



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:44 PM GMT

PDB ID : 1C41
Title : CRYSTAL STRUCTURES OF A PENTAMERIC FUNGAL AND AN ICOSAHERAL PLANT LUMAZINE SYNTHASE REVEALS THE STRUCTURAL BASIS FOR DIFFERENCES IN ASSEMBLY
Authors : Persson, K.; Schneider, G.; Jordan, D.B.; Viitanen, P.V.; Sandalova, T.
Deposited on : 1999-08-03
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 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

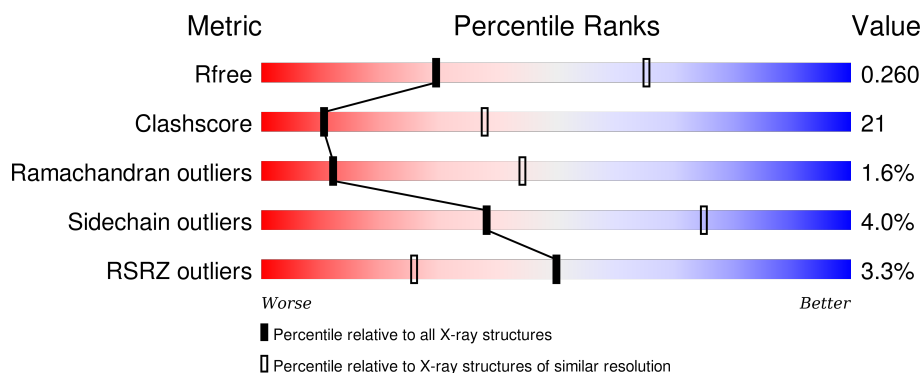
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	200	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>22%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	200	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>26%</div> <div>•</div> <div>18%</div> </div> </div>
1	C	200	<div> <div>5%</div> <div> <div></div> <div>55%</div> <div>25%</div> <div>•</div> <div>18%</div> </div> </div>
1	D	200	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>25%</div> <div>•</div> <div>18%</div> </div> </div>
1	E	200	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>25%</div> <div>•</div> <div>18%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	200	
1	G	200	
1	H	200	
1	I	200	
1	J	200	

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	SO4	A	404	-	-	-	X
2	SO4	B	401	-	-	X	-
2	SO4	J	408	-	-	-	X
3	LMZ	A	201	-	-	X	-
3	LMZ	I	209	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12740 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 LUMAZINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	5	0	0
			1243	786	222	231	4			
1	B	165	Total	C	N	O	S	5	0	0
			1243	786	222	231	4			
1	C	165	Total	C	N	O	S	4	0	0
			1243	786	222	231	4			
1	D	165	Total	C	N	O	S	5	0	0
			1243	786	222	231	4			
1	E	165	Total	C	N	O	S	7	0	0
			1243	786	222	231	4			
1	F	165	Total	C	N	O	S	5	0	0
			1243	786	222	231	4			
1	G	165	Total	C	N	O	S	7	0	0
			1243	786	222	231	4			
1	H	165	Total	C	N	O	S	7	0	0
			1243	786	222	231	4			
1	I	165	Total	C	N	O	S	5	0	0
			1243	786	222	231	4			
1	J	165	Total	C	N	O	S	7	0	0
			1243	786	222	231	4			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



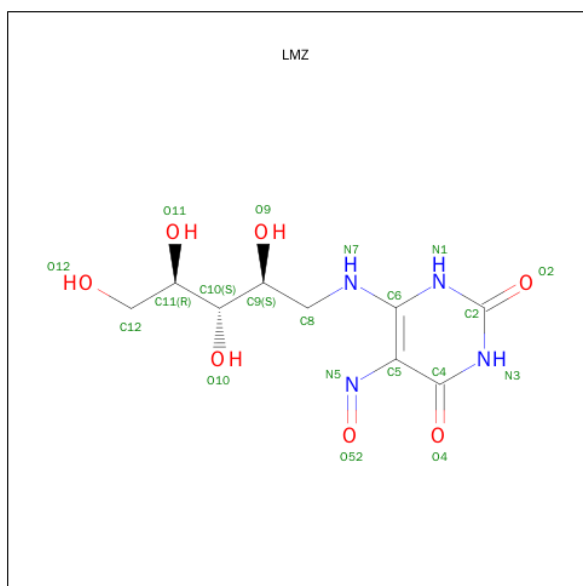
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 5-NITROSO-6-RIBITYL-AMINO-2,4(1H,3H)-PYRIMIDINEDIONE (three-letter code: LMZ) (formula: C₉H₁₄N₄O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	9	4	7		
3	B	1	Total	C	N	O	0	0
			20	9	4	7		
3	C	1	Total	C	N	O	0	0
			20	9	4	7		
3	D	1	Total	C	N	O	0	0
			20	9	4	7		
3	E	1	Total	C	N	O	0	0
			20	9	4	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			20	9	4	7		
3	G	1	Total	C	N	O	0	0
			20	9	4	7		
3	H	1	Total	C	N	O	0	0
			20	9	4	7		
3	I	1	Total	C	N	O	0	0
			20	9	4	7		
3	J	1	Total	C	N	O	0	0
			20	9	4	7		

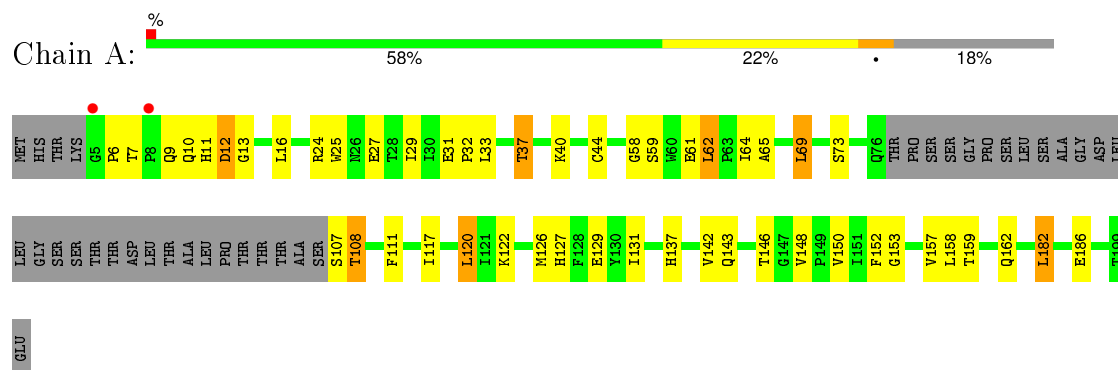
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	C	4	Total	O	0	0
			4	4		
4	G	1	Total	O	0	0
			1	1		
4	I	3	Total	O	0	0
			3	3		
4	J	1	Total	O	0	0
			1	1		

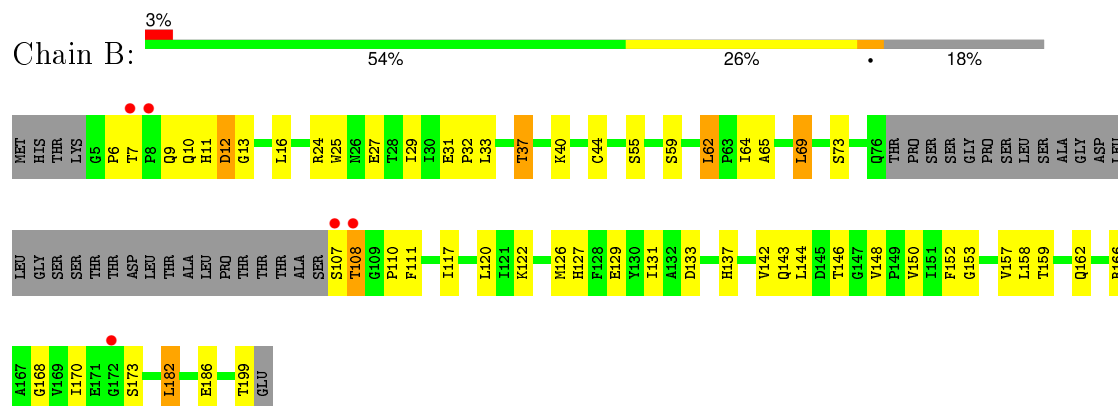
3 Residue-property plots [i](#)

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.

