.98	1.74	1.93
4	N	8704	KEG	W10-O36	-3.98	1.74	1.93
4	N	8705	KEG	W12-O14	-3.98	1.60	1.71
4	M	8703	KEG	W10-O36	-3.97	1.74	1.93
4	A	501	KEG	W10-O36	-3.97	1.74	1.93
4	M	8703	KEG	W9-O42	-3.97	1.74	1.91
4	M	8703	KEG	W12-O14	-3.97	1.60	1.71
4	N	8701	KEG	W10-O36	-3.97	1.74	1.93
4	M	8702	KEG	W10-O36	-3.97	1.74	1.93
4	N	8705	KEG	W10-O36	-3.96	1.74	1.93
4	N	8703	KEG	W10-O36	-3.96	1.74	1.93
4	A	503	KEG	W10-O36	-3.96	1.74	1.93
4	N	8704	KEG	W12-O14	-3.96	1.60	1.71
4	N	8701	KEG	W12-O14	-3.94	1.60	1.71
4	N	8703	KEG	W12-O14	-3.94	1.60	1.71
4	M	8703	KEG	W1-O17	-3.83	2.22	2.43
4	A	502	KEG	W1-O17	-3.83	2.22	2.43
4	N	8705	KEG	W1-O17	-3.82	2.22	2.43
4	M	8702	KEG	W1-O17	-3.82	2.22	2.43
4	N	8703	KEG	W1-O17	-3.82	2.22	2.43
4	M	8701	KEG	W1-O17	-3.82	2.22	2.43
4	A	501	KEG	W1-O17	-3.82	2.22	2.43
4	N	8701	KEG	W1-O17	-3.81	2.22	2.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	KEG	W1-O17	-3.81	2.22	2.43
4	N	8704	KEG	W1-O17	-3.80	2.22	2.43
4	N	8702	KEG	W1-O17	-3.79	2.22	2.43
4	A	502	KEG	W8-O10	-3.66	1.61	1.71
4	N	8704	KEG	W8-O10	-3.63	1.61	1.71
4	N	8701	KEG	W8-O10	-3.63	1.61	1.71
4	M	8701	KEG	W8-O10	-3.62	1.61	1.71
4	N	8702	KEG	W8-O10	-3.61	1.61	1.71
4	A	503	KEG	W8-O10	-3.60	1.61	1.71
4	N	8705	KEG	W8-O10	-3.59	1.61	1.71
4	M	8702	KEG	W8-O10	-3.59	1.61	1.71
4	N	8703	KEG	W8-O10	-3.58	1.61	1.71
4	A	501	KEG	W8-O10	-3.58	1.61	1.71
4	M	8703	KEG	W8-O10	-3.58	1.61	1.71
4	A	501	KEG	W6-O24	-3.52	1.76	1.93
4	M	8701	KEG	W6-O24	-3.52	1.76	1.93
4	A	502	KEG	W6-O24	-3.50	1.77	1.93
4	N	8704	KEG	W6-O24	-3.49	1.77	1.93
4	M	8702	KEG	W6-O24	-3.49	1.77	1.93
4	A	503	KEG	W6-O24	-3.49	1.77	1.93
4	M	8703	KEG	W6-O24	-3.49	1.77	1.93
4	N	8703	KEG	W6-O24	-3.48	1.77	1.93
4	N	8705	KEG	W6-O24	-3.48	1.77	1.93
4	N	8701	KEG	W6-O24	-3.47	1.77	1.93
4	N	8702	KEG	W6-O24	-3.47	1.77	1.93
4	N	8703	KEG	W2-O24	-3.25	1.78	1.93
4	N	8701	KEG	W2-O24	-3.24	1.78	1.93
4	N	8702	KEG	W2-O24	-3.23	1.78	1.93
4	N	8704	KEG	W2-O24	-3.23	1.78	1.93
4	N	8705	KEG	W2-O24	-3.22	1.78	1.93
4	A	503	KEG	W2-O24	-3.22	1.78	1.93
4	M	8703	KEG	W2-O24	-3.22	1.78	1.93
4	M	8701	KEG	W2-O24	-3.22	1.78	1.93
4	A	501	KEG	W2-O24	-3.21	1.78	1.93
4	A	502	KEG	W2-O24	-3.21	1.78	1.93
4	M	8702	KEG	W2-O24	-3.21	1.78	1.93
4	N	8701	KEG	W9-O11	-3.10	1.62	1.71
4	N	8704	KEG	W9-O11	-3.10	1.62	1.71
4	M	8703	KEG	W9-O11	-3.09	1.63	1.71
4	A	501	KEG	W9-O11	-3.09	1.63	1.71
4	M	8702	KEG	W9-O11	-3.08	1.63	1.71
4	A	502	KEG	W9-O11	-3.07	1.63	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8703	KEG	W9-O11	-3.07	1.63	1.71
4	A	503	KEG	W9-O11	-3.07	1.63	1.71
4	N	8705	KEG	W9-O11	-3.06	1.63	1.71
4	M	8701	KEG	W9-O11	-3.04	1.63	1.71
4	N	8702	KEG	W9-O11	-3.03	1.63	1.71
4	N	8702	KEG	W8-O44	-3.02	1.79	1.93
4	N	8703	KEG	W3-O25	-3.02	1.78	1.91
4	N	8705	KEG	W3-O25	-3.01	1.78	1.91
4	N	8703	KEG	W8-O44	-3.01	1.79	1.93
4	N	8704	KEG	W8-O44	-3.01	1.79	1.93
4	M	8703	KEG	W3-O25	-3.01	1.78	1.91
4	M	8701	KEG	W3-O25	-3.01	1.78	1.91
4	N	8704	KEG	W3-O25	-3.01	1.78	1.91
4	M	8701	KEG	W8-O44	-3.01	1.79	1.93
4	A	502	KEG	W8-O44	-3.00	1.79	1.93
4	M	8703	KEG	W8-O44	-3.00	1.79	1.93
4	N	8701	KEG	W3-O25	-3.00	1.78	1.91
4	A	501	KEG	W3-O25	-3.00	1.78	1.91
4	A	503	KEG	W3-O25	-3.00	1.78	1.91
