



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:08 am BST

PDB ID : 2QW7
Title : Carboxysome Subunit, CcmL
Authors : Tanaka, S.; Sawaya, M.R.; Kerfeld, C.A.; Yeates, T.O.
Deposited on : 2007-08-09
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

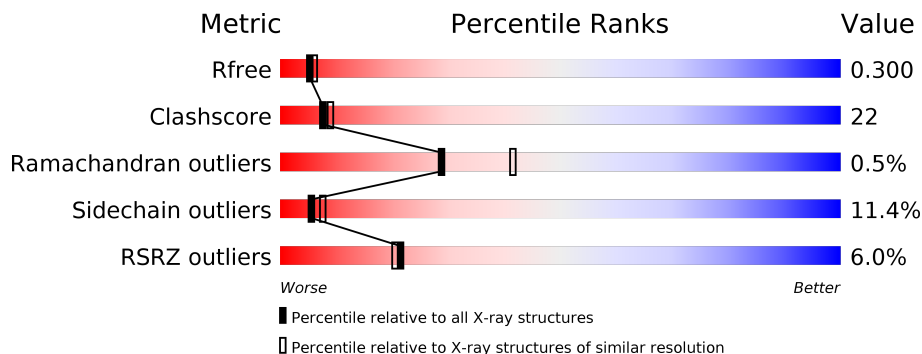
1 Overall quality at a glance i

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	111	 6% 44% 34% 6% • 14%
1	B	111	 5% 46% 35% 5% 14%
1	C	111	 9% 56% 23% 7% 14%
1	D	111	 4% 55% 29% • 14%
1	E	111	 6% 51% 29% 6% 14%
1	F	111	 9% 55% 25% 5% • 14%

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Mol	Chain	Length	Quality of chain
1	G	111	<p>2% 57% 25% 14%</p>
1	H	111	<p>4% 58% 23% 7% 12%</p>
1	I	111	<p>3% 49% 34% 14%</p>
1	J	111	<p>5% 50% 31% 5% 14%</p>

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
2	GOL	G	202	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7353 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 Carbon dioxide concentrating mechanism protein ccmL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	96	Total 726	C 457	N 129	O 137	S 3	0	2	0
1	B	96	Total 720	C 453	N 129	O 135	S 3	0	1	0
1	C	95	Total 709	C 447	N 125	O 134	S 3	0	1	0
1	D	96	Total 715	C 449	N 129	O 135	S 2	0	0	0
1	E	96	Total 715	C 449	N 129	O 135	S 2	0	0	0
1	F	96	Total 725	C 457	N 129	O 135	S 4	0	2	0
1	G	96	Total 715	C 449	N 129	O 135	S 2	0	0	0
1	H	98	Total 731	C 457	N 131	O 141	S 2	0	0	0
1	I	96	Total 715	C 449	N 129	O 135	S 2	0	0	0
1	J	96	Total 720	C 453	N 129	O 135	S 3	0	1	0

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	LEU	-	expression tag	UNP P72759
A	102	GLU	-	expression tag	UNP P72759
A	103	ALA	-	expression tag	UNP P72759
A	104	ALA	-	expression tag	UNP P72759
A	105	ALA	-	expression tag	UNP P72759
A	106	HIS	-	expression tag	UNP P72759
A	107	HIS	-	expression tag	UNP P72759
A	108	HIS	-	expression tag	UNP P72759
A	109	HIS	-	expression tag	UNP P72759

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Chain	Residue	Modelled	Actual	Comment	Reference
A	110	HIS	-	expression tag	UNP P72759
A	111	HIS	-	expression tag	UNP P72759
B	101	LEU	-	expression tag	UNP P72759
B	102	GLU	-	expression tag	UNP P72759
B	103	ALA	-	expression tag	UNP P72759
B	104	ALA	-	expression tag	UNP P72759
B	105	ALA	-	expression tag	UNP P72759
B	106	HIS	-	expression tag	UNP P72759
B	107	HIS	-	expression tag	UNP P72759
B	108	HIS	-	expression tag	UNP P72759
B	109	HIS	-	expression tag	UNP P72759
B	110	HIS	-	expression tag	UNP P72759
B	111	HIS	-	expression tag	UNP P72759
C	101	LEU	-	expression tag	UNP P72759
C	102	GLU	-	expression tag	UNP P72759
C	103	ALA	-	expression tag	UNP P72759
C	104	ALA	-	expression tag	UNP P72759
C	105	ALA	-	expression tag	UNP P72759
C	106	HIS	-	expression tag	UNP P72759
C	107	HIS	-	expression tag	UNP P72759
C	108	HIS	-	expression tag	UNP P72759
C	109	HIS	-	expression tag	UNP P72759
C	110	HIS	-	expression tag	UNP P72759
C	111	HIS	-	expression tag	UNP P72759
D	101	LEU	-	expression tag	UNP P72759
D	102	GLU	-	expression tag	UNP P72759
D	103	ALA	-	expression tag	UNP P72759
D	104	ALA	-	expression tag	UNP P72759
D	105	ALA	-	expression tag	UNP P72759
D	106	HIS	-	expression tag	UNP P72759
D	107	HIS	-	expression tag	UNP P72759
D	108	HIS	-	expression tag	UNP P72759
D	109	HIS	-	expression tag	UNP P72759
D	110	HIS	-	expression tag	UNP P72759
D	111	HIS	-	expression tag	UNP P72759
E	101	LEU	-	expression tag	UNP P72759
E	102	GLU	-	expression tag	UNP P72759
E	103	ALA	-	expression tag	UNP P72759
E	104	ALA	-	expression tag	UNP P72759
E	105	ALA	-	expression tag	UNP P72759
E	106	HIS	-	expression tag	UNP P72759
E	107	HIS	-	expression tag	UNP P72759