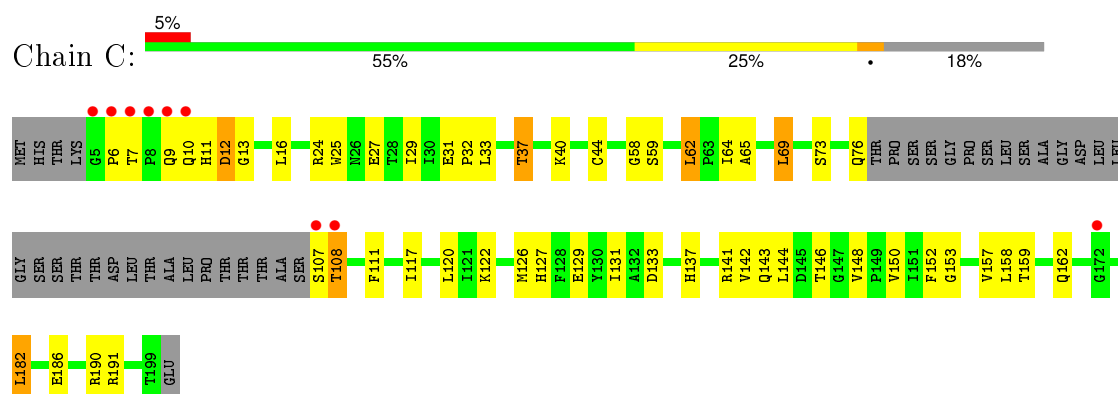
• Molecule 1: LUMAZINE SYNTHASE



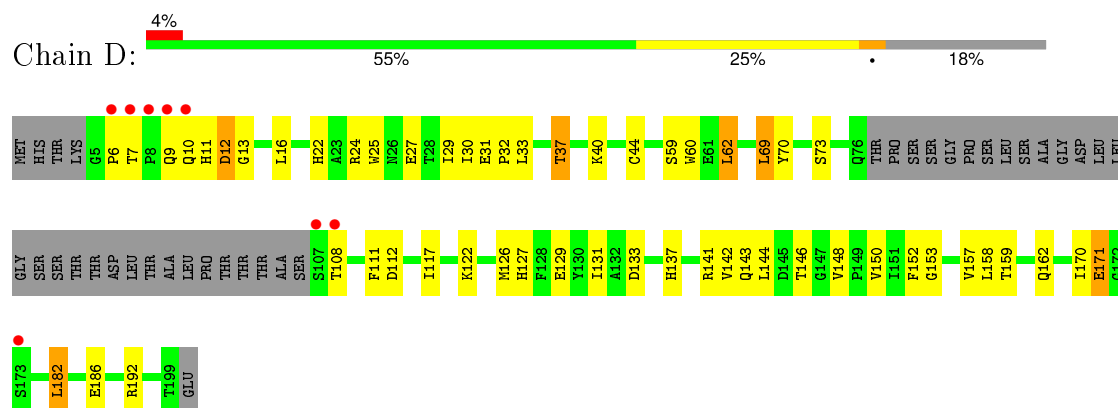
• Molecule 1: LUMAZINE SYNTHASE



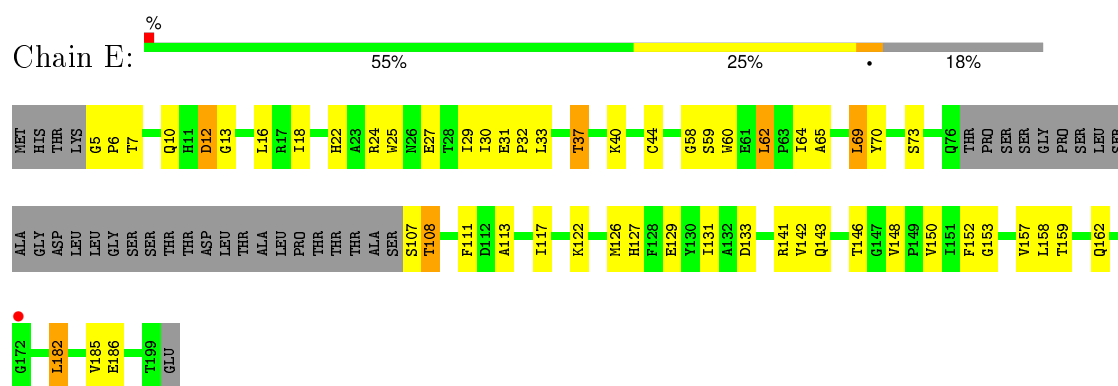
• Molecule 1: LUMAZINE SYNTHASE



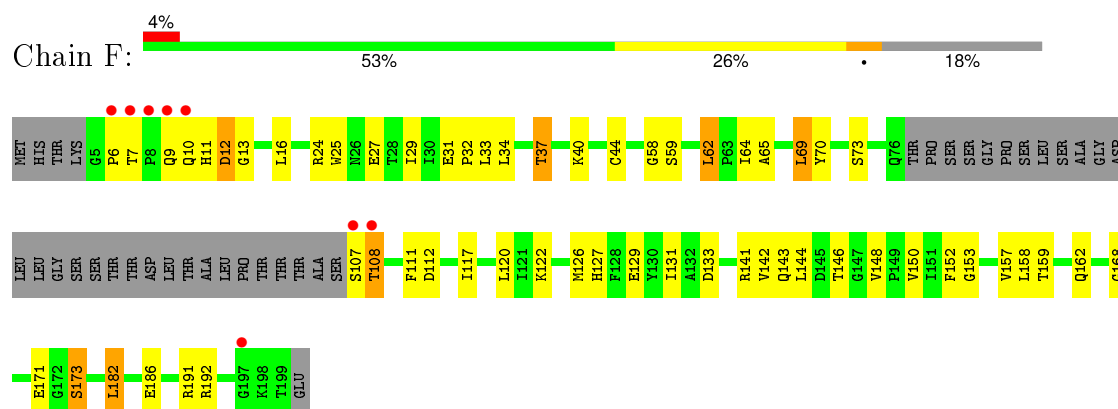
- Molecule 1: LUMAZINE SYNTHASE



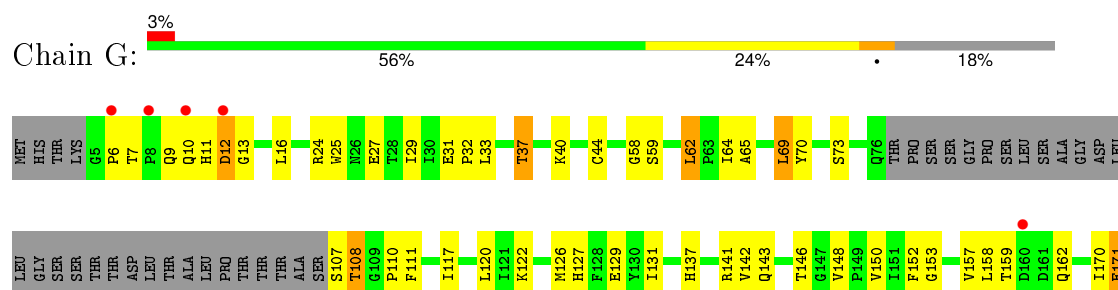
- Molecule 1: LUMAZINE SYNTHASE

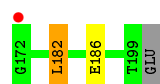


- Molecule 1: LUMAZINE SYNTHASE

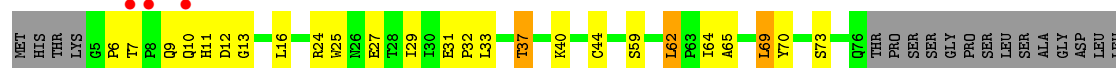


- Molecule 1: LUMAZINE SYNTHASE





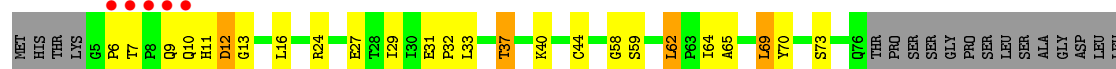
• Molecule 1: LUMAZINE SYNTHASE



• Molecule 1: LUMAZINE SYNTHASE



• Molecule 1: LUMAZINE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.80Å 124.70Å 141.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 19.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-3.10) 99.0 (19.99-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 3.09Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.248 , 0.271 0.239 , 0.260	Depositor DCC
R_{free} test set	1601 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.764	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 6.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 31795 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12740	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: LMZ, SO4