4	M	8702	KEG	W3-O25	-3.00	1.78	1.91
4	A	501	KEG	W8-O44	-3.00	1.79	1.93
4	N	8702	KEG	W3-O25	-2.99	1.78	1.91
4	A	502	KEG	W3-O25	-2.99	1.78	1.91
4	N	8701	KEG	W8-O44	-2.98	1.79	1.93
4	A	503	KEG	W8-O44	-2.98	1.79	1.93
4	M	8702	KEG	W8-O44	-2.98	1.79	1.93
4	N	8705	KEG	W8-O44	-2.96	1.79	1.93
4	N	8705	KEG	W10-O12	-2.91	1.63	1.71
4	N	8702	KEG	W10-O12	-2.91	1.63	1.71
4	N	8703	KEG	W10-O12	-2.90	1.63	1.71
4	N	8701	KEG	W10-O12	-2.90	1.63	1.71
4	M	8701	KEG	W10-O12	-2.88	1.63	1.71
4	M	8703	KEG	W10-O12	-2.87	1.63	1.71
4	N	8704	KEG	W10-O12	-2.86	1.63	1.71
4	A	501	KEG	W10-O12	-2.86	1.63	1.71
4	M	8702	KEG	W10-O12	-2.86	1.63	1.71
4	A	503	KEG	W10-O12	-2.84	1.63	1.71
4	M	8703	KEG	W6-O8	-2.83	1.63	1.71
4	A	502	KEG	W10-O12	-2.82	1.63	1.71
4	N	8704	KEG	W6-O8	-2.82	1.63	1.71
4	N	8702	KEG	W6-O8	-2.82	1.63	1.71
4	N	8703	KEG	W6-O8	-2.81	1.63	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	8701	KEG	W6-O8	-2.80	1.63	1.71
4	A	502	KEG	W6-O8	-2.80	1.63	1.71
4	N	8705	KEG	W6-O8	-2.80	1.63	1.71
4	A	501	KEG	W6-O8	-2.80	1.63	1.71
4	M	8702	KEG	W6-O8	-2.80	1.63	1.71
4	N	8701	KEG	W6-O8	-2.79	1.63	1.71
4	A	503	KEG	W6-O8	-2.77	1.63	1.71
4	N	8704	KEG	W5-O7	-2.73	1.64	1.71
4	A	502	KEG	W5-O7	-2.70	1.64	1.71
4	M	8703	KEG	W5-O7	-2.69	1.64	1.71
4	M	8701	KEG	W5-O7	-2.69	1.64	1.71
4	A	503	KEG	W5-O7	-2.69	1.64	1.71
4	M	8702	KEG	W5-O7	-2.68	1.64	1.71
4	N	8703	KEG	W5-O7	-2.68	1.64	1.71
4	N	8705	KEG	W5-O7	-2.67	1.64	1.71
4	N	8701	KEG	W5-O7	-2.65	1.64	1.71
4	N	8702	KEG	W5-O7	-2.65	1.64	1.71
4	A	501	KEG	W5-O7	-2.65	1.64	1.71
4	A	503	KEG	W1-O1	-2.54	1.64	1.71
4	N	8701	KEG	W1-O1	-2.53	1.64	1.71
4	N	8703	KEG	W1-O1	-2.52	1.64	1.71
4	N	8705	KEG	W1-O1	-2.52	1.64	1.71
4	M	8703	KEG	W11-O40	-2.51	1.80	1.91
4	A	502	KEG	W11-O40	-2.51	1.80	1.91
4	M	8701	KEG	W1-O1	-2.51	1.64	1.71
4	M	8702	KEG	W11-O40	-2.51	1.80	1.91
4	N	8703	KEG	W11-O40	-2.50	1.80	1.91
4	N	8702	KEG	W1-O1	-2.50	1.64	1.71
4	M	8701	KEG	W11-O40	-2.50	1.80	1.91
4	A	502	KEG	W1-O1	-2.50	1.64	1.71
4	A	503	KEG	W11-O40	-2.50	1.80	1.91
4	N	8701	KEG	W11-O40	-2.50	1.80	1.91
4	A	501	KEG	W11-O40	-2.50	1.80	1.91
4	N	8704	KEG	W11-O40	-2.50	1.80	1.91
4	M	8702	KEG	W1-O1	-2.49	1.64	1.71
4	N	8702	KEG	W11-O40	-2.49	1.80	1.91
4	A	501	KEG	W1-O1	-2.49	1.64	1.71
4	M	8703	KEG	W1-O1	-2.49	1.64	1.71
4	N	8705	KEG	W11-O40	-2.48	1.80	1.91
4	N	8704	KEG	W1-O1	-2.47	1.64	1.71
4	M	8702	KEG	W4-O6	-2.37	1.64	1.71
4	A	501	KEG	W4-O6	-2.35	1.65	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8702	KEG	W4-O6	-2.34	1.65	1.71
4	N	8705	KEG	W4-O6	-2.33	1.65	1.71
4	A	502	KEG	W4-O6	-2.33	1.65	1.71
4	N	8701	KEG	W4-O6	-2.32	1.65	1.71
4	A	503	KEG	W4-O6	-2.32	1.65	1.71
4	N	8704	KEG	W4-O6	-2.31	1.65	1.71
4	M	8701	KEG	W4-O6	-2.30	1.65	1.71
4	N	8703	KEG	W4-O6	-2.30	1.65	1.71
4	N	8702	KEG	W1-O25	-2.28	1.81	1.91
4	M	8703	KEG	W4-O6	-2.28	1.65	1.71
4	M	8702	KEG	W1-O25	-2.28	1.81	1.91
4	M	8701	KEG	W1-O25	-2.27	1.81	1.91
4	M	8703	KEG	W1-O25	-2.27	1.81	1.91
4	N	8705	KEG	W1-O25	-2.27	1.81	1.91
4	N	8701	KEG	W7-O33	-2.27	1.81	1.91
4	N	8704	KEG	W1-O25	-2.27	1.81	1.91
4	N	8703	KEG	W1-O25	-2.26	1.81	1.91
4	N	8702	KEG	W7-O33	-2.26	1.81	1.91
4	N	8701	KEG	W1-O25	-2.26	1.81	1.91
