Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 12:48 AM EDT

PDB ID	:	3JQJ
Title	:	Crystal structure of the molybdenum cofactor biosynthesis protein C (TTHA1789) from Thermus Theromophilus HB8
Authors	:	Kanaujia, S.P.; Jeyakanthan, J.; Nakagawa, N.; Sekar, K.; Baba, S.; Ebihara, A.; Kuramitsu, S.; Shinkai, A.; Shiro, Y.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2009-09-07
Resolution	:	1.90 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

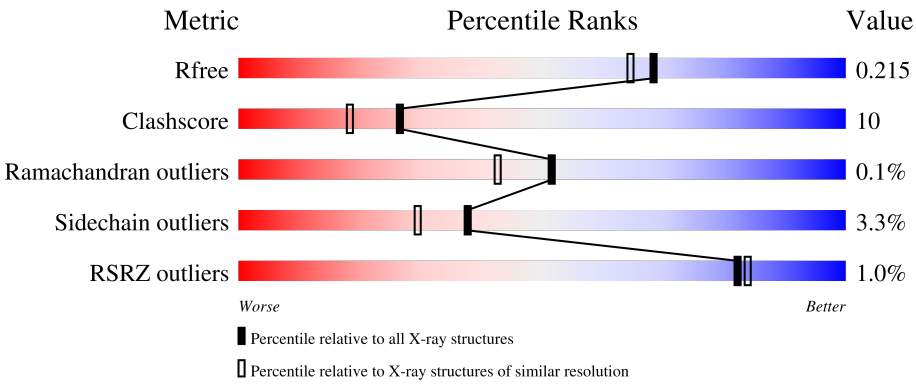
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	157	.% 73% 18% • 6%
1	B	157	2% 77% 17% • 5%
1	C	157	3% 71% 21% • 6%
1	D	157	3% 76% 16% • 6%

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Mol	Chain	Length	Quality of chain
1	E	157	% 71% 23% 6%
1	F	157	70% 22% 6%
1	G	157	81% 11% 6%
1	H	157	% 78% 13% 6%
1	I	157	74% 17% 6%
1	J	157	78% 13% 6%
1	K	157	72% 20% 6%
1	L	157	% 79% 14% 6%

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	PO4	A	161	-	X	-	-
2	PO4	B	162	-	X	-	-
2	PO4	C	163	-	X	-	-
2	PO4	D	164	-	X	-	-
2	PO4	E	165	-	X	-	-
2	PO4	F	166	-	X	-	-
2	PO4	G	167	-	X	-	-
2	PO4	H	168	-	X	-	-
2	PO4	H	171	-	X	-	-
2	PO4	I	169	-	X	-	-
2	PO4	J	170	-	X	-	-
2	PO4	L	172	-	X	-	-
4	GOL	C	333	-	-	X	-

2 Entry composition (i)

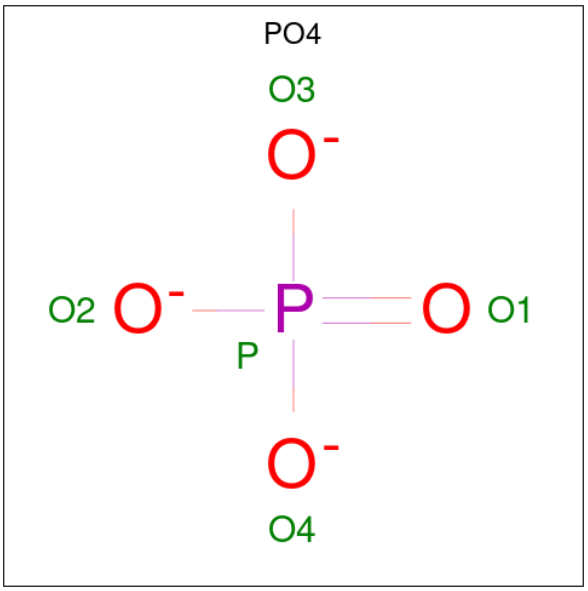
There are 5 unique types of molecules in this entry. The entry contains 14581 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Molybdenum cofactor biosynthesis protein C.

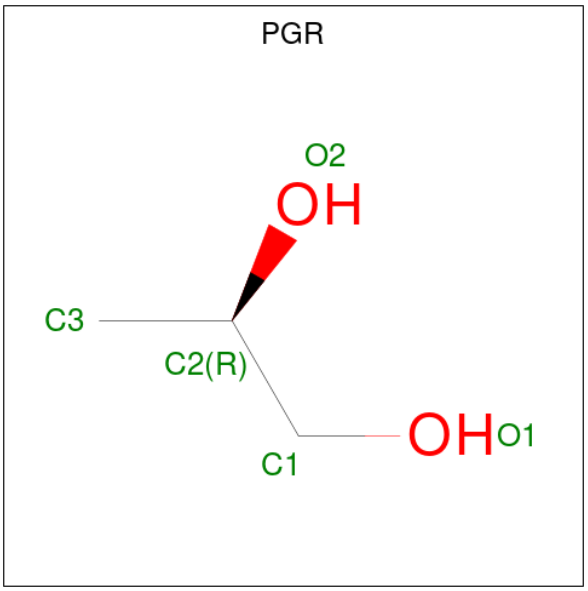
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	147	1096	692	194	204	6	0	0	0
1	B	149	1114	702	197	209	6	0	0	0
1	C	147	1096	692	194	204	6	0	0	0
1	D	147	1096	692	194	204	6	0	0	0
1	E	148	1105	697	195	207	6	0	0	0
1	F	147	1101	695	194	206	6	0	0	0
1	G	147	1096	692	194	204	6	0	0	0
1	H	148	1110	700	196	208	6	0	0	0
1	I	147	1101	695	194	206	6	0	0	0
1	J	147	1101	695	194	206	6	0	0	0
1	K	147	1101	695	194	206	6	0	0	0
1	L	147	1101	695	194	206	6	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



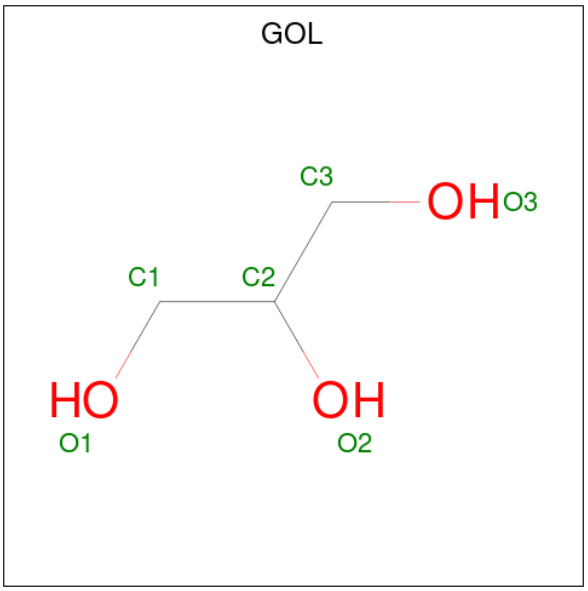
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	G	1	5	4	1	0	0
2	H	1	5	4	1	0	0
2	H	1	5	4	1	0	0
2	I	1	5	4	1	0	0
2	J	1	5	4	1	0	0
2	L	1	5	4	1	0	0