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	0.46	0/1267	0.62	1/1721 (0.1%)
1	B	0.48	0/1267	0.61	0/1721
1	C	0.47	0/1267	0.61	0/1721
1	D	0.44	0/1267	0.61	0/1721
1	E	0.47	0/1267	0.63	0/1721
1	F	0.45	0/1267	0.61	0/1721
1	G	0.43	0/1267	0.61	0/1721
1	H	0.45	0/1267	0.61	0/1721
1	I	0.45	0/1267	0.61	0/1721
1	J	0.45	0/1267	0.60	0/1721
All	All	0.46	0/12670	0.61	1/17210 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	LEU	CA-CB-CG	5.23	127.33	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1243	0	1249	63	1
1	B	1243	0	1249	65	0
1	C	1243	0	1249	69	0
1	D	1243	0	1249	64	0
1	E	1243	0	1249	76	0
1	F	1243	0	1249	67	0
1	G	1243	0	1249	62	0
1	H	1243	0	1249	62	1
1	I	1243	0	1249	53	0
1	J	1243	0	1249	61	0
2	A	10	0	0	0	0
2	B	10	0	0	2	0
2	C	15	0	0	2	0
2	D	5	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	1	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
2	I	15	0	0	0	0
2	J	10	0	0	1	0
3	A	20	0	14	8	0
3	B	20	0	14	5	0
3	C	20	0	14	4	0
3	D	20	0	14	2	0
3	E	20	0	14	3	0
3	F	20	0	14	4	0
3	G	20	0	14	4	0
3	H	20	0	14	3	0
3	I	20	0	14	3	0
3	J	20	0	14	3	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	G	1	0	0	0	0
4	I	3	0	0	0	0
4	J	1	0	0	0	0
All	All	12740	0	12630	537	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (537) 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:E:40:LYS:HD2	1:E:182:LEU:HD13	1.47	0.97
1:A:25:TRP:CE2	1:E:6:PRO:HG3	2.05	0.92
1:D:146:THR:HG23	1:D:148:VAL:H	1.40	0.86
1:H:143:GLN:HE21	1:H:150:VAL:H	1.23	0.86
1:C:40:LYS:HD2	1:C:182:LEU:HD13	1.58	0.86
1:J:143:GLN:HE21	1:J:150:VAL:H	1.23	0.86
1:B:146:THR:HG23	1:B:148:VAL:H	1.41	0.85
1:G:146:THR:HG23	1:G:148:VAL:H	1.41	0.85
1:H:40:LYS:HD2	1:H:182:LEU:HD13	1.59	0.85
1:F:40:LYS:HD2	1:F:182:LEU:HD13	1.59	0.85
1:F:143:GLN:HE21	1:F:150:VAL:H	1.25	0.85
1:D:143:GLN:HE21	1:D:150:VAL:H	1.25	0.84
1:G:40:LYS:HD2	1:G:182:LEU:HD13	1.59	0.84
1:C:146:THR:HG23	1:C:148:VAL:H	1.43	0.84
1:A:143:GLN:HE21	1:A:150:VAL:H	1.25	0.84
1:G:143:GLN:HE21	1:G:150:VAL:H	1.25	0.83
1:I:146:THR:HG23	1:I:148:VAL:H	1.42	0.83
1:A:40:LYS:HD2	1:A:182:LEU:HD13	1.60	0.83
1:J:146:THR:HG23	1:J:148:VAL:H	1.44	0.83
1:I:143:GLN:HE21	1:I:150:VAL:H	1.24	0.83
1:F:146:THR:HG23	1:F:148:VAL:H	1.43	0.83
1:E:143:GLN:HE21	1:E:150:VAL:H	1.23	0.82
1:J:40:LYS:HD2	1:J:182:LEU:HD13	1.60	0.82
1:B:7:THR:HG21	1:C:27:GLU:OE2	1.79	0.82
1:C:143:GLN:HE21	1:C:150:VAL:H	1.24	0.82
1:A:27:GLU:HG3	1:E:7:THR:CG2	2.10	0.81
1:B:40:LYS:HD2	1:B:182:LEU:HD13	1.60	0.81
1:B:143:GLN:HE21	1:B:150:VAL:H	1.27	0.81
1:D:40:LYS:HD2	1:D:182:LEU:HD13	1.60	0.81
1:H:146:THR:HG23	1:H:148:VAL:H	1.43	0.81
1:E:146:THR:HG23	1:E:148:VAL:H	1.43	0.81
1:A:146:THR:HG23	1:A:148:VAL:H	1.45	0.80
1:E:40:LYS:HD2	1:E:182:LEU:CD1	2.11	0.80
1:A:27:GLU:HG3	1:E:7:THR:HG23	1.64	0.79
1:C:33:LEU:O	1:C:37:THR:HG22	1.85	0.77
1:F:159:THR:OG1	1:F:162:GLN:HG3	1.85	0.77
1:B:7:THR:HG23	1:C:27:GLU:HG3	1.66	0.76
1:A:24:ARG:NH1	1:E:7:THR:O	2.19	0.75
1:F:33:LEU:O	1:F:37:THR:HG22	1.85	0.75
1:I:40:LYS:HD2	1:I:182:LEU:HD13	1.69	0.74
1:D:33:LEU:O	1:D:37:THR:HG22	1.87	0.74
1:B:159:THR:OG1	1:B:162:GLN:HG3	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:33:LEU:O	1:J:37:THR:HG22	1.87	0.74
1:I:159:THR:OG1	1:I:162:GLN:HG3	1.88	0.74
1:I:33:LEU:O	1:I:37:THR:HG22	1.87	0.74
1:H:33:LEU:O	1:H:37:THR:HG22	1.87	0.73
1:B:33:LEU:O	1:B:37:THR:HG22	1.89	0.72
1:G:33:LEU:O	1:G:37:THR:HG22	1.89	0.72
1:D:159:THR:OG1	1:D:162:GLN:HG3	1.90	0.72
1:A:27:GLU:OE2	1:E:7:THR:HG21	1.90	0.72
1:J:159:THR:OG1	1:J:162:GLN:HG3	1.90	0.72
1:C:37:THR:HG21	1:C:117:ILE:HD11	1.72	0.71
1:A:33:LEU:O	1:A:37:THR:HG22	1.90	0.71
1:E:33:LEU:O	1:E:37:THR:HG22	1.89	0.71
1:H:159:THR:OG1	1:H:162:GLN:HG3	1.90	0.71
1:C:159:THR:OG1	1:C:162:GLN:HG3	1.90	0.71
1:G:40:LYS:HD2	1:G:182:LEU:CD1	2.19	0.71
1:A:25:TRP:CZ2	1:E:6:PRO:HG3	2.26	0.71
1:A:159:THR:OG1	1:A:162:GLN:HG3	1.90	0.70
1:E:159:THR:OG1	1:E:162:GLN:HG3	1.89	0.70
1:J:40:LYS:HD2	1:J:182:LEU:CD1	2.21	0.70
1:G:159:THR:OG1	1:G:162:GLN:HG3	1.91	0.69
1:F:40:LYS:HD2	1:F:182:LEU:CD1	2.22	0.69
1:B:40:LYS:HD2	1:B:182:LEU:CD1	2.21	0.69
1:C:40:LYS:HD2	1:C:182:LEU:CD1	2.23	0.68
1:B:146:THR:HG23	1:B:148:VAL:N	2.08	0.68
1:E:122:LYS:HE2	1:E:129:GLU:OE2	1.93	0.68
1:D:146:THR:HG23	1:D:148:VAL:N	2.08	0.67
1:E:37:THR:HG21	1:E:117:ILE:HD11	1.75	0.67
1:H:7:THR:CG2	1:I:27:GLU:HG3	2.24	0.67
1:G:146:THR:HG23	1:G:148:VAL:N	2.08	0.67
1:D:40:LYS:HD2	1:D:182:LEU:CD1	2.24	0.67
1:E:146:THR:HG23	1:E:148:VAL:N	2.09	0.67
1:H:146:THR:HG23	1:H:148:VAL:N	2.10	0.66
1:I:146:THR:HG23	1:I:148:VAL:N	2.09	0.66
1:F:37:THR:HG21	1:F:117:ILE:HD11	1.78	0.66
1:C:146:THR:HG23	1:C:148:VAL:N	2.10	0.66
1:A:37:THR:HG21	1:A:117:ILE:HD11	1.78	0.66
1:A:122:LYS:HE2	1:A:129:GLU:OE2	1.96	0.66
1:A:40:LYS:HD2	1:A:182:LEU:CD1	2.26	0.66
1:H:122:LYS:HE2	1:H:129:GLU:OE2	1.95	0.66
1:C:122:LYS:HE2	1:C:129:GLU:OE2	1.96	0.65
1:G:122:LYS:HE2	1:G:129:GLU:OE2	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:146:THR:HG23	1:J:148:VAL:N	2.11	0.65
1:H:40:LYS:HD2	1:H:182:LEU:CD1	2.25	0.65
1:F:122:LYS:HE2	1:F:129:GLU:OE2	1.96	0.65
1:F:146:THR:HG23	1:F:148:VAL:N	2.10	0.65
1:J:122:LYS:HE2	1:J:129:GLU:OE2	1.97	0.65
1:J:59:SER:O	1:J:62:LEU:HB2	1.97	0.65
1:A:146:THR:HG23	1:A:148:VAL:N	2.11	0.64
1:H:37:THR:HG21	1:H:117:ILE:HD11	1.80	0.64
1:B:122:LYS:HE2	1:B:129:GLU:OE2	1.98	0.64
1:I:37:THR:HG21	1:I:117:ILE:HD11	1.81	0.63
1:A:131:ILE:HD13	3:A:201:LMZ:H82	1.80	0.63
1:D:122:LYS:HE2	1:D:129:GLU:OE2	1.98	0.63
1:I:59:SER:O	1:I:62:LEU:HB2	1.99	0.63
1:F:59:SER:O	1:F:62:LEU:HB2	1.99	0.63
1:I:122:LYS:HE2	1:I:129:GLU:OE2	1.99	0.63
1:G:7:THR:HG23	1:H:27:GLU:HG3	1.81	0.62
1:B:7:THR:CG2	1:C:27:GLU:HG3	2.30	0.62
1:B:37:THR:HG21	1:B:117:ILE:HD11	1.81	0.62
1:C:59:SER:O	1:C:62:LEU:HB2	2.00	0.62
1:D:37:THR:HG21	1:D:117:ILE:HD11	1.82	0.62
1:J:37:THR:HG21	1:J:117:ILE:HD11	1.81	0.62
1:D:146:THR:CG2	1:D:148:VAL:H	2.13	0.61
1:B:7:THR:OG1	1:C:24:ARG:HD2	1.99	0.61
1:D:7:THR:CG2	1:E:27:GLU:HG3	2.31	0.61
1:C:10:GLN:HG3	1:C:44:CYS:SG	2.40	0.61
1:B:59:SER:O	1:B:62:LEU:HB2	2.00	0.61
1:G:146:THR:CG2	1:G:148:VAL:H	2.13	0.61
1:I:131:ILE:HD13	3:I:209:LMZ:H82	1.81	0.61
1:J:146:THR:CG2	1:J:148:VAL:H	2.14	0.60
1:H:59:SER:O	1:H:62:LEU:HB2	2.01	0.60
1:A:59:SER:O	1:A:62:LEU:HB2	2.02	0.60
1:F:27:GLU:HG3	1:J:7:THR:HG23	1.83	0.60
1:D:6:PRO:HB3	1:E:25:TRP:CD1	2.37	0.60
1:D:59:SER:O	1:D:62:LEU:HB2	2.01	0.60
1:F:27:GLU:HG3	1:J:7:THR:CG2	2.32	0.59
1:B:131:ILE:HD13	3:B:202:LMZ:H82	1.83	0.59
1:D:13:GLY:HA3	1:D:16:LEU:HD22	1.85	0.59
1:E:59:SER:O	1:E:62:LEU:HB2	2.02	0.59
1:G:59:SER:O	1:G:62:LEU:HB2	2.01	0.59
1:D:157:VAL:HG13	1:D:162:GLN:HB2	1.84	0.59
1:A:25:TRP:CD1	1:E:6:PRO:HB3	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLU:HG3	1:E:7:THR:HG21	1.82	0.58
1:I:157:VAL:HG13	1:I:162:GLN:HB2	1.86	0.58
1:B:13:GLY:HA3	1:B:16:LEU:HD22	1.85	0.58
1:B:146:THR:CG2	1:B:148:VAL:H	2.13	0.58
1:D:7:THR:HG23	1:E:27:GLU:HG3	1.85	0.58
1:I:13:GLY:CA	1:I:16:LEU:HD22	2.34	0.58
1:G:37:THR:HG21	1:G:117:ILE:HD11	1.84	0.58
1:E:13:GLY:CA	1:E:16:LEU:HD22	2.33	0.58
1:E:146:THR:CG2	1:E:148:VAL:H	2.15	0.58
1:I:13:GLY:HA3	1:I:16:LEU:HD22	1.84	0.58
1:E:157:VAL:HG13	1:E:162:GLN:HB2	1.85	0.58
1:G:157:VAL:HG13	1:G:162:GLN:HB2	1.85	0.58
1:J:157:VAL:HG13	1:J:162:GLN:HB2	1.86	0.58
1:H:7:THR:HG21	1:I:27:GLU:HG3	1.85	0.58
1:A:152:PHE:HB3	3:B:202:LMZ:H122	1.85	0.58
1:D:13:GLY:CA	1:D:16:LEU:HD22	2.34	0.58
1:H:146:THR:CG2	1:H:148:VAL:H	2.15	0.58
1:I:40:LYS:HD2	1:I:182:LEU:CD1	2.32	0.58
1:F:13:GLY:CA	1:F:16:LEU:HD22	2.34	0.58
1:G:7:THR:CG2	1:H:27:GLU:HG3	2.34	0.57
1:F:13:GLY:HA3	1:F:16:LEU:HD22	1.86	0.57
1:A:146:THR:CG2	1:A:148:VAL:H	2.16	0.57
1:B:13:GLY:CA	1:B:16:LEU:HD22	2.35	0.57
1:J:13:GLY:CA	1:J:16:LEU:HD22	2.34	0.57
1:A:24:ARG:HB3	1:E:7:THR:OG1	2.04	0.57
1:H:13:GLY:CA	1:H:16:LEU:HD22	2.34	0.57
1:E:13:GLY:HA3	1:E:16:LEU:HD22	1.86	0.57
1:J:127:HIS:CE1	1:J:131:ILE:HD11	2.40	0.57
1:B:157:VAL:HG13	1:B:162:GLN:HB2	1.86	0.57
1:C:152:PHE:HB3	3:D:204:LMZ:H122	1.86	0.57
1:B:168:GLY:HA2	1:B:173:SER:OG	2.05	0.57
1:H:13:GLY:HA3	1:H:16:LEU:HD22	1.87	0.57
1:G:69:LEU:HD22	1:G:111:PHE:CE2	2.39	0.57
1:F:146:THR:CG2	1:F:148:VAL:H	2.15	0.57
1:D:6:PRO:HB3	1:E:25:TRP:NE1	2.19	0.57