4	M	8702	KEG	W11-O44	-2.26	1.82	1.93
4	A	502	KEG	W1-O25	-2.26	1.81	1.91
4	N	8703	KEG	W7-O33	-2.26	1.81	1.91
4	A	502	KEG	W4-O26	-2.26	1.81	1.91
4	N	8704	KEG	W8-O41	-2.26	1.82	1.93
4	N	8704	KEG	W7-O33	-2.25	1.81	1.91
4	M	8703	KEG	W7-O33	-2.25	1.81	1.91
4	N	8705	KEG	W7-O33	-2.25	1.81	1.91
4	N	8701	KEG	W4-O26	-2.25	1.81	1.91
4	N	8702	KEG	W8-O41	-2.25	1.82	1.93
4	M	8701	KEG	W4-O26	-2.25	1.81	1.91
4	M	8702	KEG	W4-O26	-2.25	1.81	1.91
4	A	503	KEG	W7-O33	-2.24	1.81	1.91
4	M	8703	KEG	W4-O26	-2.24	1.81	1.91
4	N	8705	KEG	W4-O26	-2.24	1.81	1.91
4	M	8701	KEG	W8-O41	-2.24	1.82	1.93
4	A	501	KEG	W1-O25	-2.24	1.81	1.91
4	N	8705	KEG	W8-O41	-2.24	1.83	1.93
4	N	8702	KEG	W11-O44	-2.23	1.83	1.93
4	A	502	KEG	W7-O33	-2.23	1.81	1.91
4	A	501	KEG	W8-O41	-2.23	1.83	1.93
4	N	8705	KEG	W11-O44	-2.23	1.83	1.93
4	A	501	KEG	W7-O33	-2.23	1.81	1.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8704	KEG	W4-O26	-2.23	1.81	1.91
4	A	503	KEG	W1-O25	-2.23	1.81	1.91
4	M	8701	KEG	W7-O33	-2.23	1.81	1.91
4	A	503	KEG	W11-O44	-2.23	1.83	1.93
4	N	8703	KEG	W4-O26	-2.23	1.81	1.91
4	M	8703	KEG	W11-O44	-2.23	1.83	1.93
4	A	501	KEG	W4-O26	-2.23	1.81	1.91
4	M	8702	KEG	W8-O41	-2.23	1.83	1.93
4	N	8703	KEG	W8-O41	-2.22	1.83	1.93
4	N	8702	KEG	W4-O26	-2.22	1.81	1.91
4	N	8701	KEG	W11-O44	-2.22	1.83	1.93
4	M	8703	KEG	W8-O41	-2.22	1.83	1.93
4	A	503	KEG	W4-O26	-2.22	1.81	1.91
4	A	503	KEG	W8-O41	-2.22	1.83	1.93
4	N	8701	KEG	W8-O41	-2.22	1.83	1.93
4	N	8703	KEG	W11-O44	-2.22	1.83	1.93
4	A	502	KEG	W2-O26	-2.21	1.81	1.91
4	N	8704	KEG	W11-O44	-2.21	1.83	1.93
4	A	502	KEG	W11-O44	-2.21	1.83	1.93
4	A	501	KEG	W11-O44	-2.21	1.83	1.93
4	A	502	KEG	W8-O41	-2.21	1.83	1.93
4	A	503	KEG	W2-O26	-2.21	1.81	1.91
4	M	8701	KEG	W11-O44	-2.21	1.83	1.93
4	N	8704	KEG	W2-O26	-2.21	1.81	1.91
4	M	8702	KEG	W7-O33	-2.21	1.81	1.91
4	A	501	KEG	W2-O26	-2.20	1.81	1.91
4	M	8702	KEG	W2-O26	-2.20	1.81	1.91
4	N	8701	KEG	W2-O26	-2.20	1.81	1.91
4	N	8702	KEG	W2-O26	-2.19	1.81	1.91
4	N	8705	KEG	W2-O26	-2.19	1.81	1.91
4	M	8701	KEG	W2-O26	-2.19	1.81	1.91
4	M	8703	KEG	W2-O26	-2.18	1.81	1.91
4	N	8703	KEG	W2-O26	-2.17	1.81	1.91
4	A	501	KEG	W3-O31	2.07	2.03	1.93
4	M	8701	KEG	W3-O31	2.08	2.03	1.93
4	A	503	KEG	W3-O31	2.09	2.03	1.93
4	N	8701	KEG	W3-O31	2.09	2.03	1.93
4	A	502	KEG	W3-O31	2.09	2.03	1.93
4	N	8704	KEG	W3-O31	2.09	2.03	1.93
4	M	8702	KEG	W3-O31	2.09	2.03	1.93
4	N	8702	KEG	W3-O31	2.10	2.03	1.93
4	N	8705	KEG	W3-O31	2.10	2.03	1.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8703	KEG	W3-O31	2.10	2.03	1.93
4	M	8703	KEG	W3-O31	2.11	2.03	1.93
4	N	8701	KEG	W6-O32	2.25	2.00	1.91
4	A	503	KEG	W6-O32	2.26	2.01	1.91
4	N	8702	KEG	W6-O32	2.26	2.01	1.91
4	M	8703	KEG	W6-O32	2.27	2.01	1.91
4	M	8702	KEG	W6-O32	2.27	2.01	1.91
4	N	8705	KEG	W6-O32	2.27	2.01	1.91
4	N	8703	KEG	W6-O32	2.29	2.01	1.91
4	A	502	KEG	W6-O32	2.29	2.01	1.91
4	N	8704	KEG	W6-O32	2.30	2.01	1.91
4	A	501	KEG	W6-O32	2.30	2.01	1.91
4	M	8701	KEG	W6-O32	2.31	2.01	1.91
4	N	8705	KEG	W4-O21	2.34	2.55	2.43
4	N	8704	KEG	W4-O21	2.35	2.55	2.43
4	A	503	KEG	W4-O21	2.35	2.55	2.43
4	N	8701	KEG	W4-O21	2.36	2.55	2.43
4	M	8701	KEG	W4-O21	2.36	2.55	2.43
4	A	502	KEG	W4-O21	2.36	2.55	2.43
4	N	8703	KEG	W4-O21	2.36	2.55	2.43