- Molecule 3 is R-1,2-PROPANEDIOL (three-letter code: PGR) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	5	3	2	0	0
3	C	1	5	3	2	0	0
3	D	1	5	3	2	0	0
3	E	1	5	3	2	0	0
3	F	1	5	3	2	0	0
3	G	1	5	3	2	0	0
3	I	1	5	3	2	0	0
3	K	1	5	3	2	0	0
3	K	1	5	3	2	0	0
3	L	1	5	3	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

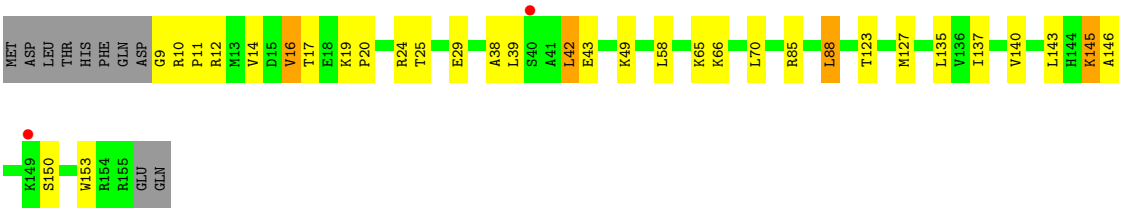
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	92	92	92	0	0
			Total	O		
5	B	94	94	94	0	0
			Total	O		
5	C	88	88	88	0	0
			Total	O		
5	D	97	97	97	0	0
			Total	O		
5	E	75	75	75	0	0
			Total	O		
5	F	83	83	83	0	0
			Total	O		
5	G	110	110	110	0	0
			Total	O		
5	H	111	111	111	0	0
			Total	O		
5	I	110	110	110	0	0
			Total	O		
5	J	114	114	114	0	0
			Total	O		
5	K	94	94	94	0	0
			Total	O		
5	L	113	113	113	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

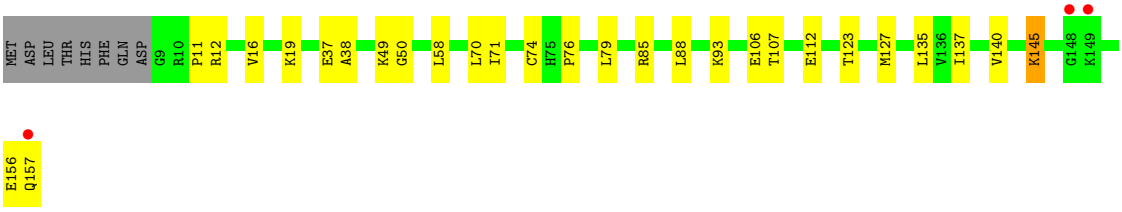
• Molecule 1: Molybdenum cofactor biosynthesis protein C

Chain A:



• Molecule 1: Molybdenum cofactor biosynthesis protein C

Chain B:

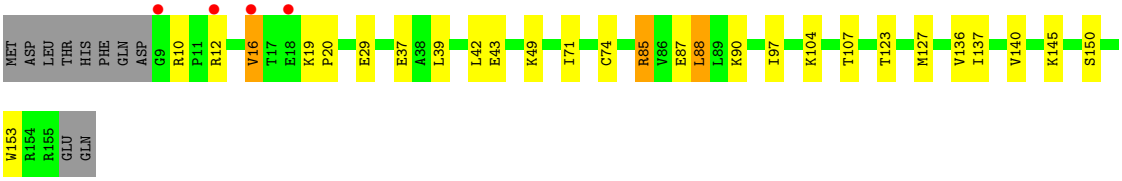


• Molecule 1: Molybdenum cofactor biosynthesis protein C

Chain C:

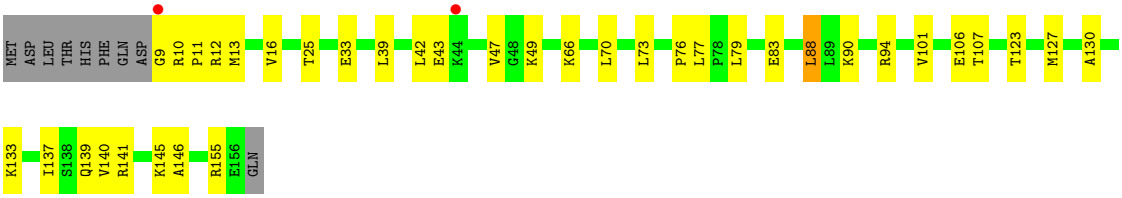
• Molecule 1: Molybdenum cofactor biosynthesis protein C

Chain D:



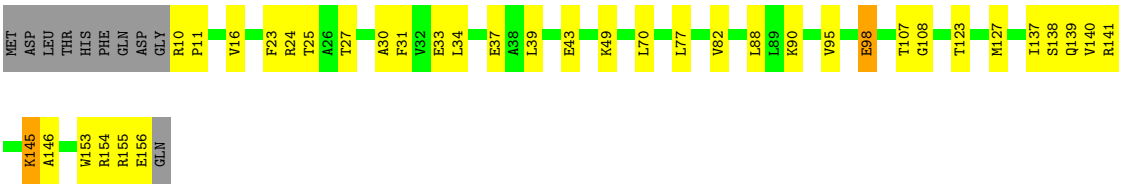
• Molecule 1: Molybdenum cofactor biosynthesis protein C

Chain E:



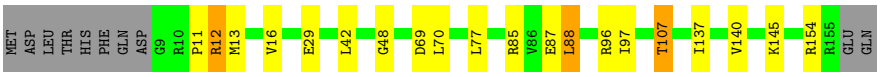
• Molecule 1: Molybdenum cofactor biosynthesis protein C

Chain F:



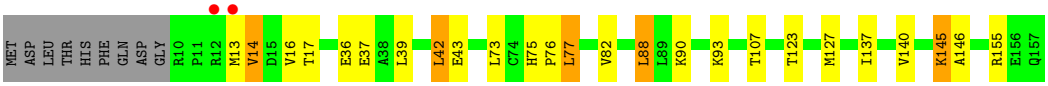
• Molecule 1: Molybdenum cofactor biosynthesis protein C

Chain G:



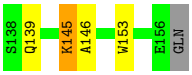
• Molecule 1: Molybdenum cofactor biosynthesis protein C

Chain H:



• Molecule 1: Molybdenum cofactor biosynthesis protein C

Chain I:

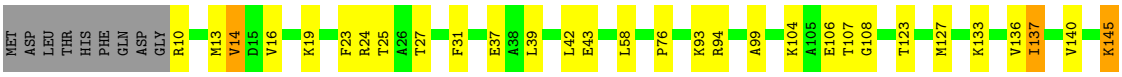


• Molecule 1: Molybdenum cofactor biosynthesis protein C

Chain J:

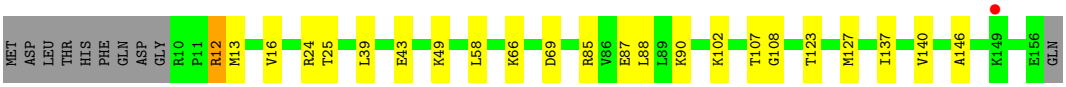
• Molecule 1: Molybdenum cofactor biosynthesis protein C

Chain K:



• Molecule 1: Molybdenum cofactor biosynthesis protein C

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.81Å 109.84Å 115.19Å 90.00° 104.86° 90.00°	Depositor
Resolution (Å)	49.66 – 1.90 49.66 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.66-1.90) 98.7 (49.66-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	4.61 (at 1.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.188 , 0.219 0.186 , 0.215	Depositor DCC
R_{free} test set	6078 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14581	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.47 % 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 2.6183e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PGR, PO4, 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	0.28	0/1108	0.62	0/1495
1	B	0.29	0/1126	0.63	0/1519
1	C	0.29	0/1108	0.62	0/1495
1	D	0.29	0/1108	0.63	0/1495
1	E	0.28	0/1117	0.61	0/1507
1	F	0.28	0/1113	0.60	0/1502
1	G	0.30	0/1108	0.62	0/1495
1	H	0.30	0/1122	0.64	0/1514
1	I	0.31	0/1113	0.66	1/1502 (0.1%)
1	J	0.30	0/1113	0.63	0/1502
1	K	0.30	0/1113	0.63	1/1502 (0.1%)
1	L	0.30	0/1113	0.66	0/1502
All	All	0.29	0/13362	0.63	2/18030 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	137	ILE	N-CA-C	-5.30	96.70	111.00
1	K	137	ILE	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1096	0	1166	33	0
1	B	1114	0	1180	25	0
1	C	1096	0	1166	30	0
1	D	1096	0	1166	32	0
1	E	1105	0	1172	33	0
1	F	1101	0	1169	31	0
1	G	1096	0	1166	19	0
1	H	1110	0	1177	21	0
1	I	1101	0	1169	36	0
1	J	1101	0	1169	29	0
1	K	1101	0	1169	30	0
1	L	1101	0	1169	24	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	L	5	0	0	0	0
3	A	5	0	8	0	0
3	C	5	0	8	0	0
3	D	5	0	8	0	0
3	E	5	0	8	0	0
3	F	5	0	8	0	0
3	G	5	0	8	3	0
3	I	5	0	8	0	0
3	K	10	0	16	0	0
3	L	5	0	8	0	0
4	A	6	0	8	2	0
4	B	6	0	8	0	0
4	C	6	0	8	4	0
4	D	6	0	8	1	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
4	G	6	0	8	0	0
4	H	6	0	8	0	0
4	I	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	6	0	8	3	0
4	K	6	0	8	1	0
4	L	6	0	8	1	0
5	A	92	0	0	2	0
5	B	94	0	0	0	0
5	C	88	0	0	3	0
5	D	97	0	0	2	0
5	E	75	0	0	3	0
5	F	83	0	0	4	0
5	G	110	0	0	2	0
5	H	111	0	0	0	0
5	I	110	0	0	4	0
5	J	114	0	0	1	0
5	K	94	0	0	3	0
5	L	113	0	0	4	0
All	All	14581	0	14214	283	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 10.