1:D:10:GLN:HG3	1:D:44:CYS:SG	2.45	0.57
1:H:7:THR:HG23	1:I:27:GLU:HG3	1.86	0.56
1:H:173:SER:O	1:H:174:HIS:HB3	2.05	0.56
1:G:127:HIS:CE1	1:G:131:ILE:HD11	2.40	0.56
1:C:146:THR:CG2	1:C:148:VAL:H	2.15	0.56
1:G:7:THR:HG21	1:H:27:GLU:OE2	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLY:CA	1:C:16:LEU:HD22	2.36	0.56
1:J:13:GLY:HA3	1:J:16:LEU:HD22	1.87	0.56
1:G:69:LEU:HD22	1:G:111:PHE:HE2	1.70	0.56
1:G:131:ILE:HD13	3:G:207:LMZ:H82	1.88	0.56
1:C:13:GLY:HA3	1:C:16:LEU:HD22	1.88	0.56
1:F:7:THR:HG23	1:G:27:GLU:HG3	1.87	0.56
1:I:146:THR:CG2	1:I:148:VAL:H	2.15	0.56
1:B:10:GLN:HG3	1:B:44:CYS:SG	2.45	0.56
1:A:13:GLY:CA	1:A:16:LEU:HD22	2.36	0.56
1:B:69:LEU:HD22	1:B:111:PHE:CE2	2.41	0.56
1:I:10:GLN:HG3	1:I:44:CYS:SG	2.46	0.56
1:B:12:ASP:O	1:B:44:CYS:O	2.24	0.56
1:B:157:VAL:CG1	1:B:158:LEU:N	2.69	0.55
1:A:127:HIS:CE1	1:A:131:ILE:HD11	2.42	0.55
3:A:201:LMZ:H122	1:E:152:PHE:HB3	1.87	0.55
1:H:10:GLN:HG3	1:H:44:CYS:SG	2.45	0.55
1:F:7:THR:CG2	1:G:27:GLU:HG3	2.36	0.55
1:B:186:GLU:OE1	1:C:24:ARG:NH2	2.36	0.55
1:D:157:VAL:CG1	1:D:162:GLN:HB2	2.37	0.55
1:H:186:GLU:OE2	1:I:24:ARG:NH2	2.40	0.55
1:F:27:GLU:OE2	1:J:7:THR:HG21	2.07	0.55
1:G:157:VAL:CG1	1:G:162:GLN:HB2	2.36	0.55
1:D:152:PHE:HB3	3:E:205:LMZ:H122	1.89	0.55
1:I:137:HIS:HE1	1:J:133:ASP:OD2	1.89	0.55
1:I:73:SER:HB3	1:I:111:PHE:CE2	2.42	0.55
1:D:69:LEU:HD22	1:D:111:PHE:CE2	2.41	0.55
1:F:157:VAL:HG13	1:F:162:GLN:HB2	1.88	0.54
1:J:157:VAL:CG1	1:J:162:GLN:HB2	2.37	0.54
1:H:157:VAL:CG1	1:H:158:LEU:N	2.68	0.54
1:C:157:VAL:HG13	1:C:162:GLN:HB2	1.89	0.54
1:A:157:VAL:HG13	1:A:162:GLN:HB2	1.89	0.54
1:F:7:THR:HG21	1:G:27:GLU:OE2	2.06	0.54
1:B:55:SER:N	2:B:401:SO4:O2	2.39	0.54
1:C:127:HIS:CE1	1:C:131:ILE:HD11	2.42	0.54
1:B:157:VAL:CG1	1:B:162:GLN:HB2	2.37	0.54
1:B:69:LEU:HD22	1:B:111:PHE:HE2	1.72	0.54
1:I:157:VAL:CG1	1:I:162:GLN:HB2	2.37	0.54
1:C:157:VAL:CG1	1:C:158:LEU:N	2.70	0.54
1:E:157:VAL:CG1	1:E:162:GLN:HB2	2.38	0.54
1:I:12:ASP:O	1:I:44:CYS:O	2.25	0.54
1:E:131:ILE:HD13	3:E:205:LMZ:H82	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:PHE:HB3	3:I:209:LMZ:H122	1.90	0.54
1:F:127:HIS:CE1	1:F:131:ILE:HD11	2.43	0.54
1:H:69:LEU:HD22	1:H:111:PHE:CE2	2.43	0.54
1:A:157:VAL:CG1	1:A:158:LEU:N	2.71	0.54
1:G:157:VAL:CG1	1:G:158:LEU:N	2.71	0.54
1:D:127:HIS:CE1	1:D:131:ILE:HD11	2.43	0.54
1:H:127:HIS:CE1	1:H:131:ILE:HD11	2.42	0.54
1:C:12:ASP:O	1:C:44:CYS:O	2.26	0.54
1:H:73:SER:HB3	1:H:111:PHE:CE2	2.43	0.54
1:J:10:GLN:HG3	1:J:44:CYS:SG	2.48	0.54
1:H:157:VAL:HG13	1:H:162:GLN:HB2	1.90	0.53
1:E:127:HIS:CE1	1:E:131:ILE:HD11	2.44	0.53
1:D:69:LEU:HD22	1:D:111:PHE:HE2	1.73	0.53
1:G:13:GLY:CA	1:G:16:LEU:HD22	2.38	0.53
1:A:13:GLY:HA3	1:A:16:LEU:HD22	1.89	0.53
1:D:73:SER:HB3	1:D:111:PHE:CE2	2.44	0.53
1:F:157:VAL:CG1	1:F:158:LEU:N	2.71	0.53
1:G:13:GLY:HA3	1:G:16:LEU:HD22	1.89	0.53
1:A:69:LEU:HD22	1:A:111:PHE:CE2	2.43	0.53
1:I:157:VAL:CG1	1:I:158:LEU:N	2.72	0.53
1:G:137:HIS:HE1	1:H:133:ASP:OD2	1.92	0.53
1:I:137:HIS:CE1	1:J:133:ASP:OD2	2.62	0.53
1:J:12:ASP:O	1:J:44:CYS:O	2.26	0.53
1:J:69:LEU:HD22	1:J:111:PHE:CE2	2.44	0.53
1:F:157:VAL:CG1	1:F:162:GLN:HB2	2.39	0.52
1:F:29:ILE:C	1:F:32:PRO:HD2	2.30	0.52
1:A:24:ARG:NH2	1:E:186:GLU:OE1	2.38	0.52
1:A:24:ARG:HD2	1:E:7:THR:OG1	2.09	0.52
1:A:69:LEU:HD22	1:A:111:PHE:HE2	1.74	0.52
1:G:29:ILE:C	1:G:32:PRO:HD2	2.30	0.52
1:H:29:ILE:C	1:H:32:PRO:HD2	2.30	0.52
1:J:157:VAL:CG1	1:J:158:LEU:N	2.72	0.52
1:J:73:SER:HB3	1:J:111:PHE:CE2	2.45	0.52
1:I:127:HIS:CE1	1:I:131:ILE:HD11	2.45	0.52
1:H:69:LEU:HD22	1:H:111:PHE:HE2	1.75	0.52
1:D:12:ASP:O	1:D:44:CYS:O	2.28	0.52
1:E:12:ASP:O	1:E:44:CYS:O	2.28	0.52
1:D:157:VAL:CG1	1:D:158:LEU:N	2.72	0.51
1:E:69:LEU:HD22	1:E:111:PHE:CE2	2.45	0.51
1:C:157:VAL:CG1	1:C:162:GLN:HB2	2.40	0.51
1:A:120:LEU:HD13	3:A:201:LMZ:N3	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:LEU:HD22	1:E:111:PHE:HE2	1.76	0.51
1:F:131:ILE:HD13	3:F:206:LMZ:H82	1.92	0.51
1:B:127:HIS:CE1	1:B:131:ILE:HD11	2.45	0.51
1:B:152:PHE:HB3	3:C:203:LMZ:H122	1.92	0.51
1:D:29:ILE:C	1:D:32:PRO:HD2	2.31	0.51
1:G:58:GLY:HA3	3:G:207:LMZ:O9	2.09	0.51
1:G:12:ASP:O	1:G:44:CYS:O	2.28	0.51
1:G:117:ILE:HA	1:G:153:GLY:O	2.11	0.51
1:J:69:LEU:HD22	1:J:111:PHE:HE2	1.76	0.51
1:D:7:THR:HG21	1:E:27:GLU:OE2	2.10	0.51
1:A:186:GLU:OE2	1:B:24:ARG:NH2	2.44	0.51
1:C:6:PRO:HB3	1:D:25:TRP:NE1	2.26	0.51
1:A:157:VAL:CG1	1:A:162:GLN:HB2	2.41	0.50
1:C:29:ILE:C	1:C:32:PRO:HD2	2.31	0.50
1:E:29:ILE:C	1:E:32:PRO:HD2	2.31	0.50
1:F:25:TRP:CD1	1:J:6:PRO:HB3	2.46	0.50
1:D:117:ILE:HA	1:D:153:GLY:O	2.11	0.50
1:F:10:GLN:HG3	1:F:44:CYS:SG	2.51	0.50
1:A:29:ILE:C	1:A:32:PRO:HD2	2.31	0.50
1:E:157:VAL:CG1	1:E:158:LEU:N	2.74	0.50
1:G:186:GLU:OE2	1:H:24:ARG:NH2	2.45	0.50
1:G:137:HIS:CE1	1:H:133:ASP:OD2	2.65	0.50
1:H:157:VAL:CG1	1:H:162:GLN:HB2	2.42	0.50
1:H:6:PRO:HB3	1:I:25:TRP:NE1	2.26	0.50
1:B:29:ILE:C	1:B:32:PRO:HD2	2.32	0.50
1:F:120:LEU:HD13	3:F:206:LMZ:N3	2.27	0.50
1:J:170:ILE:CG2	1:J:171:GLU:N	2.74	0.50
1:B:120:LEU:HD13	3:B:202:LMZ:N3	2.27	0.50
1:I:29:ILE:C	1:I:32:PRO:HD2	2.32	0.50
1:B:137:HIS:HE1	1:C:133:ASP:OD2	1.94	0.50
1:F:117:ILE:HA	1:F:153:GLY:O	2.12	0.50
1:D:152:PHE:HB2	1:E:60:TRP:CE2	2.47	0.50
1:J:170:ILE:HG22	1:J:173:SER:H	1.75	0.50
1:A:137:HIS:HE1	1:B:133:ASP:OD2	1.95	0.50
1:D:13:GLY:HA2	1:D:16:LEU:HD13	1.94	0.49
1:H:12:ASP:O	1:H:44:CYS:O	2.30	0.49
1:F:12:ASP:O	1:F:44:CYS:O	2.29	0.49
1:A:12:ASP:O	1:A:44:CYS:O	2.29	0.49
1:C:37:THR:HG21	1:C:117:ILE:CD1	2.42	0.49
1:I:69:LEU:HD22	1:I:111:PHE:CE2	2.47	0.49
1:I:142:VAL:O	1:I:146:THR:HG22	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:VAL:O	1:E:146:THR:HG22	2.12	0.49
1:C:117:ILE:HA	1:C:153:GLY:O	2.13	0.49
1:J:117:ILE:HA	1:J:153:GLY:O	2.12	0.49
1:G:6:PRO:HB3	1:H:25:TRP:CD1	2.48	0.49
1:H:120:LEU:HD13	3:H:208:LMZ:N3	2.28	0.49
1:E:73:SER:HB3	1:E:111:PHE:CE2	2.47	0.49
1:A:6:PRO:HB3	1:B:25:TRP:NE1	2.27	0.49
1:C:69:LEU:HD22	1:C:111:PHE:HE2	1.77	0.49
1:G:73:SER:HB3	1:G:111:PHE:CE2	2.48	0.49
1:F:73:SER:HB3	1:F:111:PHE:CE2	2.47	0.49
1:J:29:ILE:C	1:J:32:PRO:HD2	2.32	0.49
1:F:69:LEU:HD22	1:F:111:PHE:CE2	2.48	0.49
1:H:6:PRO:HB3	1:I:25:TRP:CD1	2.47	0.49
1:C:69:LEU:HD22	1:C:111:PHE:CE2	2.48	0.49
1:A:73:SER:HB3	1:A:111:PHE:CE2	2.47	0.49
1:C:6:PRO:HB3	1:D:25:TRP:CD1	2.48	0.48
1:J:24:ARG:O	1:J:27:GLU:HG2	2.13	0.48
1:A:61:GLU:OE2	3:A:201:LMZ:O12	2.31	0.48
1:G:29:ILE:O	1:G:32:PRO:HD2	2.13	0.48
1:I:117:ILE:HA	1:I:153:GLY:O	2.13	0.48
1:A:10:GLN:HG3	1:A:44:CYS:SG	2.54	0.48
1:F:69:LEU:HD22	1:F:111:PHE:HE2	1.78	0.48
1:C:131:ILE:HD13	3:C:203:LMZ:H82	1.94	0.48
1:F:6:PRO:HB3	1:G:25:TRP:CD1	2.49	0.48
1:C:137:HIS:HE1	1:D:133:ASP:OD2	1.96	0.48
1:B:142:VAL:O	1:B:146:THR:HG22	2.14	0.48
1:H:131:ILE:HD13	3:H:208:LMZ:H82	1.95	0.48
1:A:126:MET:O	1:A:129:GLU:HG2	2.14	0.47
1:A:13:GLY:HA2	1:A:16:LEU:HD13	1.96	0.47
1:H:29:ILE:O	1:H:32:PRO:HD2	2.14	0.47
1:D:144:LEU:CD1	1:E:141:ARG:HD3	2.44	0.47
1:D:142:VAL:O	1:D:146:THR:HG22	2.13	0.47
1:D:144:LEU:HD12	1:E:141:ARG:HD3	1.96	0.47
1:A:117:ILE:HA	1:A:153:GLY:O	2.14	0.47
1:I:69:LEU:HD22	1:I:111:PHE:HE2	1.79	0.47
1:C:7:THR:HG21	1:D:27:GLU:OE2	2.14	0.47
1:C:144:LEU:HD12	1:D:141:ARG:HD3	1.96	0.47
1:A:24:ARG:NH2	1:E:186:GLU:OE2	2.47	0.47
1:H:117:ILE:HA	1:H:153:GLY:O	2.15	0.47
1:G:186:GLU:OE1	1:H:24:ARG:NH2	2.43	0.47
1:A:59:SER:HA	1:A:62:LEU:HD22	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:206:LMZ:H122	1:J:152:PHE:HB3	1.96	0.47
1:C:73:SER:HB3	1:C:111:PHE:CE2	2.49	0.47
1:C:137:HIS:CE1	1:D:133:ASP:OD2	2.68	0.47
1:H:142:VAL:O	1:H:146:THR:HG22	2.14	0.47
1:F:24:ARG:HD2	1:J:7:THR:OG1	2.15	0.47
1:F:6:PRO:HB3	1:G:25:TRP:NE1	2.30	0.47
1:F:25:TRP:NE1	1:J:6:PRO:HB3	2.30	0.47
3:A:201:LMZ:H122	1:E:152:PHE:H	1.80	0.47
1:F:13:GLY:HA2	1:F:16:LEU:HD13	1.97	0.47
1:G:10:GLN:HG3	1:G:44:CYS:SG	2.56	0.47
1:D:186:GLU:OE2	1:E:24:ARG:NH2	2.48	0.46
1:F:24:ARG:NH2	1:J:186:GLU:OE1	2.42	0.46
1:I:13:GLY:HA2	1:I:16:LEU:HD13	1.96	0.46
1:J:13:GLY:HA2	1:J:16:LEU:HD13	1.97	0.46
1:C:142:VAL:O	1:C:146:THR:HG22	2.16	0.46
1:B:137:HIS:CE1	1:C:133:ASP:OD2	2.68	0.46
1:B:107:SER:O	1:B:108:THR:O	2.34	0.46
1:B:13:GLY:HA2	1:B:16:LEU:HD13	1.98	0.46
1:G:120:LEU:HD13	3:G:207:LMZ:N3	2.31	0.46