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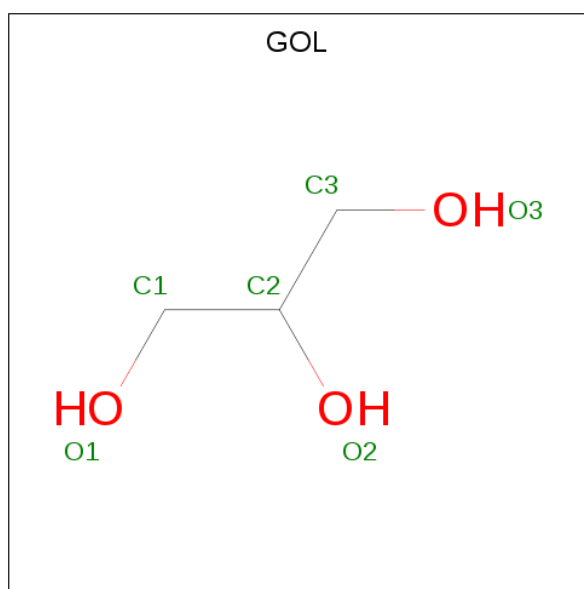
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E	108	HIS	-	expression tag	UNP P72759
E	109	HIS	-	expression tag	UNP P72759
E	110	HIS	-	expression tag	UNP P72759
E	111	HIS	-	expression tag	UNP P72759
F	101	LEU	-	expression tag	UNP P72759
F	102	GLU	-	expression tag	UNP P72759
F	103	ALA	-	expression tag	UNP P72759
F	104	ALA	-	expression tag	UNP P72759
F	105	ALA	-	expression tag	UNP P72759
F	106	HIS	-	expression tag	UNP P72759
F	107	HIS	-	expression tag	UNP P72759
F	108	HIS	-	expression tag	UNP P72759
F	109	HIS	-	expression tag	UNP P72759
F	110	HIS	-	expression tag	UNP P72759
F	111	HIS	-	expression tag	UNP P72759
G	101	LEU	-	expression tag	UNP P72759
G	102	GLU	-	expression tag	UNP P72759
G	103	ALA	-	expression tag	UNP P72759
G	104	ALA	-	expression tag	UNP P72759
G	105	ALA	-	expression tag	UNP P72759
G	106	HIS	-	expression tag	UNP P72759
G	107	HIS	-	expression tag	UNP P72759
G	108	HIS	-	expression tag	UNP P72759
G	109	HIS	-	expression tag	UNP P72759
G	110	HIS	-	expression tag	UNP P72759
G	111	HIS	-	expression tag	UNP P72759
H	101	LEU	-	expression tag	UNP P72759
H	102	GLU	-	expression tag	UNP P72759
H	103	ALA	-	expression tag	UNP P72759
H	104	ALA	-	expression tag	UNP P72759
H	105	ALA	-	expression tag	UNP P72759
H	106	HIS	-	expression tag	UNP P72759
H	107	HIS	-	expression tag	UNP P72759
H	108	HIS	-	expression tag	UNP P72759
H	109	HIS	-	expression tag	UNP P72759
H	110	HIS	-	expression tag	UNP P72759
H	111	HIS	-	expression tag	UNP P72759
I	101	LEU	-	expression tag	UNP P72759
I	102	GLU	-	expression tag	UNP P72759
I	103	ALA	-	expression tag	UNP P72759
I	104	ALA	-	expression tag	UNP P72759
I	105	ALA	-	expression tag	UNP P72759

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Chain	Residue	Modelled	Actual	Comment	Reference
I	106	HIS	-	expression tag	UNP P72759
I	107	HIS	-	expression tag	UNP P72759
I	108	HIS	-	expression tag	UNP P72759
I	109	HIS	-	expression tag	UNP P72759
I	110	HIS	-	expression tag	UNP P72759
I	111	HIS	-	expression tag	UNP P72759
J	101	LEU	-	expression tag	UNP P72759
J	102	GLU	-	expression tag	UNP P72759
J	103	ALA	-	expression tag	UNP P72759
J	104	ALA	-	expression tag	UNP P72759
J	105	ALA	-	expression tag	UNP P72759
J	106	HIS	-	expression tag	UNP P72759
J	107	HIS	-	expression tag	UNP P72759
J	108	HIS	-	expression tag	UNP P72759
J	109	HIS	-	expression tag	UNP P72759
J	110	HIS	-	expression tag	UNP P72759
J	111	HIS	-	expression tag	UNP P72759

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	C O	0	1
			30	15 15		
2	B	1	Total	C O	0	0
			6	3 3		
2	G	1	Total	C O	0	1
			30	15 15		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	C O	0	0
			6	3 3		

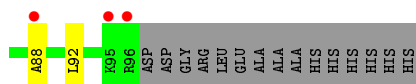
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		
3	B	11	Total	O	0	0
			11	11		
3	C	5	Total	O	0	0
			5	5		
3	D	7	Total	O	0	0
			7	7		
3	E	11	Total	O	0	0
			11	11		
3	F	8	Total	O	0	0
			8	8		
3	G	9	Total	O	0	0
			9	9		
3	H	10	Total	O	0	0
			10	10		
3	I	4	Total	O	0	0
			4	4		
3	J	12	Total	O	0	0
			12	12		

GLY
ARG
LEU
GLU
ALA
ALA
ALA
HIS
HIS
HIS
HIS
HIS
HIS

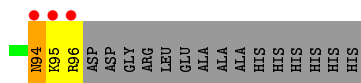
• Molecule 1: Carbon dioxide concentrating mechanism protein ccml

Chain E: 



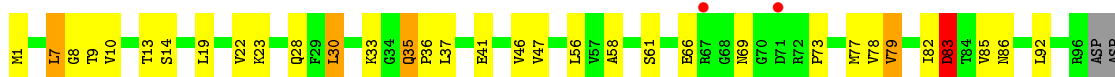
• Molecule 1: Carbon dioxide concentrating mechanism protein ccml

Chain F: 



• Molecule 1: Carbon dioxide concentrating mechanism protein ccml

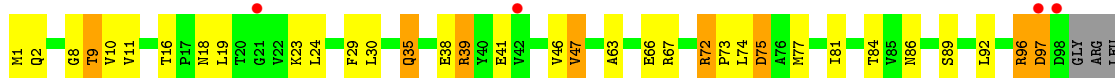
Chain G: 



GLY
ARG
LEU
GLU
ALA
ALA
ALA
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Carbon dioxide concentrating mechanism protein ccml

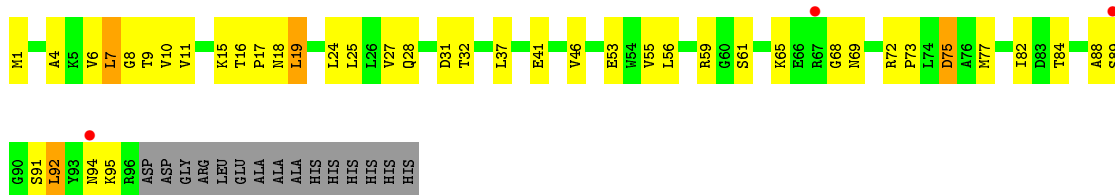
Chain H: 



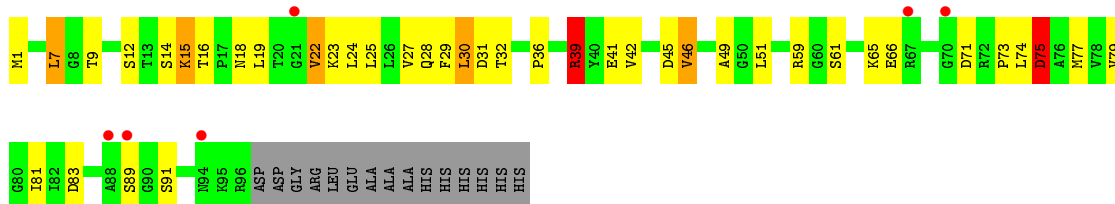
GLU
ALA
ALA
ALA
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Carbon dioxide concentrating mechanism protein ccml

Chain I: 



- Molecule 1: Carbon dioxide concentrating mechanism protein ccML



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.43Å 107.44Å 72.26Å 90.00° 96.51° 90.00°	Depositor
Resolution (Å)	19.90 – 2.40 19.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	78.9 (19.90-2.40) 78.8 (19.95-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.41Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.240 , 0.296 0.243 , 0.300	Depositor DCC
R_{free} test set	1512 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtrriage
Anisotropy	0.150	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7353	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.5502e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

