Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:05 PM GMT

PDB ID	:	3SOM
Title	:	crystal structure of human MMACHC
Authors	:	Krojer, T.; Froese, D.S.; von Delft, F.; Muniz, J.R.; Gileadi, C.; Vollmar, M.; Bountra, C.; Arrowsmith, C.H.; Weigelt, J.; Edwards, A.; Gravel, R.A.; Yue, W.W.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on	:	2011-06-30
Resolution	:	2.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

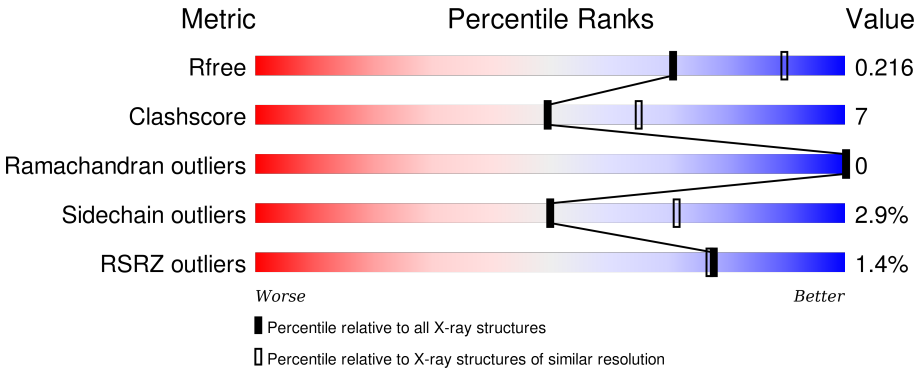
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 <=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	286	2% 70% 9% 21%
1	B	286	2% 69% 10% 20%
1	C	286	3% 69% 10% • 20%
1	D	286	% 70% 9% • 20%
1	E	286	72% 8% 20%

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Mol	Chain	Length	Quality of chain
1	F	286	71% 9% 20%
1	G	286	70% 9% 20%
1	H	286	69% 10% 21%
1	I	286	69% 10% 20%
1	J	286	69% 10% 21%
1	K	286	70% 9% 21%
1	L	286	72% 9% 19%
1	M	286	73% 8% 19%
1	N	286	70% 10% 19%
1	O	286	70% 9% 20%
1	P	286	70% 10% 20%

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	DHL	C	601	-	-	-	X
4	DHL	D	601	-	-	-	X
4	DHL	I	601	-	-	-	X
4	DHL	J	601	-	-	-	X
4	DHL	K	601	-	-	-	X
4	DHL	N	601	-	-	-	X
4	DHL	O	601	-	-	-	X
5	5AD	A	401	X	-	-	-
5	5AD	B	401	X	-	-	-
5	5AD	C	401	X	-	-	-
5	5AD	D	401	X	-	-	-
5	5AD	E	401	X	-	-	-
5	5AD	F	401	X	-	-	-
5	5AD	G	283	X	-	-	X
5	5AD	G	401	X	-	-	-
5	5AD	H	401	X	-	-	-
5	5AD	I	283	X	-	-	X
5	5AD	I	401	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	5AD	J	401	X	-	-	-
5	5AD	K	401	X	-	-	-
5	5AD	L	401	X	-	-	-
5	5AD	M	401	X	-	-	-
5	5AD	N	401	X	-	-	-
5	5AD	O	401	X	-	-	-
5	5AD	P	401	X	-	-	-
6	EDO	P	284	-	-	X	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 33236 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 Methylmalonic aciduria and homocystinuria type C protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	Se	0	0	0
			1837	1193	319	318	5	2			
1	B	228	Total	C	N	O	S	Se	0	0	0
			1837	1193	319	318	5	2			
1	C	228	Total	C	N	O	S	Se	0	2	0
			1832	1190	318	316	6	2			
1	D	229	Total	C	N	O	S	Se	0	1	0
			1848	1200	320	320	6	2			
1	E	230	Total	C	N	O	S	Se	0	1	0
			1849	1201	321	319	6	2			
1	F	228	Total	C	N	O	S	Se	0	3	0
			1857	1203	324	322	6	2			
1	G	228	Total	C	N	O	S	Se	0	0	0
			1843	1195	322	319	5	2			
1	H	227	Total	C	N	O	S	Se	0	0	0
			1833	1190	317	319	5	2			
1	I	228	Total	C	N	O	S	Se	0	1	0
			1844	1196	321	319	6	2			
1	J	227	Total	C	N	O	S	Se	0	2	0
			1844	1196	321	319	5	3			
1	K	227	Total	C	N	O	S	Se	0	1	0
			1832	1189	318	318	5	2			
1	L	231	Total	C	N	O	S	Se	0	2	0
			1868	1213	325	322	6	2			
1	M	231	Total	C	N	O	S	Se	0	1	0
			1861	1206	321	326	6	2			
1	N	232	Total	C	N	O	S	Se	0	0	0
			1853	1204	324	318	5	2			
1	O	228	Total	C	N	O	S	Se	0	1	0
			1836	1194	316	318	6	2			
1	P	230	Total	C	N	O	S	Se	0	0	0
			1860	1208	322	323	5	2			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
A	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
A	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
A	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
B	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
B	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
B	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
B	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
C	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
C	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
C	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
C	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
D	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
D	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
D	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
D	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
E	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
E	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
E	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
E	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
F	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
F	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
F	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
F	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
G	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
G	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
G	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
G	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
H	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
H	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
H	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
H	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
I	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
I	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
I	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
I	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
J	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
J	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
J	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
J	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
K	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
K	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1

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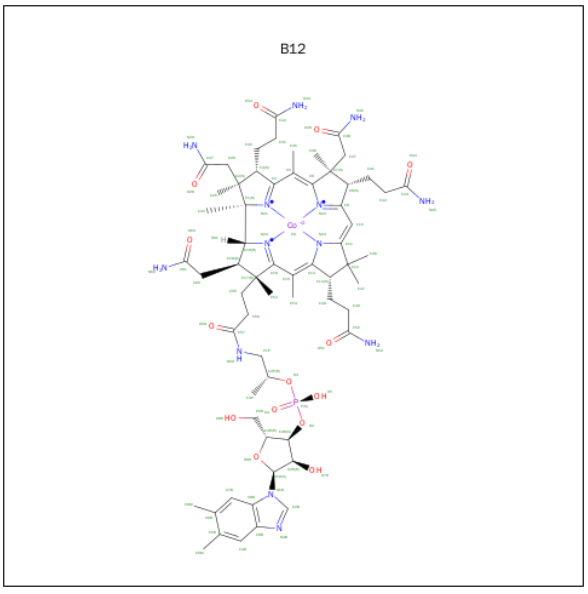
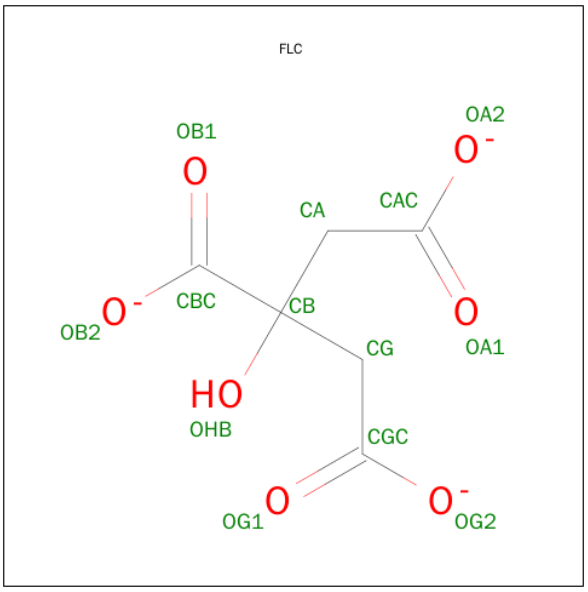
Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
K	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
L	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
L	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
L	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
L	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
M	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
M	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
M	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
M	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
N	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
N	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
N	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
N	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
O	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
O	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
O	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
O	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1
P	-3	TYR	-	EXPRESSION TAG	UNP Q9Y4U1
P	-2	PHE	-	EXPRESSION TAG	UNP Q9Y4U1
P	-1	GLN	-	EXPRESSION TAG	UNP Q9Y4U1
P	0	SER	-	EXPRESSION TAG	UNP Q9Y4U1

- Molecule 2 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	D	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	E	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	F	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	G	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	H	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	I	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	J	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	K	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	L	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	M	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	N	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	O	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	P	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0
3	D	1	Total C O 13 6 7	0	0
3	E	1	Total C O 13 6 7	0	0
3	F	1	Total C O 13 6 7	0	0
3	G	1	Total C O 13 6 7	0	0
3	H	1	Total C O 13 6 7	0	0
3	I	1	Total C O 13 6 7	0	0
3	J	1	Total C O 13 6 7	0	0
3	K	1	Total C O 13 6 7	0	0
3	L	1	Total C O 13 6 7	0	0
3	M	1	Total C O 13 6 7	0	0
3	N	1	Total C O 13 6 7	0	0

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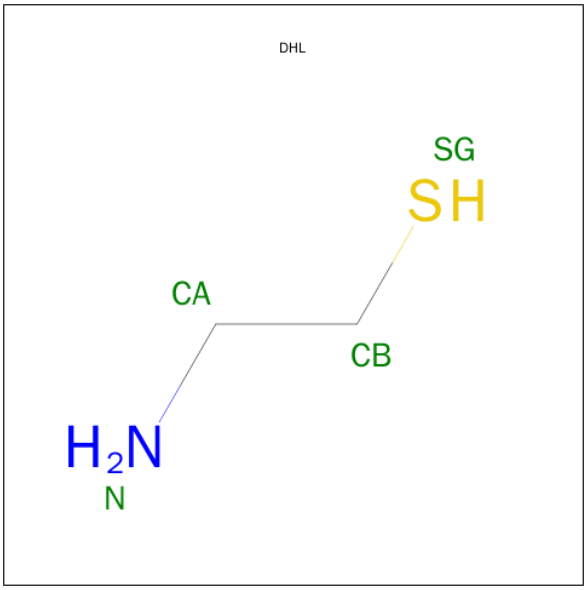
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total C O 13 6 7	0	0
3	P	1	Total C O 13 6 7	0	0

- Molecule 4 is 2-AMINO-ETHANETHIOL (three-letter code: DHL) (formula: C_2H_7NS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N S 4 2 1 1	0	0
4	C	1	Total C N S 4 2 1 1	0	0
4	D	1	Total C N S 4 2 1 1	0	0
4	F	1	Total C N S 4 2 1 1	0	0
4	G	1	Total C N S 4 2 1 1	0	0
4	H	1	Total C N S 4 2 1 1	0	0
4	I	1	Total C N S 4 2 1 1	0	0
4	J	1	Total C N S 4 2 1 1	0	0
4	K	1	Total C N S 4 2 1 1	0	0

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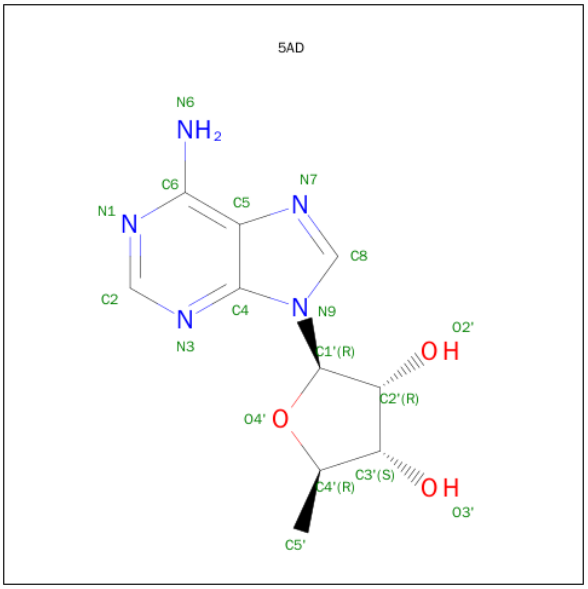
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C N S 4 2 1 1	0	0
4	M	1	Total C N S 4 2 1 1	0	0
4	N	1	Total C N S 4 2 1 1	0	0
4	O	1	Total C N S 4 2 1 1	0	0
4	P	1	Total C N S 4 2 1 1	0	0

- Molecule 5 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 18 10 5 3	0	0
5	B	1	Total C N O 18 10 5 3	0	0
5	C	1	Total C N O 18 10 5 3	0	0
5	D	1	Total C N O 18 10 5 3	0	0
5	E	1	Total C N O 18 10 5 3	0	0
5	F	1	Total C N O 18 10 5 3	0	0

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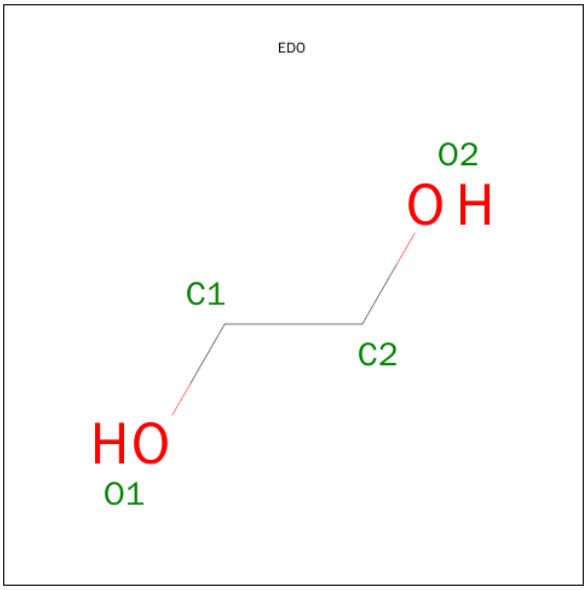
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			18	10	5	3		
5	G	1	Total	C	N	O	0	0
			18	10	5	3		
5	H	1	Total	C	N	O	0	0
			18	10	5	3		
5	I	1	Total	C	N	O	0	0
			18	10	5	3		
5	I	1	Total	C	N	O	0	0
			18	10	5	3		
5	J	1	Total	C	N	O	0	0
			18	10	5	3		
5	K	1	Total	C	N	O	0	0
			18	10	5	3		
5	L	1	Total	C	N	O	0	0
			18	10	5	3		
5	M	1	Total	C	N	O	0	0
			18	10	5	3		
5	N	1	Total	C	N	O	0	0
			18	10	5	3		
5	O	1	Total	C	N	O	0	0
			18	10	5	3		
5	P	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is water.

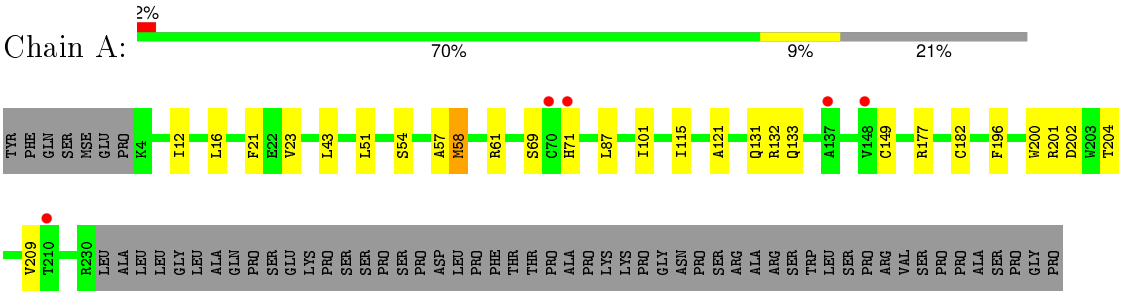
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	70	Total O 70 70	0	0
7	B	63	Total O 63 63	0	0
7	C	63	Total O 63 63	0	0
7	D	79	Total O 79 79	0	0
7	E	105	Total O 105 105	0	0
7	F	111	Total O 111 111	0	0
7	G	125	Total O 125 125	0	0
7	H	124	Total O 124 124	0	0
7	I	122	Total O 122 122	0	0
7	J	111	Total O 111 111	0	0
7	K	100	Total O 100 100	0	0
7	L	130	Total O 130 130	0	0
7	M	125	Total O 125 125	0	0
7	N	100	Total O 100 100	0	0
7	O	124	Total O 124 124	0	0
7	P	94	Total O 94 94	0	0

3 Residue-property plots (i)

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.