All (283) 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:I:133:LYS:HE2	1:J:145:LYS:HE2	1.45	0.98
1:A:16:VAL:HG22	1:A:19:LYS:HD2	1.55	0.88
1:I:85:ARG:HH21	1:I:85:ARG:HB3	1.38	0.87
1:J:24:ARG:HH22	4:J:340:GOL:H32	1.37	0.87
1:H:16:VAL:HG11	1:H:107:THR:CG2	2.09	0.83
1:K:31:PHE:CD2	1:K:94:ARG:HD3	2.13	0.82
1:A:17:THR:O	1:D:104:LYS:HE2	1.81	0.80
1:D:16:VAL:HG21	1:D:107:THR:HG23	1.63	0.79
1:D:16:VAL:HG23	1:D:19:LYS:HD2	1.65	0.77
1:I:85:ARG:HB3	1:I:85:ARG:NH2	2.00	0.76
1:K:16:VAL:HG11	1:K:107:THR:CG2	2.16	0.75
1:A:85:ARG:HG2	1:E:10:ARG:NH1	2.05	0.72
1:L:16:VAL:HG11	1:L:107:THR:HG23	1.72	0.72
1:L:69:ASP:HB2	5:L:1508:HOH:O	1.88	0.72
1:H:16:VAL:HG11	1:H:107:THR:HG23	1.70	0.71
1:H:82:VAL:HG23	1:L:13:MET:HE1	1.75	0.69
1:D:90:LYS:HB2	1:D:90:LYS:NZ	2.07	0.68
1:A:85:ARG:HH11	1:E:10:ARG:NH1	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:ARG:HH12	4:J:340:GOL:H11	1.58	0.68
1:J:43:GLU:OE2	1:J:90:LYS:HE2	1.94	0.68
1:F:39:LEU:O	1:F:43:GLU:HG3	1.94	0.67
1:G:77:LEU:H	3:G:187:PGR:H31	1.60	0.67
1:L:12:ARG:HG3	1:L:12:ARG:HH11	1.60	0.66
1:D:19:LYS:HB3	5:D:1002:HOH:O	1.95	0.65
1:K:39:LEU:O	1:K:43:GLU:HG3	1.97	0.65
1:I:16:VAL:HG11	1:I:107:THR:CG2	2.26	0.65
1:G:145:LYS:HE3	5:G:1030:HOH:O	1.97	0.64
1:E:47:VAL:HG21	1:E:130:ALA:HB3	1.80	0.64
1:H:145:LYS:HE2	1:K:133:LYS:HE2	1.79	0.63
1:H:42:LEU:HD13	1:H:88:LEU:HG	1.79	0.63
1:L:24:ARG:HH12	4:L:342:GOL:H32	1.63	0.63
1:B:85:ARG:HD3	1:F:10:ARG:NH1	2.15	0.62
1:K:23:PHE:CE1	1:K:104:LYS:HE2	2.35	0.62
1:J:139:GLN:HE21	1:J:141:ARG:HH11	1.47	0.62
1:G:16:VAL:HG11	1:G:107:THR:HG23	1.83	0.61
1:K:31:PHE:HD2	1:K:94:ARG:HD3	1.64	0.60
1:G:12:ARG:HG2	1:G:12:ARG:HH11	1.66	0.60
1:D:145:LYS:HG3	1:D:153:TRP:HB3	1.83	0.60
1:I:31:PHE:HB3	1:I:94:ARG:HD2	1.83	0.60
1:E:77:LEU:O	1:E:77:LEU:HD12	2.02	0.60
1:A:24:ARG:HH12	4:A:331:GOL:H32	1.66	0.60
1:B:140:VAL:HB	1:E:137:ILE:HB	1.82	0.60
1:D:20:PRO:HB3	1:I:23:PHE:CG	2.36	0.59
1:K:156:GLU:CD	1:K:156:GLU:H	2.06	0.59
1:L:39:LEU:O	1:L:43:GLU:HG3	2.02	0.59
1:C:133:LYS:HD3	1:D:145:LYS:HD3	1.83	0.59
1:G:48:GLY:O	1:L:12:ARG:HD3	2.03	0.59
1:J:16:VAL:HG11	1:J:107:THR:CG2	2.32	0.58
1:A:140:VAL:HB	1:F:137:ILE:HB	1.84	0.58
1:D:90:LYS:HB2	1:D:90:LYS:HZ2	1.67	0.58
1:D:16:VAL:CG2	1:D:19:LYS:HD2	2.32	0.58
1:B:19:LYS:HE2	1:B:106:GLU:O	2.03	0.57
1:I:37:GLU:HG3	5:I:1068:HOH:O	2.03	0.57
1:G:140:VAL:HB	1:L:137:ILE:HB	1.84	0.57
1:L:16:VAL:HG11	1:L:107:THR:CG2	2.33	0.57
1:A:16:VAL:CG2	1:A:19:LYS:HD2	2.32	0.57
1:I:85:ARG:HH21	1:I:85:ARG:CB	2.13	0.57
1:D:39:LEU:O	1:D:43:GLU:HG3	2.05	0.56
1:K:148:GLY:HA3	4:K:341:GOL:H2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:VAL:HG11	1:C:107:THR:HG22	1.88	0.56
1:L:85:ARG:HH21	1:L:87:GLU:CD	2.10	0.56
1:F:25:THR:HG22	1:F:146:ALA:HB3	1.87	0.56
1:I:16:VAL:HG21	1:I:107:THR:HG23	1.87	0.55
1:F:156:GLU:HG3	5:F:650:HOH:O	2.06	0.55
1:I:139:GLN:HA	1:J:137:ILE:O	2.07	0.55
1:K:24:ARG:HD3	1:K:108:GLY:HA2	1.89	0.55
1:C:16:VAL:HG11	1:C:107:THR:CG2	2.36	0.55
1:C:140:VAL:HB	1:D:137:ILE:HB	1.89	0.55
1:A:20:PRO:HG3	1:I:18:GLU:HB3	1.87	0.54
1:G:87:GLU:OE1	1:G:96:ARG:NH2	2.41	0.54
1:A:65:LYS:HD3	1:E:13:MET:CE	2.37	0.54
1:E:33:GLU:OE1	1:E:94:ARG:HG2	2.07	0.54
1:B:38:ALA:HB2	1:B:135:LEU:HD21	1.90	0.54
1:A:25:THR:HG22	1:A:146:ALA:HB3	1.90	0.53
1:B:123:THR:O	1:B:127:MET:HG2	2.08	0.53
1:C:44:LYS:HB3	5:C:1398:HOH:O	2.07	0.53
1:H:17:THR:HG21	1:I:23:PHE:CE1	2.44	0.53
1:J:39:LEU:O	1:J:43:GLU:HG3	2.09	0.53
1:H:17:THR:HG21	1:I:23:PHE:HE1	1.74	0.52
1:A:42:LEU:HD13	1:A:88:LEU:HG	1.91	0.52
1:H:145:LYS:HD2	1:H:145:LYS:C	2.29	0.52
1:J:123:THR:O	1:J:127:MET:HG2	2.09	0.52
1:L:43:GLU:OE2	1:L:90:LYS:HE3	2.10	0.52
1:G:16:VAL:HG11	1:G:107:THR:CG2	2.39	0.52
1:C:148:GLY:HA3	4:C:333:GOL:H32	1.92	0.52
1:I:16:VAL:HG11	1:I:107:THR:HG22	1.91	0.52
1:K:25:THR:HG22	1:K:146:ALA:HB3	1.92	0.51
1:E:88:LEU:HD22	1:E:90:LYS:N	2.24	0.51
1:E:16:VAL:HG11	1:E:107:THR:CG2	2.41	0.51
1:F:145:LYS:HG3	1:F:153:TRP:HB3	1.92	0.51
1:K:37:GLU:OE1	1:K:37:GLU:N	2.44	0.51
1:B:145:LYS:C	1:B:145:LYS:HD2	2.31	0.51
5:I:1185:HOH:O	1:J:77:LEU:HD11	2.10	0.51
1:C:137:ILE:HB	1:D:140:VAL:HB	1.92	0.51
1:B:11:PRO:HA	1:E:49:LYS:O	2.11	0.51
1:E:39:LEU:O	1:E:43:GLU:HG3	2.11	0.51
1:D:16:VAL:HG22	1:D:19:LYS:HB2	1.92	0.50
1:K:93:LYS:HD2	5:K:908:HOH:O	2.11	0.50
1:K:156:GLU:CD	1:K:156:GLU:N	2.64	0.50