4	M	8703	KEG	W4-O21	2.36	2.55	2.43
4	M	8702	KEG	W4-O21	2.37	2.55	2.43
4	A	501	KEG	W4-O21	2.37	2.55	2.43
4	N	8702	KEG	W4-O21	2.38	2.55	2.43
4	N	8705	KEG	W5-O32	2.39	2.01	1.91
4	N	8704	KEG	W5-O32	2.39	2.01	1.91
4	A	501	KEG	W5-O32	2.40	2.01	1.91
4	N	8702	KEG	W5-O32	2.40	2.01	1.91
4	N	8701	KEG	W5-O32	2.41	2.01	1.91
4	M	8701	KEG	W5-O32	2.41	2.01	1.91
4	M	8702	KEG	W5-O32	2.41	2.01	1.91
4	N	8703	KEG	W5-O32	2.41	2.01	1.91
4	M	8703	KEG	W5-O32	2.42	2.01	1.91
4	A	503	KEG	W5-O32	2.43	2.01	1.91
4	A	502	KEG	W5-O32	2.43	2.01	1.91
4	A	502	KEG	P1-O21	2.51	1.63	1.54
4	M	8701	KEG	P1-O21	2.51	1.63	1.54
4	A	501	KEG	P1-O21	2.52	1.63	1.54
4	N	8705	KEG	P1-O21	2.52	1.63	1.54
4	M	8703	KEG	P1-O21	2.53	1.63	1.54
4	A	503	KEG	P1-O21	2.53	1.63	1.54
4	N	8701	KEG	P1-O21	2.53	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8702	KEG	P1-O21	2.54	1.63	1.54
4	M	8702	KEG	P1-O21	2.54	1.63	1.54
4	N	8703	KEG	P1-O21	2.54	1.63	1.54
4	N	8704	KEG	P1-O21	2.56	1.63	1.54
4	N	8702	KEG	W3-O37	2.88	2.07	1.93
4	M	8702	KEG	W3-O37	2.89	2.07	1.93
4	N	8701	KEG	W3-O37	2.89	2.07	1.93
4	A	503	KEG	W3-O37	2.89	2.07	1.93
4	M	8703	KEG	W3-O37	2.90	2.07	1.93
4	A	502	KEG	W3-O37	2.90	2.07	1.93
4	M	8701	KEG	W3-O37	2.91	2.07	1.93
4	N	8705	KEG	W3-O37	2.91	2.07	1.93
4	N	8703	KEG	W3-O37	2.91	2.07	1.93
4	N	8704	KEG	W3-O37	2.92	2.07	1.93
4	A	501	KEG	W3-O37	2.92	2.07	1.93
4	N	8702	KEG	W3-O21	3.35	2.61	2.43
4	M	8702	KEG	W3-O21	3.35	2.61	2.43
4	M	8703	KEG	W3-O21	3.35	2.61	2.43
4	N	8703	KEG	W3-O21	3.37	2.61	2.43
4	A	501	KEG	W3-O21	3.37	2.61	2.43
4	N	8701	KEG	W3-O21	3.37	2.61	2.43
4	N	8704	KEG	W3-O21	3.37	2.61	2.43
4	M	8701	KEG	W3-O21	3.38	2.61	2.43
4	A	503	KEG	W3-O21	3.38	2.61	2.43
4	N	8705	KEG	W3-O21	3.38	2.61	2.43
4	A	502	KEG	W3-O21	3.40	2.61	2.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	8701	KEG	O19-P1-O18	-3.99	104.65	109.11
4	N	8705	KEG	O19-P1-O18	-3.99	104.65	109.11
4	N	8702	KEG	O19-P1-O18	-3.96	104.68	109.11
4	A	502	KEG	O19-P1-O18	-3.93	104.71	109.11
4	M	8703	KEG	O19-P1-O18	-3.91	104.74	109.11
4	N	8704	KEG	O19-P1-O18	-3.91	104.74	109.11
4	A	501	KEG	O19-P1-O18	-3.90	104.74	109.11
4	M	8702	KEG	O19-P1-O18	-3.90	104.75	109.11
4	N	8703	KEG	O19-P1-O18	-3.90	104.75	109.11
4	N	8701	KEG	O19-P1-O18	-3.88	104.77	109.11
4	A	503	KEG	O19-P1-O18	-3.86	104.79	109.11
4	N	8702	KEG	O21-P1-O18	3.37	112.89	109.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	KEG	O21-P1-O18	3.37	112.89	109.11
4	M	8702	KEG	O21-P1-O18	3.38	112.90	109.11
4	A	503	KEG	O21-P1-O18	3.39	112.90	109.11
4	N	8703	KEG	O21-P1-O18	3.39	112.91	109.11
4	N	8701	KEG	O21-P1-O18	3.40	112.92	109.11
4	A	501	KEG	O21-P1-O18	3.41	112.93	109.11
4	N	8704	KEG	O21-P1-O18	3.41	112.93	109.11
4	N	8705	KEG	O21-P1-O18	3.42	112.94	109.11
4	M	8703	KEG	O21-P1-O18	3.43	112.95	109.11
4	M	8701	KEG	O21-P1-O18	3.45	112.97	109.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 101 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	KEG	24	0
4	A	502	KEG	13	0
4	A	503	KEG	16	0
4	M	8701	KEG	6	0
4	M	8702	KEG	6	0
4	M	8703	KEG	6	0
4	N	8701	KEG	6	0
4	N	8702	KEG	6	0
4	N	8703	KEG	6	0
4	N	8704	KEG	6	0
4	N	8705	KEG	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	N	126