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	1.06	2/739 (0.3%)	1.32	7/999 (0.7%)
1	B	0.92	1/730 (0.1%)	1.27	4/987 (0.4%)
1	C	0.77	1/719 (0.1%)	1.17	3/973 (0.3%)
1	D	0.77	0/722	1.19	2/977 (0.2%)
1	E	0.93	1/722 (0.1%)	1.17	2/977 (0.2%)
1	F	0.77	0/738	1.20	3/997 (0.3%)
1	G	0.71	0/722	1.11	2/977 (0.2%)
1	H	0.89	0/738	1.26	3/999 (0.3%)
1	I	0.81	0/722	1.20	3/977 (0.3%)
1	J	0.78	0/730	1.25	5/987 (0.5%)
All	All	0.85	5/7282 (0.1%)	1.22	34/9850 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	ASP	CB-CG	-6.92	1.37	1.51
1	A	53	GLU	CG-CD	5.64	1.60	1.51
1	E	27	VAL	CB-CG2	5.40	1.64	1.52
1	B	76	ALA	CA-CB	5.39	1.63	1.52
1	A	57	VAL	CB-CG2	5.32	1.64	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	75	ASP	CB-CG-OD1	-9.80	109.47	118.30
1	H	75	ASP	CB-CA-C	-8.67	93.05	110.40
1	H	72	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	D	75	ASP	CB-CA-C	-7.81	94.78	110.40
1	J	75	ASP	CB-CA-C	-7.73	94.94	110.40
1	C	75	ASP	CB-CA-C	-7.57	95.26	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	75	ASP	N-CA-CB	-7.54	97.03	110.60
1	E	75	ASP	CB-CA-C	-7.46	95.47	110.40
1	A	75	ASP	CB-CA-C	-7.40	95.60	110.40
1	J	39	ARG	NE-CZ-NH2	7.23	123.92	120.30
1	C	75	ASP	CB-CG-OD1	-7.21	111.81	118.30
1	D	19	LEU	CB-CG-CD2	-6.94	99.20	111.00
1	F	75	ASP	N-CA-CB	-6.92	98.14	110.60
1	H	72	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	B	59	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	59	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	J	39	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	F	75	ASP	CB-CA-C	-5.98	98.43	110.40
1	A	26	LEU	CB-CG-CD2	-5.85	101.06	111.00
1	A	64	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	J	15	LYS	CB-CA-C	-5.80	98.80	110.40
1	A	56	LEU	CB-CG-CD1	-5.66	101.38	111.00
1	F	83	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	59	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	3	LEU	CA-CB-CG	5.42	127.77	115.30
1	I	19	LEU	CB-CG-CD1	-5.35	101.90	111.00
1	G	83	ASP	N-CA-CB	5.26	120.07	110.60
1	B	42	VAL	N-CA-C	-5.22	96.90	111.00
1	A	26	LEU	CA-CB-CG	5.20	127.27	115.30
1	J	31	ASP	CB-CG-OD1	5.18	122.96	118.30
1	C	95	LYS	CA-CB-CG	5.15	124.74	113.40
1	G	79	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	B	56	LEU	CA-CB-CG	5.06	126.94	115.30
1	E	15	LYS	CB-CA-C	-5.02	100.36	110.40

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	726	0	769	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	720	0	763	51	0
1	C	709	0	750	28	0
1	D	715	0	752	33	0
1	E	715	0	752	34	0
1	F	725	0	772	39	0
1	G	715	0	752	29	0
1	H	731	0	760	34	0
1	I	715	0	752	39	0
1	J	720	0	763	38	0
2	B	36	0	48	10	0
2	G	36	0	48	10	0
3	A	13	0	0	1	0
3	B	11	0	0	2	0
3	C	5	0	0	0	0
3	D	7	0	0	0	0
3	E	11	0	0	0	0
3	F	8	0	0	1	0
3	G	9	0	0	0	0
3	H	10	0	0	1	0
3	I	4	0	0	0	0
3	J	12	0	0	1	0
All	All	7353	0	7681	329	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 22.