1:F:133:ASP:OD2	1:J:137:HIS:HE1	1.97	0.46
1:A:142:VAL:O	1:A:146:THR:HG22	2.15	0.46
1:F:152:PHE:HB3	3:G:207:LMZ:H122	1.98	0.46
1:D:137:HIS:HE1	1:E:133:ASP:OD2	1.98	0.46
1:C:7:THR:CG2	1:D:27:GLU:HG3	2.46	0.46
1:G:152:PHE:HB3	3:H:208:LMZ:H122	1.97	0.46
1:G:126:MET:O	1:G:129:GLU:HG2	2.16	0.46
1:B:73:SER:HB3	1:B:111:PHE:CE2	2.51	0.46
1:B:24:ARG:O	1:B:27:GLU:HG2	2.15	0.46
1:J:131:ILE:HD13	3:J:210:LMZ:H82	1.98	0.46
1:A:137:HIS:CE1	1:B:133:ASP:OD2	2.69	0.46
1:H:9:GLN:NE2	1:H:11:HIS:NE2	2.64	0.46
1:C:24:ARG:O	1:C:27:GLU:HG2	2.17	0.45
1:B:143:GLN:HG2	1:C:64:ILE:HB	1.97	0.45
1:B:117:ILE:HA	1:B:153:GLY:O	2.15	0.45
1:F:186:GLU:OE2	1:G:24:ARG:NH2	2.49	0.45
1:E:29:ILE:O	1:E:32:PRO:HD2	2.15	0.45
1:E:64:ILE:HG23	1:E:65:ALA:N	2.31	0.45
1:F:9:GLN:NE2	1:F:11:HIS:NE2	2.64	0.45
1:J:9:GLN:NE2	1:J:11:HIS:NE2	2.64	0.45
1:C:120:LEU:HD13	3:C:203:LMZ:N3	2.30	0.45
1:B:166:ARG:NH2	2:C:303:SO4:O3	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:THR:HG23	1:D:27:GLU:HG3	1.98	0.45
1:C:191:ARG:HG2	1:C:191:ARG:HH11	1.80	0.45
1:E:24:ARG:O	1:E:27:GLU:HG2	2.17	0.45
1:H:59:SER:HA	1:H:62:LEU:HD22	1.98	0.45
1:I:152:PHE:HB3	3:J:210:LMZ:H122	1.97	0.45
1:G:13:GLY:HA2	1:G:16:LEU:HD13	1.99	0.45
1:J:59:SER:HA	1:J:62:LEU:HD22	1.99	0.45
1:D:29:ILE:O	1:D:32:PRO:HD2	2.16	0.45
1:B:29:ILE:O	1:B:32:PRO:HD2	2.17	0.45
1:C:144:LEU:CD1	1:D:141:ARG:HD3	2.46	0.45
1:E:117:ILE:HA	1:E:153:GLY:O	2.17	0.45
1:D:59:SER:HA	1:D:62:LEU:HD22	1.97	0.45
1:A:29:ILE:O	1:A:32:PRO:HD2	2.17	0.45
1:G:9:GLN:NE2	1:G:11:HIS:NE2	2.65	0.45
1:G:142:VAL:O	1:G:146:THR:HG22	2.17	0.45
1:A:7:THR:CG2	1:B:27:GLU:HG3	2.47	0.45
1:I:126:MET:O	1:I:129:GLU:HG2	2.16	0.45
1:J:143:GLN:NE2	1:J:150:VAL:H	2.04	0.45
1:C:58:GLY:HA3	3:C:203:LMZ:O9	2.17	0.45
1:J:64:ILE:HG23	1:J:65:ALA:N	2.32	0.45
1:E:5:GLY:HA2	1:E:6:PRO:HD3	1.75	0.45
1:E:126:MET:O	1:E:129:GLU:HG2	2.17	0.45
1:H:186:GLU:OE1	1:I:24:ARG:NH2	2.40	0.45
1:D:7:THR:HG21	1:E:27:GLU:HG3	1.99	0.45
1:H:143:GLN:NE2	1:H:150:VAL:H	2.03	0.44
1:F:59:SER:HA	1:F:62:LEU:HD22	1.99	0.44
1:F:126:MET:O	1:F:129:GLU:HG2	2.17	0.44
1:E:59:SER:HA	1:E:62:LEU:HD22	1.99	0.44
1:D:131:ILE:HD13	3:D:204:LMZ:H82	1.99	0.44
1:I:29:ILE:O	1:I:32:PRO:HD2	2.17	0.44
1:I:186:GLU:OE2	1:J:24:ARG:NH2	2.49	0.44
1:A:9:GLN:NE2	1:A:11:HIS:NE2	2.66	0.44
1:C:9:GLN:NE2	1:C:11:HIS:NE2	2.66	0.44
1:D:126:MET:O	1:D:129:GLU:HG2	2.18	0.44
1:H:13:GLY:HA2	1:H:16:LEU:HD13	2.00	0.44
1:H:24:ARG:O	1:H:27:GLU:HG2	2.17	0.44
1:F:142:VAL:O	1:F:146:THR:HG22	2.16	0.44
1:F:24:ARG:O	1:F:27:GLU:HG2	2.17	0.44
1:I:120:LEU:HD13	3:I:209:LMZ:N3	2.32	0.44
1:F:133:ASP:OD2	1:J:137:HIS:CE1	2.70	0.44
1:J:107:SER:O	1:J:108:THR:O	2.36	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:LEU:HD12	1:F:182:LEU:HA	1.88	0.44
3:A:201:LMZ:C12	1:E:152:PHE:H	2.31	0.43
1:D:7:THR:OG1	1:E:24:ARG:HD2	2.18	0.43
1:G:73:SER:OG	1:G:110:PRO:HA	2.18	0.43
1:C:29:ILE:O	1:C:32:PRO:HD2	2.18	0.43
1:B:64:ILE:HG23	1:B:65:ALA:N	2.33	0.43
1:H:7:THR:OG1	1:I:24:ARG:HB3	2.18	0.43
1:G:24:ARG:O	1:G:27:GLU:HG2	2.19	0.43
1:J:142:VAL:O	1:J:146:THR:HG22	2.17	0.43
1:A:24:ARG:HD2	1:E:7:THR:HG1	1.83	0.43
1:J:126:MET:O	1:J:129:GLU:HG2	2.18	0.43
1:I:59:SER:HA	1:I:62:LEU:HD22	1.99	0.43
1:G:59:SER:HA	1:G:62:LEU:HD22	1.99	0.43
1:G:127:HIS:NE2	1:G:131:ILE:CD1	2.82	0.43
1:D:182:LEU:HA	1:D:182:LEU:HD12	1.88	0.43
1:G:7:THR:OG1	1:H:24:ARG:HD2	2.18	0.43
1:A:107:SER:O	1:A:108:THR:O	2.37	0.43
1:F:70:TYR:CE1	1:F:148:VAL:HG21	2.53	0.43
1:H:126:MET:O	1:H:129:GLU:HG2	2.18	0.43
1:I:24:ARG:O	1:I:27:GLU:HG2	2.19	0.43
1:F:58:GLY:HA3	3:F:206:LMZ:O9	2.19	0.43
1:D:137:HIS:CE1	1:E:133:ASP:OD2	2.72	0.43
1:F:24:ARG:NH2	1:J:186:GLU:OE2	2.50	0.43
1:F:7:THR:OG1	1:G:24:ARG:HD2	2.19	0.43
1:F:29:ILE:O	1:F:32:PRO:HD2	2.18	0.43
1:F:141:ARG:HD3	1:J:144:LEU:CD1	2.49	0.43
1:F:141:ARG:HD3	1:J:144:LEU:HD12	2.01	0.43
1:G:70:TYR:CE1	1:G:148:VAL:HG21	2.53	0.43
1:H:13:GLY:HA3	1:H:185:VAL:HG13	2.01	0.43
1:B:186:GLU:OE2	1:C:24:ARG:NH2	2.52	0.43
1:H:186:GLU:CD	1:I:24:ARG:NH2	2.72	0.43
1:A:6:PRO:HB3	1:B:25:TRP:CD1	2.54	0.43
1:D:9:GLN:NE2	1:D:11:HIS:NE2	2.66	0.43
1:B:59:SER:HA	1:B:62:LEU:HD22	2.00	0.42
1:B:73:SER:OG	1:B:110:PRO:HA	2.19	0.42
1:H:64:ILE:HG23	1:H:65:ALA:N	2.34	0.42
1:C:190:ARG:NH2	2:C:402:SO4:O1	2.49	0.42
1:E:13:GLY:HA2	1:E:16:LEU:HD13	1.99	0.42
1:A:24:ARG:O	1:A:27:GLU:HG2	2.18	0.42
1:H:70:TYR:CE1	1:H:148:VAL:HG21	2.54	0.42
1:A:127:HIS:NE2	1:A:131:ILE:CD1	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ILE:O	1:B:173:SER:HB3	2.19	0.42
1:B:9:GLN:NE2	1:B:11:HIS:NE2	2.67	0.42
1:I:144:LEU:HD12	1:J:141:ARG:HD3	2.01	0.42
1:B:126:MET:O	1:B:129:GLU:HG2	2.20	0.42
3:A:201:LMZ:H122	1:E:152:PHE:N	2.34	0.42
1:C:13:GLY:HA2	1:C:16:LEU:HD13	2.00	0.42
1:J:29:ILE:O	1:J:32:PRO:HD2	2.20	0.42
1:A:182:LEU:HD12	1:A:182:LEU:HA	1.90	0.42
1:J:70:TYR:CE1	1:J:148:VAL:HG21	2.54	0.42
1:F:37:THR:HG21	1:F:117:ILE:CD1	2.48	0.42
1:G:6:PRO:HB3	1:H:25:TRP:NE1	2.35	0.42
2:F:306:SO4:O3	1:J:166:ARG:NH2	2.47	0.42
1:C:62:LEU:HA	1:C:62:LEU:HD12	1.88	0.42
1:J:123:GLY:HA3	2:J:310:SO4:O1	2.19	0.42
1:E:70:TYR:CE1	1:E:148:VAL:HG21	2.55	0.42
1:E:13:GLY:HA2	1:E:16:LEU:HD22	2.01	0.42
1:F:64:ILE:HG23	1:F:65:ALA:N	2.35	0.42
1:C:126:MET:O	1:C:129:GLU:HG2	2.19	0.42
1:G:64:ILE:HG23	1:G:65:ALA:N	2.35	0.42
1:B:199:THR:HG23	1:C:76:GLN:NE2	2.34	0.42
1:D:70:TYR:CE1	1:D:148:VAL:HG21	2.55	0.41
1:C:186:GLU:OE1	1:D:24:ARG:NH2	2.48	0.41
1:E:182:LEU:HD12	1:E:182:LEU:HA	1.89	0.41
1:H:7:THR:HG21	1:I:27:GLU:OE2	2.21	0.41
1:I:170:ILE:HG22	1:I:171:GLU:N	2.36	0.41
1:B:6:PRO:HB3	1:C:25:TRP:CD1	2.55	0.41
1:A:37:THR:HG21	1:A:117:ILE:CD1	2.47	0.41
1:C:59:SER:HA	1:C:62:LEU:HD22	2.02	0.41
1:J:13:GLY:HA2	1:J:16:LEU:HD22	2.02	0.41
1:C:186:GLU:OE2	1:D:24:ARG:NH2	2.53	0.41
1:F:191:ARG:HG2	1:F:191:ARG:HH11	1.86	0.41
1:F:168:GLY:HA2	1:F:173:SER:O	2.20	0.41
1:H:157:VAL:HG13	1:H:158:LEU:N	2.35	0.41
1:B:131:ILE:HD13	3:B:202:LMZ:C8	2.49	0.41
1:D:170:ILE:O	1:D:171:GLU:C	2.59	0.41
1:I:107:SER:O	1:I:108:THR:O	2.38	0.41
1:C:64:ILE:HG23	1:C:65:ALA:N	2.35	0.41
1:E:37:THR:HG21	1:E:117:ILE:CD1	2.47	0.41
1:B:120:LEU:HD13	3:B:202:LMZ:C2	2.50	0.41
1:G:107:SER:O	1:G:108:THR:O	2.38	0.41
1:C:107:SER:O	1:C:108:THR:O	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:64:ILE:HG23	1:I:65:ALA:N	2.35	0.41
1:B:144:LEU:HD12	1:C:141:ARG:HD3	2.03	0.41
1:I:182:LEU:HA	1:I:182:LEU:HD12	1.89	0.41
1:E:13:GLY:HA3	1:E:185:VAL:HG13	2.02	0.41
1:H:13:GLY:HA2	1:H:16:LEU:HD22	2.02	0.41
1:D:24:ARG:O	1:D:27:GLU:HG2	2.21	0.41
1:E:107:SER:O	1:E:108:THR:O	2.38	0.41
1:E:22:HIS:CD2	1:E:30:ILE:HG21	2.55	0.41
1:E:143:GLN:NE2	1:E:150:VAL:H	2.03	0.41
1:F:144:LEU:CD1	1:G:141:ARG:HD3	2.51	0.41
1:I:9:GLN:NE2	1:I:11:HIS:NE2	2.67	0.41
1:J:112:ASP:OD1	1:J:192:ARG:NH1	2.54	0.41
1:A:58:GLY:HA3	3:A:201:LMZ:O9	2.21	0.41
1:F:186:GLU:OE1	1:G:24:ARG:NH2	2.46	0.41
1:J:170:ILE:HG23	1:J:171:GLU:N	2.36	0.41
1:F:107:SER:O	1:F:108:THR:O	2.39	0.41
1:H:191:ARG:HG2	1:H:191:ARG:HH11	1.86	0.41
1:A:27:GLU:CG	1:E:7:THR:HG21	2.49	0.41
1:F:34:LEU:O	1:F:37:THR:HG23	2.20	0.41
1:C:7:THR:OG1	1:D:24:ARG:HD2	2.21	0.41
1:E:62:LEU:HD12	1:E:62:LEU:HA	1.88	0.41
1:G:127:HIS:NE2	1:G:131:ILE:HD12	2.36	0.41
1:D:22:HIS:CD2	1:D:30:ILE:HG21	2.56	0.41
1:B:157:VAL:HG13	1:B:158:LEU:N	2.36	0.40
1:F:13:GLY:HA2	1:F:16:LEU:HD22	2.03	0.40
1:J:58:GLY:HA3	3:J:210:LMZ:O9	2.22	0.40
1:C:152:PHE:HB2	1:D:60:TRP:CE2	2.56	0.40
1:E:58:GLY:HA3	3:E:205:LMZ:O9	2.21	0.40
1:C:191:ARG:HG2	1:C:191:ARG:NH1	2.35	0.40
1:E:18:ILE:HD12	1:E:113:ALA:HB3	2.02	0.40
1:B:182:LEU:HA	1:B:182:LEU:HD12	1.88	0.40
1:B:126:MET:CE	1:B:129:GLU:HG3	2.51	0.40
1:C:13:GLY:HA2	1:C:16:LEU:HD22	2.04	0.40
1:C:9:GLN:HB3	1:C:9:GLN:HE21	1.67	0.40
1:F:144:LEU:HD12	1:G:141:ARG:HD3	2.02	0.40
1:F:112:ASP:OD1	1:F:192:ARG:NH1	2.54	0.40
1:A:64:ILE:HG23	1:A:65:ALA:N	2.35	0.40
1:B:55:SER:OG	2:B:401:SO4:O2	2.30	0.40
1:D:112:ASP:OD1	1:D:192:ARG:NH1	2.54	0.40
1:G:170:ILE:CG2	1:G:171:GLU:N	2.84	0.40
1:A:25:TRP:HA	1:E:6:PRO:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:37:THR:HG21	1:I:117:ILE:CD1	2.50	0.40
1:A:62:LEU:HA	1:A:62:LEU:HD12	1.88	0.40
1:E:10:GLN:HG3	1:E:44:CYS:SG	2.61	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLU:OE2	1:H:12:ASP:OD2[2_565]	2.15	0.05