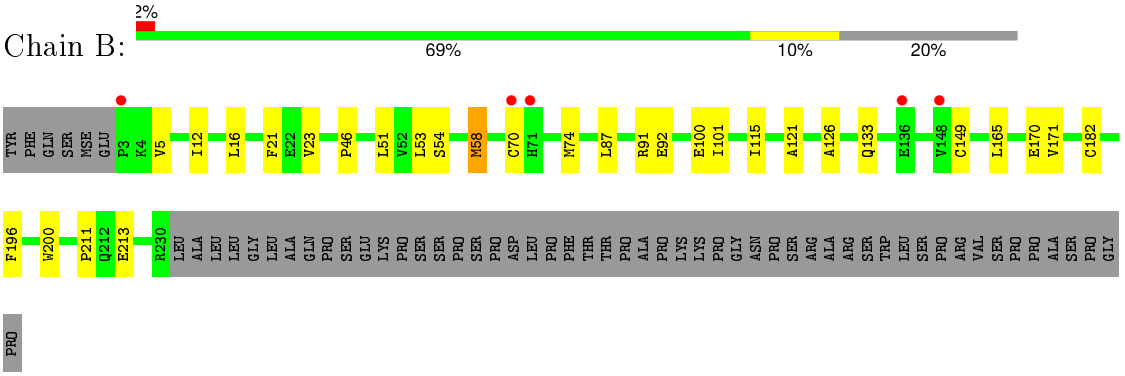
- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain A:



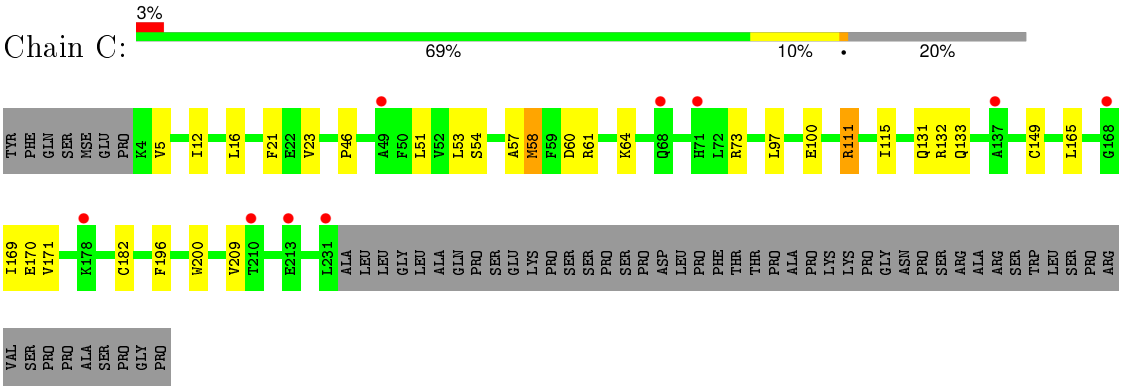
- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain B:



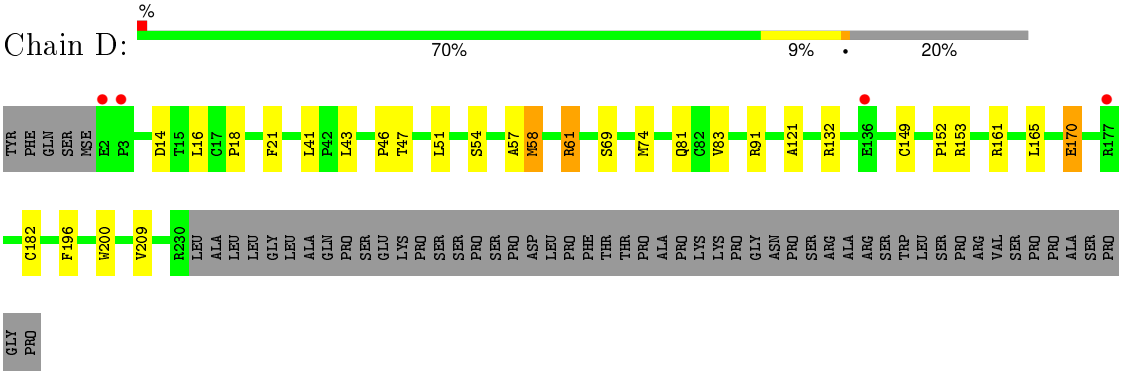
- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain C:



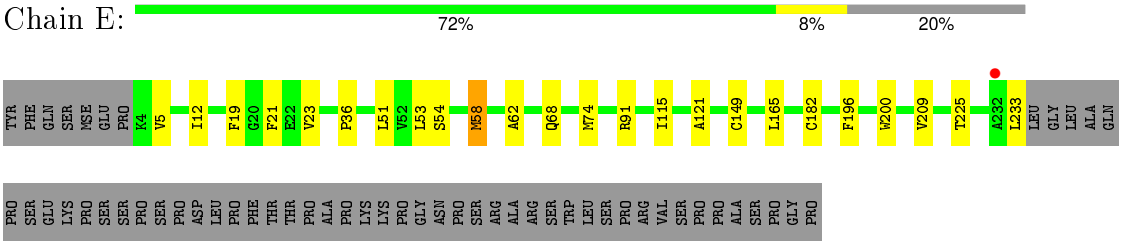
- Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain D:



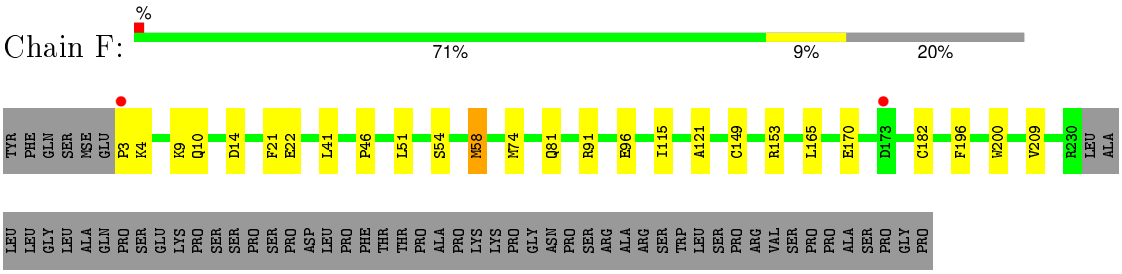
• Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain E:



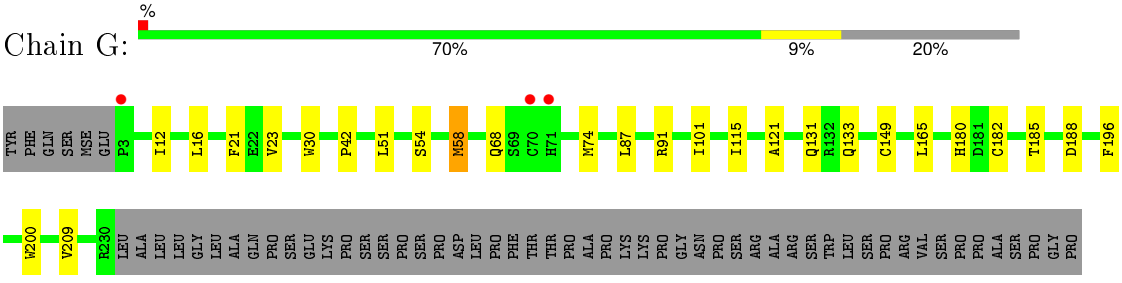
• Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain F:



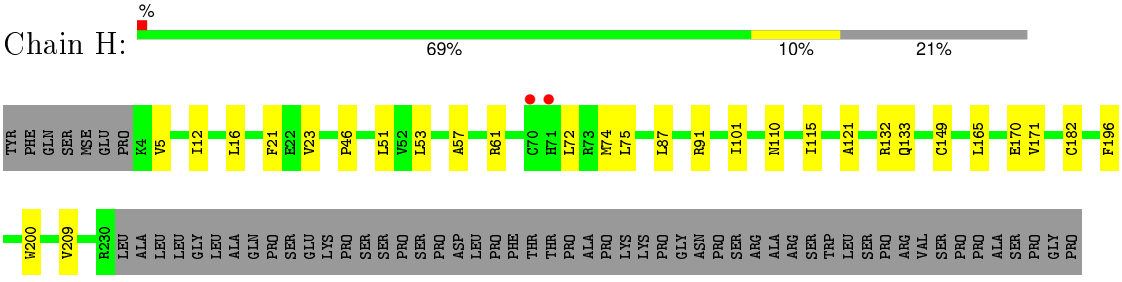
• Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain G:



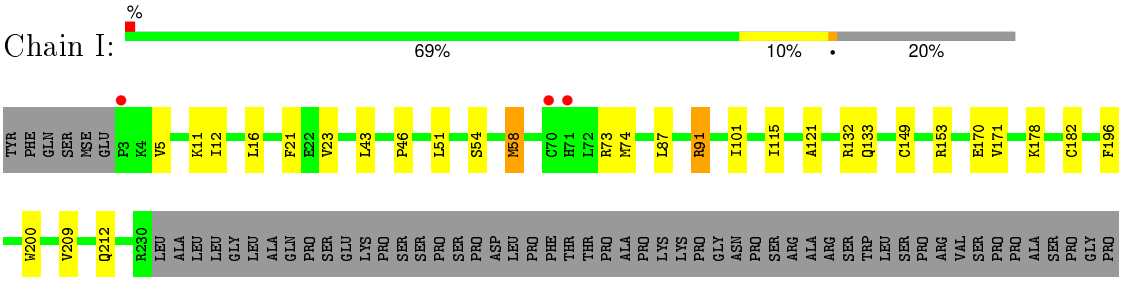
• Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain H:



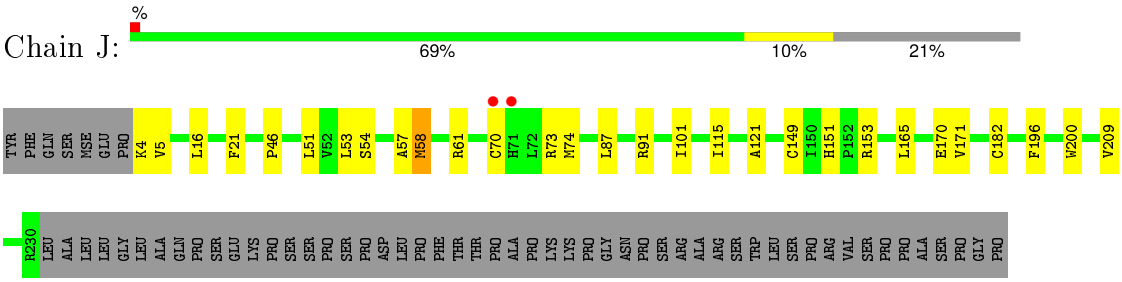
• Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain I:



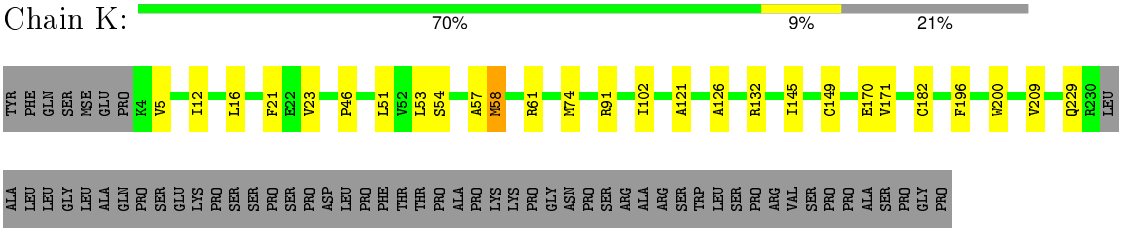
• Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain J:



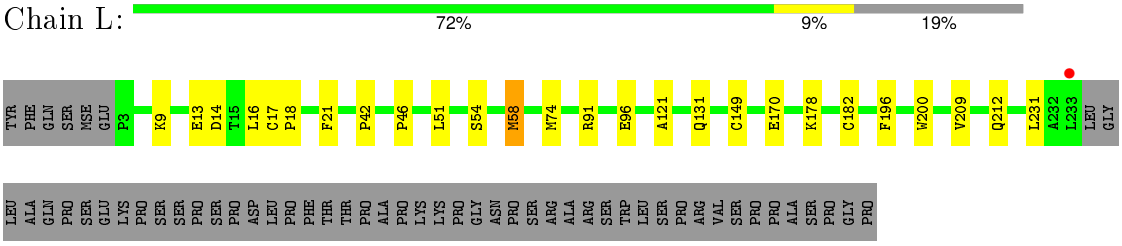
• Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain K:



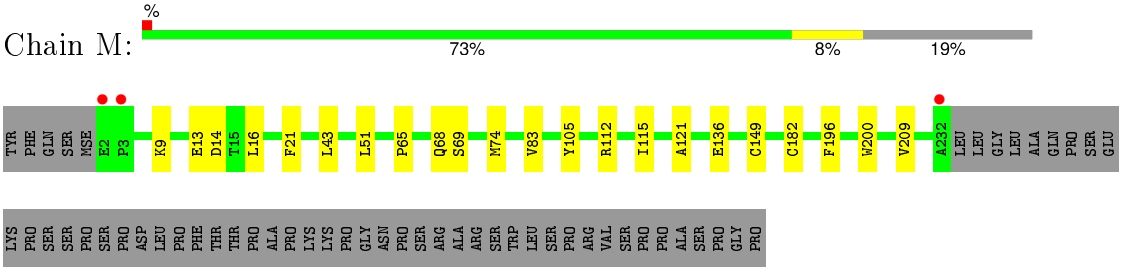
• Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain L:



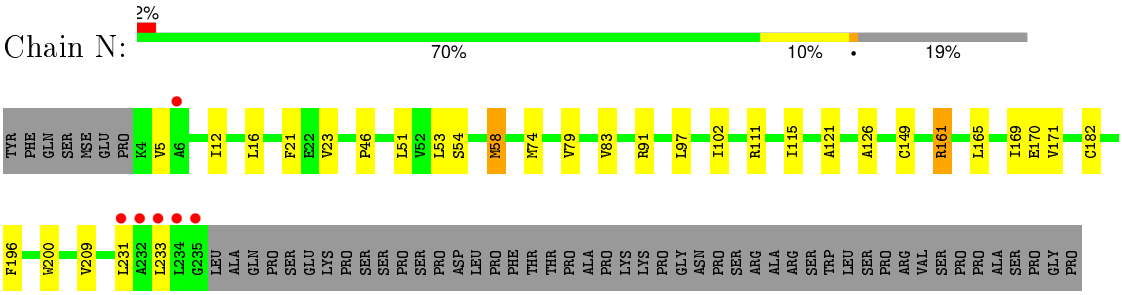
• Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain M:



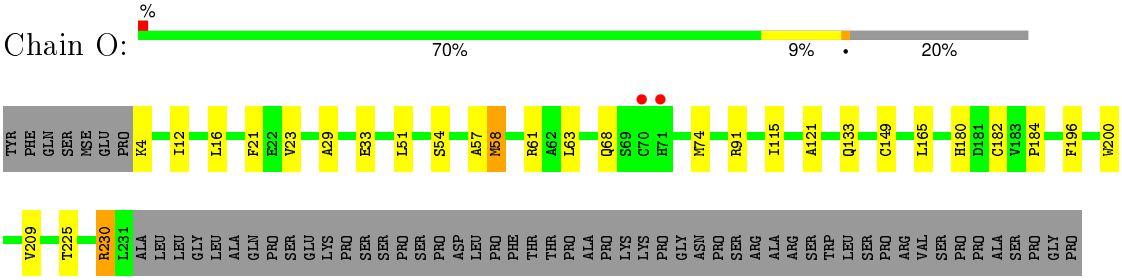
• Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain N:



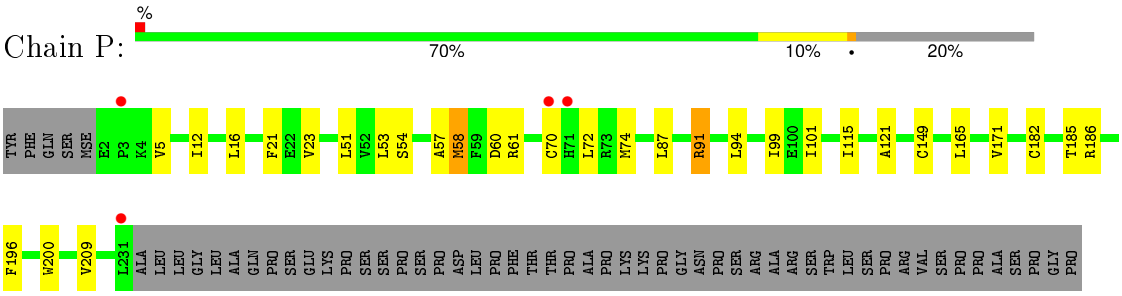
• Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain O:



• Molecule 1: Methylmalonic aciduria and homocystinuria type C protein

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.66Å 71.96Å 300.06Å 88.53° 85.25° 83.76°	Depositor
Resolution (Å)	19.86 – 2.40 19.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.86-2.40) 98.2 (19.84-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.41Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.182 , 0.206 0.190 , 0.216	Depositor DCC
R_{free} test set	11473 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.7	EDS
Estimated twinning fraction	0.007 for -h,-k,-h+l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 228734 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	33236	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FLC, DHL, B12, EDO, 5AD