1:C:93:LYS:HD3	5:C:1397:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ARG:HG2	1:B:12:ARG:HH11	1.77	0.50
1:H:43:GLU:OE2	1:H:90:LYS:HE2	2.11	0.50
1:H:13:MET:O	1:H:14:VAL:C	2.50	0.50
1:C:129:LYS:NZ	1:C:129:LYS:HB3	2.27	0.49
1:D:37:GLU:CD	1:D:37:GLU:H	2.16	0.49
1:A:70:LEU:HD11	1:F:70:LEU:HD21	1.93	0.49
1:B:137:ILE:HB	1:E:140:VAL:HB	1.95	0.49
5:D:974:HOH:O	1:E:66:LYS:HD3	2.13	0.49
1:E:9:GLY:HA3	5:E:1380:HOH:O	2.13	0.49
1:H:137:ILE:HB	1:K:140:VAL:HB	1.94	0.49
1:H:36:GLU:OE2	1:H:93:LYS:HE3	2.12	0.49
1:H:145:LYS:HD2	1:H:146:ALA:N	2.28	0.49
1:G:11:PRO:HA	1:L:49:LYS:O	2.13	0.49
1:I:137:ILE:HB	1:J:140:VAL:HB	1.93	0.49
1:L:107:THR:HG22	5:L:1444:HOH:O	2.12	0.49
1:B:70:LEU:HA	1:E:66:LYS:NZ	2.28	0.49
1:B:79:LEU:HD21	1:B:112:GLU:HG2	1.95	0.49
1:A:16:VAL:HG13	1:A:16:VAL:O	2.12	0.49
1:A:137:ILE:HB	1:F:140:VAL:HB	1.95	0.49
1:E:47:VAL:HG22	1:E:47:VAL:O	2.13	0.49
1:J:42:LEU:HD13	1:J:88:LEU:HG	1.94	0.49
1:A:145:LYS:HG3	1:A:153:TRP:HB3	1.94	0.48
1:F:123:THR:O	1:F:127:MET:HG2	2.13	0.48
1:J:37:GLU:H	1:J:37:GLU:CD	2.17	0.48
1:B:85:ARG:HG3	1:B:85:ARG:HH11	1.78	0.48
1:E:141:ARG:HB2	1:E:155:ARG:NH2	2.28	0.48
1:J:139:GLN:HE21	1:J:141:ARG:NH1	2.11	0.48
1:L:24:ARG:HD3	1:L:108:GLY:HA2	1.95	0.48
1:A:39:LEU:O	1:A:43:GLU:HG3	2.14	0.48
1:B:49:LYS:O	1:E:11:PRO:HA	2.13	0.48
1:E:139:GLN:HE22	1:E:141:ARG:HH11	1.61	0.48
1:I:145:LYS:HD2	1:I:145:LYS:C	2.34	0.48
4:C:333:GOL:H11	5:C:518:HOH:O	2.14	0.48
1:B:127:MET:SD	1:E:73:LEU:HD12	2.54	0.48
1:I:106:GLU:OE1	1:I:106:GLU:N	2.47	0.48
1:A:29:GLU:OE2	1:A:143:LEU:HD21	2.13	0.48
1:D:123:THR:O	1:D:127:MET:HG2	2.13	0.48
5:G:1164:HOH:O	1:K:76:PRO:HB2	2.14	0.48
1:C:150:SER:OG	4:C:333:GOL:H12	2.14	0.48
1:L:12:ARG:O	1:L:12:ARG:HG2	2.13	0.47
1:G:77:LEU:N	3:G:187:PGR:H31	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49:LYS:O	1:J:11:PRO:HA	2.15	0.47
1:L:12:ARG:HG3	1:L:12:ARG:NH1	2.29	0.47
1:E:123:THR:O	1:E:127:MET:HG2	2.14	0.47
1:I:11:PRO:HA	1:J:49:LYS:O	2.15	0.47
1:A:65:LYS:HD2	1:E:76:PRO:HG3	1.97	0.47
1:B:16:VAL:HG21	1:B:107:THR:HG23	1.95	0.47
1:C:17:THR:HG21	1:F:23:PHE:CE1	2.50	0.47
1:C:34:LEU:HD11	1:C:95:VAL:HG23	1.96	0.47
1:A:85:ARG:HD2	5:E:1518:HOH:O	2.14	0.47
1:F:16:VAL:HG11	1:F:107:THR:CG2	2.44	0.47
1:F:31:PHE:HB2	1:F:138:SER:OG	2.15	0.47
1:F:37:GLU:OE1	1:F:37:GLU:N	2.42	0.47
1:J:35:THR:HB	1:J:37:GLU:OE2	2.14	0.47
1:C:101:VAL:HG21	1:C:112:GLU:HB3	1.97	0.47
1:C:11:PRO:HA	1:D:49:LYS:O	2.15	0.47
1:A:66:LYS:HD3	5:F:1361:HOH:O	2.15	0.47
1:F:156:GLU:HG2	5:F:1523:HOH:O	2.14	0.47
1:K:19:LYS:HE2	1:K:149:LYS:NZ	2.30	0.47
1:F:30:ALA:HA	1:F:139:GLN:O	2.15	0.46
1:K:149:LYS:HB2	5:K:904:HOH:O	2.14	0.46
1:B:70:LEU:HA	1:E:66:LYS:HZ1	1.81	0.46
1:E:47:VAL:HG21	1:E:130:ALA:CB	2.44	0.46
1:G:13:MET:CE	1:J:65:LYS:HD3	2.44	0.46
1:H:73:LEU:HD12	1:K:127:MET:SD	2.56	0.46
1:A:11:PRO:HA	1:F:49:LYS:O	2.15	0.46
1:C:29:GLU:OE2	1:C:143:LEU:HD21	2.15	0.46
1:E:133:LYS:HD2	5:E:1009:HOH:O	2.16	0.46
1:I:123:THR:O	1:I:127:MET:HG2	2.16	0.46
1:A:9:GLY:N	5:A:1018:HOH:O	2.48	0.46
1:A:20:PRO:HB3	1:I:18:GLU:O	2.14	0.46
1:K:123:THR:O	1:K:127:MET:HG2	2.16	0.46
1:C:145:LYS:HG3	1:C:153:TRP:HB3	1.97	0.46
1:D:20:PRO:HB3	1:I:23:PHE:CB	2.46	0.46
1:A:10:ARG:HH11	1:D:85:ARG:CZ	2.29	0.46
1:F:24:ARG:HD3	1:F:108:GLY:HA2	1.98	0.46
1:H:123:THR:O	1:H:127:MET:HG2	2.15	0.46
1:A:137:ILE:O	1:F:139:GLN:HA	2.16	0.46
1:I:133:LYS:HE3	5:I:1490:HOH:O	2.16	0.46
1:L:25:THR:HG22	1:L:146:ALA:HB3	1.98	0.45
1:A:85:ARG:HH11	1:E:10:ARG:HH11	1.59	0.45
1:C:71:ILE:HB	1:C:74:CYS:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:VAL:HB	1:K:137:ILE:HB	1.99	0.45
1:D:10:ARG:NH1	1:D:12:ARG:HH21	2.15	0.45
1:C:139:GLN:HA	1:D:137:ILE:O	2.17	0.45
1:A:123:THR:O	1:A:127:MET:HG2	2.17	0.45
1:C:13:MET:HB2	1:F:82:VAL:HB	1.99	0.45
1:C:37:GLU:HG2	1:C:132:SER:HG	1.82	0.45
1:D:16:VAL:HG21	1:D:107:THR:CG2	2.41	0.45
1:F:154:ARG:NH2	1:F:154:ARG:HB3	2.32	0.45
1:G:29:GLU:HA	1:G:97:ILE:O	2.17	0.45
1:I:133:LYS:HB2	1:I:133:LYS:NZ	2.32	0.45
1:K:10:ARG:N	5:K:741:HOH:O	2.49	0.45
1:H:77:LEU:H	1:H:77:LEU:HD12	1.82	0.44
1:B:38:ALA:CB	1:B:135:LEU:HD21	2.47	0.44
1:J:139:GLN:NE2	1:J:141:ARG:HH11	2.14	0.44
1:G:77:LEU:H	3:G:187:PGR:C3	2.29	0.44
1:F:141:ARG:HD2	1:F:155:ARG:NE	2.32	0.44
1:I:102:LYS:HE2	5:I:784:HOH:O	2.16	0.44
1:A:12:ARG:HG2	1:A:12:ARG:HH11	1.83	0.44