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	161/200 (80%)	155 (96%)	4 (2%)	2 (1%)	16	52
1	B	161/200 (80%)	155 (96%)	4 (2%)	2 (1%)	16	52
1	C	161/200 (80%)	154 (96%)	5 (3%)	2 (1%)	16	52
1	D	161/200 (80%)	153 (95%)	5 (3%)	3 (2%)	10	40
1	E	161/200 (80%)	154 (96%)	5 (3%)	2 (1%)	16	52
1	F	161/200 (80%)	154 (96%)	4 (2%)	3 (2%)	10	40
1	G	161/200 (80%)	153 (95%)	5 (3%)	3 (2%)	10	40
1	H	161/200 (80%)	154 (96%)	6 (4%)	1 (1%)	30	68
1	I	161/200 (80%)	154 (96%)	5 (3%)	2 (1%)	16	52
1	J	161/200 (80%)	152 (94%)	4 (2%)	5 (3%)	5	27
All	All	1610/2000 (80%)	1538 (96%)	47 (3%)	25 (2%)	12	44

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	THR
1	B	108	THR
1	C	108	THR
1	D	108	THR
1	E	108	THR
1	F	108	THR
1	F	171	GLU
1	G	108	THR
1	G	171	GLU
1	H	108	THR
1	I	108	THR
1	J	108	THR
1	J	171	GLU
1	J	173	SER
1	D	12	ASP
1	I	12	ASP
1	B	12	ASP
1	C	12	ASP
1	D	171	GLU
1	E	12	ASP
1	G	12	ASP
1	J	12	ASP
1	A	12	ASP
1	F	12	ASP
1	J	170	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/159 (82%)	125 (96%)	5 (4%)	40	76
1	B	130/159 (82%)	125 (96%)	5 (4%)	40	76
1	C	130/159 (82%)	125 (96%)	5 (4%)	40	76
1	D	130/159 (82%)	125 (96%)	5 (4%)	40	76
1	E	130/159 (82%)	125 (96%)	5 (4%)	40	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	130/159 (82%)	124 (95%)	6 (5%)	33	70
1	G	130/159 (82%)	125 (96%)	5 (4%)	40	76
1	H	130/159 (82%)	125 (96%)	5 (4%)	40	76
1	I	130/159 (82%)	124 (95%)	6 (5%)	33	70
1	J	130/159 (82%)	125 (96%)	5 (4%)	40	76
All	All	1300/1590 (82%)	1248 (96%)	52 (4%)	38	75