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	0.47	0/1898	0.63	0/2592
1	B	0.45	0/1899	0.64	0/2595
1	C	0.46	0/1899	0.64	0/2598
1	D	0.47	0/1913	0.64	0/2616
1	E	0.47	0/1913	0.65	0/2615
1	F	0.50	0/1928	0.67	0/2635
1	G	0.48	0/1905	0.64	0/2603
1	H	0.48	0/1894	0.65	0/2588
1	I	0.46	0/1909	0.64	0/2609
1	J	0.48	0/1911	0.66	0/2610
1	K	0.49	0/1899	0.66	0/2596
1	L	0.49	0/1936	0.68	0/2646
1	M	0.49	0/1926	0.66	0/2635
1	N	0.48	0/1914	0.67	0/2618
1	O	0.49	0/1900	0.67	0/2596
1	P	0.48	0/1922	0.65	0/2626
All	All	0.48	0/30566	0.65	0/41778

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1837	0	1791	15	0
1	B	1837	0	1792	15	0
1	C	1832	0	1779	18	0
1	D	1848	0	1798	20	0
1	E	1849	0	1802	18	0
1	F	1857	0	1813	19	0
1	G	1843	0	1797	21	0
1	H	1833	0	1782	22	0
1	I	1844	0	1796	22	0
1	J	1844	0	1804	16	0
1	K	1832	0	1783	21	0
1	L	1868	0	1826	17	0
1	M	1861	0	1800	19	0
1	N	1853	0	1806	21	0
1	O	1836	0	1786	23	0
1	P	1860	0	1817	22	0
2	A	91	0	88	14	0
2	B	91	0	88	13	0
2	C	91	0	88	15	0
2	D	91	0	88	12	0
2	E	91	0	88	14	0
2	F	91	0	88	13	0
2	G	91	0	88	15	0
2	H	91	0	88	13	0
2	I	91	0	88	14	0
2	J	91	0	88	12	0
2	K	91	0	88	12	0
2	L	91	0	88	13	0
2	M	91	0	88	12	0
2	N	91	0	88	13	0
2	O	91	0	88	15	0
2	P	91	0	88	16	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
3	C	13	0	5	0	0
3	D	13	0	5	0	0
3	E	13	0	5	0	0
3	F	13	0	5	0	0
3	G	13	0	5	0	0
3	H	13	0	5	0	0
3	I	13	0	5	0	0
3	J	13	0	5	0	0
3	K	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	13	0	5	0	0
3	M	13	0	5	0	0
3	N	13	0	5	0	0
3	O	13	0	5	0	0
3	P	13	0	5	0	0
4	A	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	2	0
4	F	4	0	6	0	0
4	G	4	0	6	1	0
4	H	4	0	6	0	0
4	I	4	0	7	3	0
4	J	4	0	7	1	0
4	K	4	0	7	3	0
4	L	4	0	6	0	0
4	M	4	0	6	0	0
4	N	4	0	7	1	0
4	O	4	0	6	1	0
4	P	4	0	6	0	0
5	A	18	0	13	3	0
5	B	18	0	13	3	0
5	C	18	0	13	4	0
5	D	18	0	13	3	0
5	E	18	0	13	3	0
5	F	18	0	13	3	0
5	G	36	0	26	4	0
5	H	18	0	13	4	0
5	I	36	0	26	4	0
5	J	18	0	13	3	0
5	K	18	0	13	3	0
5	L	18	0	13	3	0
5	M	18	0	13	3	0
5	N	18	0	13	4	0
5	O	18	0	13	3	0
5	P	18	0	13	3	0
6	E	4	0	6	2	0
6	P	8	0	12	7	0
7	A	70	0	0	0	0
7	B	63	0	0	1	0
7	C	63	0	0	0	0
7	D	79	0	0	0	0
7	E	105	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	111	0	0	0	0
7	G	125	0	0	1	0
7	H	124	0	0	0	0
7	I	122	0	0	2	0
7	J	111	0	0	0	0
7	K	100	0	0	0	0
7	L	130	0	0	0	0
7	M	125	0	0	3	0
7	N	100	0	0	0	0
7	O	124	0	0	1	0
7	P	94	0	0	0	0
All	All	33236	0	30600	442	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 7.