1:H:39:LEU:O	1:H:43:GLU:HG3	2.18	0.44
1:B:137:ILE:O	1:E:139:GLN:HA	2.18	0.44
1:D:16:VAL:HG13	1:D:16:VAL:O	2.17	0.44
1:E:106:GLU:OE1	1:E:106:GLU:N	2.48	0.43
1:G:137:ILE:HB	1:L:140:VAL:HB	1.99	0.43
1:H:37:GLU:H	1:H:37:GLU:CD	2.21	0.43
1:G:70:LEU:HD23	1:L:66:LYS:HD2	2.00	0.43
1:I:73:LEU:HD12	1:J:127:MET:SD	2.57	0.43
1:A:14:VAL:HG23	1:F:49:LYS:HG2	2.00	0.43
1:G:42:LEU:CD2	1:G:88:LEU:HG	2.48	0.43
1:A:145:LYS:HD2	1:A:145:LYS:C	2.37	0.43
1:D:12:ARG:O	1:D:12:ARG:HG3	2.18	0.43
1:C:73:LEU:HD12	1:D:127:MET:SD	2.58	0.43
1:D:150:SER:H	4:D:334:GOL:H12	1.83	0.43
1:E:25:THR:HG22	1:E:146:ALA:HB3	2.01	0.43
1:D:71:ILE:HB	1:D:74:CYS:HB2	2.01	0.43
1:E:79:LEU:HD22	1:E:101:VAL:CG1	2.49	0.43
1:I:42:LEU:HD13	1:I:88:LEU:HG	2.00	0.43
1:C:24:ARG:HH12	4:C:333:GOL:H31	1.84	0.43
1:J:42:LEU:CD1	1:J:88:LEU:HG	2.49	0.43
1:K:13:MET:O	1:K:14:VAL:C	2.57	0.43
1:L:12:ARG:NH2	5:L:1451:HOH:O	2.51	0.43
1:C:77:LEU:HD23	5:F:618:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:LYS:HD2	1:F:145:LYS:C	2.40	0.42
1:J:24:ARG:HH12	4:J:340:GOL:C1	2.28	0.42
1:K:24:ARG:NH1	1:K:108:GLY:N	2.67	0.42
1:A:49:LYS:O	1:F:11:PRO:HA	2.18	0.42
1:A:145:LYS:NZ	1:A:150:SER:OG	2.49	0.42
1:F:34:LEU:HD11	1:F:95:VAL:HG23	2.01	0.42
1:H:155:ARG:NH1	1:K:136:VAL:CG2	2.82	0.42
1:K:31:PHE:CD2	1:K:94:ARG:CD	2.95	0.42
1:K:37:GLU:H	1:K:37:GLU:CD	2.22	0.42
1:L:123:THR:O	1:L:127:MET:HG2	2.19	0.42
1:C:53:LEU:HD22	1:C:86:VAL:HG12	2.00	0.42
1:E:12:ARG:HH11	1:E:12:ARG:HG2	1.84	0.42
1:I:77:LEU:HD23	1:I:77:LEU:O	2.20	0.42
1:J:16:VAL:HG21	1:J:107:THR:HG23	2.02	0.42
1:K:27:THR:HA	1:K:99:ALA:O	2.19	0.42
1:B:37:GLU:OE1	1:B:37:GLU:N	2.46	0.42
1:C:37:GLU:HG2	1:C:132:SER:OG	2.19	0.42
1:C:155:ARG:NH1	1:D:136:VAL:CG2	2.83	0.42
1:G:13:MET:HE1	1:J:65:LYS:HD3	2.02	0.42
1:I:42:LEU:CD1	1:I:88:LEU:HG	2.48	0.42
1:C:16:VAL:HG21	1:C:107:THR:HG23	2.01	0.42
1:D:42:LEU:CD2	1:D:88:LEU:HG	2.50	0.42
1:J:133:LYS:NZ	5:J:1225:HOH:O	2.52	0.42
1:I:77:LEU:N	1:I:77:LEU:HD22	2.35	0.42
1:B:76:PRO:HG3	1:C:65:LYS:HD2	2.02	0.41
1:B:156:GLU:O	1:B:157:GLN:C	2.57	0.41
1:F:77:LEU:HD12	1:F:77:LEU:C	2.40	0.41
1:F:154:ARG:NH2	1:F:154:ARG:CB	2.83	0.41
1:F:154:ARG:CB	1:F:154:ARG:HH21	2.33	0.41
1:K:16:VAL:HG11	1:K:107:THR:HG21	1.99	0.41
1:G:85:ARG:CZ	1:G:87:GLU:OE2	2.68	0.41
1:I:25:THR:HG22	1:I:146:ALA:HB3	2.02	0.41
1:I:71:ILE:HB	1:I:74:CYS:HB2	2.01	0.41
1:I:145:LYS:HG3	1:I:153:TRP:HB3	2.02	0.41
1:C:17:THR:HG21	1:F:23:PHE:CD1	2.55	0.41
1:F:27:THR:CG2	1:F:98:GLU:OE2	2.69	0.41
1:J:12:ARG:HH11	1:J:12:ARG:HG2	1.85	0.41
1:J:145:LYS:HD2	1:J:145:LYS:C	2.40	0.41
1:B:93:LYS:HE2	1:B:93:LYS:HB3	1.89	0.41
1:D:29:GLU:HA	1:D:97:ILE:O	2.21	0.41
1:D:42:LEU:HD21	1:D:88:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ALA:HB2	1:A:135:LEU:HD21	2.02	0.41
1:C:123:THR:O	1:C:127:MET:HG2	2.20	0.41
1:K:19:LYS:HB2	1:K:106:GLU:HB3	2.02	0.41
1:B:50:GLY:HA2	1:E:9:GLY:O	2.21	0.41
1:I:12:ARG:HG2	1:I:12:ARG:HH11	1.86	0.41
1:L:12:ARG:NH1	1:L:12:ARG:CG	2.84	0.41
1:D:19:LYS:HA	1:D:20:PRO:HD3	1.89	0.41
1:H:75:HIS:HA	1:H:76:PRO:HD3	1.93	0.40
1:L:12:ARG:HH11	1:L:12:ARG:CG	2.30	0.40
4:A:331:GOL:H31	5:A:1365:HOH:O	2.20	0.40
1:B:70:LEU:HD21	1:E:70:LEU:HD21	2.03	0.40
1:I:83:GLU:HG2	1:I:100:THR:HB	2.04	0.40
1:J:145:LYS:HG3	1:J:153:TRP:HB3	2.03	0.40
1:L:102:LYS:HE2	5:L:1096:HOH:O	2.21	0.40
1:F:90:LYS:HB2	1:F:90:LYS:HE3	1.81	0.40
1:G:42:LEU:HD23	1:G:88:LEU:HG	2.03	0.40
1:I:133:LYS:NZ	1:J:153:TRP:CG	2.90	0.40
1:B:71:ILE:HB	1:B:74:CYS:HB2	2.03	0.40
1:K:145:LYS:HE2	1:K:145:LYS:HB2	1.88	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	145/157 (92%)	141 (97%)	4 (3%)	0	100	100
1	B	147/157 (94%)	143 (97%)	4 (3%)	0	100	100
1	C	145/157 (92%)	141 (97%)	4 (3%)	0	100	100
1	D	145/157 (92%)	143 (99%)	2 (1%)	0	100	100
1	E	146/157 (93%)	139 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	145/157 (92%)	141 (97%)	4 (3%)	0	100	100
1	G	145/157 (92%)	143 (99%)	2 (1%)	0	100	100
1	H	146/157 (93%)	143 (98%)	2 (1%)	1 (1%)	22	12
1	I	145/157 (92%)	141 (97%)	4 (3%)	0	100	100
1	J	145/157 (92%)	142 (98%)	3 (2%)	0	100	100
1	K	145/157 (92%)	143 (99%)	1 (1%)	1 (1%)	22	12
1	L	145/157 (92%)	141 (97%)	4 (3%)	0	100	100
All	All	1744/1884 (93%)	1701 (98%)	41 (2%)	2 (0%)	51	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	14	VAL
1	K	14	VAL