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	37	THR
1	A	62	LEU
1	A	69	LEU
1	A	182	LEU
1	B	31	GLU
1	B	37	THR
1	B	62	LEU
1	B	69	LEU
1	B	182	LEU
1	C	31	GLU
1	C	37	THR
1	C	62	LEU
1	C	69	LEU
1	C	182	LEU
1	D	31	GLU
1	D	37	THR
1	D	62	LEU
1	D	69	LEU
1	D	182	LEU
1	E	31	GLU
1	E	37	THR
1	E	62	LEU
1	E	69	LEU
1	E	182	LEU
1	F	31	GLU
1	F	37	THR
1	F	62	LEU
1	F	69	LEU
1	F	173	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	182	LEU
1	G	31	GLU
1	G	37	THR
1	G	62	LEU
1	G	69	LEU
1	G	182	LEU
1	H	31	GLU
1	H	37	THR
1	H	62	LEU
1	H	69	LEU
1	H	182	LEU
1	I	31	GLU
1	I	37	THR
1	I	62	LEU
1	I	69	LEU
1	I	171	GLU
1	I	182	LEU
1	J	31	GLU
1	J	37	THR
1	J	62	LEU
1	J	69	LEU
1	J	182	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	22	HIS
1	A	50	ASN
1	A	143	GLN
1	B	9	GLN
1	B	22	HIS
1	B	50	ASN
1	B	143	GLN
1	C	9	GLN
1	C	22	HIS
1	C	50	ASN
1	C	143	GLN
1	D	9	GLN
1	D	22	HIS
1	D	50	ASN
1	D	143	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	9	GLN
1	E	22	HIS
1	E	50	ASN
1	E	143	GLN
1	F	9	GLN
1	F	22	HIS
1	F	50	ASN
1	F	143	GLN
1	G	9	GLN
1	G	22	HIS
1	G	50	ASN
1	G	143	GLN
1	H	9	GLN
1	H	22	HIS
1	H	50	ASN
1	H	143	GLN
1	I	9	GLN
1	I	22	HIS
1	I	50	ASN
1	I	137	HIS
1	I	143	GLN
1	J	9	GLN
1	J	22	HIS
1	J	50	ASN
1	J	143	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 ⓘ