All (442) 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:D:182:CYS:SG	4:D:601:DHL:SG	2.33	1.26
2:A:301:B12:H362	2:A:301:B12:H351	1.37	1.06
2:P:301:B12:H362	2:P:301:B12:H351	1.37	1.05
2:D:301:B12:H362	2:D:301:B12:H351	1.39	1.03
2:O:301:B12:H351	2:O:301:B12:H362	1.40	1.03
2:G:301:B12:H362	2:G:301:B12:H351	1.37	1.03
2:M:301:B12:H362	2:M:301:B12:H351	1.39	1.03
2:I:301:B12:H351	2:I:301:B12:H362	1.38	1.02
2:K:301:B12:H362	2:K:301:B12:H351	1.38	1.02
2:L:301:B12:H362	2:L:301:B12:H351	1.39	1.02
2:F:301:B12:H362	2:F:301:B12:H351	1.39	1.01
2:E:301:B12:H351	2:E:301:B12:H362	1.39	1.01
2:C:301:B12:H351	2:C:301:B12:H362	1.40	1.01
2:J:301:B12:H351	2:J:301:B12:H362	1.41	1.00
2:B:301:B12:H362	2:B:301:B12:H351	1.42	1.00
2:H:301:B12:H351	2:H:301:B12:H362	1.39	1.00
2:N:301:B12:H351	2:N:301:B12:H362	1.40	0.99
1:E:36:PRO:HD3	6:E:283:EDO:H12	1.47	0.94
1:D:149:CYS:H	2:D:301:B12:H332	1.18	0.92
1:K:149:CYS:H	2:K:301:B12:H332	1.18	0.91
1:B:149:CYS:H	2:B:301:B12:H332	1.19	0.91
1:L:149:CYS:H	2:L:301:B12:H332	1.16	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:CYS:H	2:H:301:B12:H332	1.17	0.90
1:P:149:CYS:H	2:P:301:B12:H332	1.19	0.89
1:J:149:CYS:H	2:J:301:B12:H332	1.16	0.89
1:E:149:CYS:H	2:E:301:B12:H332	1.18	0.88
1:K:51:LEU:HD22	1:K:121:ALA:HA	1.55	0.88
1:A:149:CYS:H	2:A:301:B12:H332	1.18	0.88
1:M:149:CYS:H	2:M:301:B12:H332	1.17	0.88
1:I:149:CYS:H	2:I:301:B12:H332	1.18	0.88
1:N:149:CYS:H	2:N:301:B12:H332	1.18	0.88
1:G:149:CYS:H	2:G:301:B12:H332	1.18	0.87
2:N:301:B12:H531	2:N:301:B12:H552	1.57	0.87
2:F:301:B12:H552	2:F:301:B12:H531	1.57	0.86
1:F:149:CYS:H	2:F:301:B12:H332	1.19	0.86
1:O:230:ARG:HH11	1:O:230:ARG:HG2	1.38	0.86
1:O:149:CYS:H	2:O:301:B12:H332	1.18	0.86
2:I:301:B12:H531	2:I:301:B12:H552	1.57	0.86
2:E:301:B12:H531	2:E:301:B12:H552	1.58	0.86
2:A:301:B12:H531	2:A:301:B12:H552	1.59	0.85
2:G:301:B12:H552	2:G:301:B12:H531	1.58	0.85
1:E:74:MSE:HE1	1:F:165:LEU:HD13	1.55	0.85
2:H:301:B12:H531	2:H:301:B12:H552	1.59	0.85
2:K:301:B12:H552	2:K:301:B12:H531	1.60	0.84
2:D:301:B12:H552	2:D:301:B12:H531	1.60	0.84
1:K:182:CYS:HG	4:K:601:DHL:HS	0.86	0.84
1:C:149:CYS:H	2:C:301:B12:H332	1.26	0.83
2:J:301:B12:H552	2:J:301:B12:H531	1.60	0.83
2:C:301:B12:H552	2:C:301:B12:H531	1.60	0.83
2:P:301:B12:H531	2:P:301:B12:H552	1.60	0.83
2:O:301:B12:H552	2:O:301:B12:H531	1.60	0.82
2:M:301:B12:H552	2:M:301:B12:H531	1.60	0.82
2:L:301:B12:H531	2:L:301:B12:H552	1.59	0.82
2:B:301:B12:H531	2:B:301:B12:H552	1.60	0.82
1:K:74:MSE:HE3	1:L:42:PRO:HD2	1.63	0.80
1:P:91:ARG:HG2	6:P:284:EDO:H11	1.64	0.79
1:G:165:LEU:HD13	1:H:74:MSE:HE1	1.63	0.78
1:K:54:SER:HB2	1:K:58:MSE:HG2	1.67	0.77
2:G:301:B12:C36	2:G:301:B12:H351	2.16	0.76
1:D:46:PRO:HB2	1:D:170:GLU:HG3	1.68	0.75
2:A:301:B12:H351	2:A:301:B12:C36	2.16	0.75
1:E:54:SER:HB2	1:E:58:MSE:HG2	1.66	0.75
1:J:54:SER:HB2	1:J:58:MSE:HG2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:301:B12:H351	2:I:301:B12:C36	2.16	0.75
2:M:301:B12:C36	2:M:301:B12:H351	2.17	0.74
2:J:301:B12:H351	2:J:301:B12:C36	2.17	0.74
2:H:301:B12:H351	2:H:301:B12:C36	2.17	0.74
1:H:74:MSE:HG2	1:H:75:LEU:HD12	1.68	0.74
2:L:301:B12:H351	2:L:301:B12:C36	2.17	0.74
1:C:54:SER:HB2	1:C:58:MSE:HG2	1.70	0.74
1:G:74:MSE:HE1	1:H:165:LEU:HD13	1.68	0.74
1:G:54:SER:HB2	1:G:58:MSE:HG2	1.70	0.73
2:D:301:B12:H351	2:D:301:B12:C36	2.17	0.73
1:B:54:SER:HB2	1:B:58:MSE:HG2	1.70	0.73
5:A:401:5AD:C8	2:B:301:B12:H532	2.20	0.72
2:E:301:B12:H351	2:E:301:B12:C36	2.17	0.72
1:A:43:LEU:HD21	1:B:74:MSE:HE1	1.70	0.72
2:P:301:B12:C36	2:P:301:B12:H351	2.15	0.71
2:O:301:B12:H351	2:O:301:B12:C36	2.18	0.71
2:I:301:B12:H532	5:J:401:5AD:C8	2.21	0.71
2:K:301:B12:H532	5:L:401:5AD:C8	2.21	0.71
5:M:401:5AD:C8	2:N:301:B12:H532	2.20	0.71
5:M:401:5AD:H8	2:N:301:B12:H532	1.72	0.71
2:C:301:B12:H532	5:D:401:5AD:C8	2.21	0.71
2:G:301:B12:H532	5:H:401:5AD:C8	2.21	0.71
2:A:301:B12:H532	5:B:401:5AD:C8	2.20	0.71
1:F:54:SER:HB2	1:F:58:MSE:HG2	1.73	0.71
2:F:301:B12:H351	2:F:301:B12:C36	2.17	0.70
2:K:301:B12:H532	5:L:401:5AD:H8	1.73	0.70
1:N:54:SER:HB2	1:N:58:MSE:HG2	1.73	0.70
5:A:401:5AD:H8	2:B:301:B12:H532	1.72	0.70
2:O:301:B12:H203	2:O:301:B12:H301	1.73	0.70
5:O:401:5AD:C8	2:P:301:B12:H532	2.22	0.69
1:C:46:PRO:HB2	1:C:170:GLU:HG2	1.72	0.69
1:D:54:SER:HB2	1:D:58:MSE:HG2	1.74	0.69
1:O:58:MSE:HE1	1:O:63:LEU:HB2	1.73	0.69
2:N:301:B12:C36	2:N:301:B12:H351	2.17	0.69
2:B:301:B12:H301	2:B:301:B12:H203	1.74	0.69
1:L:54:SER:HB2	1:L:58:MSE:HG2	1.73	0.69
2:A:301:B12:H301	2:A:301:B12:H203	1.74	0.69
2:F:301:B12:H301	2:F:301:B12:H203	1.75	0.69
2:E:301:B12:H532	5:F:401:5AD:H8	1.74	0.69
2:E:301:B12:H532	5:F:401:5AD:C8	2.23	0.69
2:C:301:B12:H203	2:C:301:B12:H301	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:301:B12:H203	2:I:301:B12:H301	1.74	0.68
2:L:301:B12:H301	2:L:301:B12:H203	1.75	0.68
2:J:301:B12:H203	2:J:301:B12:H301	1.75	0.68
1:H:74:MSE:HE3	1:H:75:LEU:HD13	1.74	0.68
2:M:301:B12:H532	5:N:401:5AD:H8	1.75	0.68
5:I:401:5AD:C8	2:J:301:B12:H532	2.24	0.68
2:D:301:B12:H301	2:D:301:B12:H203	1.75	0.68
5:G:401:5AD:C8	2:H:301:B12:H532	2.22	0.68
2:M:301:B12:H301	2:M:301:B12:H203	1.75	0.68
2:N:301:B12:H203	2:N:301:B12:H301	1.75	0.68
1:P:54:SER:HB2	1:P:58:MSE:HG2	1.75	0.68
5:C:401:5AD:C8	2:D:301:B12:H532	2.23	0.68
2:A:301:B12:H532	5:B:401:5AD:H8	1.74	0.68
2:G:301:B12:H301	2:G:301:B12:H203	1.74	0.68
5:K:401:5AD:C8	2:L:301:B12:H532	2.24	0.68
5:E:401:5AD:C8	2:F:301:B12:H532	2.24	0.68
2:E:301:B12:H301	2:E:301:B12:H203	1.76	0.68
5:C:401:5AD:H8	2:D:301:B12:H532	1.74	0.68
2:O:301:B12:H532	5:P:401:5AD:C8	2.24	0.68
2:G:301:B12:H532	5:H:401:5AD:H8	1.76	0.68
1:N:58:MSE:HE1	1:N:79:VAL:HG13	1.75	0.68
2:K:301:B12:H203	2:K:301:B12:H301	1.76	0.67
2:H:301:B12:H301	2:H:301:B12:H203	1.76	0.67
2:C:301:B12:H532	5:D:401:5AD:H8	1.75	0.67
1:O:182[A]:CYS:HB3	1:O:209:VAL:HG21	1.76	0.67
2:C:301:B12:H351	2:C:301:B12:C36	2.17	0.67
1:L:46:PRO:HB2	1:L:170:GLU:HG2	1.77	0.67
1:O:58:MSE:CE	1:O:63:LEU:HB2	2.25	0.67
2:I:301:B12:H532	5:J:401:5AD:H8	1.77	0.67
5:E:401:5AD:H8	2:F:301:B12:H532	1.77	0.67
1:K:51:LEU:CD2	1:K:121:ALA:HA	2.23	0.67
2:M:301:B12:H532	5:N:401:5AD:C8	2.24	0.66
2:P:301:B12:H203	2:P:301:B12:H301	1.77	0.66
5:O:401:5AD:H8	2:P:301:B12:H532	1.77	0.66
5:K:401:5AD:H8	2:L:301:B12:H532	1.76	0.66
1:F:46:PRO:HB2	1:F:170:GLU:HG2	1.78	0.66
2:K:301:B12:C36	2:K:301:B12:H351	2.16	0.66
1:E:21:PHE:CZ	1:E:58:MSE:HE3	2.31	0.66
1:A:54:SER:HB2	1:A:58:MSE:HG2	1.76	0.65
5:I:401:5AD:H8	2:J:301:B12:H532	1.77	0.65
1:N:46:PRO:HB2	1:N:170:GLU:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:GLU:OE2	1:F:153[A]:ARG:NH1	2.30	0.65
2:B:301:B12:C36	2:B:301:B12:H351	2.19	0.65
5:G:401:5AD:H8	2:H:301:B12:H532	1.77	0.65
1:J:46:PRO:HB2	1:J:170:GLU:HG2	1.79	0.65
1:I:46:PRO:HB2	1:I:170:GLU:HG2	1.78	0.65
2:O:301:B12:H532	5:P:401:5AD:H8	1.78	0.65
1:J:182:CYS:SG	4:J:601:DHL:SG	2.96	0.64
1:G:185:THR:HG21	7:G:1246:HOH:O	1.97	0.64
1:B:46:PRO:HB2	1:B:170:GLU:HG2	1.78	0.64
1:H:46:PRO:HB2	1:H:170:GLU:HG2	1.79	0.64
1:K:46:PRO:HB2	1:K:170:GLU:HG2	1.81	0.63
1:K:182:CYS:HB3	1:K:209:VAL:HG21	1.81	0.63
1:G:182:CYS:HB3	1:G:209:VAL:HG21	1.81	0.62
1:C:165:LEU:HD13	1:D:74:MSE:HE1	1.81	0.62
1:F:182:CYS:HB3	1:F:209:VAL:HG21	1.80	0.62
1:B:12:ILE:HG22	1:B:23:VAL:HG21	1.81	0.62
1:I:54:SER:HB2	1:I:58:MSE:HG2	1.82	0.61
1:D:182:CYS:HB3	1:D:209:VAL:HG21	1.82	0.61
2:L:301:B12:H601	2:L:301:B12:H252	1.81	0.61
1:G:165:LEU:CD1	1:H:74:MSE:HE1	2.30	0.61
1:L:182:CYS:HB3	1:L:209:VAL:HG21	1.82	0.60
1:O:182[B]:CYS:HB3	1:O:209:VAL:HG21	1.82	0.60
1:I:74:MSE:HE1	1:J:165:LEU:HD13	1.84	0.60
1:O:225:THR:O	1:O:230:ARG:NE	2.35	0.60
2:M:301:B12:H601	2:M:301:B12:H252	1.84	0.59
2:D:301:B12:H252	2:D:301:B12:H601	1.84	0.59
1:C:97:LEU:HD21	1:C:169:ILE:HD11	1.85	0.59
2:F:301:B12:H601	2:F:301:B12:H252	1.85	0.58
1:O:165:LEU:HD13	1:P:74:MSE:HE1	1.84	0.58
2:J:301:B12:H252	2:J:301:B12:H601	1.85	0.58
2:G:301:B12:H601	2:G:301:B12:H252	1.84	0.58
1:N:182:CYS:HB3	1:N:209:VAL:HG21	1.86	0.58
2:H:301:B12:H252	2:H:301:B12:H601	1.86	0.58
1:F:21:PHE:CZ	1:F:58:MSE:HE3	2.39	0.58
2:I:301:B12:N22	5:J:401:5AD:H5'1	2.19	0.58
1:O:230:ARG:HG2	1:O:230:ARG:NH1	2.14	0.58
1:E:182[B]:CYS:HB2	1:E:209:VAL:HG21	1.85	0.58
2:M:301:B12:N22	5:N:401:5AD:H5'1	2.20	0.57
2:C:301:B12:H601	2:C:301:B12:H252	1.85	0.57
1:P:182:CYS:HB3	1:P:209:VAL:HG21	1.86	0.57
1:P:186:ARG:HB3	6:P:283:EDO:H11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:12:ILE:HG22	1:O:23:VAL:HG21	1.86	0.57
1:A:202:ASP:OD1	1:A:204:THR:HB	2.04	0.57
5:A:401:5AD:H5'1	2:B:301:B12:N22	2.19	0.57
1:P:99:ILE:HG12	6:P:284:EDO:H12	1.87	0.57
5:K:401:5AD:H5'1	2:L:301:B12:N22	2.19	0.57
2:E:301:B12:N22	5:F:401:5AD:H5'1	2.20	0.57
5:I:401:5AD:H5'1	2:J:301:B12:N22	2.20	0.57
1:M:182:CYS:HB3	1:M:209:VAL:HG21	1.86	0.57
2:A:301:B12:N22	5:B:401:5AD:H5'1	2.19	0.57
2:K:301:B12:N22	5:L:401:5AD:H5'1	2.20	0.57
5:C:401:5AD:H5'1	2:D:301:B12:N22	2.20	0.56
1:H:182:CYS:HB3	1:H:209:VAL:HG21	1.87	0.56
2:A:301:B12:H601	2:A:301:B12:H252	1.86	0.56
5:E:401:5AD:H5'1	2:F:301:B12:N22	2.21	0.56
1:M:43:LEU:HD21	1:N:74:MSE:HE1	1.87	0.56
2:I:301:B12:H601	2:I:301:B12:H252	1.88	0.56
2:C:301:B12:N22	5:D:401:5AD:H5'1	2.20	0.56
2:P:301:B12:H601	2:P:301:B12:H252	1.87	0.56
1:G:74:MSE:HE1	1:H:165:LEU:CD1	2.35	0.56
5:G:401:5AD:H5'1	2:H:301:B12:N22	2.20	0.55
1:J:182:CYS:HB3	1:J:209:VAL:HG21	1.87	0.55
5:M:401:5AD:H5'1	2:N:301:B12:N22	2.21	0.55
1:G:42:PRO:CD	1:H:75:LEU:HD11	2.35	0.55
5:O:401:5AD:H5'1	2:P:301:B12:N22	2.21	0.55
1:I:43:LEU:HD21	1:J:74[B]:MSE:HE1	1.88	0.55
2:G:301:B12:N22	5:H:401:5AD:H5'1	2.20	0.55
2:O:301:B12:H252	2:O:301:B12:H601	1.88	0.55
2:N:301:B12:H252	2:N:301:B12:H601	1.88	0.55
1:A:182:CYS:HB3	1:A:209:VAL:HG21	1.88	0.55
2:O:301:B12:N22	5:P:401:5AD:H5'1	2.21	0.55
2:K:301:B12:H252	2:K:301:B12:H601	1.89	0.55
1:O:54:SER:HB2	1:O:58:MSE:HG2	1.88	0.54
1:D:57:ALA:O	1:D:61:ARG:HG2	2.07	0.54
2:B:301:B12:H601	2:B:301:B12:H252	1.90	0.54
1:L:13:GLU:HG2	1:L:17[A]:CYS:SG	2.49	0.53
1:I:182[B]:CYS:HB2	1:I:209:VAL:HG21	1.90	0.53
1:K:5:VAL:HG22	1:K:171:VAL:HG11	1.90	0.53
1:A:200:TRP:CD1	2:A:301:B12:H412	2.44	0.53
1:C:5:VAL:HG22	1:C:171:VAL:HG11	1.91	0.53
1:O:16:LEU:HB3	1:O:21:PHE:HB2	1.91	0.53
1:N:5:VAL:HG22	1:N:171:VAL:HG11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:12:ILE:HG22	1:I:23:VAL:HG21	1.92	0.52
1:C:111:ARG:CZ	5:C:401:5AD:H8	2.40	0.52
1:C:131:GLN:NE2	2:C:301:B12:O7R	2.37	0.52
1:A:196:PHE:CZ	2:A:301:B12:H422	2.45	0.52
2:E:301:B12:H601	2:E:301:B12:H252	1.90	0.52
1:G:42:PRO:HD2	1:H:75:LEU:HD11	1.92	0.52
1:N:53:LEU:HD11	1:N:126:ALA:HB1	1.92	0.52
1:F:196:PHE:CZ	2:F:301:B12:H422	2.45	0.51
1:H:196:PHE:CZ	2:H:301:B12:H422	2.46	0.51
1:P:196:PHE:CZ	2:P:301:B12:H422	2.45	0.51
1:K:196:PHE:CZ	2:K:301:B12:H422	2.46	0.51
1:E:196:PHE:CZ	2:E:301:B12:H422	2.46	0.51
1:I:196:PHE:CZ	2:I:301:B12:H422	2.46	0.51
1:H:74:MSE:HE3	1:H:75:LEU:CD1	2.40	0.51
1:A:69:SER:HB2	1:A:71:HIS:CD2	2.45	0.51
1:M:196:PHE:CZ	2:M:301:B12:H422	2.46	0.51
1:D:69:SER:OG	1:F:96:GLU:HA	2.10	0.51
1:O:196:PHE:CZ	2:O:301:B12:H422	2.46	0.51
1:C:57:ALA:HB1	1:C:61:ARG:HD2	1.92	0.51
1:L:196:PHE:CZ	2:L:301:B12:H422	2.46	0.50
1:B:16:LEU:HB3	1:B:21:PHE:HB2	1.92	0.50
1:K:12:ILE:HG22	1:K:23:VAL:HG21	1.93	0.50
1:B:196:PHE:CZ	2:B:301:B12:H422	2.46	0.50
1:K:182:CYS:HG	4:K:601:DHL:CB	2.25	0.50
1:J:57:ALA:HB1	1:J:61:ARG:HD2	1.93	0.50
1:P:12:ILE:HG22	1:P:23:VAL:HG21	1.93	0.50
1:H:57:ALA:HB1	1:H:61:ARG:HD2	1.93	0.50
1:D:196:PHE:CZ	2:D:301:B12:H422	2.46	0.50
1:O:182[A]:CYS:HB3	1:O:209:VAL:CG2	2.42	0.50
1:I:182[A]:CYS:HG	4:I:601:DHL:CB	2.25	0.50
1:J:196:PHE:CZ	2:J:301:B12:H422	2.47	0.49
1:N:196:PHE:CZ	2:N:301:B12:H422	2.47	0.49
1:C:196:PHE:CZ	2:C:301:B12:H422	2.47	0.49
1:L:96:GLU:HA	1:M:69:SER:OG	2.12	0.49
1:B:53:LEU:HD11	1:B:126:ALA:HB1	1.94	0.49
1:B:100:GLU:HB2	1:B:165:LEU:HB2	1.95	0.49
1:F:200:TRP:CD1	2:F:301:B12:H412	2.48	0.49
2:J:301:B12:H552	2:J:301:B12:C53	2.38	0.49
1:E:12:ILE:HG22	1:E:23:VAL:HG21	1.94	0.49
1:E:74:MSE:CE	1:F:165:LEU:HD13	2.35	0.49
1:L:200:TRP:CD1	2:L:301:B12:H412	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:105:TYR:HE2	7:M:661:HOH:O	1.95	0.49
1:L:14:ASP:O	1:M:14:ASP:HB3	2.14	0.48
1:C:200:TRP:CD1	2:C:301:B12:H412	2.48	0.48
1:H:12:ILE:HG22	1:H:23:VAL:HG21	1.95	0.48
1:P:200:TRP:CD1	2:P:301:B12:H412	2.48	0.48
1:A:12:ILE:HG22	1:A:23:VAL:HG21	1.95	0.48
1:C:12:ILE:HG22	1:C:23:VAL:HG21	1.95	0.48
1:N:97:LEU:HD21	1:N:169:ILE:HD11	1.96	0.48
2:K:301:B12:H552	2:K:301:B12:C53	2.40	0.48
1:N:54:SER:OG	1:N:161:ARG:HD2	2.13	0.48
1:K:51:LEU:HD22	1:K:121:ALA:CA	2.34	0.48
1:A:69:SER:HB2	1:A:71:HIS:HD2	1.79	0.48
1:I:182[A]:CYS:HB3	1:I:209:VAL:HG21	1.96	0.47
1:G:196:PHE:CZ	2:G:301:B12:H422	2.49	0.47
1:F:182:CYS:HB3	1:F:209:VAL:CG2	2.44	0.47
1:P:185:THR:HB	6:P:283:EDO:H22	1.95	0.47
1:M:200:TRP:CD1	2:M:301:B12:H412	2.50	0.47
1:J:200:TRP:CD1	2:J:301:B12:H412	2.50	0.47
1:P:5:VAL:HG22	1:P:171:VAL:HG11	1.97	0.47
1:P:16:LEU:HB3	1:P:21:PHE:HB2	1.95	0.47
1:M:74:MSE:HE1	1:N:165:LEU:HD13	1.97	0.47
2:N:301:B12:C55	2:N:301:B12:H531	2.36	0.47
1:O:29:ALA:O	1:O:33:GLU:HG3	2.15	0.47
1:I:153:ARG:NH1	1:I:212:GLN:HE22	2.12	0.47
2:D:301:B12:H552	2:D:301:B12:C53	2.40	0.47
1:I:200:TRP:CD1	2:I:301:B12:H412	2.49	0.47
2:F:301:B12:H552	2:F:301:B12:C53	2.36	0.47
1:M:83:VAL:HG11	7:M:483:HOH:O	2.15	0.47
1:O:74:MSE:HE1	1:P:165:LEU:HD13	1.96	0.47
2:C:301:B12:C53	2:C:301:B12:H552	2.40	0.47
1:K:182:CYS:HB3	1:K:209:VAL:CG2	2.44	0.47
1:C:100:GLU:HB2	1:C:165:LEU:HB2	1.97	0.47
1:L:51:LEU:HD22	1:L:121:ALA:HA	1.97	0.47
1:A:51:LEU:HD22	1:A:121:ALA:HA	1.97	0.47
1:I:5:VAL:HG22	1:I:171:VAL:HG11	1.97	0.47
2:A:301:B12:C53	2:A:301:B12:H552	2.38	0.46
1:D:200:TRP:CD1	2:D:301:B12:H412	2.50	0.46
1:I:182[A]:CYS:SG	4:I:601:DHL:SG	3.07	0.46
1:M:51:LEU:HD22	1:M:121:ALA:HA	1.98	0.46
1:B:51:LEU:HD22	1:B:121:ALA:HA	1.97	0.46
2:N:301:B12:C53	2:N:301:B12:H552	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:TRP:CD1	2:G:301:B12:H412	2.50	0.46
2:G:301:B12:C53	2:G:301:B12:H552	2.38	0.46
1:A:16:LEU:HB3	1:A:21:PHE:HB2	1.96	0.46
1:E:165:LEU:HD13	1:F:74:MSE:HE1	1.98	0.46
1:J:51:LEU:HD22	1:J:121:ALA:HA	1.98	0.46
2:P:301:B12:H552	2:P:301:B12:C53	2.40	0.46
1:B:200:TRP:CD1	2:B:301:B12:H412	2.51	0.46
1:H:51:LEU:HD22	1:H:121:ALA:HA	1.97	0.46
1:P:51:LEU:HD22	1:P:121:ALA:HA	1.98	0.46
1:G:182:CYS:HB3	1:G:209:VAL:CG2	2.45	0.46
1:G:87:LEU:HB3	1:G:101:ILE:HG21	1.98	0.46
1:G:12:ILE:HG22	1:G:23:VAL:HG21	1.97	0.46
1:G:30:TRP:CG	5:G:283:5AD:N6	2.84	0.46
1:B:211:PRO:HB2	1:B:213:GLU:O	2.16	0.46
1:E:182[B]:CYS:HB2	1:E:209:VAL:CG2	2.46	0.45
1:M:43:LEU:CD2	1:N:74:MSE:HE1	2.46	0.45
1:I:16:LEU:HB3	1:I:21:PHE:HB2	1.98	0.45
1:O:57:ALA:HB1	1:O:61:ARG:HD2	1.97	0.45
1:K:57:ALA:HB1	1:K:61:ARG:HD2	1.98	0.45
1:O:200:TRP:CD1	2:O:301:B12:H412	2.51	0.45
1:N:111:ARG:CZ	5:N:401:5AD:H8	2.46	0.45
1:J:5:VAL:HG22	1:J:171:VAL:HG11	1.98	0.45
1:B:5:VAL:HG22	1:B:171:VAL:HG11	1.97	0.45
1:H:87:LEU:HB3	1:H:101:ILE:HG21	1.97	0.45
1:D:61:ARG:NH2	1:F:10:GLN:OE1	2.49	0.45
1:N:51:LEU:HD22	1:N:121:ALA:HA	1.98	0.45
2:A:301:B12:H362	2:A:301:B12:C35	2.28	0.45
1:P:57:ALA:HB1	1:P:61:ARG:HD2	1.99	0.45
1:D:152:PRO:O	4:D:601:DHL:N	2.50	0.45
1:J:16:LEU:HB3	1:J:21:PHE:HB2	1.98	0.45
1:D:41:LEU:HD13	1:D:165:LEU:HD21	1.99	0.45
2:P:301:B12:C35	2:P:301:B12:C36	2.91	0.45
1:K:200:TRP:CD1	2:K:301:B12:H412	2.51	0.45
1:C:200:TRP:CG	2:C:301:B12:H412	2.52	0.45
1:D:18:PRO:HG3	1:F:14:ASP:OD2	2.16	0.45
1:E:225:THR:HG21	1:E:233:LEU:CD2	2.47	0.45
1:H:110:ASN:HA	5:H:401:5AD:C2	2.47	0.45
1:D:16:LEU:HB3	1:D:21:PHE:HB2	1.98	0.45
1:K:16:LEU:HB3	1:K:21:PHE:HB2	1.99	0.45
1:I:87:LEU:HB3	1:I:101:ILE:HG21	1.98	0.45
1:P:87:LEU:HB3	1:P:101:ILE:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:301:B12:C35	2:G:301:B12:C36	2.92	0.44
2:E:301:B12:H2B	6:E:283:EDO:H11	1.99	0.44
1:P:94:LEU:O	6:P:284:EDO:O1	2.34	0.44
1:N:12:ILE:HG22	1:N:23:VAL:HG21	1.98	0.44
1:N:83:VAL:HG21	1:N:161:ARG:HD3	2.00	0.44
1:M:16:LEU:HB3	1:M:21:PHE:HB2	2.00	0.44
2:L:301:B12:C53	2:L:301:B12:H552	2.38	0.44
1:J:87:LEU:HB3	1:J:101:ILE:HG21	1.99	0.44
1:N:200:TRP:CD1	2:N:301:B12:H412	2.52	0.44
1:G:185:THR:HG22	1:G:188:ASP:H	1.82	0.44
1:H:16:LEU:HB3	1:H:21:PHE:HB2	2.00	0.44
1:A:87:LEU:HB3	1:A:101:ILE:HG21	1.99	0.44
1:C:60:ASP:HA	1:C:64:LYS:HD2	1.98	0.44
1:L:16:LEU:HB3	1:L:21:PHE:HB2	1.99	0.44
1:G:51:LEU:HD22	1:G:121:ALA:HA	2.00	0.44
1:A:131:GLN:NE2	2:A:301:B12:O7R	2.37	0.44
2:O:301:B12:H552	2:O:301:B12:C53	2.40	0.44
1:K:182:CYS:SG	4:K:601:DHL:SG	2.79	0.44
2:I:301:B12:H531	2:I:301:B12:C55	2.36	0.44
2:H:301:B12:H552	2:H:301:B12:C53	2.39	0.44
1:G:16:LEU:HB3	1:G:21:PHE:HB2	2.00	0.44
2:I:301:B12:C53	2:I:301:B12:H552	2.38	0.43
1:L:131:GLN:NE2	2:L:301:B12:O7R	2.42	0.43
1:E:21:PHE:CZ	1:E:58:MSE:CE	3.01	0.43
1:I:182[B]:CYS:HB3	4:I:601:DHL:HB2	1.99	0.43
2:P:301:B12:C35	2:P:301:B12:H362	2.28	0.43
1:F:51:LEU:HD22	1:F:121:ALA:HA	2.00	0.43
1:D:51:LEU:HD22	1:D:121:ALA:HA	1.99	0.43
1:E:19:PHE:HB3	1:E:62:ALA:HB2	1.99	0.43
2:P:301:B12:H601	2:P:301:B12:H262	2.01	0.43
1:O:182[B]:CYS:HB3	1:O:209:VAL:CG2	2.47	0.43
1:B:87:LEU:HB3	1:B:101:ILE:HG21	1.99	0.43
2:F:301:B12:H362	2:F:301:B12:C35	2.29	0.43
1:N:16:LEU:HB3	1:N:21:PHE:HB2	2.00	0.43
1:M:112:ARG:NH2	7:M:1374:HOH:O	2.50	0.43
1:E:200:TRP:CD1	2:E:301:B12:H412	2.54	0.43
1:C:16:LEU:HB3	1:C:21:PHE:HB2	2.01	0.43
2:M:301:B12:C55	2:M:301:B12:H531	2.38	0.43
1:I:51:LEU:HD22	1:I:121:ALA:HA	2.01	0.43
2:C:301:B12:H302	2:C:301:B12:H353	2.00	0.43
1:H:182:CYS:HB3	1:H:209:VAL:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:ASP:O	1:F:14:ASP:HB3	2.18	0.43
1:C:182[A]:CYS:HB3	1:C:209:VAL:HG21	2.00	0.43
1:O:165:LEU:CD1	1:P:74:MSE:HE1	2.48	0.42
1:K:53:LEU:HD11	1:K:126:ALA:HB1	2.01	0.42
1:O:51:LEU:HG	1:O:121:ALA:HA	2.00	0.42
1:I:178:LYS:HA	5:I:283:5AD:H2	2.02	0.42
1:L:182:CYS:HB3	1:L:209:VAL:CG2	2.48	0.42
1:N:182:CYS:HG	4:N:601:DHL:HS	0.56	0.42
1:D:182:CYS:HB3	1:D:209:VAL:CG2	2.49	0.42
1:G:131:GLN:NE2	2:G:301:B12:O7R	2.41	0.42
1:O:184:PRO:HD2	7:O:2012:HOH:O	2.19	0.42
2:I:301:B12:H601	2:I:301:B12:H262	2.02	0.42
1:D:83:VAL:HG11	1:D:161:ARG:HB3	2.02	0.42
1:H:200:TRP:CD1	2:H:301:B12:H412	2.54	0.42
2:H:301:B12:C35	2:H:301:B12:C36	2.93	0.42
1:P:99:ILE:HG23	6:P:284:EDO:H12	2.02	0.41
1:E:58:MSE:HE2	1:E:62:ALA:HB3	2.02	0.41
1:M:74:MSE:HE2	1:N:102:ILE:HD11	2.02	0.41
1:M:182:CYS:HB3	1:M:209:VAL:CG2	2.49	0.41
1:M:9:LYS:O	1:M:13:GLU:HB2	2.21	0.41
1:F:41:LEU:HD13	1:F:165:LEU:HD21	2.03	0.41
2:O:301:B12:H262	2:O:301:B12:H601	2.03	0.41
1:F:3:PRO:HB2	1:F:4:LYS:H	1.68	0.41
1:G:180:HIS:HB3	4:G:601:DHL:SG	2.61	0.41
2:O:301:B12:C35	2:O:301:B12:C36	2.94	0.41
1:P:99:ILE:HG12	6:P:284:EDO:C1	2.50	0.41
2:P:301:B12:H353	2:P:301:B12:H302	2.03	0.41
1:E:182[A]:CYS:HB3	1:E:209:VAL:HG21	2.02	0.41
1:L:17[B]:CYS:SG	1:L:18:PRO:HD3	2.61	0.41
1:L:14:ASP:HB3	1:M:14:ASP:O	2.21	0.41
2:B:301:B12:H601	2:B:301:B12:H262	2.03	0.41
1:K:102:ILE:HD11	1:L:74:MSE:HE2	2.03	0.41
1:I:91:ARG:HH21	1:J:73:ARG:HH21	1.68	0.41
1:I:11:LYS:HA	7:I:396:HOH:O	2.21	0.41
1:J:151:HIS:CE1	1:J:153:ARG:HB3	2.55	0.41
1:O:180:HIS:HB3	4:O:601:DHL:SG	2.61	0.41
1:B:70:CYS:HB2	7:B:1664:HOH:O	2.21	0.41
1:D:43:LEU:HD13	1:D:47:THR:HG21	2.02	0.41
2:B:301:B12:C53	2:B:301:B12:H552	2.40	0.41
1:P:182:CYS:HB3	1:P:209:VAL:CG2	2.50	0.41
1:E:51:LEU:HD22	1:E:121:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:PHE:O	1:C:200:TRP:HB3	2.20	0.40
1:H:5:VAL:HG22	1:H:171:VAL:HG11	2.03	0.40
2:O:301:B12:H203	2:O:301:B12:C30	2.48	0.40
2:E:301:B12:H262	2:E:301:B12:H601	2.02	0.40
2:G:301:B12:C30	2:G:301:B12:H203	2.47	0.40
2:E:301:B12:H552	2:E:301:B12:C53	2.38	0.40
1:A:57:ALA:HB1	1:A:61:ARG:HD2	2.03	0.40
1:K:132:ARG:HD2	1:K:145:ILE:HB	2.04	0.40
1:I:132:ARG:HG3	7:I:287:HOH:O	2.22	0.40
1:M:65:PRO:HA	1:M:68:GLN:HE21	1.86	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	225/286 (79%)	222 (99%)	3 (1%)	0	100	100
1	B	226/286 (79%)	222 (98%)	4 (2%)	0	100	100
1	C	228/286 (80%)	226 (99%)	2 (1%)	0	100	100
1	D	228/286 (80%)	224 (98%)	4 (2%)	0	100	100
1	E	229/286 (80%)	227 (99%)	2 (1%)	0	100	100
1	F	229/286 (80%)	225 (98%)	4 (2%)	0	100	100
1	G	226/286 (79%)	223 (99%)	3 (1%)	0	100	100
1	H	225/286 (79%)	224 (100%)	1 (0%)	0	100	100
1	I	227/286 (79%)	223 (98%)	4 (2%)	0	100	100
1	J	227/286 (79%)	224 (99%)	3 (1%)	0	100	100
1	K	226/286 (79%)	224 (99%)	2 (1%)	0	100	100
1	L	231/286 (81%)	228 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	230/286 (80%)	228 (99%)	2 (1%)	0	100	100
1	N	230/286 (80%)	229 (100%)	1 (0%)	0	100	100
1	O	227/286 (79%)	224 (99%)	3 (1%)	0	100	100
1	P	228/286 (80%)	227 (100%)	1 (0%)	0	100	100
All	All	3642/4576 (80%)	3600 (99%)	42 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/243 (79%)	187 (97%)	6 (3%)	47	69
1	B	193/243 (79%)	187 (97%)	6 (3%)	47	69
1	C	192/243 (79%)	184 (96%)	8 (4%)	36	56
1	D	194/243 (80%)	187 (96%)	7 (4%)	42	63
1	E	193/243 (79%)	187 (97%)	6 (3%)	47	69
1	F	197/243 (81%)	192 (98%)	5 (2%)	55	76
1	G	194/243 (80%)	189 (97%)	5 (3%)	54	74
1	H	192/243 (79%)	186 (97%)	6 (3%)	47	69
1	I	194/243 (80%)	189 (97%)	5 (3%)	54	74
1	J	195/243 (80%)	189 (97%)	6 (3%)	47	69
1	K	192/243 (79%)	189 (98%)	3 (2%)	70	86
1	L	196/243 (81%)	190 (97%)	6 (3%)	47	69
1	M	195/243 (80%)	193 (99%)	2 (1%)	82	93
1	N	192/243 (79%)	186 (97%)	6 (3%)	47	69
1	O	192/243 (79%)	185 (96%)	7 (4%)	42	63
1	P	196/243 (81%)	189 (96%)	7 (4%)	42	63
All	All	3100/3888 (80%)	3009 (97%)	91 (3%)	50	71