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	114/124 (92%)	109 (96%)	5 (4%)	28	19
1	B	116/124 (94%)	113 (97%)	3 (3%)	46	39
1	C	114/124 (92%)	112 (98%)	2 (2%)	59	55
1	D	114/124 (92%)	110 (96%)	4 (4%)	36	27
1	E	115/124 (93%)	111 (96%)	4 (4%)	36	27
1	F	115/124 (93%)	111 (96%)	4 (4%)	36	27
1	G	114/124 (92%)	109 (96%)	5 (4%)	28	19
1	H	116/124 (94%)	112 (97%)	4 (3%)	37	28
1	I	115/124 (93%)	110 (96%)	5 (4%)	29	19
1	J	115/124 (93%)	112 (97%)	3 (3%)	46	39
1	K	115/124 (93%)	112 (97%)	3 (3%)	46	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	115/124 (93%)	112 (97%)	3 (3%)	46	39
All	All	1378/1488 (93%)	1333 (97%)	45 (3%)	38	29

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	42	LEU
1	A	58	LEU
1	A	88	LEU
1	A	145	LYS
1	B	58	LEU
1	B	88	LEU
1	B	145	LYS
1	C	37	GLU
1	C	145	LYS
1	D	16	VAL
1	D	85	ARG
1	D	87	GLU
1	D	88	LEU
1	E	42	LEU
1	E	83	GLU
1	E	88	LEU
1	E	145	LYS
1	F	33	GLU
1	F	88	LEU
1	F	98	GLU
1	F	145	LYS
1	G	12	ARG
1	G	69	ASP
1	G	88	LEU
1	G	107	THR
1	G	154	ARG
1	H	42	LEU
1	H	77	LEU
1	H	88	LEU
1	H	145	LYS
1	I	42	LEU
1	I	58	LEU
1	I	77	LEU
1	I	88	LEU
1	I	145	LYS