All (329) 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:H:84:THR:HG22	1:I:11:VAL:HB	1.39	1.05
1:A:11:VAL:HB	1:E:84:THR:HG22	1.41	1.03
1:I:69:ASN:HD22	1:I:77:MET:HE1	1.23	1.02
1:B:92:LEU:O	1:B:92:LEU:HD13	1.66	0.95
1:B:27:VAL:HG23	1:B:27:VAL:O	1.68	0.93
1:C:19:LEU:O	1:C:22:VAL:HG12	1.71	0.90
1:E:19:LEU:HD12	1:E:22:VAL:HG11	1.53	0.89
1:F:46:VAL:HG21	1:F:77[B]:MET:HE3	1.55	0.88
2:G:203[D]:GOL:HO1	1:I:61:SER:HG	1.25	0.83
1:A:94:ASN:N	1:A:94:ASN:HD22	1.77	0.82
1:B:19:LEU:CD1	1:B:73:PRO:HG2	2.09	0.82
1:I:69:ASN:HD22	1:I:77:MET:CE	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1[B]:MET:HE2	1:C:75:ASP:HB2	1.60	0.82
1:F:83:ASP:OD2	1:G:13:THR:HG23	1.85	0.77
1:B:23:LYS:HE2	1:B:25:LEU:HD21	1.68	0.76
1:E:33:LYS:O	1:E:35:GLN:NE2	2.18	0.76
1:I:69:ASN:ND2	1:I:77:MET:HE1	2.01	0.74
1:B:46:VAL:HG12	1:B:77:MET:CE	2.19	0.73
1:H:75:ASP:OD2	3:H:120:HOH:O	2.05	0.73
1:B:46:VAL:CG1	1:B:77:MET:HE2	2.18	0.73
1:B:19:LEU:HD13	1:B:73:PRO:CG	2.20	0.72
1:I:69:ASN:ND2	1:I:77:MET:CE	2.53	0.72
1:H:9:THR:HB	1:H:23:LYS:HZ1	1.54	0.72
1:J:25:LEU:HD12	1:J:45:ASP:HB2	1.71	0.72
1:A:51:LEU:HD21	1:E:88:ALA:HB2	1.72	0.71
1:B:19:LEU:HD13	1:B:73:PRO:HG2	1.72	0.71
1:D:87:VAL:HG12	1:D:88:ALA:H	1.56	0.71
1:A:10:VAL:HG22	1:E:85:VAL:HG22	1.71	0.71
1:G:66:GLU:HB2	1:G:69:ASN:ND2	2.07	0.70
1:F:46:VAL:HG21	1:F:77[B]:MET:CE	2.21	0.70
1:E:92:LEU:O	1:E:92:LEU:HD13	1.92	0.70
1:J:25:LEU:CD1	1:J:45:ASP:HB2	2.21	0.69
2:G:203[C]:GOL:HO1	1:J:61:SER:HG	1.38	0.69
1:I:1:MET:CE	1:J:24:LEU:HD21	2.23	0.69
1:H:2:GLN:NE2	1:I:41:GLU:OE1	2.25	0.69
1:J:46:VAL:HG13	1:J:46:VAL:O	1.91	0.69
1:A:61:SER:HG	2:B:200[B]:GOL:HO1	1.39	0.69
1:H:41:GLU:HA	1:H:41:GLU:OE1	1.93	0.68
1:A:75:ASP:OD2	1:E:59:ARG:NH1	2.26	0.68
1:B:19:LEU:HD11	1:B:73:PRO:HG2	1.74	0.68
1:F:61:SER:HG	2:G:203[B]:GOL:HO1	1.41	0.68
1:C:74:LEU:HD13	1:C:77:MET:HE2	1.77	0.67
1:F:94:ASN:N	1:F:94:ASN:OD1	2.29	0.66
1:A:1[A]:MET:HE2	1:A:1[A]:MET:H1	1.60	0.66
1:B:46:VAL:CG1	1:B:77:MET:CE	2.73	0.66
1:G:85:VAL:HG22	1:H:10:VAL:HG13	1.77	0.66
1:B:31:ASP:HB3	1:B:37:LEU:HD21	1.78	0.66
1:H:19:LEU:CD1	1:H:73:PRO:HD2	2.26	0.66
1:B:91:SER:OG	1:B:94:ASN:OD1	2.04	0.66
1:F:75:ASP:OD2	1:J:59:ARG:NH1	2.30	0.65
1:B:61:SER:HG	2:B:200[C]:GOL:H32	1.62	0.65
1:J:24:LEU:HD22	1:J:42:VAL:HG12	1.78	0.65
1:D:87:VAL:HG12	1:D:88:ALA:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:ALA:HB2	1:G:79:VAL:HG11	1.79	0.64
1:J:9:THR:HG21	1:J:23:LYS:NZ	2.13	0.64
1:E:22:VAL:HB	1:E:72:ARG:NH1	2.13	0.64
1:A:46:VAL:HG21	1:A:77:MET:CE	2.28	0.64
1:B:27:VAL:CG2	1:B:27:VAL:O	2.45	0.63
1:C:3:LEU:HD22	1:C:82:ILE:HD13	1.79	0.63
1:A:35:GLN:HG3	1:A:36:PRO:HD2	1.80	0.63
1:D:5:LYS:HB2	1:D:30:LEU:HD11	1.79	0.63
1:I:7:LEU:HD22	1:I:28:GLN:HB2	1.80	0.63
1:G:66:GLU:HB2	1:G:69:ASN:HD22	1.63	0.63
1:C:87:VAL:HG13	1:C:88:ALA:H	1.62	0.63
2:G:203[C]:GOL:HO2	2:G:202:GOL:HO2	1.43	0.63
1:J:30:LEU:HD12	1:J:36:PRO:HA	1.81	0.63
1:J:24:LEU:HD22	1:J:42:VAL:CG1	2.28	0.62
1:A:56:LEU:HD23	1:A:82:ILE:HD11	1.79	0.62
1:F:31:ASP:HB3	1:F:37:LEU:HD21	1.82	0.61
1:H:9:THR:HB	1:H:23:LYS:NZ	2.16	0.61
1:I:15:LYS:NZ	1:I:19:LEU:O	2.23	0.61
1:B:33:LYS:O	1:B:35:GLN:NE2	2.34	0.61
1:B:92:LEU:HD13	1:B:92:LEU:C	2.21	0.61
1:E:12:SER:HB3	1:E:15:LYS:HD3	1.82	0.61
1:C:1[B]:MET:CE	1:D:74:LEU:HD22	2.31	0.61
1:C:1[B]:MET:HE2	1:D:74:LEU:HD22	1.83	0.61
1:H:19:LEU:HD11	1:H:73:PRO:HG2	1.83	0.60
1:A:94:ASN:N	1:A:94:ASN:ND2	2.48	0.60
1:E:12:SER:O	1:E:15:LYS:HE2	2.00	0.60
1:H:63:ALA:O	1:H:77:MET:HE3	2.01	0.60
1:D:7:LEU:HD22	1:D:28:GLN:HB2	1.83	0.60
1:I:88:ALA:HB2	1:J:51:LEU:HD11	1.81	0.60
1:B:86:ASN:O	1:C:8:GLY:HA3	2.01	0.59
1:G:83:ASP:OD1	1:H:11:VAL:HG12	2.02	0.59
1:F:46:VAL:CG1	1:F:46:VAL:O	2.50	0.59
1:D:31:ASP:HB3	1:D:37:LEU:HD21	1.85	0.59
1:E:46:VAL:HG11	1:E:66:GLU:HG3	1.85	0.59
1:H:9:THR:CB	1:H:23:LYS:HZ1	2.15	0.59
1:A:93:TYR:C	1:A:94:ASN:HD22	2.06	0.59
1:J:19:LEU:HD13	1:J:73:PRO:HD2	1.84	0.59
1:J:46:VAL:CG1	1:J:46:VAL:O	2.51	0.58
1:A:44:GLY:O	1:A:77:MET:SD	2.61	0.58
2:G:203[A]:GOL:HO2	2:G:202:GOL:HO2	1.51	0.58
1:I:84:THR:HG22	1:I:94:ASN:HD22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LEU:HD13	1:A:73:PRO:HG2	1.86	0.58
1:J:74:LEU:HD13	1:J:77:MET:CE	2.34	0.58
1:J:9:THR:HG21	1:J:23:LYS:HZ2	1.69	0.58
1:G:86:ASN:O	1:H:8:GLY:HA3	2.03	0.58
1:B:12:SER:O	1:B:15:LYS:HE2	2.03	0.58
1:H:74:LEU:HD13	1:H:77:MET:HE1	1.86	0.58
1:H:47:VAL:HG11	1:H:81:ILE:HG13	1.86	0.58
1:J:74:LEU:HD13	1:J:77:MET:HE2	1.84	0.58
1:D:28:GLN:NE2	1:D:37:LEU:O	2.29	0.57
1:E:19:LEU:O	1:E:22:VAL:HG12	2.04	0.57
1:A:46:VAL:CG2	1:A:77:MET:CE	2.82	0.57
1:G:30:LEU:HD12	1:G:36:PRO:HA	1.86	0.57
2:B:200[A]:GOL:O2	2:B:201:GOL:O2	2.21	0.57
1:E:66:GLU:OE2	1:E:67:ARG:N	2.38	0.57
1:F:46:VAL:HG23	1:F:77[A]:MET:SD	2.45	0.57
1:J:9:THR:CG2	1:J:23:LYS:NZ	2.68	0.57
1:A:46:VAL:HG21	1:A:77:MET:HE3	1.86	0.57