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	MSE
1	A	115	ILE
1	A	132	ARG
1	A	133	GLN
1	A	177	ARG
1	A	201	ARG
1	B	58	MSE
1	B	91	ARG
1	B	92	GLU
1	B	115	ILE
1	B	133	GLN
1	B	182	CYS
1	C	51	LEU
1	C	53	LEU
1	C	58	MSE
1	C	73	ARG
1	C	111	ARG
1	C	115	ILE
1	C	132	ARG
1	C	133	GLN
1	D	58	MSE
1	D	61	ARG
1	D	81	GLN
1	D	91	ARG
1	D	132	ARG
1	D	153	ARG
1	D	170	GLU
1	E	5	VAL
1	E	53	LEU
1	E	58	MSE
1	E	68	GLN
1	E	91	ARG
1	E	115	ILE
1	F	9	LYS
1	F	58	MSE
1	F	81	GLN
1	F	91	ARG
1	F	115	ILE
1	G	58	MSE
1	G	68	GLN
1	G	91	ARG
1	G	115	ILE

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Mol	Chain	Res	Type
1	G	133	GLN
1	H	53	LEU
1	H	72	LEU
1	H	91	ARG
1	H	115	ILE
1	H	132	ARG
1	H	133	GLN
1	I	58	MSE
1	I	73	ARG
1	I	91	ARG
1	I	115	ILE
1	I	133	GLN
1	J	4	LYS
1	J	53	LEU
1	J	58	MSE
1	J	70	CYS
1	J	91	ARG
1	J	115	ILE
1	K	58	MSE
1	K	91	ARG
1	K	229	GLN
1	L	9	LYS
1	L	58	MSE
1	L	91	ARG
1	L	178	LYS
1	L	212	GLN
1	L	231	LEU
1	M	115	ILE
1	M	136	GLU
1	N	58	MSE
1	N	91	ARG
1	N	115	ILE
1	N	161	ARG
1	N	231	LEU
1	N	233	LEU
1	O	4	LYS
1	O	58	MSE
1	O	68	GLN
1	O	91	ARG
1	O	115	ILE
1	O	133	GLN
1	O	230	ARG

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Mol	Chain	Res	Type
1	P	53	LEU
1	P	58	MSE
1	P	60	ASP
1	P	70	CYS
1	P	72	LEU
1	P	91	ARG
1	P	115	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	131	GLN
1	B	131	GLN
1	C	131	GLN
1	D	131	GLN
1	G	131	GLN
1	I	131	GLN
1	I	199	HIS
1	I	212	GLN
1	J	81	GLN
1	L	131	GLN
1	M	68	GLN
1	M	131	GLN
1	P	98	GLN

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 (i)

67 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	B12	A	301	5	74,101,101	1.21	7 (9%)	111,166,166	1.87	15 (13%)
5	5AD	A	401	2	15,20,20	1.24	1 (6%)	14,30,30	2.26	4 (28%)
3	FLC	A	501	-	3,12,12	0.57	0	3,17,17	0.89	0
4	DHL	A	601	1	3,3,3	1.38	0	2,2,2	0.77	0
2	B12	B	301	5	74,101,101	1.23	7 (9%)	111,166,166	1.90	16 (14%)
5	5AD	B	401	2	15,20,20	1.19	2 (13%)	14,30,30	2.45	4 (28%)
3	FLC	B	501	-	3,12,12	1.14	0	3,17,17	0.51	0
2	B12	C	301	5	74,101,101	1.21	6 (8%)	111,166,166	1.96	16 (14%)
5	5AD	C	401	2	15,20,20	1.27	2 (13%)	14,30,30	2.31	3 (21%)
3	FLC	C	501	-	3,12,12	0.91	0	3,17,17	0.56	0
4	DHL	C	601	-	3,3,3	1.19	0	2,2,2	0.95	0
2	B12	D	301	5	74,101,101	1.16	6 (8%)	111,166,166	1.89	15 (13%)
5	5AD	D	401	2	15,20,20	1.30	2 (13%)	14,30,30	2.42	4 (28%)
3	FLC	D	501	-	3,12,12	1.74	1 (33%)	3,17,17	1.10	0
4	DHL	D	601	-	3,3,3	1.75	1 (33%)	2,2,2	1.14	0
6	EDO	E	283	-	3,3,3	0.53	0	2,2,2	0.20	0
2	B12	E	301	5	74,101,101	1.21	7 (9%)	111,166,166	1.96	16 (14%)
5	5AD	E	401	2	15,20,20	1.25	2 (13%)	14,30,30	2.58	4 (28%)
3	FLC	E	501	-	3,12,12	1.31	1 (33%)	3,17,17	1.06	0
2	B12	F	301	5	74,101,101	1.17	6 (8%)	111,166,166	1.91	15 (13%)
5	5AD	F	401	2	15,20,20	1.23	1 (6%)	14,30,30	2.40	3 (21%)
3	FLC	F	501	-	3,12,12	1.02	0	3,17,17	1.10	0
4	DHL	F	601	1	3,3,3	1.46	1 (33%)	2,2,2	1.02	0
5	5AD	G	283	-	15,20,20	1.44	3 (20%)	14,30,30	2.64	3 (21%)
2	B12	G	301	5	74,101,101	1.18	6 (8%)	111,166,166	1.87	16 (14%)
5	5AD	G	401	2	15,20,20	1.28	2 (13%)	14,30,30	2.51	4 (28%)
3	FLC	G	501	-	3,12,12	0.97	0	3,17,17	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	DHL	G	601	1	3,3,3	1.18	0	2,2,2	2.51	1 (50%)
2	B12	H	301	5	74,101,101	1.20	7 (9%)	111,166,166	1.91	17 (15%)
5	5AD	H	401	2	15,20,20	1.22	1 (6%)	14,30,30	2.45	4 (28%)
3	FLC	H	501	-	3,12,12	0.31	0	3,17,17	0.79	0
4	DHL	H	601	1	3,3,3	1.38	1 (33%)	2,2,2	0.90	0
5	5AD	I	283	-	15,20,20	1.37	3 (20%)	14,30,30	2.33	2 (14%)
2	B12	I	301	5	74,101,101	1.24	7 (9%)	111,166,166	1.88	16 (14%)
5	5AD	I	401	2	15,20,20	1.31	2 (13%)	14,30,30	2.37	4 (28%)
3	FLC	I	501	-	3,12,12	0.93	0	3,17,17	0.90	0
4	DHL	I	601	-	3,3,3	1.41	1 (33%)	2,2,2	3.23	1 (50%)
2	B12	J	301	5	74,101,101	1.24	7 (9%)	111,166,166	1.87	17 (15%)
5	5AD	J	401	2	15,20,20	1.19	2 (13%)	14,30,30	2.40	4 (28%)
3	FLC	J	501	-	3,12,12	0.99	0	3,17,17	0.96	0
4	DHL	J	601	-	3,3,3	1.72	1 (33%)	2,2,2	0.41	0
2	B12	K	301	5	74,101,101	1.17	7 (9%)	111,166,166	1.91	16 (14%)
5	5AD	K	401	2	15,20,20	1.29	2 (13%)	14,30,30	2.34	4 (28%)
3	FLC	K	501	-	3,12,12	1.29	1 (33%)	3,17,17	0.96	0
4	DHL	K	601	-	3,3,3	1.76	1 (33%)	2,2,2	0.14	0
2	B12	L	301	5	74,101,101	1.16	6 (8%)	111,166,166	1.91	15 (13%)
5	5AD	L	401	2	15,20,20	1.25	2 (13%)	14,30,30	2.43	3 (21%)
3	FLC	L	501	-	3,12,12	1.14	0	3,17,17	0.71	0
4	DHL	L	601	-	3,3,3	1.81	1 (33%)	2,2,2	0.37	0
2	B12	M	301	5	74,101,101	1.21	6 (8%)	111,166,166	1.87	15 (13%)
5	5AD	M	401	2	15,20,20	1.21	1 (6%)	14,30,30	2.36	4 (28%)
3	FLC	M	501	-	3,12,12	1.51	0	3,17,17	1.08	0
4	DHL	M	601	-	3,3,3	1.54	1 (33%)	2,2,2	0.41	0
2	B12	N	301	5	74,101,101	1.20	6 (8%)	111,166,166	1.91	15 (13%)
5	5AD	N	401	2	15,20,20	1.14	1 (6%)	14,30,30	2.53	4 (28%)
3	FLC	N	501	-	3,12,12	0.61	0	3,17,17	0.71	0
4	DHL	N	601	-	3,3,3	1.76	1 (33%)	2,2,2	1.85	1 (50%)
2	B12	O	301	5	74,101,101	1.19	6 (8%)	111,166,166	1.87	15 (13%)
5	5AD	O	401	2	15,20,20	1.27	1 (6%)	14,30,30	2.38	4 (28%)
3	FLC	O	501	-	3,12,12	0.60	0	3,17,17	0.77	0
4	DHL	O	601	1	3,3,3	1.39	1 (33%)	2,2,2	0.40	0
6	EDO	P	283	-	3,3,3	0.56	0	2,2,2	0.19	0
6	EDO	P	284	-	3,3,3	0.42	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	B12	P	301	5	74,101,101	1.23	7 (9%)	111,166,166	1.88	16 (14%)
5	5AD	P	401	2	15,20,20	1.21	1 (6%)	14,30,30	2.27	4 (28%)
3	FLC	P	501	-	3,12,12	0.55	0	3,17,17	0.76	0
4	DHL	P	601	-	3,3,3	1.23	0	2,2,2	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B12	A	301	5	-	0/51/223/223	0/3/11/11
5	5AD	A	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	A	501	-	-	0/6/16/16	0/0/0/0
4	DHL	A	601	1	-	0/1/1/1	0/0/0/0
2	B12	B	301	5	-	0/51/223/223	0/3/11/11
5	5AD	B	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	B	501	-	-	0/6/16/16	0/0/0/0
2	B12	C	301	5	-	0/51/223/223	0/3/11/11
5	5AD	C	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	C	501	-	-	0/6/16/16	0/0/0/0
4	DHL	C	601	-	-	0/1/1/1	0/0/0/0
2	B12	D	301	5	-	0/51/223/223	0/3/11/11
5	5AD	D	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	D	501	-	-	0/6/16/16	0/0/0/0
4	DHL	D	601	-	-	0/1/1/1	0/0/0/0
6	EDO	E	283	-	-	0/1/1/1	0/0/0/0
2	B12	E	301	5	-	0/51/223/223	0/3/11/11
5	5AD	E	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	E	501	-	-	0/6/16/16	0/0/0/0
2	B12	F	301	5	-	0/51/223/223	0/3/11/11
5	5AD	F	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	F	501	-	-	0/6/16/16	0/0/0/0
4	DHL	F	601	1	-	0/1/1/1	0/0/0/0
5	5AD	G	283	-	1/1/4/4	0/0/20/20	0/3/3/3
2	B12	G	301	5	-	0/51/223/223	0/3/11/11
5	5AD	G	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	G	501	-	-	0/6/16/16	0/0/0/0
4	DHL	G	601	1	-	0/1/1/1	0/0/0/0
2	B12	H	301	5	-	0/51/223/223	0/3/11/11
5	5AD	H	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	H	501	-	-	0/6/16/16	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DHL	H	601	1	-	0/1/1/1	0/0/0/0
5	5AD	I	283	-	1/1/4/4	0/0/20/20	0/3/3/3
2	B12	I	301	5	-	0/51/223/223	0/3/11/11
5	5AD	I	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	I	501	-	-	0/6/16/16	0/0/0/0
4	DHL	I	601	-	-	0/1/1/1	0/0/0/0
2	B12	J	301	5	-	0/51/223/223	0/3/11/11
5	5AD	J	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	J	501	-	-	0/6/16/16	0/0/0/0
4	DHL	J	601	-	-	0/1/1/1	0/0/0/0
2	B12	K	301	5	-	0/51/223/223	0/3/11/11
5	5AD	K	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	K	501	-	-	0/6/16/16	0/0/0/0
4	DHL	K	601	-	-	0/1/1/1	0/0/0/0
2	B12	L	301	5	-	0/51/223/223	0/3/11/11
5	5AD	L	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	L	501	-	-	0/6/16/16	0/0/0/0
4	DHL	L	601	-	-	0/1/1/1	0/0/0/0
2	B12	M	301	5	-	0/51/223/223	0/3/11/11
5	5AD	M	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	M	501	-	-	0/6/16/16	0/0/0/0
4	DHL	M	601	-	-	0/1/1/1	0/0/0/0
2	B12	N	301	5	-	0/51/223/223	0/3/11/11
5	5AD	N	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	N	501	-	-	0/6/16/16	0/0/0/0
4	DHL	N	601	-	-	0/1/1/1	0/0/0/0
2	B12	O	301	5	-	0/51/223/223	0/3/11/11
5	5AD	O	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	O	501	-	-	0/6/16/16	0/0/0/0
4	DHL	O	601	1	-	0/1/1/1	0/0/0/0
6	EDO	P	283	-	-	0/1/1/1	0/0/0/0
6	EDO	P	284	-	-	0/1/1/1	0/0/0/0
2	B12	P	301	5	-	0/51/223/223	0/3/11/11
5	5AD	P	401	2	1/1/4/4	0/0/20/20	0/3/3/3
3	FLC	P	501	-	-	0/6/16/16	0/0/0/0
4	DHL	P	601	-	-	0/1/1/1	0/0/0/0