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Mol	Chain	Number of breaks
3	M	126
2	B	27
2	D	27

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	5289:UNK	C	6033:UNK	N	143.88
1	M	5289:UNK	C	6033:UNK	N	142.81
1	N	5148:UNK	C	5197:UNK	N	119.38
1	M	5148:UNK	C	5197:UNK	N	119.33
1	N	492:UNK	C	2104:UNK	N	118.52
1	M	492:UNK	C	2104:UNK	N	116.29
1	N	2121:UNK	C	2503:UNK	N	113.46
1	M	2121:UNK	C	2503:UNK	N	110.84
1	M	4017:UNK	C	4063:UNK	N	96.53
1	N	4017:UNK	C	4063:UNK	N	96.53
1	N	3052:UNK	C	3180:UNK	N	87.26
1	M	3052:UNK	C	3180:UNK	N	87.14
1	M	2992:UNK	C	3011:UNK	N	66.88
1	N	2992:UNK	C	3011:UNK	N	66.88
1	N	7362:UNK	C	8092:UNK	N	66.56
1	M	7362:UNK	C	8092:UNK	N	66.31
1	M	6744:UNK	C	6808:UNK	N	65.65
1	N	6744:UNK	C	6808:UNK	N	65.65
1	M	2846:UNK	C	2857:UNK	N	58.81
1	N	2846:UNK	C	2857:UNK	N	58.81
1	M	2958:UNK	C	2971:UNK	N	58.36
1	N	2958:UNK	C	2971:UNK	N	58.36
1	M	2927:UNK	C	2938:UNK	N	56.61
1	M	221:UNK	C	232:UNK	N	56.04
1	N	221:UNK	C	232:UNK	N	56.04
1	N	2927:UNK	C	2938:UNK	N	55.65
1	M	3200:UNK	C	4002:UNK	N	55.11
1	N	3200:UNK	C	4002:UNK	N	54.88
1	M	7079:UNK	C	7103:UNK	N	52.41
1	N	7079:UNK	C	7103:UNK	N	52.41
1	M	6081:UNK	C	6092:UNK	N	49.92
1	N	6081:UNK	C	6092:UNK	N	49.92
1	M	6871:UNK	C	6877:UNK	N	43.24
1	N	6871:UNK	C	6877:UNK	N	43.24
1	M	8498:UNK	C	8539:UNK	N	41.00
1	N	8498:UNK	C	8539:UNK	N	41.00

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	6502:UNK	C	6514:UNK	N	39.49
1	N	6502:UNK	C	6514:UNK	N	39.49
1	M	4105:UNK	C	4110:UNK	N	38.22
1	N	4105:UNK	C	4110:UNK	N	38.21
1	M	2681:UNK	C	2800:UNK	N	38.17
1	M	4618:UNK	C	4629:UNK	N	38.07
1	N	4618:UNK	C	4629:UNK	N	38.07
1	M	4734:UNK	C	4746:UNK	N	37.66
1	N	4734:UNK	C	4746:UNK	N	37.66
1	M	2523:UNK	C	2537:UNK	N	36.92
1	N	2523:UNK	C	2537:UNK	N	36.92
1	N	8253:UNK	C	8256:UNK	N	36.58
1	M	4688:UNK	C	4690:UNK	N	36.49
1	N	4688:UNK	C	4690:UNK	N	36.49
1	N	2681:UNK	C	2800:UNK	N	36.35
1	M	8253:UNK	C	8256:UNK	N	36.29
1	M	2895:UNK	C	2906:UNK	N	36.08
1	N	2895:UNK	C	2906:UNK	N	36.08
1	M	471:UNK	C	482:UNK	N	35.36
1	N	471:UNK	C	482:UNK	N	35.36
1	M	8126:UNK	C	8133:UNK	N	35.02
1	N	8126:UNK	C	8133:UNK	N	35.02
1	M	6114:UNK	C	6123:UNK	N	34.38
1	N	6114:UNK	C	6123:UNK	N	34.38
1	M	4353:UNK	C	4366:UNK	N	34.34
1	N	4353:UNK	C	4366:UNK	N	34.34
1	M	6826:UNK	C	6830:UNK	N	34.23
1	N	6826:UNK	C	6830:UNK	N	34.23
1	M	6680:UNK	C	6692:UNK	N	33.69
1	N	6680:UNK	C	6692:UNK	N	33.69
1	M	411:UNK	C	425:UNK	N	33.36
1	N	411:UNK	C	425:UNK	N	33.36
1	M	6053:UNK	C	6066:UNK	N	32.68
1	N	6053:UNK	C	6066:UNK	N	32.68
1	M	4567:UNK	C	4578:UNK	N	31.33
1	N	4567:UNK	C	4578:UNK	N	31.33
1	M	4895:UNK	C	4905:UNK	N	30.94
1	N	4895:UNK	C	4905:UNK	N	30.94
1	M	4709:UNK	C	4720:UNK	N	30.88
1	N	4709:UNK	C	4720:UNK	N	30.88
1	M	4217:UNK	C	4230:UNK	N	30.33
1	N	4217:UNK	C	4230:UNK	N	30.33

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	6647:UNK	C	6659:UNK	N	29.73
1	N	6647:UNK	C	6659:UNK	N	29.73
1	M	4273:UNK	C	4286:UNK	N	29.70
1	N	4273:UNK	C	4286:UNK	N	29.70
1	M	4187:UNK	C	4199:UNK	N	29.38
1	N	4187:UNK	C	4199:UNK	N	29.38
1	M	4443:UNK	C	4454:UNK	N	29.37
1	M	4763:UNK	C	4780:UNK	N	29.37
1	N	4443:UNK	C	4454:UNK	N	29.37
1	N	4763:UNK	C	4780:UNK	N	29.37