1:E:56:LEU:HD23	1:E:82:ILE:HD11	1.86	0.57
1:H:9:THR:CG2	1:H:23:LYS:HZ1	2.18	0.57
1:J:18:ASN:ND2	1:J:71:ASP:O	2.37	0.56
1:B:59:ARG:NE	3:B:202:HOH:O	2.38	0.56
1:C:87:VAL:CG1	1:C:88:ALA:N	2.68	0.56
1:A:19:LEU:HD13	1:A:73:PRO:CG	2.35	0.56
1:F:25:LEU:HD12	1:F:45:ASP:HB2	1.87	0.56
1:B:1[B]:MET:H1	1:B:1[B]:MET:HE2	1.71	0.55
1:F:75:ASP:HB2	1:J:1[B]:MET:HG3	1.88	0.55
1:D:87:VAL:CG1	1:D:88:ALA:H	2.19	0.55
1:B:10:VAL:HG12	1:B:24:LEU:HD23	1.88	0.55
1:F:7:LEU:HD22	1:F:28:GLN:HB2	1.88	0.55
1:G:58:ALA:CB	1:G:79:VAL:HG11	2.36	0.55
1:B:46:VAL:HG12	1:B:77:MET:HE3	1.87	0.55
1:C:22:VAL:O	1:C:22:VAL:HG13	2.06	0.55
1:C:87:VAL:HG13	1:C:88:ALA:N	2.20	0.55
1:A:65:LYS:HD3	1:B:71:ASP:HA	1.88	0.54
1:H:84:THR:CG2	1:I:11:VAL:HB	2.25	0.54
1:B:7:LEU:HD22	1:B:28:GLN:HB2	1.88	0.54
2:B:200[B]:GOL:O2	2:B:201:GOL:O2	2.25	0.54
1:A:1[A]:MET:SD	1:B:74:LEU:HD23	2.47	0.54
1:G:19:LEU:HD13	1:G:73:PRO:HG2	1.90	0.54
1:A:84:THR:HG22	1:A:94:ASN:HA	1.88	0.54
1:E:47:VAL:O	1:E:47:VAL:CG1	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:HB	1:E:84:THR:CG2	2.25	0.54
1:A:1[A]:MET:HE2	1:A:1[A]:MET:H3	1.70	0.54
1:G:61:SER:HG	2:G:203[C]:GOL:H32	1.72	0.54
1:B:64:ARG:O	3:B:211:HOH:O	2.18	0.53
1:I:1:MET:HE1	1:J:24:LEU:HD21	1.90	0.53
1:A:88:ALA:HB2	1:B:51:LEU:HD21	1.89	0.53
1:F:3:LEU:HD22	1:F:82:ILE:HD13	1.91	0.53
1:G:7:LEU:HD22	1:G:28:GLN:HB2	1.89	0.53
1:I:16:THR:CG2	1:I:19:LEU:HG	2.38	0.53
1:B:51:LEU:O	1:B:52:ASN:HB2	2.09	0.53
1:F:86:ASN:O	1:G:8:GLY:HA3	2.08	0.53
1:I:27:VAL:O	1:I:27:VAL:HG23	2.10	0.52
1:D:86:ASN:O	1:E:8:GLY:HA3	2.10	0.52
1:G:9:THR:HG22	1:G:10:VAL:N	2.23	0.52
1:A:53:GLU:OE1	1:A:81:ILE:HD13	2.10	0.52
1:F:66:GLU:HB2	1:F:77[B]:MET:CE	2.39	0.52
1:I:16:THR:OG1	1:I:17:PRO:HD2	2.09	0.52
1:I:18:ASN:HB2	1:I:73:PRO:HD3	1.92	0.52
1:B:61:SER:HG	2:B:200[A]:GOL:HO1	1.57	0.52
1:F:83:ASP:OD1	1:F:95:LYS:HE3	2.09	0.52
1:I:69:ASN:ND2	1:I:77:MET:HE3	2.24	0.52
1:F:22:VAL:HG12	1:F:24:LEU:HD23	1.92	0.52
1:F:66:GLU:HB3	1:F:69:ASN:ND2	2.25	0.52
1:C:65:LYS:HE2	1:D:64:ARG:CZ	2.40	0.51
1:D:4:ALA:HA	1:D:30:LEU:HD13	1.92	0.51
1:I:6:VAL:HG11	1:I:25:LEU:HD13	1.92	0.51
1:A:46:VAL:CG2	1:A:77:MET:HE1	2.40	0.51
1:D:16:THR:HG22	1:D:19:LEU:HB2	1.93	0.51
1:J:7:LEU:HD22	1:J:28:GLN:HB2	1.91	0.51
1:F:46:VAL:HG12	1:F:46:VAL:O	2.09	0.51
1:A:25:LEU:HD12	1:A:45:ASP:HB2	1.92	0.51
1:I:59:ARG:N	1:J:75:ASP:OD1	2.40	0.51
1:E:47:VAL:O	1:E:47:VAL:HG12	2.09	0.51
1:B:5:LYS:HE3	1:B:52:ASN:HA	1.93	0.51
1:B:65:LYS:HG2	1:C:71:ASP:HA	1.93	0.50
1:D:66:GLU:HG3	1:E:16:THR:HG21	1.93	0.50
1:B:46:VAL:HG11	1:B:77:MET:HE2	1.93	0.50
2:G:203[A]:GOL:H32	1:I:61:SER:HG	1.76	0.50
1:C:84:THR:HG22	1:D:11:VAL:HB	1.93	0.50
1:H:35:GLN:HE21	1:H:35:GLN:CA	2.24	0.50
1:A:46:VAL:HG11	1:A:66[B]:GLU:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200[D]:GOL:HO1	1:D:61:SER:HG	1.58	0.50
1:J:9:THR:CG2	1:J:23:LYS:HZ1	2.25	0.50
1:A:22:VAL:HG12	1:A:24:LEU:HD23	1.94	0.50
1:A:31:ASP:OD1	1:A:31:ASP:C	2.50	0.49
1:G:33:LYS:O	1:G:35:GLN:NE2	2.45	0.49
1:E:72:ARG:HB2	1:E:74:LEU:HD12	1.93	0.49
1:A:23:LYS:HB3	3:A:121:HOH:O	2.13	0.49
1:C:74:LEU:HD13	1:C:77:MET:CE	2.42	0.49
1:D:6:VAL:HG13	1:D:25:LEU:HD22	1.94	0.49
1:F:74:LEU:HD23	1:J:1[B]:MET:CE	2.42	0.49
1:J:7:LEU:CD2	1:J:28:GLN:HB2	2.42	0.49
1:H:74:LEU:HD13	1:H:77:MET:CE	2.42	0.49
1:H:86:ASN:O	1:I:8:GLY:HA3	2.11	0.49
1:D:64:ARG:HD2	1:D:70:GLY:O	2.12	0.49
1:A:1[A]:MET:CE	1:A:1[A]:MET:H3	2.25	0.49
1:E:72:ARG:HD3	1:E:74:LEU:HD11	1.95	0.49
1:B:63:ALA:HB1	1:B:77:MET:HB2	1.95	0.49
1:B:92:LEU:CD1	1:B:92:LEU:C	2.80	0.49
1:A:56:LEU:CD2	1:A:82:ILE:HD11	2.42	0.48
1:B:46:VAL:O	1:B:46:VAL:HG22	2.13	0.48
1:H:74:LEU:CD1	1:H:77:MET:HE1	2.43	0.48
1:B:46:VAL:CG2	1:B:46:VAL:O	2.61	0.48
1:C:7:LEU:CD2	1:C:28:GLN:HB2	2.43	0.48
1:D:7:LEU:CD2	1:D:28:GLN:HB2	2.44	0.48
1:G:61:SER:HG	2:G:203[A]:GOL:HO1	1.60	0.48
1:D:27:VAL:O	1:D:27:VAL:HG23	2.14	0.48
2:B:200[C]:GOL:HO2	2:B:201:GOL:HO2	1.62	0.47
1:I:1:MET:HG3	3:J:112:HOH:O	2.13	0.47
1:F:19:LEU:HD22	1:J:79:VAL:HG22	1.96	0.47
1:E:41:GLU:OE1	1:E:41:GLU:HA	2.14	0.47
1:B:66:GLU:O	1:B:67:ARG:C	2.52	0.47
1:D:16:THR:HG21	1:D:73:PRO:HG3	1.96	0.47
1:H:19:LEU:HD13	1:H:73:PRO:HD2	1.95	0.47
1:F:81:ILE:HG13	1:G:14:SER:HB2	1.97	0.47
1:C:47:VAL:CG1	1:C:47:VAL:O	2.61	0.47
1:D:64:ARG:HB2	1:D:69:ASN:O	2.14	0.47
1:I:68:GLY:O	1:I:72:ARG:HD2	2.15	0.47
1:D:20:THR:O	1:D:72:ARG:NH2	2.47	0.47
1:F:24:LEU:HD22	1:J:1[A]:MET:CE	2.45	0.47
1:F:39:ARG:NH1	3:F:119:HOH:O	2.47	0.47
1:I:84:THR:CG2	1:I:94:ASN:HD22	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:LEU:HA	1:H:19:LEU:HD12	1.57	0.47
2:B:200[C]:GOL:HO1	1:E:61:SER:HG	1.63	0.46
1:H:72:ARG:HD2	1:H:74:LEU:HD11	1.98	0.46
1:C:92:LEU:O	1:C:92:LEU:HD22	2.15	0.46
1:F:3:LEU:HD22	1:F:82:ILE:CD1	2.46	0.46
1:B:46:VAL:HB	1:B:77:MET:CE	2.46	0.46
1:D:6:VAL:CG1	1:D:25:LEU:HD22	2.46	0.46