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	301	B12	C11-C10	-4.48	1.33	1.41
2	B	301	B12	C11-C10	-4.42	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	B12	C11-C10	-4.38	1.33	1.41
2	M	301	B12	C11-C10	-4.37	1.33	1.41
2	E	301	B12	C11-C10	-4.35	1.33	1.41
2	J	301	B12	C11-C10	-4.34	1.33	1.41
2	I	301	B12	C11-C10	-4.33	1.33	1.41
2	G	301	B12	C11-C10	-4.32	1.33	1.41
2	K	301	B12	C11-C10	-4.29	1.33	1.41
2	N	301	B12	C11-C10	-4.29	1.33	1.41
2	F	301	B12	C11-C10	-4.28	1.33	1.41
2	A	301	B12	C11-C10	-4.23	1.33	1.41
2	C	301	B12	C11-C10	-4.22	1.33	1.41
2	P	301	B12	C11-C10	-4.10	1.33	1.41
2	H	301	B12	C11-C10	-4.10	1.33	1.41
2	D	301	B12	C11-C10	-3.90	1.34	1.41
2	E	301	B12	C8B-N1B	-3.84	1.33	1.38
2	P	301	B12	C8B-N1B	-3.61	1.34	1.38
2	A	301	B12	C8B-N1B	-3.47	1.34	1.38
2	O	301	B12	C8B-N1B	-3.44	1.34	1.38
2	J	301	B12	C18-C19	-3.42	1.46	1.53
2	N	301	B12	C8B-N1B	-3.37	1.34	1.38
2	M	301	B12	C8B-N1B	-3.36	1.34	1.38
2	B	301	B12	C18-C19	-3.30	1.46	1.53
2	I	301	B12	C8B-N1B	-3.26	1.34	1.38
2	J	301	B12	C8B-N1B	-3.24	1.34	1.38
2	L	301	B12	C18-C19	-3.19	1.46	1.53
2	D	301	B12	C18-C19	-3.17	1.46	1.53
2	H	301	B12	C8B-N1B	-3.17	1.34	1.38
2	A	301	B12	C18-C19	-3.15	1.46	1.53
2	B	301	B12	C8B-N1B	-3.13	1.34	1.38
2	O	301	B12	C18-C19	-3.13	1.46	1.53
2	P	301	B12	C18-C19	-3.12	1.46	1.53
2	E	301	B12	C18-C19	-3.11	1.46	1.53
2	F	301	B12	C18-C19	-3.11	1.46	1.53
2	C	301	B12	C8B-N1B	-3.10	1.34	1.38
2	G	301	B12	C18-C19	-3.05	1.47	1.53
2	C	301	B12	C18-C19	-3.04	1.47	1.53
2	I	301	B12	C18-C19	-3.03	1.47	1.53
2	D	301	B12	C8B-N1B	-3.00	1.34	1.38
2	K	301	B12	C18-C19	-3.00	1.47	1.53
2	N	301	B12	C18-C19	-2.99	1.47	1.53
4	N	601	DHL	CB-CA	-2.98	1.39	1.51
2	M	301	B12	C18-C19	-2.98	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301	B12	C8B-N1B	-2.95	1.34	1.38
2	H	301	B12	C18-C19	-2.95	1.47	1.53
2	F	301	B12	C8B-N1B	-2.92	1.34	1.38
2	L	301	B12	C8B-N1B	-2.79	1.35	1.38
2	G	301	B12	C8B-N1B	-2.73	1.35	1.38
4	D	601	DHL	CB-CA	-2.36	1.41	1.51
4	I	601	DHL	CB-CA	-2.27	1.41	1.51
4	K	601	DHL	CB-CA	-2.25	1.41	1.51
4	F	601	DHL	CB-CA	-2.24	1.42	1.51
4	H	601	DHL	CB-CA	-2.21	1.42	1.51
4	O	601	DHL	CB-CA	-2.19	1.42	1.51
4	M	601	DHL	CB-CA	-2.05	1.42	1.51
2	K	301	B12	O6R-C1R	2.01	1.43	1.41
2	H	301	B12	O6R-C1R	2.01	1.43	1.41
5	G	401	5AD	C2-N3	2.05	1.35	1.32
5	B	401	5AD	C2-N3	2.05	1.35	1.32
5	I	283	5AD	C2-N3	2.06	1.35	1.32
3	K	501	FLC	CA-CB	2.07	1.57	1.54
3	E	501	FLC	CA-CB	2.10	1.57	1.54
5	C	401	5AD	C2-N3	2.12	1.35	1.32
5	L	401	5AD	C2-N3	2.19	1.36	1.32
2	J	301	B12	O6R-C1R	2.23	1.44	1.41
5	D	401	5AD	C2-N3	2.24	1.36	1.32
5	E	401	5AD	C2-N3	2.27	1.36	1.32
5	G	283	5AD	C2-N3	2.30	1.36	1.32
5	J	401	5AD	C2-N3	2.30	1.36	1.32
5	I	401	5AD	C2-N3	2.32	1.36	1.32
5	K	401	5AD	C2-N3	2.33	1.36	1.32
2	I	301	B12	O6R-C1R	2.37	1.44	1.41
2	B	301	B12	O6R-C1R	2.39	1.44	1.41
2	E	301	B12	O6R-C1R	2.41	1.44	1.41
2	P	301	B12	O6R-C1R	2.47	1.44	1.41
4	J	601	DHL	CB-SG	2.52	1.89	1.80
2	E	301	B12	C17-C18	2.53	1.58	1.54
5	I	283	5AD	O4'-C1'	2.55	1.44	1.41
3	D	501	FLC	CA-CB	2.58	1.58	1.54
2	A	301	B12	O6R-C1R	2.64	1.44	1.41
2	A	301	B12	C17-C18	2.69	1.58	1.54
2	K	301	B12	C17-C18	2.74	1.58	1.54
2	O	301	B12	C17-C18	2.75	1.58	1.54
4	L	601	DHL	CB-SG	2.80	1.90	1.80
2	L	301	B12	C17-C18	2.82	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	B12	C17-C18	2.84	1.58	1.54
2	M	301	B12	C17-C18	2.86	1.58	1.54
2	D	301	B12	C17-C18	2.96	1.58	1.54
5	N	401	5AD	C5-C4	2.98	1.47	1.40
2	N	301	B12	C17-C18	2.99	1.58	1.54
2	C	301	B12	C17-C18	3.03	1.58	1.54
2	F	301	B12	C17-C18	3.03	1.58	1.54
2	P	301	B12	C17-C18	3.06	1.58	1.54
2	B	301	B12	C17-C18	3.07	1.58	1.54
2	H	301	B12	C17-C18	3.07	1.58	1.54
5	G	283	5AD	C5-C4	3.07	1.47	1.40
5	G	283	5AD	O4'-C1'	3.08	1.45	1.41
5	J	401	5AD	C5-C4	3.09	1.47	1.40
2	I	301	B12	C17-C18	3.13	1.58	1.54
5	E	401	5AD	C5-C4	3.16	1.47	1.40
5	H	401	5AD	C5-C4	3.17	1.47	1.40
5	B	401	5AD	C5-C4	3.17	1.47	1.40
5	L	401	5AD	C5-C4	3.29	1.47	1.40
5	I	283	5AD	C5-C4	3.29	1.47	1.40
5	O	401	5AD	C5-C4	3.32	1.48	1.40
2	L	301	B12	C6B-C5B	3.34	1.49	1.41
5	P	401	5AD	C5-C4	3.36	1.48	1.40
5	M	401	5AD	C5-C4	3.37	1.48	1.40
5	A	401	5AD	C5-C4	3.39	1.48	1.40
5	D	401	5AD	C5-C4	3.39	1.48	1.40
5	I	401	5AD	C5-C4	3.40	1.48	1.40
2	M	301	B12	C6B-C5B	3.42	1.50	1.41
5	F	401	5AD	C5-C4	3.43	1.48	1.40
5	G	401	5AD	C5-C4	3.44	1.48	1.40
2	J	301	B12	C17-C18	3.45	1.59	1.54
2	P	301	B12	C6B-C5B	3.46	1.50	1.41
2	O	301	B12	C6B-C5B	3.46	1.50	1.41
2	B	301	B12	C6B-C5B	3.48	1.50	1.41
2	A	301	B12	C6B-C5B	3.48	1.50	1.41
5	K	401	5AD	C5-C4	3.49	1.48	1.40
5	C	401	5AD	C5-C4	3.51	1.48	1.40
2	K	301	B12	C6B-C5B	3.53	1.50	1.41
2	D	301	B12	C6B-C5B	3.56	1.50	1.41
2	H	301	B12	C6B-C5B	3.56	1.50	1.41
2	J	301	B12	C6B-C5B	3.62	1.50	1.41
2	F	301	B12	C6B-C5B	3.64	1.50	1.41
2	E	301	B12	C6B-C5B	3.65	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	B12	C6B-C5B	3.65	1.50	1.41
2	N	301	B12	C6B-C5B	3.70	1.50	1.41
2	G	301	B12	C6B-C5B	3.74	1.51	1.41
2	L	301	B12	C8B-C9B	3.83	1.48	1.40
2	I	301	B12	C6B-C5B	3.83	1.51	1.41
2	K	301	B12	C8B-C9B	3.87	1.48	1.40
2	G	301	B12	C8B-C9B	3.92	1.48	1.40
2	E	301	B12	C8B-C9B	3.99	1.48	1.40
2	D	301	B12	C8B-C9B	4.08	1.48	1.40
2	M	301	B12	C8B-C9B	4.10	1.48	1.40
2	O	301	B12	C8B-C9B	4.12	1.48	1.40
2	F	301	B12	C8B-C9B	4.16	1.48	1.40
2	H	301	B12	C8B-C9B	4.20	1.48	1.40
2	P	301	B12	C8B-C9B	4.22	1.48	1.40
2	A	301	B12	C8B-C9B	4.22	1.48	1.40
2	J	301	B12	C8B-C9B	4.23	1.49	1.40
2	N	301	B12	C8B-C9B	4.23	1.49	1.40
2	I	301	B12	C8B-C9B	4.27	1.49	1.40
2	C	301	B12	C8B-C9B	4.32	1.49	1.40
2	B	301	B12	C8B-C9B	4.56	1.49	1.40