1	M	5238:UNK	C	5251:UNK	N	28.59
1	N	5238:UNK	C	5251:UNK	N	28.59
1	M	4244:UNK	C	4255:UNK	N	28.49
1	N	4244:UNK	C	4255:UNK	N	28.49
1	M	7222:UNK	C	7342:UNK	N	28.20
1	N	7222:UNK	C	7342:UNK	N	28.20
1	M	4472:UNK	C	4484:UNK	N	28.19
1	N	4472:UNK	C	4484:UNK	N	28.19
1	M	8299:UNK	C	8311:UNK	N	28.06
1	N	8299:UNK	C	8311:UNK	N	28.06
1	M	8226:UNK	C	8234:UNK	N	28.03
1	N	8226:UNK	C	8234:UNK	N	28.03
1	M	4076:UNK	C	4089:UNK	N	27.97
1	N	4076:UNK	C	4089:UNK	N	27.97
1	M	6468:UNK	C	6480:UNK	N	27.60
1	N	6468:UNK	C	6480:UNK	N	27.60
1	M	8442:UNK	C	8449:UNK	N	26.57
1	N	8442:UNK	C	8449:UNK	N	26.57
1	M	4325:UNK	C	4337:UNK	N	26.47
1	N	4325:UNK	C	4337:UNK	N	26.46
1	M	8106:UNK	C	8109:UNK	N	25.92
1	N	8106:UNK	C	8109:UNK	N	25.92
1	M	6283:UNK	C	6296:UNK	N	25.90
1	N	6283:UNK	C	6296:UNK	N	25.90
1	M	292:UNK	C	303:UNK	N	25.77
1	N	292:UNK	C	303:UNK	N	25.77
1	M	8483:UNK	C	8485:UNK	N	24.83
1	N	8483:UNK	C	8485:UNK	N	24.83
1	M	4875:UNK	C	4886:UNK	N	24.81
1	N	4875:UNK	C	4886:UNK	N	24.81
1	M	186:UNK	C	200:UNK	N	24.57
1	N	186:UNK	C	200:UNK	N	24.57

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	4540:UNK	C	4552:UNK	N	24.41
1	N	4540:UNK	C	4552:UNK	N	24.41
1	M	5211:UNK	C	5225:UNK	N	24.30
1	M	8325:UNK	C	8338:UNK	N	24.29
1	N	5211:UNK	C	5225:UNK	N	24.29
1	N	8325:UNK	C	8338:UNK	N	24.29
1	M	134:UNK	C	138:UNK	N	23.96
1	M	350:UNK	C	365:UNK	N	23.96
1	N	134:UNK	C	138:UNK	N	23.96
1	N	350:UNK	C	365:UNK	N	23.96
1	M	6711:UNK	C	6724:UNK	N	23.79
1	N	6711:UNK	C	6724:UNK	N	23.79
1	M	6845:UNK	C	6856:UNK	N	23.48
1	N	6845:UNK	C	6856:UNK	N	23.48
1	M	6935:UNK	C	7068:UNK	N	23.38
1	N	6935:UNK	C	7068:UNK	N	23.38
1	M	4931:UNK	C	4942:UNK	N	23.35
1	N	4931:UNK	C	4942:UNK	N	23.35
1	M	2558:UNK	C	2569:UNK	N	23.23
1	N	2558:UNK	C	2569:UNK	N	23.23
1	M	8156:UNK	C	8166:UNK	N	23.07
1	N	8156:UNK	C	8166:UNK	N	23.07
1	M	6350:UNK	C	6372:UNK	N	22.69
1	N	6350:UNK	C	6372:UNK	N	22.69
1	M	4417:UNK	C	4431:UNK	N	22.67
1	N	4417:UNK	C	4431:UNK	N	22.67
1	M	117:UNK	C	119:UNK	N	22.35
1	N	117:UNK	C	119:UNK	N	22.35
1	M	4380:UNK	C	4386:UNK	N	21.94
1	N	4380:UNK	C	4386:UNK	N	21.94
1	M	4644:UNK	C	4671:UNK	N	21.42
1	N	4644:UNK	C	4671:UNK	N	21.42
1	M	6888:UNK	C	6900:UNK	N	20.85
1	N	6888:UNK	C	6900:UNK	N	20.85
1	M	8427:UNK	C	8432:UNK	N	20.71
1	N	8427:UNK	C	8432:UNK	N	20.71
1	M	264:UNK	C	276:UNK	N	20.62
1	N	264:UNK	C	276:UNK	N	20.62
1	M	63:UNK	C	69:UNK	N	20.54
1	N	63:UNK	C	69:UNK	N	20.54
1	M	17:UNK	C	24:UNK	N	20.40
1	N	17:UNK	C	24:UNK	N	20.40

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	150:UNK	C	158:UNK	N	19.85
1	N	150:UNK	C	158:UNK	N	19.85
1	M	4950:UNK	C	5137:UNK	N	19.70
1	N	4950:UNK	C	5137:UNK	N	19.70
1	M	4794:UNK	C	4804:UNK	N	19.52
1	N	4794:UNK	C	4804:UNK	N	19.52
1	M	8204:UNK	C	8211:UNK	N	19.44
1	N	8204:UNK	C	8211:UNK	N	19.43
1	M	4399:UNK	C	4407:UNK	N	19.41
1	N	4399:UNK	C	4407:UNK	N	19.41
1	M	4163:UNK	C	4173:UNK	N	19.34
1	N	4163:UNK	C	4173:UNK	N	19.34
1	M	2647:UNK	C	2663:UNK	N	19.24
1	N	2647:UNK	C	2663:UNK	N	19.24
1	M	98:UNK	C	108:UNK	N	19.08
1	N	98:UNK	C	108:UNK	N	19.08
1	M	4854:UNK	C	4865:UNK	N	19.05
1	N	4854:UNK	C	4865:UNK	N	19.05
1	M	6557:UNK	C	6601:UNK	N	18.71
1	N	6557:UNK	C	6601:UNK	N	18.71