1:G:47:VAL:CG2	1:G:78:VAL:HG12	2.46	0.46
1:A:86:ASN:O	1:B:8:GLY:HA3	2.16	0.46
1:C:27:VAL:HG23	1:C:27:VAL:O	2.15	0.46
1:I:31:ASP:HB3	1:I:37:LEU:HD21	1.97	0.46
1:D:87:VAL:CG1	1:D:88:ALA:N	2.77	0.46
1:D:69:ASN:ND2	1:D:77:MET:CE	2.78	0.46
1:I:46:VAL:HG11	1:J:16:THR:HG21	1.98	0.46
1:D:69:ASN:ND2	1:D:77:MET:HE1	2.31	0.46
1:A:22:VAL:CG2	1:A:72:ARG:NE	2.79	0.46
1:E:18:ASN:O	1:E:72:ARG:HG2	2.15	0.46
1:A:46:VAL:O	1:A:46:VAL:HG12	2.16	0.45
1:E:30:LEU:HD12	1:E:36:PRO:HA	1.97	0.45
1:H:19:LEU:CD1	1:H:73:PRO:HG2	2.46	0.45
1:I:69:ASN:HA	1:I:72:ARG:CD	2.47	0.45
1:I:53:GLU:OE2	1:I:95:LYS:NZ	2.49	0.45
1:I:56:LEU:CD2	1:I:82:ILE:HD11	2.46	0.45
1:A:29:PHE:HD1	1:A:39:ARG:HB3	1.81	0.45
1:A:66[B]:GLU:HB3	1:A:69:ASN:HD22	1.82	0.45
1:A:67:ARG:HD3	1:A:67:ARG:C	2.36	0.45
1:F:13:THR:HG23	1:J:83:ASP:OD1	2.17	0.45
1:F:81:ILE:CG1	1:G:14:SER:HB2	2.47	0.45
1:H:19:LEU:CD1	1:H:73:PRO:CG	2.95	0.45
1:E:72:ARG:CD	1:E:74:LEU:HD11	2.47	0.45
1:E:7:LEU:HD22	1:E:28:GLN:HB2	1.99	0.45
1:B:66:GLU:HB2	1:B:69:ASN:ND2	2.32	0.45
1:C:3:LEU:CD2	1:C:82:ILE:HD13	2.45	0.45
2:G:203[E]:GOL:HO2	2:G:202:GOL:HO2	1.64	0.44
1:J:27:VAL:HG23	1:J:27:VAL:O	2.17	0.44
1:G:28:GLN:NE2	1:G:37:LEU:O	2.38	0.44
1:D:2:GLN:HG3	1:D:59:ARG:NH1	2.32	0.44
1:D:3:LEU:N	1:E:40:TYR:OH	2.41	0.44
1:A:7:LEU:CD2	1:A:28:GLN:HB2	2.47	0.44
1:E:3:LEU:HD22	1:E:82:ILE:CD1	2.48	0.44
2:G:203[B]:GOL:O2	2:G:202:GOL:O2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:LEU:CD1	1:F:45:ASP:HB2	2.48	0.44
1:F:81:ILE:O	1:F:81:ILE:HD12	2.18	0.44
1:H:29:PHE:CD1	1:H:39:ARG:HB3	2.52	0.44
1:G:9:THR:CG2	1:G:10:VAL:N	2.81	0.44
1:G:1:MET:HE1	1:H:24:LEU:HD22	2.00	0.44
1:A:22:VAL:HG21	1:A:72:ARG:CD	2.47	0.44
1:E:2:GLN:HG2	1:E:59:ARG:NH1	2.33	0.44
1:I:4:ALA:O	1:I:55:VAL:HG22	2.17	0.44
1:J:29:PHE:CD1	1:J:39:ARG:HG2	2.53	0.43
1:B:9:THR:CG2	1:B:10:VAL:N	2.81	0.43
1:C:87:VAL:HG12	1:C:89:SER:H	1.83	0.43
1:C:35:GLN:HA	1:C:36:PRO:HD3	1.86	0.43
1:I:16:THR:HG22	1:I:19:LEU:HG	2.00	0.43
1:F:19:LEU:HD13	1:F:73:PRO:HG2	2.01	0.43
1:I:46:VAL:CG1	1:J:16:THR:CG2	2.97	0.43
1:B:66:GLU:OE1	1:B:77:MET:CE	2.67	0.43
1:J:25:LEU:HD11	1:J:45:ASP:HB2	2.00	0.43
1:A:61:SER:HG	2:B:200[B]:GOL:C1	2.31	0.42
1:J:22:VAL:HG21	1:J:74:LEU:HD11	2.01	0.42
1:B:2:GLN:HG2	1:B:59:ARG:NH1	2.34	0.42
1:G:37:LEU:CD2	1:H:38:GLU:OE1	2.68	0.42
1:A:7:LEU:HD22	1:A:28:GLN:HB2	2.02	0.42
1:B:1[B]:MET:HE3	1:B:1[B]:MET:H3	1.84	0.42
1:A:46:VAL:CG1	1:A:46:VAL:O	2.68	0.42
1:C:74:LEU:HA	1:C:74:LEU:HD23	1.83	0.42
1:D:2:GLN:NE2	1:E:40:TYR:O	2.53	0.42
1:I:9:THR:HG22	1:I:10:VAL:N	2.35	0.42
1:A:22:VAL:HG23	1:A:72:ARG:NE	2.34	0.42
1:C:83:ASP:HA	1:C:95:LYS:HD2	2.01	0.42
1:F:65:LYS:HA	1:F:65:LYS:HE3	2.00	0.42
1:F:66:GLU:HB2	1:F:77[B]:MET:HE3	2.00	0.42
1:H:19:LEU:CD1	1:H:73:PRO:CD	2.96	0.42
1:F:81:ILE:HD12	1:F:81:ILE:C	2.40	0.42
1:C:86:ASN:O	1:D:8:GLY:HA3	2.19	0.42
1:G:56:LEU:HD23	1:G:82:ILE:HD11	2.01	0.42
1:A:1[A]:MET:HE2	1:B:75:ASP:OD2	2.20	0.41
1:C:3:LEU:HD22	1:C:82:ILE:CD1	2.47	0.41
1:F:7:LEU:CD2	1:F:28:GLN:HB2	2.50	0.41
1:E:9:THR:HG23	1:F:96:ARG:HG2	2.02	0.41
1:G:7:LEU:CD2	1:G:28:GLN:HB2	2.49	0.41
1:B:1[B]:MET:H1	1:B:1[B]:MET:CE	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:PRO:O	1:C:20:THR:OG1	2.36	0.41
1:F:47:VAL:HG11	1:F:81:ILE:HG23	2.02	0.41
1:D:87:VAL:O	1:F:96:ARG:C	2.59	0.41
1:H:19:LEU:HD11	1:H:73:PRO:CG	2.49	0.41
1:A:7:LEU:O	1:A:51:LEU:HD11	2.20	0.41
1:J:49:ALA:HA	1:J:81:ILE:HD11	2.03	0.41
1:A:18:ASN:O	1:A:72:ARG:HD3	2.21	0.41
1:E:25:LEU:CD1	1:E:45:ASP:HB2	2.50	0.41
1:G:46:VAL:HG13	1:H:16:THR:HG22	2.03	0.41
1:A:61:SER:HG	2:B:200[D]:GOL:H32	1.85	0.41
1:G:56:LEU:O	1:G:79:VAL:HG22	2.21	0.41
1:H:1:MET:HE3	1:I:24:LEU:HD22	2.02	0.40
1:I:19:LEU:CD2	1:I:73:PRO:HD2	2.51	0.40
1:I:92:LEU:O	1:I:92:LEU:HD22	2.20	0.40
1:E:65:LYS:HA	1:E:65:LYS:HD3	1.92	0.40
1:H:96:ARG:C	1:H:97:ASP:OD2	2.59	0.40
1:I:6:VAL:CG1	1:I:25:LEU:HD13	2.52	0.40
1:J:12:SER:O	1:J:15:LYS:HE2	2.21	0.40
1:J:39:ARG:NH1	1:J:41:GLU:OE2	2.54	0.40
1:C:66:GLU:O	1:C:67:ARG:C	2.60	0.40
1:F:83:ASP:OD2	1:G:13:THR:CG2	2.64	0.40
1:J:65:LYS:HD3	1:J:65:LYS:HA	1.95	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	95/111 (86%)	92 (97%)	2 (2%)	1 (1%)	14 20
1	B	94/111 (85%)	91 (97%)	3 (3%)	0	100 100
1	C	93/111 (84%)	91 (98%)	1 (1%)	1 (1%)	14 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	94/111 (85%)	91 (97%)	3 (3%)	0	100	100
1	E	94/111 (85%)	91 (97%)	2 (2%)	1 (1%)	14	20
1	F	95/111 (86%)	92 (97%)	2 (2%)	1 (1%)	14	20
1	G	94/111 (85%)	91 (97%)	3 (3%)	0	100	100
1	H	96/111 (86%)	91 (95%)	4 (4%)	1 (1%)	15	23
1	I	94/111 (85%)	92 (98%)	2 (2%)	0	100	100
1	J	94/111 (85%)	92 (98%)	2 (2%)	0	100	100
All	All	943/1110 (85%)	914 (97%)	24 (2%)	5 (0%)	29	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	67	ARG
1	F	67	ARG
1	H	67	ARG
1	A	67	ARG
1	E	67	ARG