All (320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	B12	C20-C1-C19	-8.79	100.75	109.38
5	G	283	5AD	N3-C2-N1	-8.49	122.39	128.89
2	K	301	B12	C20-C1-C19	-8.28	101.25	109.38
2	H	301	B12	C20-C1-C19	-8.26	101.28	109.38
2	B	301	B12	C20-C1-C19	-8.14	101.39	109.38
2	M	301	B12	C20-C1-C19	-8.03	101.51	109.38
2	A	301	B12	C20-C1-C19	-7.95	101.58	109.38
2	E	301	B12	C20-C1-C19	-7.94	101.59	109.38
2	D	301	B12	C20-C1-C19	-7.91	101.62	109.38
2	L	301	B12	C20-C1-C19	-7.87	101.66	109.38
5	E	401	5AD	N3-C2-N1	-7.87	122.87	128.89
2	P	301	B12	C20-C1-C19	-7.83	101.70	109.38
2	N	301	B12	C20-C1-C19	-7.80	101.73	109.38
5	I	283	5AD	N3-C2-N1	-7.76	122.95	128.89
5	N	401	5AD	N3-C2-N1	-7.76	122.95	128.89
5	G	401	5AD	N3-C2-N1	-7.72	122.99	128.89
2	F	301	B12	C20-C1-C19	-7.70	101.83	109.38
5	B	401	5AD	N3-C2-N1	-7.58	123.09	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	301	B12	C20-C1-C19	-7.53	101.99	109.38
5	D	401	5AD	N3-C2-N1	-7.43	123.21	128.89
5	L	401	5AD	N3-C2-N1	-7.40	123.22	128.89
2	O	301	B12	C20-C1-C19	-7.35	102.17	109.38
5	I	401	5AD	N3-C2-N1	-7.27	123.33	128.89
5	H	401	5AD	N3-C2-N1	-7.21	123.37	128.89
5	F	401	5AD	N3-C2-N1	-7.20	123.38	128.89
2	G	301	B12	C20-C1-C19	-7.19	102.33	109.38
2	H	301	B12	C17-C18-C19	-7.14	90.46	102.38
2	J	301	B12	C20-C1-C19	-7.13	102.39	109.38
2	N	301	B12	C17-C18-C19	-7.11	90.51	102.38
5	K	401	5AD	N3-C2-N1	-7.09	123.46	128.89
2	P	301	B12	C17-C18-C19	-7.07	90.58	102.38
5	J	401	5AD	N3-C2-N1	-7.06	123.48	128.89
5	O	401	5AD	N3-C2-N1	-7.01	123.52	128.89
5	M	401	5AD	N3-C2-N1	-7.01	123.53	128.89
2	K	301	B12	C17-C18-C19	-7.00	90.70	102.38
2	L	301	B12	C17-C18-C19	-6.98	90.72	102.38
2	C	301	B12	C17-C18-C19	-6.97	90.74	102.38
5	A	401	5AD	N3-C2-N1	-6.97	123.56	128.89
2	B	301	B12	C17-C18-C19	-6.97	90.75	102.38
2	O	301	B12	C17-C18-C19	-6.94	90.79	102.38
2	G	301	B12	C17-C18-C19	-6.93	90.80	102.38
2	F	301	B12	C17-C18-C19	-6.92	90.82	102.38
2	I	301	B12	C17-C18-C19	-6.92	90.83	102.38
2	M	301	B12	C17-C18-C19	-6.92	90.84	102.38
2	E	301	B12	C17-C18-C19	-6.90	90.87	102.38
2	A	301	B12	C17-C18-C19	-6.89	90.88	102.38
5	C	401	5AD	N3-C2-N1	-6.86	123.64	128.89
2	J	301	B12	C17-C18-C19	-6.78	91.06	102.38
5	P	401	5AD	N3-C2-N1	-6.77	123.71	128.89
2	D	301	B12	C17-C18-C19	-6.77	91.07	102.38
4	I	601	DHL	CA-CB-SG	-4.54	97.66	112.79
2	K	301	B12	C9-C10-C11	-4.39	121.27	132.28
2	G	301	B12	C9-C10-C11	-4.34	121.39	132.28
2	F	301	B12	C9-C10-C11	-4.32	121.44	132.28
2	E	301	B12	C9-C10-C11	-4.31	121.47	132.28
2	I	301	B12	C9-C10-C11	-4.30	121.50	132.28
2	A	301	B12	C9-C10-C11	-4.30	121.50	132.28
2	C	301	B12	C9-C10-C11	-4.27	121.58	132.28
2	H	301	B12	C9-C10-C11	-4.25	121.62	132.28
2	M	301	B12	C9-C10-C11	-4.25	121.62	132.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	301	B12	C9-C10-C11	-4.24	121.64	132.28
2	J	301	B12	C9-C10-C11	-4.22	121.70	132.28
2	N	301	B12	C9-C10-C11	-4.21	121.73	132.28
2	D	301	B12	C9-C10-C11	-4.19	121.77	132.28
2	L	301	B12	C9-C10-C11	-4.11	121.97	132.28
2	O	301	B12	C9-C10-C11	-4.08	122.04	132.28
2	B	301	B12	C9-C10-C11	-4.03	122.17	132.28
4	G	601	DHL	CA-CB-SG	-3.55	100.95	112.79
2	G	301	B12	C20-C1-C2	-3.40	107.07	113.26
5	G	283	5AD	C2'-C1'-N9	-3.25	109.33	114.29
5	N	401	5AD	C5'-C4'-C3'	-3.24	112.41	115.80
5	H	401	5AD	C5'-C4'-C3'	-3.23	112.42	115.80
2	F	301	B12	C20-C1-C2	-3.16	107.50	113.26
2	O	301	B12	C20-C1-C2	-3.15	107.52	113.26
5	J	401	5AD	C5'-C4'-C3'	-3.11	112.54	115.80
2	N	301	B12	C20-C1-C2	-3.07	107.67	113.26
2	E	301	B12	C20-C1-C2	-3.06	107.68	113.26
5	E	401	5AD	C5'-C4'-C3'	-3.02	112.65	115.80
2	P	301	B12	C20-C1-C2	-3.01	107.77	113.26
5	K	401	5AD	C5'-C4'-C3'	-3.00	112.66	115.80
2	B	301	B12	C20-C1-C2	-3.00	107.80	113.26
2	L	301	B12	C25-C2-C1	-2.99	109.06	113.79
2	A	301	B12	C20-C1-C2	-2.98	107.82	113.26
2	C	301	B12	C20-C1-C2	-2.95	107.88	113.26
2	D	301	B12	C20-C1-C2	-2.95	107.88	113.26
2	M	301	B12	C25-C2-C1	-2.95	109.14	113.79
2	I	301	B12	C20-C1-C2	-2.94	107.90	113.26
2	H	301	B12	C20-C1-C2	-2.92	107.93	113.26
2	M	301	B12	C20-C1-C2	-2.92	107.94	113.26
5	M	401	5AD	C5'-C4'-C3'	-2.88	112.79	115.80
5	F	401	5AD	C5'-C4'-C3'	-2.85	112.82	115.80
5	C	401	5AD	C5'-C4'-C3'	-2.85	112.82	115.80
2	N	301	B12	C25-C2-C1	-2.84	109.31	113.79
5	L	401	5AD	C5'-C4'-C3'	-2.82	112.85	115.80
2	A	301	B12	O5-P-O4	-2.82	110.31	118.70
2	K	301	B12	C20-C1-C2	-2.81	108.14	113.26
2	L	301	B12	C20-C1-C2	-2.80	108.16	113.26
2	J	301	B12	C20-C1-C2	-2.79	108.17	113.26
2	G	301	B12	C37-C7-C8	-2.77	100.54	108.27
2	F	301	B12	C25-C2-C1	-2.76	109.42	113.79
2	D	301	B12	C25-C2-C1	-2.74	109.46	113.79
2	O	301	B12	C25-C2-C1	-2.74	109.46	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	401	5AD	C4-C5-N7	-2.74	106.96	109.48
5	O	401	5AD	C5'-C4'-C3'	-2.72	112.96	115.80
2	C	301	B12	O5-P-O4	-2.71	110.63	118.70
2	C	301	B12	C37-C7-C8	-2.71	100.71	108.27
2	O	301	B12	O5-P-O4	-2.69	110.68	118.70
5	I	283	5AD	C4-C5-N7	-2.69	107.00	109.48
2	A	301	B12	C25-C2-C1	-2.69	109.54	113.79
5	D	401	5AD	C5'-C4'-C3'	-2.69	112.99	115.80
2	P	301	B12	O5-P-O4	-2.64	110.83	118.70
2	J	301	B12	C37-C7-C8	-2.64	100.90	108.27
2	E	301	B12	C25-C2-C1	-2.64	109.62	113.79
5	I	401	5AD	C5'-C4'-C3'	-2.63	113.05	115.80
2	A	301	B12	C30-C3-C2	-2.63	113.91	119.11
2	K	301	B12	C25-C2-C1	-2.62	109.65	113.79
2	C	301	B12	C25-C2-C1	-2.62	109.65	113.79
2	O	301	B12	C37-C7-C8	-2.62	100.96	108.27
2	M	301	B12	C30-C3-C2	-2.62	113.93	119.11
2	G	301	B12	C30-C3-C2	-2.62	113.94	119.11
2	N	301	B12	C30-C3-C2	-2.61	113.94	119.11
2	D	301	B12	C37-C7-C8	-2.61	101.00	108.27
2	J	301	B12	C25-C2-C1	-2.59	109.70	113.79
2	D	301	B12	C30-C3-C2	-2.59	113.99	119.11
5	B	401	5AD	C5'-C4'-C3'	-2.59	113.09	115.80
2	B	301	B12	C25-C2-C1	-2.58	109.71	113.79
2	A	301	B12	C20-C1-N21	-2.58	100.75	108.29
2	P	301	B12	C25-C2-C1	-2.58	109.72	113.79
2	N	301	B12	C20-C1-N21	-2.56	100.80	108.29
5	A	401	5AD	C5'-C4'-C3'	-2.56	113.12	115.80
2	P	301	B12	C37-C7-C8	-2.56	101.13	108.27
5	G	401	5AD	C5'-C4'-C3'	-2.54	113.14	115.80
2	I	301	B12	C25-C2-C1	-2.54	109.77	113.79
2	H	301	B12	C25-C2-C1	-2.53	109.79	113.79
2	H	301	B12	C37-C7-C8	-2.53	101.21	108.27
2	F	301	B12	C37-C7-C8	-2.53	101.22	108.27
2	A	301	B12	C37-C7-C8	-2.53	101.22	108.27
2	B	301	B12	O5-P-O4	-2.53	111.17	118.70
2	M	301	B12	C37-C7-C8	-2.52	101.22	108.27
2	J	301	B12	O5-P-O4	-2.51	111.23	118.70
4	N	601	DHL	CA-CB-SG	-2.49	104.47	112.79
2	G	301	B12	C25-C2-C1	-2.49	109.85	113.79
2	K	301	B12	C20-C1-N21	-2.49	101.00	108.29
2	D	301	B12	C20-C1-N21	-2.49	101.02	108.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	B12	C2R-C1R-N1B	-2.48	110.50	114.29
2	I	301	B12	C20-C1-N21	-2.48	101.03	108.29
2	N	301	B12	C37-C7-C8	-2.46	101.39	108.27
2	B	301	B12	C20-C1-N21	-2.46	101.09	108.29
2	J	301	B12	C20-C1-N21	-2.46	101.10	108.29
2	J	301	B12	C2R-C1R-N1B	-2.44	110.56	114.29
2	E	301	B12	C30-C3-C2	-2.44	114.29	119.11
2	F	301	B12	C30-C3-C2	-2.43	114.30	119.11
2	I	301	B12	C37-C7-C8	-2.42	101.52	108.27
5	P	401	5AD	C5'-C4'-C3'	-2.42	113.27	115.80
2	K	301	B12	C37-C7-C8	-2.42	101.53	108.27
2	B	301	B12	C37-C7-C8	-2.41	101.55	108.27
2	H	301	B12	O5-P-O4	-2.41	111.53	118.70
2	O	301	B12	C30-C3-C2	-2.41	114.35	119.11
2	H	301	B12	C20-C1-N21	-2.40	101.27	108.29
2	B	301	B12	C30-C3-C2	-2.39	114.38	119.11
2	E	301	B12	C37-C7-C8	-2.39	101.61	108.27
2	P	301	B12	C20-C1-N21	-2.39	101.32	108.29
2	I	301	B12	O5-P-O4	-2.38	111.60	118.70
2	E	301	B12	C20-C1-N21	-2.38	101.34	108.29
2	I	301	B12	C30-C3-C2	-2.37	114.42	119.11
2	L	301	B12	C20-C1-N21	-2.35	101.41	108.29
5	G	401	5AD	C4-C5-N7	-2.34	107.33	109.48
2	O	301	B12	C20-C1-N21	-2.33	101.47	108.29
2	C	301	B12	C20-C1-N21	-2.32	101.49	108.29
2	K	301	B12	C30-C3-C2	-2.31	114.54	119.11
2	F	301	B12	O5-P-O4	-2.30	111.86	118.70
2	C	301	B12	C30-C3-C2	-2.29	114.58	119.11
2	M	301	B12	C20-C1-N21	-2.28	101.61	108.29
2	E	301	B12	O5-P-O4	-2.28	111.90	118.70
5	C	401	5AD	C4-C5-N7	-2.28	107.38	109.48
2	H	301	B12	C2R-C1R-N1B	-2.28	110.81	114.29
2	I	301	B12	C2R-C1R-N1B	-2.24	110.86	114.29
2	L	301	B12	C30-C3-C2	-2.24	114.68	119.11
2	H	301	B12	C30-C3-C2	-2.23	114.69	119.11
2	P	301	B12	C30-C3-C2	-2.23	114.70	119.11
2	G	301	B12	O5-P-O4	-2.23	112.06	118.70
2	K	301	B12	C2R-C1R-N1B	-2.22	110.89	114.29
5	N	401	5AD	C4-C5-N7	-2.21	107.45	109.48
2	F	301	B12	C20-C1-N21	-2.20	101.85	108.29
2	G	301	B12	C20-C1-N21	-2.20	101.85	108.29
2	N	301	B12	O5-P-O4	-2.19	112.17	118.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	301	B12	O5-P-O4	-2.18	112.21	118.70
2	E	301	B12	C2R-C1R-N1B	-2.16	111.00	114.29
2	J	301	B12	C30-C3-C2	-2.15	114.86	119.11
2	L	301	B12	C37-C7-C8	-2.14	102.31	108.27
5	D	401	5AD	C4-C5-N7	-2.11	107.54	109.48
5	A	401	5AD	C4-C5-N7	-2.10	107.55	109.48
2	K	301	B12	O5-P-O4	-2.09	112.47	118.70
5	K	401	5AD	C4-C5-N7	-2.06	107.58	109.48
2	D	301	B12	O5-P-O4	-2.06	112.57	118.70
2	L	301	B12	C2R-C1R-N1B	-2.05	111.15	114.29
2	B	301	B12	C60-C18-C17	-2.04	111.72	115.68
5	I	401	5AD	C4-C5-N7	-2.01	107.63	109.48
5	M	401	5AD	C4'-O4'-C1'	2.01	111.92	109.72
5	K	401	5AD	C2'-C1'-N9	2.02	117.38	114.29
2	C	301	B12	C1-C19-N24	2.03	108.67	106.20
2	P	301	B12	C53-C15-C16	2.05	121.92	118.25
5	E	401	5AD	C2'-C1'-N9	2.05	117.42	114.29
5	D	401	5AD	C2'-C1'-N9	2.07	117.46	114.29
5	A	401	5AD	C2'-C1'-N9	2.08	117.48	114.29
5	G	283	5AD	N6-C6-N1	2.11	123.73	119.20
5	N	401	5AD	C2'-C1'-N9	2.13	117.55	114.29
2	H	301	B12	C53-C15-C16	2.15	122.09	118.25
2	J	301	B12	C53-C15-C16	2.23	122.25	118.25
5	H	401	5AD	C2'-C1'-N9	2.26	117.75	114.29
5	J	401	5AD	N6-C6-N1	2.27	124.08	119.20
5	L	401	5AD	C2'-C1'-N9	2.30	117.80	114.29
5	B	401	5AD	N6-C6-N1	2.33	124.20	119.20
5	G	401	5AD	C2'-C1'-N9	2.41	117.97	114.29
5	P	401	5AD	C2'-C1'-N9	2.43	118.00	114.29
5	I	401	5AD	C2'-C1'-N9	2.44	118.02	114.29
5	B	401	5AD	C2'-C1'-N9	2.52	118.14	114.29
5	O	401	5AD	C2'-C1'-N9	2.54	118.17	114.29
5	M	401	5AD	C2'-C1'-N9	2.55	118.19	114.29
5	E	401	5AD	N6-C6-N1	2.62	124.83	119.20
2	P	301	B12	C41-C8-C7	2.62	121.64	114.16
2	H	301	B12	C41-C8-C7	2.67	121.76	114.16
5	H	401	5AD	N6-C6-N1	2.67	124.93	119.20
2	B	301	B12	C41-C8-C7	2.70	121.84	114.16
2	E	301	B12	C41-C8-C7	2.70	121.86	114.16
2	G	301	B12	C41-C8-C7	2.72	121.91	114.16
2	D	301	B12	C41-C8-C7	2.74	121.96	114.16
2	J	301	B12	C41-C8-C7	2.78	122.09	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	301	B12	C41-C8-C7	2.79	122.10	114.16
2	J	301	B12	C35-C5-C6	2.84	123.33	118.25
2	N	301	B12	C35-C5-C6	2.84	123.33	118.25
2	C	301	B12	C41-C8-C7	2.88	122.36	114.16
2	N	301	B12	C41-C8-C7	2.88	122.37	114.16
5	F	401	5AD	C2'-C1'-N9	2.88	118.69	114.29
5	O	401	5AD	N6-C6-N1	2.88	125.39	119.20
2	O	301	B12	C41-C8-C7	2.89	122.39	114.16
2	A	301	B12	C41-C8-C7	2.92	122.48	114.16
2	M	301	B12	C35-C5-C6	2.94	123.51	118.25
5	J	401	5AD	C2'-C1'-N9	2.97	118.83	114.29
2	D	301	B12	C35-C5-C6	3.00	123.61	118.25
2	K	301	B12	C35-C5-C6	3.00	123.62	118.25
2	P	301	B12	C35-C5-C6	3.01	123.64	118.25
2	E	301	B12	C35-C5-C6	3.02	123.66	118.25
2	M	301	B12	C41-C8-C7	3.04	122.83	114.16
2	C	301	B12	C35-C5-C6	3.07	123.74	118.25
2	L	301	B12	C41-C8-C7	3.07	122.92	114.16
2	G	301	B12	C35-C5-C6	3.11	123.81	118.25
2	I	301	B12	C41-C8-C7	3.12	123.04	114.16
2	H	301	B12	C35-C5-C6	3.12	123.84	118.25
2	O	301	B12	C35-C5-C6	3.13	123.86	118.25
2	I	301	B12	C35-C5-C6	3.13	123.86	118.25
2	A	301	B12	C35-C5-C6	3.14	123.88	118.25
2	B	301	B12	C35-C5-C6	3.15	123.90	118.25
2	F	301	B12	C35-C5-C6	3.16	123.91	118.25
2	F	301	B12	C41-C8-C7	3.17	123.19	114.16
2	L	301	B12	C35-C5-C6	3.31	124.17	118.25
2	F	301	B12	C19-C1-N21	3.70	105.93	102.16
2	G	301	B12	C19-C1-N21	3.72	105.94	102.16
2	O	301	B12	C19-C1-N21	3.75	105.97	102.16
2	K	301	B12	C19-C1-N21	3.75	105.98	102.16
2	P	301	B12	C19-C1-N21	3.80	106.02	102.16
2	I	301	B12	C19-C1-N21	3.81	106.03	102.16
2	E	301	B12	C19-C1-N21	3.86	106.08	102.16
2	L	301	B12	C19-C1-N21	3.91	106.13	102.16
2	J	301	B12	C19-C1-N21	4.04	106.27	102.16
2	A	301	B12	C19-C1-N21	4.09	106.32	102.16
2	M	301	B12	C19-C1-N21	4.10	106.33	102.16
2	C	301	B12	C19-C1-N21	4.12	106.35	102.16
2	N	301	B12	C19-C1-N21	4.17	106.41	102.16
2	B	301	B12	C19-C1-N21	4.21	106.44	102.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	301	B12	C19-C1-N21	4.31	106.54	102.16
2	D	301	B12	C19-C1-N21	4.50	106.73	102.16
2	I	301	B12	C18-C17-C16	4.82	107.06	100.54
2	D	301	B12	C18-C17-C16	4.84	107.09	100.54
2	C	301	B12	C18-C17-C16	4.90	107.17	100.54
2	J	301	B12	C18-C17-C16	4.96	107.24	100.54
2	F	301	B12	C18-C17-C16	4.99	107.29	100.54
2	O	301	B12	C18-C17-C16	4.99	107.29	100.54
2	H	301	B12	C18-C17-C16	5.05	107.37	100.54
2	B	301	B12	C18-C17-C16	5.06	107.38	100.54
2	E	301	B12	C18-C17-C16	5.06	107.39	100.54
2	M	301	B12	C18-C17-C16	5.07	107.39	100.54
2	K	301	B12	C18-C17-C16	5.11	107.45	100.54
2	L	301	B12	C18-C17-C16	5.12	107.47	100.54
2	N	301	B12	C18-C17-C16	5.14	107.49	100.54
2	A	301	B12	C18-C17-C16	5.15	107.51	100.54
2	G	301	B12	C18-C17-C16	5.16	107.52	100.54
2	P	301	B12	O2-P-O3	5.22	105.03	100.07
2	P	301	B12	C18-C17-C16	5.23	107.61	100.54
2	M	301	B12	O2-P-O3	5.51	105.31	100.07
2	A	301	B12	O2-P-O3	5.66	105.45	100.07
2	O	301	B12	O2-P-O3	6.09	105.86	100.07
2	G	301	B12	O2-P-O3	6.17	105.94	100.07
2	B	301	B12	O2-P-O3	6.27	106.03	100.07
2	H	301	B12	O2-P-O3	6.30	106.06	100.07
2	I	301	B12	O2-P-O3	6.30	106.06	100.07
2	J	301	B12	C2-C1-C19	6.77	130.25	118.56
2	N	301	B12	O2-P-O3	6.82	106.56	100.07
2	D	301	B12	C2-C1-C19	6.89	130.44	118.56
2	K	301	B12	O2-P-O3	6.94	106.67	100.07
2	L	301	B12	C2-C1-C19	6.98	130.61	118.56
2	C	301	B12	O2-P-O3	6.98	106.71	100.07
2	H	301	B12	C2-C1-C19	7.01	130.66	118.56
2	I	301	B12	C2-C1-C19	7.06	130.74	118.56
2	J	301	B12	O2-P-O3	7.10	106.82	100.07
2	A	301	B12	C2-C1-C19	7.11	130.83	118.56
2	M	301	B12	C2-C1-C19	7.11	130.83	118.56
2	E	301	B12	C2-C1-C19	7.13	130.86	118.56
2	N	301	B12	C2-C1-C19	7.16	130.92	118.56
2	F	301	B12	C2-C1-C19	7.17	130.94	118.56
2	P	301	B12	C2-C1-C19	7.20	130.98	118.56
2	O	301	B12	C2-C1-C19	7.22	131.03	118.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	B12	C2-C1-C19	7.23	131.03	118.56
2	D	301	B12	O2-P-O3	7.27	106.98	100.07
2	B	301	B12	C2-C1-C19	7.28	131.12	118.56
2	K	301	B12	C2-C1-C19	7.29	131.13	118.56
2	C	301	B12	C2-C1-C19	7.40	131.34	118.56
2	F	301	B12	O2-P-O3	7.46	107.16	100.07
2	L	301	B12	O2-P-O3	7.62	107.32	100.07
2	E	301	B12	O2-P-O3	8.22	107.88	100.07