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Mol	Chain	Res	Type
1	J	42	LEU
1	J	88	LEU
1	J	145	LYS
1	K	42	LEU
1	K	58	LEU
1	K	145	LYS
1	L	12	ARG
1	L	58	LEU
1	L	88	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	139	GLN
1	G	139	GLN
1	I	139	GLN
1	J	139	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

34 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	$\#\|Z\| > 2$
3	PGR	I	189	-	3,4,4	0.17	0	1,4,4	0.39	0
2	PO4	I	169	-	4,4,4	2.82	4 (100%)	6,6,6	0.57	0
3	PGR	K	202	-	3,4,4	0.17	0	1,4,4	0.52	0
3	PGR	L	192	-	3,4,4	0.31	0	1,4,4	0.42	0
2	PO4	A	161	-	4,4,4	2.89	4 (100%)	6,6,6	0.59	0
3	PGR	E	185	-	3,4,4	0.23	0	1,4,4	0.30	0
4	GOL	G	337	-	5,5,5	0.71	0	5,5,5	0.74	0
2	PO4	H	171	-	4,4,4	2.74	4 (100%)	6,6,6	0.59	0
3	PGR	D	201	-	3,4,4	0.16	0	1,4,4	0.38	0
4	GOL	F	336	-	5,5,5	0.72	0	5,5,5	0.75	0
3	PGR	C	183	-	3,4,4	0.18	0	1,4,4	0.34	0
2	PO4	L	172	-	4,4,4	2.74	4 (100%)	6,6,6	0.62	0
2	PO4	C	163	-	4,4,4	2.83	4 (100%)	6,6,6	0.61	0
3	PGR	K	191	-	3,4,4	0.27	0	1,4,4	0.39	0
2	PO4	D	164	-	4,4,4	2.80	4 (100%)	6,6,6	0.55	0
2	PO4	F	166	-	4,4,4	2.88	4 (100%)	6,6,6	0.53	0
2	PO4	G	167	-	4,4,4	2.82	4 (100%)	6,6,6	0.60	0
4	GOL	B	339	-	5,5,5	0.67	0	5,5,5	0.73	0
4	GOL	E	335	-	5,5,5	0.70	0	5,5,5	0.74	0
2	PO4	E	165	-	4,4,4	2.83	4 (100%)	6,6,6	0.54	0
3	PGR	F	186	-	3,4,4	0.23	0	1,4,4	0.37	0
4	GOL	C	333	-	5,5,5	0.66	0	5,5,5	0.76	0
4	GOL	H	338	-	5,5,5	0.68	0	5,5,5	0.72	0
4	GOL	A	331	-	5,5,5	0.66	0	5,5,5	0.75	0
2	PO4	J	170	-	4,4,4	2.77	4 (100%)	6,6,6	0.52	0
2	PO4	B	162	-	4,4,4	2.88	4 (100%)	6,6,6	0.54	0
3	PGR	A	181	-	3,4,4	0.20	0	1,4,4	0.37	0
4	GOL	D	334	-	5,5,5	0.73	0	5,5,5	0.80	0
4	GOL	K	341	-	5,5,5	0.77	0	5,5,5	0.80	0
3	PGR	G	187	-	3,4,4	0.23	0	1,4,4	0.44	0
2	PO4	H	168	-	4,4,4	2.81	4 (100%)	6,6,6	0.57	0
4	GOL	J	340	-	5,5,5	0.69	0	5,5,5	0.82	0
4	GOL	I	332	-	5,5,5	0.68	0	5,5,5	0.74	0
4	GOL	L	342	-	5,5,5	0.69	0	5,5,5	0.76	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
3	PGR	I	189	-	-	1/2/2/2	-
3	PGR	K	202	-	-	2/2/2/2	-
3	PGR	L	192	-	-	1/2/2/2	-
3	PGR	E	185	-	-	0/2/2/2	-
4	GOL	G	337	-	-	4/4/4/4	-
3	PGR	D	201	-	-	0/2/2/2	-
4	GOL	F	336	-	-	4/4/4/4	-
3	PGR	C	183	-	-	0/2/2/2	-
3	PGR	K	191	-	-	0/2/2/2	-
4	GOL	B	339	-	-	4/4/4/4	-
4	GOL	E	335	-	-	0/4/4/4	-
3	PGR	F	186	-	-	0/2/2/2	-
4	GOL	C	333	-	-	1/4/4/4	-
4	GOL	H	338	-	-	2/4/4/4	-
4	GOL	A	331	-	-	2/4/4/4	-
3	PGR	A	181	-	-	0/2/2/2	-
4	GOL	D	334	-	-	2/4/4/4	-
4	GOL	K	341	-	-	2/4/4/4	-
3	PGR	G	187	-	-	2/2/2/2	-
4	GOL	J	340	-	-	4/4/4/4	-
4	GOL	I	332	-	-	3/4/4/4	-
4	GOL	L	342	-	-	0/4/4/4	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	161	PO4	P-O4	-3.36	1.44	1.54
2	J	170	PO4	P-O4	-3.34	1.44	1.54
2	H	168	PO4	P-O4	-3.33	1.44	1.54
2	F	166	PO4	P-O4	-3.31	1.44	1.54
2	B	162	PO4	P-O1	-3.31	1.43	1.50
2	C	163	PO4	P-O4	-3.28	1.44	1.54
2	H	171	PO4	P-O4	-3.24	1.44	1.54
2	I	169	PO4	P-O4	-3.22	1.44	1.54
2	F	166	PO4	P-O1	-3.22	1.43	1.50
2	G	167	PO4	P-O4	-3.20	1.45	1.54
2	E	165	PO4	P-O4	-3.19	1.45	1.54
2	D	164	PO4	P-O4	-3.18	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	162	PO4	P-O4	-3.17	1.45	1.54
2	G	167	PO4	P-O1	-3.15	1.43	1.50
2	L	172	PO4	P-O4	-3.14	1.45	1.54
2	E	165	PO4	P-O1	-3.14	1.43	1.50
2	A	161	PO4	P-O1	-3.13	1.43	1.50
2	I	169	PO4	P-O1	-3.12	1.43	1.50
2	D	164	PO4	P-O1	-3.10	1.43	1.50
2	C	163	PO4	P-O1	-3.07	1.43	1.50
2	J	170	PO4	P-O1	-3.02	1.43	1.50
2	H	168	PO4	P-O1	-2.97	1.43	1.50
2	L	172	PO4	P-O1	-2.97	1.43	1.50
2	H	171	PO4	P-O1	-2.88	1.44	1.50
2	F	166	PO4	P-O3	-2.53	1.47	1.54
2	B	162	PO4	P-O3	-2.52	1.47	1.54
2	A	161	PO4	P-O3	-2.50	1.47	1.54
2	H	168	PO4	P-O3	-2.50	1.47	1.54
2	I	169	PO4	P-O2	-2.47	1.47	1.54
2	H	171	PO4	P-O3	-2.46	1.47	1.54
2	E	165	PO4	P-O2	-2.44	1.47	1.54
2	C	163	PO4	P-O3	-2.44	1.47	1.54
2	G	167	PO4	P-O3	-2.44	1.47	1.54
2	L	172	PO4	P-O2	-2.44	1.47	1.54
2	A	161	PO4	P-O2	-2.44	1.47	1.54
2	E	165	PO4	P-O3	-2.44	1.47	1.54
2	D	164	PO4	P-O2	-2.43	1.47	1.54
2	C	163	PO4	P-O2	-2.43	1.47	1.54
2	D	164	PO4	P-O3	-2.41	1.47	1.54
2	B	162	PO4	P-O2	-2.41	1.47	1.54
2	G	167	PO4	P-O2	-2.39	1.47	1.54
2	I	169	PO4	P-O3	-2.36	1.47	1.54
2	L	172	PO4	P-O3	-2.34	1.47	1.54
2	H	168	PO4	P-O2	-2.34	1.47	1.54
2	J	170	PO4	P-O2	-2.34	1.47	1.54
2	F	166	PO4	P-O2	-2.33	1.47	1.54
2	H	171	PO4	P-O2	-2.27	1.47	1.54
2	J	170	PO4	P-O3	-2.21	1.47	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	187	PGR	O1-C1-C2-C3
3	K	202	PGR	O1-C1-C2-C3
3	K	202	PGR	O1-C1-C2-O2
3	L	192	PGR	O1-C1-C2-C3
4	A	331	GOL	O1-C1-C2-C3
4	B	339	GOL	O1-C1-C2-C3
4	F	336	GOL	O1-C1-C2-C3
4	F	336	GOL	C1-C2-C3-O3
4	F	336	GOL	O2-C2-C3-O3
4	G	337	GOL	O1-C1-C2-C3
4	I	332	GOL	O1-C1-C2-C3
4	J	340	GOL	O1-C1-C2-O2
4	J	340	GOL	O1-C1-C2-C3
4	K	341	GOL	C1-C2-C3-O3
4	G	337	GOL	O1-C1-C2-O2
4	B	339	GOL	C1-C2-C3-O3
4	D	334	GOL	C1-C2-C3-O3
4	G	337	GOL	C1-C2-C3-O3
4	I	332	GOL	C1-C2-C3-O3
4	J	340	GOL	C1-C2-C3-O3
4	D	334	GOL	O2-C2-C3-O3
4	F	336	GOL	O1-C1-C2-O2
4	G	337	GOL	O2-C2-C3-O3
4	K	341	GOL	O2-C2-C3-O3
4	A	331	GOL	O1-C1-C2-O2
4	I	332	GOL	O2-C2-C3-O3
4	J	340	GOL	O2-C2-C3-O3
4	B	339	GOL	O2-C2-C3-O3
4	H	338	GOL	O1-C1-C2-C3
4	H	338	GOL	O2-C2-C3-O3
4	B	339	GOL	O1-C1-C2-O2
4	C	333	GOL	O2-C2-C3-O3
3	G	187	PGR	O1-C1-C2-O2
3	I	189	PGR	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	333	GOL	4	0
4	A	331	GOL	2	0
4	D	334	GOL	1	0
4	K	341	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	187	PGR	3	0
4	J	340	GOL	3	0
4	L	342	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	147/157 (93%)	-0.00	2 (1%)	75	77	14, 25, 43, 54	0
1	B	149/157 (94%)	0.03	3 (2%)	65	68	12, 23, 40, 61	0
1	C	147/157 (93%)	0.18	4 (2%)	54	57	12, 24, 43, 53	0
1	D	147/157 (93%)	-0.02	4 (2%)	54	57	11, 22, 43, 58	0
1	E	148/157 (94%)	0.16	2 (1%)	75	77	14, 26, 41, 58	0
1	F	147/157 (93%)	-0.06	0	100	100	12, 23, 38, 63	0
1	G	147/157 (93%)	-0.12	0	100	100	9, 20, 36, 50	0
1	H	148/157 (94%)	-0.19	2 (1%)	75	77	9, 19, 36, 56	0
1	I	147/157 (93%)	-0.20	0	100	100	8, 18, 34, 50	0
1	J	147/157 (93%)	-0.24	0	100	100	8, 18, 32, 47	0
1	K	147/157 (93%)	-0.23	0	100	100	9, 19, 36, 52	0
1	L	147/157 (93%)	-0.19	1 (0%)	87	88	9, 19, 33, 50	0
All	All	1768/1884 (93%)	-0.07	18 (1%)	82	84	8, 21, 40, 63	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	GLU	4.3
1	C	44	LYS	3.0
1	B	157	GLN	3.0
1	C	48	GLY	2.8
1	C	148	GLY	2.8
1	D	16	VAL	2.7
1	A	149	LYS	2.7
1	E	9	GLY	2.7
1	D	12	ARG	2.5
1	L	149	LYS	2.5
1	B	148	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	91	ALA	2.4
1	D	9	GLY	2.3
1	A	40	SER	2.2
1	H	12	ARG	2.2
1	B	149	LYS	2.2
1	H	13	MET	2.1
1	E	44	LYS	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	GOL	H	338	6/6	0.59	0.21	48,51,52,53	0
3	PGR	D	201	5/5	0.62	0.20	42,43,44,44	0
4	GOL	A	331	6/6	0.68	0.13	58,58,58,59	0
4	GOL	E	335	6/6	0.69	0.20	50,53,53,53	0
4	GOL	J	340	6/6	0.69	0.21	49,50,50,50	0
4	GOL	C	333	6/6	0.70	0.17	51,52,53,54	0
4	GOL	K	341	6/6	0.70	0.18	51,51,51,51	0
4	GOL	G	337	6/6	0.72	0.19	51,51,51,53	0
4	GOL	L	342	6/6	0.73	0.17	51,52,53,53	0
3	PGR	K	202	5/5	0.75	0.14	40,40,42,42	0
4	GOL	I	332	6/6	0.76	0.15	49,49,49,49	0
4	GOL	D	334	6/6	0.76	0.14	58,59,59,60	0
4	GOL	F	336	6/6	0.80	0.12	51,52,53,55	0
3	PGR	K	191	5/5	0.82	0.19	26,33,36,38	0
4	GOL	B	339	6/6	0.82	0.12	49,51,52,53	0
3	PGR	A	181	5/5	0.84	0.16	39,39,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PGR	F	186	5/5	0.85	0.15	29,33,34,35	0
3	PGR	E	185	5/5	0.86	0.20	36,40,41,42	0
3	PGR	G	187	5/5	0.87	0.14	26,32,34,35	0
3	PGR	L	192	5/5	0.87	0.19	27,31,32,35	0
3	PGR	I	189	5/5	0.89	0.14	17,25,27,29	0
3	PGR	C	183	5/5	0.90	0.13	25,26,29,29	0
2	PO4	B	162	5/5	0.92	0.11	30,34,35,36	0
2	PO4	H	168	5/5	0.93	0.10	45,45,47,48	0
2	PO4	L	172	5/5	0.93	0.10	31,31,36,37	0
2	PO4	I	169	5/5	0.95	0.09	33,37,38,40	0
2	PO4	D	164	5/5	0.95	0.09	29,32,33,34	0
2	PO4	G	167	5/5	0.95	0.10	37,39,41,41	0
2	PO4	C	163	5/5	0.95	0.09	34,36,37,38	0
2	PO4	J	170	5/5	0.96	0.07	23,24,26,28	0
2	PO4	F	166	5/5	0.96	0.08	31,33,33,35	0
2	PO4	A	161	5/5	0.97	0.09	33,34,36,37	0
2	PO4	H	171	5/5	0.98	0.06	24,26,28,28	0
2	PO4	E	165	5/5	0.98	0.07	29,32,32,35	0

6.5 Other polymers (i)

There are no such residues in this entry.