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	79/88 (90%)	67 (85%)	12 (15%)	3	3
1	B	78/88 (89%)	70 (90%)	8 (10%)	7	10
1	C	77/88 (88%)	68 (88%)	9 (12%)	5	7
1	D	77/88 (88%)	72 (94%)	5 (6%)	17	27
1	E	77/88 (88%)	70 (91%)	7 (9%)	9	14
1	F	79/88 (90%)	69 (87%)	10 (13%)	4	5
1	G	77/88 (88%)	69 (90%)	8 (10%)	7	10
1	H	79/88 (90%)	67 (85%)	12 (15%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	77/88 (88%)	70 (91%)	7 (9%)	9	14
1	J	78/88 (89%)	67 (86%)	11 (14%)	3	4
All	All	778/880 (88%)	689 (89%)	89 (11%)	5	7

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1[A]	MET
1	A	1[B]	MET
1	A	9	THR
1	A	18	ASN
1	A	47	VAL
1	A	59	ARG
1	A	65	LYS
1	A	67	ARG
1	A	71	ASP
1	A	75	ASP
1	A	83	ASP
1	A	94	ASN
1	B	7	LEU
1	B	19	LEU
1	B	24	LEU
1	B	32	THR
1	B	35	GLN
1	B	46	VAL
1	B	84	THR
1	B	89	SER
1	C	13	THR
1	C	35	GLN
1	C	39	ARG
1	C	46	VAL
1	C	53	GLU
1	C	84	THR
1	C	87	VAL
1	C	89	SER
1	C	92	LEU
1	D	7	LEU
1	D	14	SER
1	D	16	THR
1	D	32	THR
1	D	65	LYS