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	I	401	5AD	C4'
5	M	401	5AD	C4'
5	J	401	5AD	C4'
5	G	401	5AD	C4'
5	K	401	5AD	C4'
5	I	283	5AD	C4'
5	H	401	5AD	C4'
5	L	401	5AD	C4'
5	G	283	5AD	C4'
5	O	401	5AD	C4'
5	F	401	5AD	C4'
5	P	401	5AD	C4'
5	E	401	5AD	C4'
5	B	401	5AD	C4'
5	C	401	5AD	C4'
5	N	401	5AD	C4'
5	A	401	5AD	C4'
5	D	401	5AD	C4'

There are no torsion outliers.

There are no ring outliers.

44 monomers are involved in 241 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	B12	14	0
5	A	401	5AD	3	0
2	B	301	B12	13	0
5	B	401	5AD	3	0
2	C	301	B12	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	401	5AD	4	0
2	D	301	B12	12	0
5	D	401	5AD	3	0
4	D	601	DHL	2	0
6	E	283	EDO	2	0
2	E	301	B12	14	0
5	E	401	5AD	3	0
2	F	301	B12	13	0
5	F	401	5AD	3	0
5	G	283	5AD	1	0
2	G	301	B12	15	0
5	G	401	5AD	3	0
4	G	601	DHL	1	0
2	H	301	B12	13	0
5	H	401	5AD	4	0
5	I	283	5AD	1	0
2	I	301	B12	14	0
5	I	401	5AD	3	0
4	I	601	DHL	3	0
2	J	301	B12	12	0
5	J	401	5AD	3	0
4	J	601	DHL	1	0
2	K	301	B12	12	0
5	K	401	5AD	3	0
4	K	601	DHL	3	0
2	L	301	B12	13	0
5	L	401	5AD	3	0
2	M	301	B12	12	0
5	M	401	5AD	3	0
2	N	301	B12	13	0
5	N	401	5AD	4	0
4	N	601	DHL	1	0
2	O	301	B12	15	0
5	O	401	5AD	3	0
4	O	601	DHL	1	0
6	P	283	EDO	2	0
6	P	284	EDO	5	0
2	P	301	B12	16	0
5	P	401	5AD	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	225/286 (78%)	-0.19	5 (2%)	65	64	24, 40, 57, 70	0
1	B	226/286 (79%)	-0.17	5 (2%)	65	64	26, 40, 59, 70	0
1	C	226/286 (79%)	0.05	9 (3%)	42	43	29, 43, 60, 76	0
1	D	227/286 (79%)	-0.30	4 (1%)	71	71	23, 35, 52, 73	0
1	E	228/286 (79%)	-0.41	1 (0%)	93	93	18, 31, 51, 72	0
1	F	226/286 (79%)	-0.46	2 (0%)	85	85	16, 29, 47, 63	0
1	G	226/286 (79%)	-0.48	3 (1%)	79	79	16, 27, 48, 68	0
1	H	225/286 (78%)	-0.51	2 (0%)	85	85	17, 27, 47, 66	0
1	I	226/286 (79%)	-0.42	3 (1%)	79	79	19, 30, 51, 71	0
1	J	225/286 (78%)	-0.49	2 (0%)	85	85	19, 28, 50, 71	0
1	K	225/286 (78%)	-0.39	0	100	100	19, 32, 51, 67	0
1	L	229/286 (80%)	-0.45	1 (0%)	93	93	16, 28, 45, 71	0
1	M	229/286 (80%)	-0.45	3 (1%)	79	79	16, 28, 45, 63	0
1	N	230/286 (80%)	-0.29	6 (2%)	59	58	20, 33, 51, 76	0
1	O	226/286 (79%)	-0.49	2 (0%)	85	85	19, 30, 47, 68	0
1	P	228/286 (79%)	-0.42	4 (1%)	71	71	18, 31, 51, 68	0
All	All	3627/4576 (79%)	-0.37	52 (1%)	78	77	16, 32, 54, 76	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	CYS	5.0
1	H	70	CYS	4.7
1	M	3	PRO	4.3
1	I	71	HIS	4.1
1	E	232	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	70	CYS	3.9
1	B	3	PRO	3.7
1	P	3	PRO	3.5
1	J	70	CYS	3.5
1	H	71	HIS	3.5
1	G	71	HIS	3.4
1	P	71	HIS	3.4
1	N	232	ALA	3.4
1	P	70	CYS	3.4
1	D	177	ARG	3.3
1	D	3	PRO	3.2
1	B	71	HIS	3.1
1	B	70	CYS	3.0
1	A	137	ALA	3.0
1	C	49	ALA	2.9
1	O	70	CYS	2.8
1	A	71	HIS	2.8
1	I	70	CYS	2.8
1	G	3	PRO	2.8
1	P	231	LEU	2.7
1	C	137	ALA	2.7
1	C	213	GLU	2.6
1	L	233	LEU	2.5
1	N	6	ALA	2.5
1	B	148	VAL	2.5
1	C	168	GLY	2.5
1	J	71	HIS	2.5
1	A	210	THR	2.5
1	N	231	LEU	2.4
1	C	231	LEU	2.3
1	C	210	THR	2.3
1	D	136	GLU	2.3
1	C	71	HIS	2.3
1	A	148	VAL	2.2
1	F	3	PRO	2.2
1	N	234	LEU	2.2
1	O	71	HIS	2.2
1	N	233	LEU	2.2
1	D	2	GLU	2.2
1	I	3	PRO	2.2
1	M	2	GLU	2.1
1	M	232	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	136	GLU	2.1
1	F	173	ASP	2.1
1	C	178	LYS	2.0
1	N	235	GLY	2.0
1	C	68	GLN	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^{th} 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(Å^2)	Q<0.9
4	DHL	O	601	4/4	0.80	0.27	8.96	29,30,32,35	4
5	5AD	G	283	18/18	0.75	0.43	6.89	55,68,72,72	0
4	DHL	I	601	4/4	0.70	0.38	6.03	41,42,42,42	4
5	5AD	I	283	18/18	0.71	0.40	4.98	59,64,71,73	0
4	DHL	D	601	4/4	0.87	0.40	4.73	62,62,63,64	0
4	DHL	N	601	4/4	0.92	0.23	4.49	51,55,58,61	0
4	DHL	K	601	4/4	0.92	0.19	3.50	50,51,51,53	0
4	DHL	J	601	4/4	0.91	0.24	2.74	43,47,51,54	0
6	EDO	P	284	4/4	0.82	0.31	2.30	48,49,49,53	0
4	DHL	C	601	4/4	0.90	0.24	2.09	22,23,25,30	4
3	FLC	B	501	13/13	0.93	0.18	1.88	53,54,55,55	0
4	DHL	F	601	4/4	0.89	0.28	1.76	52,52,53,54	0
4	DHL	H	601	4/4	0.96	0.14	1.55	39,40,41,42	0
4	DHL	A	601	4/4	0.82	0.27	1.48	79,79,79,80	0
4	DHL	P	601	4/4	0.96	0.14	1.31	38,38,38,40	0
3	FLC	D	501	13/13	0.91	0.14	1.30	43,44,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FLC	C	501	13/13	0.91	0.17	1.09	61,62,63,63	0
3	FLC	G	501	13/13	0.93	0.15	0.83	33,34,35,36	0
3	FLC	P	501	13/13	0.92	0.15	0.79	39,40,41,42	0
3	FLC	H	501	13/13	0.95	0.14	0.78	37,38,39,39	0
3	FLC	K	501	13/13	0.93	0.14	0.46	37,38,39,39	0
3	FLC	E	501	13/13	0.93	0.13	0.40	36,37,38,38	0
3	FLC	O	501	13/13	0.95	0.14	0.38	36,37,38,38	0
3	FLC	J	501	13/13	0.95	0.13	0.35	35,36,37,38	0
3	FLC	N	501	13/13	0.94	0.14	0.11	38,39,40,41	0
2	B12	N	301	91/91	0.96	0.12	0.10	15,23,29,32	0
3	FLC	A	501	13/13	0.95	0.14	0.01	43,44,45,46	0
3	FLC	L	501	13/13	0.95	0.12	-0.05	35,35,36,37	0
2	B12	K	301	91/91	0.96	0.11	-0.11	17,25,29,34	0
2	B12	J	301	91/91	0.96	0.12	-0.12	18,23,30,32	0
2	B12	P	301	91/91	0.96	0.12	-0.17	17,24,29,31	0
2	B12	D	301	91/91	0.96	0.13	-0.18	17,28,37,38	0
2	B12	M	301	91/91	0.96	0.12	-0.18	10,21,28,31	0
3	FLC	I	501	13/13	0.96	0.12	-0.25	34,34,35,36	0
2	B12	I	301	91/91	0.96	0.12	-0.28	17,23,30,33	0
2	B12	E	301	91/91	0.97	0.11	-0.31	17,23,30,32	0
2	B12	G	301	91/91	0.96	0.12	-0.32	15,21,28,29	0
2	B12	L	301	91/91	0.96	0.11	-0.33	14,20,28,30	0
2	B12	A	301	91/91	0.94	0.12	-0.35	27,33,41,44	0
2	B12	O	301	91/91	0.96	0.11	-0.38	15,22,29,32	0
3	FLC	F	501	13/13	0.96	0.11	-0.46	31,32,33,33	0
2	B12	B	301	91/91	0.94	0.12	-0.47	29,35,42,49	0
2	B12	F	301	91/91	0.97	0.11	-0.49	12,21,28,30	0
2	B12	C	301	91/91	0.95	0.12	-0.53	28,35,46,55	0
2	B12	H	301	91/91	0.96	0.11	-0.55	16,22,26,29	0
3	FLC	M	501	13/13	0.95	0.12	-0.78	35,36,37,37	0
5	5AD	K	401	18/18	0.91	0.17	-	23,32,34,35	0
5	5AD	F	401	18/18	0.94	0.16	-	24,31,35,38	0
5	5AD	J	401	18/18	0.93	0.18	-	22,28,37,38	0
5	5AD	H	401	18/18	0.91	0.17	-	23,29,38,38	0
5	5AD	L	401	18/18	0.93	0.17	-	24,32,44,47	0
6	EDO	E	283	4/4	0.86	0.40	-	55,55,55,59	0
4	DHL	M	601	4/4	0.80	0.29	-	54,55,56,56	0
5	5AD	I	401	18/18	0.93	0.15	-	28,34,38,39	0
4	DHL	L	601	4/4	0.92	0.19	-	51,51,51,51	0
5	5AD	G	401	18/18	0.94	0.17	-	28,32,38,39	0
5	5AD	B	401	18/18	0.91	0.17	-	35,40,43,43	0
5	5AD	P	401	18/18	0.93	0.16	-	26,32,36,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	5AD	C	401	18/18	0.91	0.18	-	31,39,46,46	0
5	5AD	N	401	18/18	0.93	0.17	-	22,31,39,40	0
6	EDO	P	283	4/4	0.89	0.42	-	43,44,45,48	0
5	5AD	M	401	18/18	0.93	0.17	-	26,34,40,43	0
5	5AD	A	401	18/18	0.92	0.19	-	41,44,47,49	0
5	5AD	O	401	18/18	0.90	0.17	-	25,31,35,39	0
5	5AD	E	401	18/18	0.92	0.15	-	24,31,38,38	0
5	5AD	D	401	18/18	0.93	0.22	-	31,35,47,48	0
4	DHL	G	601	4/4	0.73	0.34	-	57,59,61,64	0

6.5 Other polymers (i)

There are no such residues in this entry.