1	M	6911:UNK	C	6924:UNK	N	18.05
1	N	6911:UNK	C	6924:UNK	N	18.05
1	M	2809:UNK	C	2822:UNK	N	17.92
1	N	2809:UNK	C	2822:UNK	N	17.92
1	N	4828:UNK	C	4841:UNK	N	17.16
1	M	4828:UNK	C	4841:UNK	N	17.15
1	M	8179:UNK	C	8193:UNK	N	17.14
1	N	8179:UNK	C	8193:UNK	N	17.14
1	M	6194:UNK	C	6210:UNK	N	15.76
1	N	6194:UNK	C	6210:UNK	N	15.76
1	B	254:UNK	C	261:UNK	N	15.57
1	D	254:UNK	C	261:UNK	N	15.57
1	M	382:UNK	C	394:UNK	N	15.53
1	N	382:UNK	C	394:UNK	N	15.53
1	M	6161:UNK	C	6172:UNK	N	15.30
1	N	6161:UNK	C	6172:UNK	N	15.30
1	M	79:UNK	C	83:UNK	N	15.14
1	N	79:UNK	C	83:UNK	N	15.14
1	M	8355:UNK	C	8367:UNK	N	15.11
1	N	8355:UNK	C	8367:UNK	N	15.11
1	M	6416:UNK	C	6431:UNK	N	14.90
1	N	6416:UNK	C	6431:UNK	N	14.90

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	7167:UNK	C	7201:UNK	N	14.22
1	M	7167:UNK	C	7201:UNK	N	14.21
1	M	8269:UNK	C	8274:UNK	N	14.20
1	N	8269:UNK	C	8274:UNK	N	14.20
1	M	442:UNK	C	455:UNK	N	14.03
1	N	442:UNK	C	455:UNK	N	14.03
1	M	4128:UNK	C	4136:UNK	N	14.01
1	N	4128:UNK	C	4136:UNK	N	14.01
1	M	6316:UNK	C	6327:UNK	N	13.82
1	N	6316:UNK	C	6327:UNK	N	13.82
1	M	38:UNK	C	44:UNK	N	13.50
1	N	38:UNK	C	44:UNK	N	13.50
1	B	84:UNK	C	91:UNK	N	12.91
1	D	84:UNK	C	91:UNK	N	12.91
1	M	2608:UNK	C	2630:UNK	N	12.79
1	N	2608:UNK	C	2630:UNK	N	12.79
1	B	42:UNK	C	49:UNK	N	12.40
1	D	42:UNK	C	49:UNK	N	12.40
1	M	6532:UNK	C	6542:UNK	N	12.09
1	N	6532:UNK	C	6542:UNK	N	12.09
1	M	4588:UNK	C	4598:UNK	N	11.91
1	N	4588:UNK	C	4598:UNK	N	11.90
1	B	168:UNK	C	175:UNK	N	11.88
1	D	168:UNK	C	175:UNK	N	11.88
1	M	6622:UNK	C	6636:UNK	N	11.62
1	N	6622:UNK	C	6636:UNK	N	11.61
1	M	6242:UNK	C	6267:UNK	N	11.55
1	N	6242:UNK	C	6267:UNK	N	11.55
1	M	8407:UNK	C	8415:UNK	N	11.17
1	N	8407:UNK	C	8415:UNK	N	11.16
1	N	4303:UNK	C	4314:UNK	N	11.14
1	M	4303:UNK	C	4314:UNK	N	11.13
1	B	127:UNK	C	133:UNK	N	11.04
1	D	127:UNK	C	133:UNK	N	11.04
1	M	4499:UNK	C	4511:UNK	N	10.80
1	N	4499:UNK	C	4511:UNK	N	10.80
1	M	8379:UNK	C	8393:UNK	N	10.75
1	N	8379:UNK	C	8393:UNK	N	10.75
1	M	5262:UNK	C	5273:UNK	N	10.22
1	N	5262:UNK	C	5273:UNK	N	10.22
1	B	211:UNK	C	216:UNK	N	10.20
1	D	211:UNK	C	216:UNK	N	10.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	6389:UNK	C	6402:UNK	N	10.15
1	N	6389:UNK	C	6402:UNK	N	10.15
1	M	319:UNK	C	332:UNK	N	10.11
1	N	319:UNK	C	332:UNK	N	10.11
1	M	169:UNK	C	175:UNK	N	10.01
1	N	169:UNK	C	175:UNK	N	10.01
1	M	8460:UNK	C	8471:UNK	N	9.97
1	N	8460:UNK	C	8471:UNK	N	9.97
1	M	7143:UNK	C	7147:UNK	N	9.83
1	N	7143:UNK	C	7147:UNK	N	9.83
1	B	299:UNK	C	304:UNK	N	9.31
1	D	299:UNK	C	304:UNK	N	9.31
1	M	4145:UNK	C	4151:UNK	N	8.71
1	N	4145:UNK	C	4151:UNK	N	8.71
1	M	6442:UNK	C	6453:UNK	N	8.69
1	N	6442:UNK	C	6453:UNK	N	8.69
1	B	320:UNK	C	327:UNK	N	7.11
1	D	320:UNK	C	327:UNK	N	7.11
1	B	97:UNK	C	101:UNK	N	7.02
1	D	97:UNK	C	101:UNK	N	7.02
1	N	4525:UNK	C	4529:UNK	N	6.93
1	M	4525:UNK	C	4529:UNK	N	6.92
1	B	287:UNK	C	293:UNK	N	6.66
1	D	287:UNK	C	293:UNK	N	6.66
1	B	199:UNK	C	205:UNK	N	6.62
1	D	199:UNK	C	205:UNK	N	6.62
1	B	179:UNK	C	184:UNK	N	6.48
1	D	179:UNK	C	184:UNK	N	6.48
1	B	309:UNK	C	315:UNK	N	5.88
1	D	309:UNK	C	315:UNK	N	5.88
1	B	268:UNK	C	272:UNK	N	5.87
1	D	268:UNK	C	272:UNK	N	5.86
1	B	222:UNK	C	228:UNK	N	5.63
1	D	222:UNK	C	228:UNK	N	5.63