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Mol	Chain	Res	Type
1	E	7	LEU
1	E	14	SER
1	E	16	THR
1	E	30	LEU
1	E	32	THR
1	E	46	VAL
1	E	59	ARG
1	F	7	LEU
1	F	16	THR
1	F	18	ASN
1	F	35	GLN
1	F	59	ARG
1	F	65	LYS
1	F	66	GLU
1	F	67	ARG
1	F	75	ASP
1	F	94	ASN
1	G	7	LEU
1	G	22	VAL
1	G	23	LYS
1	G	30	LEU
1	G	35	GLN
1	G	77	MET
1	G	83	ASP
1	G	92	LEU
1	H	9	THR
1	H	18	ASN
1	H	30	LEU
1	H	35	GLN
1	H	39	ARG
1	H	46	VAL
1	H	47	VAL
1	H	66	GLU
1	H	89	SER
1	H	92	LEU
1	H	96	ARG
1	H	97	ASP
1	I	7	LEU
1	I	32	THR
1	I	65	LYS
1	I	75	ASP
1	I	89	SER

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Mol	Chain	Res	Type
1	I	91	SER
1	I	92	LEU
1	J	7	LEU
1	J	14	SER
1	J	22	VAL
1	J	30	LEU
1	J	32	THR
1	J	39	ARG
1	J	46	VAL
1	J	66	GLU
1	J	75	ASP
1	J	89	SER
1	J	91	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	35	GLN
1	A	69	ASN
1	A	86	ASN
1	A	94	ASN
1	B	35	GLN
1	B	69	ASN
1	B	86	ASN
1	D	69	ASN
1	E	86	ASN
1	F	35	GLN
1	F	52	ASN
1	G	69	ASN
1	G	86	ASN
1	H	2	GLN
1	H	35	GLN
1	I	69	ASN
1	I	94	ASN
1	J	35	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	GOL	B	200[D]	-	5,5,5	0.44	0	5,5,5	0.68	0
2	GOL	B	200[E]	-	5,5,5	0.43	0	5,5,5	0.61	0
2	GOL	G	203[D]	-	5,5,5	0.49	0	5,5,5	0.78	0
2	GOL	G	203[E]	-	5,5,5	0.52	0	5,5,5	0.65	0
2	GOL	G	203[A]	-	5,5,5	0.51	0	5,5,5	0.65	0
2	GOL	G	202	-	5,5,5	0.70	0	5,5,5	1.09	0
2	GOL	G	203[B]	-	5,5,5	0.93	0	5,5,5	0.52	0
2	GOL	G	203[C]	-	5,5,5	0.48	0	5,5,5	0.76	0
2	GOL	B	200[A]	-	5,5,5	0.43	0	5,5,5	0.57	0
2	GOL	B	201	-	5,5,5	0.47	0	5,5,5	0.71	0
2	GOL	B	200[B]	-	5,5,5	0.49	0	5,5,5	0.56	0
2	GOL	B	200[C]	-	5,5,5	0.42	0	5,5,5	0.61	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	200[D]	-	-	0/4/4/4	-
2	GOL	B	200[E]	-	-	0/4/4/4	-
2	GOL	G	203[D]	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	G	203[E]	-	-	0/4/4/4	-
2	GOL	G	203[A]	-	-	0/4/4/4	-
2	GOL	G	202	-	-	3/4/4/4	-
2	GOL	G	203[B]	-	-	0/4/4/4	-
2	GOL	G	203[C]	-	-	0/4/4/4	-
2	GOL	B	200[A]	-	-	0/4/4/4	-
2	GOL	B	201	-	-	4/4/4/4	-
2	GOL	B	200[B]	-	-	0/4/4/4	-
2	GOL	B	200[C]	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	202	GOL	O1-C1-C2-C3
2	G	202	GOL	C1-C2-C3-O3
2	B	201	GOL	O1-C1-C2-C3
2	B	201	GOL	C1-C2-C3-O3
2	G	202	GOL	O2-C2-C3-O3
2	B	201	GOL	O1-C1-C2-O2
2	G	203[D]	GOL	C1-C2-C3-O3
2	B	201	GOL	O2-C2-C3-O3

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	200[D]	GOL	2	0
2	G	203[D]	GOL	1	0
2	G	203[E]	GOL	1	0
2	G	203[A]	GOL	3	0
2	G	202	GOL	4	0
2	G	203[B]	GOL	2	0
2	G	203[C]	GOL	3	0
2	B	200[A]	GOL	2	0
2	B	201	GOL	3	0
2	B	200[B]	GOL	3	0
2	B	200[C]	GOL	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	96/111 (86%)	0.36	7 (7%) 15 13	21, 29, 47, 55	0
1	B	96/111 (86%)	0.39	5 (5%) 27 26	21, 29, 47, 55	0
1	C	95/111 (85%)	0.43	10 (10%) 6 5	21, 29, 48, 53	0
1	D	96/111 (86%)	0.36	4 (4%) 36 35	21, 30, 48, 55	0
1	E	96/111 (86%)	0.45	7 (7%) 15 13	21, 29, 49, 54	0
1	F	96/111 (86%)	0.64	10 (10%) 6 6	21, 30, 49, 58	0
1	G	96/111 (86%)	0.28	2 (2%) 63 61	21, 29, 49, 56	0
1	H	98/111 (88%)	0.17	4 (4%) 37 36	20, 30, 49, 65	0
1	I	96/111 (86%)	0.08	3 (3%) 49 47	20, 30, 47, 56	0
1	J	96/111 (86%)	0.55	6 (6%) 20 18	19, 30, 48, 54	0
All	All	961/1110 (86%)	0.37	58 (6%) 21 20	19, 29, 49, 65	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	90	GLY	5.9
1	B	88	ALA	5.5
1	F	94	ASN	5.4
1	J	67	ARG	5.1
1	J	88	ALA	5.0
1	F	89	SER	5.0
1	F	88	ALA	4.8
1	A	67	ARG	4.6
1	E	67	ARG	4.5
1	D	89	SER	4.4
1	D	67	ARG	4.3
1	C	95	LYS	4.1
1	B	67	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	67	ARG	3.5
1	B	1[A]	MET	3.5
1	I	67	ARG	3.4
1	D	94	ASN	3.2
1	H	98	ASP	3.2
1	F	96	ARG	3.2
1	A	1[A]	MET	3.1
1	F	1[A]	MET	3.1
1	F	95	LYS	3.1
1	E	88	ALA	3.1
1	F	67	ARG	3.0
1	A	90	GLY	3.0
1	A	96	ARG	2.9
1	C	1[A]	MET	2.9
1	A	89	SER	2.9
1	C	71	ASP	2.8
1	A	88	ALA	2.8
1	H	97	ASP	2.8
1	J	70	GLY	2.8
1	C	67	ARG	2.7
1	D	1	MET	2.7
1	J	21	GLY	2.7
1	I	94	ASN	2.7
1	J	89	SER	2.7
1	E	95	LYS	2.7
1	A	57	VAL	2.6
1	C	89	SER	2.6
1	C	88	ALA	2.5
1	B	89	SER	2.5
1	I	89	SER	2.5
1	E	13	THR	2.4
1	G	71	ASP	2.3
1	C	93	TYR	2.3
1	J	94	ASN	2.3
1	B	43	ALA	2.3
1	F	87	VAL	2.3
1	C	94	ASN	2.3
1	C	79	VAL	2.2
1	E	96	ARG	2.2
1	E	39	ARG	2.2
1	F	4	ALA	2.2
1	C	92	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	42	VAL	2.1
1	E	21	GLY	2.1
1	H	21	GLY	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	B	201	6/6	0.66	0.22	36,42,48,54	0
2	GOL	G	202	6/6	0.77	0.18	37,40,43,50	0
2	GOL	B	200[D]	6/6	0.86	0.39	25,25,25,25	6
2	GOL	B	200[A]	6/6	0.86	0.39	25,25,25,25	6
2	GOL	B	200[E]	6/6	0.86	0.39	25,25,25,25	6
2	GOL	B	200[B]	6/6	0.86	0.39	25,25,25,25	6
2	GOL	B	200[C]	6/6	0.86	0.39	25,25,25,25	6
2	GOL	G	203[C]	6/6	0.87	0.42	24,25,25,25	6
2	GOL	G	203[E]	6/6	0.87	0.42	24,25,25,25	6
2	GOL	G	203[A]	6/6	0.87	0.42	24,25,25,25	6
2	GOL	G	203[D]	6/6	0.87	0.42	24,25,25,25	6
2	GOL	G	203[B]	6/6	0.87	0.42	24,25,25,25	6

6.5 Other polymers [i](#)

There are no such residues in this entry.