1	B	138:UNK	C	142:UNK	N	5.56
1	D	138:UNK	C	142:UNK	N	5.56
1	B	277:UNK	C	283:UNK	N	5.52
1	D	277:UNK	C	283:UNK	N	5.52
1	B	54:UNK	C	58:UNK	N	5.34
1	D	54:UNK	C	58:UNK	N	5.34
1	B	157:UNK	C	162:UNK	N	4.74
1	D	157:UNK	C	162:UNK	N	4.74

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	233:UNK	C	237:UNK	N	4.70
1	D	233:UNK	C	237:UNK	N	4.70
1	B	73:UNK	C	78:UNK	N	4.64
1	D	73:UNK	C	78:UNK	N	4.64
1	B	64:UNK	C	67:UNK	N	3.96
1	D	64:UNK	C	67:UNK	N	3.96
1	M	8287:UNK	C	8289:UNK	N	3.95
1	N	8287:UNK	C	8289:UNK	N	3.95
1	B	106:UNK	C	109:UNK	N	3.94
1	D	106:UNK	C	109:UNK	N	3.94
1	B	242:UNK	C	246:UNK	N	3.91
1	D	242:UNK	C	246:UNK	N	3.91
1	B	190:UNK	C	193:UNK	N	3.80
1	D	190:UNK	C	193:UNK	N	3.80
1	B	148:UNK	C	151:UNK	N	3.75
1	D	148:UNK	C	151:UNK	N	3.74
1	B	116:UNK	C	119:UNK	N	3.73
1	D	116:UNK	C	119:UNK	N	3.73

## 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	374/446 (83%)	0.64	42 (11%) <b>7</b> <b>12</b>	200, 200, 200, 200	0
1	C	374/446 (83%)	0.51	29 (7%) <b>16</b> <b>19</b>	200, 200, 200, 200	0
2	B	0/400	-	-	-	-
2	D	0/400	-	-	-	-
3	M	0/2300	-	-	-	-
3	N	0/2300	-	-	-	-
All	All	748/6292 (11%)	0.58	71 (9%) <b>10</b> <b>14</b>	200, 200, 200, 200	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	335	THR	5.4
1	A	384	THR	5.4
1	A	108	SER	5.0
1	A	267	GLU	4.9
1	A	104	CYS	4.5
1	A	106	ALA	4.3
1	C	362	SER	4.2
1	A	397	ALA	4.1
1	A	411	SER	4.0
1	C	336	VAL	3.9
1	C	397	ALA	3.9
1	C	399	ARG	3.9
1	A	424	GLU	3.8
1	C	337	HIS	3.7
1	A	305	GLU	3.6
1	C	398	GLY	3.6
1	A	435	GLU	3.5
1	C	283	GLN	3.5
1	A	386	GLU	3.4
1	A	179	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	286	ILE	3.3
1	C	390	TYR	3.2
1	A	335	THR	3.2
1	A	287	LYS	3.1
1	A	385	ASN	3.0
1	A	164	VAL	3.0
1	C	411	SER	3.0
1	C	246	PHE	2.9
1	A	407	ILE	2.9
1	C	302	ASP	2.8
1	A	107	LYS	2.8
1	A	368	ARG	2.7
1	A	396	ARG	2.6
1	A	105	GLN	2.6
1	C	394	VAL	2.6
1	A	304	LEU	2.6
1	A	268	ILE	2.6
1	C	107	LYS	2.5
1	A	410	VAL	2.5
1	C	395	GLY	2.4
1	C	410	VAL	2.4
1	A	395	GLY	2.4
1	A	103	LEU	2.3
1	C	258	CYS	2.3
1	C	363	THR	2.3
1	C	301	LEU	2.3
1	A	433	PHE	2.3
1	A	399	ARG	2.2
1	C	108	SER	2.2
1	A	159	ASP	2.2
1	A	248	ALA	2.2
1	A	377	LEU	2.2
1	C	287	LYS	2.2
1	C	371	ASP	2.2
1	A	263	GLN	2.2
1	C	111	GLY	2.2
1	C	126	PRO	2.1
1	C	140	ARG	2.1
1	A	163	ALA	2.1
1	C	162	THR	2.1
1	A	84	HIS	2.1
1	A	175	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	ALA	2.1
1	C	320	ASN	2.1
1	C	444	LEU	2.1
1	A	95	GLN	2.0
1	A	301	LEU	2.0
1	A	165	PHE	2.0
1	C	361	VAL	2.0
1	A	383	LEU	2.0
1	A	62	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	KEG	A	503	53/53	0.86	0.36	-0.51	200,200,200,200	53
4	KEG	A	502	53/53	0.88	0.25	-0.86	200,200,200,200	53
4	KEG	A	501	53/53	0.92	0.17	-0.89	200,200,200,200	53
4	KEG	M	8703	53/53	0.97	0.19	-	200,200,200,200	53
4	KEG	M	8701	53/53	0.98	0.14	-	200,200,200,200	53
4	KEG	N	8701	53/53	0.98	0.08	-	200,200,200,200	53
4	KEG	N	8705	53/53	0.98	0.11	-	200,200,200,200	53
4	KEG	M	8702	53/53	0.98	0.08	-	200,200,200,200	53
4	KEG	N	8702	53/53	0.97	0.14	-	200,200,200,200	53
4	KEG	N	8704	53/53	0.97	0.14	-	200,200,200,200	53
4	KEG	N	8703	53/53	0.89	0.19	-	200,200,200,200	53

## 6.5 Other polymers

There are no such residues in this entry.