30 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	LMZ	A	201	-	15,20,20	2.77	9 (60%)	18,27,27	3.98	8 (44%)
2	SO4	A	301	-	4,4,4	0.25	0	6,6,6	0.28	0
2	SO4	A	404	-	4,4,4	1.06	0	6,6,6	0.33	0
3	LMZ	B	202	-	15,20,20	2.93	8 (53%)	18,27,27	3.91	8 (44%)
2	SO4	B	302	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	B	401	-	4,4,4	0.68	0	6,6,6	0.28	0
3	LMZ	C	203	-	15,20,20	2.87	9 (60%)	18,27,27	3.98	8 (44%)
2	SO4	C	303	-	4,4,4	0.16	0	6,6,6	0.08	0
2	SO4	C	402	-	4,4,4	0.68	0	6,6,6	0.29	0
2	SO4	C	410	-	4,4,4	1.58	1 (25%)	6,6,6	0.50	0
3	LMZ	D	204	-	15,20,20	2.83	9 (60%)	18,27,27	3.99	8 (44%)
2	SO4	D	304	-	4,4,4	0.15	0	6,6,6	0.11	0
3	LMZ	E	205	-	15,20,20	2.93	9 (60%)	18,27,27	3.92	8 (44%)
2	SO4	E	305	-	4,4,4	0.08	0	6,6,6	0.15	0
2	SO4	E	403	-	4,4,4	1.05	0	6,6,6	0.10	0
3	LMZ	F	206	-	15,20,20	2.85	8 (53%)	18,27,27	3.96	8 (44%)
2	SO4	F	306	-	4,4,4	0.17	0	6,6,6	0.10	0
2	SO4	F	405	-	4,4,4	0.85	0	6,6,6	0.17	0
3	LMZ	G	207	-	15,20,20	2.87	9 (60%)	18,27,27	3.93	8 (44%)
2	SO4	G	307	-	4,4,4	0.12	0	6,6,6	0.06	0
3	LMZ	H	208	-	15,20,20	2.92	8 (53%)	18,27,27	3.98	8 (44%)
2	SO4	H	308	-	4,4,4	0.11	0	6,6,6	0.12	0
2	SO4	H	406	-	4,4,4	0.85	0	6,6,6	0.27	0
3	LMZ	I	209	-	15,20,20	2.79	9 (60%)	18,27,27	4.00	8 (44%)
2	SO4	I	309	-	4,4,4	0.09	0	6,6,6	0.15	0
2	SO4	I	407	-	4,4,4	0.70	0	6,6,6	0.16	0
2	SO4	I	409	-	4,4,4	1.58	1 (25%)	6,6,6	0.50	0
3	LMZ	J	210	-	15,20,20	2.94	9 (60%)	18,27,27	3.95	8 (44%)
2	SO4	J	310	-	4,4,4	0.15	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	J	408	-	4,4,4	1.16	0	6,6,6	0.13	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	LMZ	A	201	-	-	0/17/17/17	0/1/1/1
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	A	404	-	-	0/0/0/0	0/0/0/0
3	LMZ	B	202	-	-	0/17/17/17	0/1/1/1
2	SO4	B	302	-	-	0/0/0/0	0/0/0/0
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
3	LMZ	C	203	-	-	0/17/17/17	0/1/1/1
2	SO4	C	303	-	-	0/0/0/0	0/0/0/0
2	SO4	C	402	-	-	0/0/0/0	0/0/0/0
2	SO4	C	410	-	-	0/0/0/0	0/0/0/0
3	LMZ	D	204	-	-	0/17/17/17	0/1/1/1
2	SO4	D	304	-	-	0/0/0/0	0/0/0/0
3	LMZ	E	205	-	-	0/17/17/17	0/1/1/1
2	SO4	E	305	-	-	0/0/0/0	0/0/0/0
2	SO4	E	403	-	-	0/0/0/0	0/0/0/0
3	LMZ	F	206	-	-	0/17/17/17	0/1/1/1
2	SO4	F	306	-	-	0/0/0/0	0/0/0/0
2	SO4	F	405	-	-	0/0/0/0	0/0/0/0
3	LMZ	G	207	-	-	0/17/17/17	0/1/1/1
2	SO4	G	307	-	-	0/0/0/0	0/0/0/0
3	LMZ	H	208	-	-	0/17/17/17	0/1/1/1
2	SO4	H	308	-	-	0/0/0/0	0/0/0/0
2	SO4	H	406	-	-	0/0/0/0	0/0/0/0
3	LMZ	I	209	-	-	0/17/17/17	0/1/1/1
2	SO4	I	309	-	-	0/0/0/0	0/0/0/0
2	SO4	I	407	-	-	0/0/0/0	0/0/0/0
2	SO4	I	409	-	-	0/0/0/0	0/0/0/0
3	LMZ	J	210	-	-	0/17/17/17	0/1/1/1
2	SO4	J	310	-	-	0/0/0/0	0/0/0/0
2	SO4	J	408	-	-	0/0/0/0	0/0/0/0

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	210	LMZ	C6-N7	2.06	1.37	1.34
3	F	206	LMZ	C6-N7	2.09	1.37	1.34
3	D	204	LMZ	C6-N7	2.14	1.37	1.34
3	I	209	LMZ	C6-N7	2.16	1.37	1.34
3	J	210	LMZ	C8-N7	2.18	1.49	1.45
3	B	202	LMZ	C5-N5	2.19	1.42	1.35
3	H	208	LMZ	C5-N5	2.19	1.42	1.35
3	C	203	LMZ	C5-N5	2.22	1.42	1.35
2	C	410	SO4	O3-S	2.24	1.55	1.47
2	I	409	SO4	O3-S	2.24	1.55	1.47
3	H	208	LMZ	C12-C11	2.25	1.58	1.52
3	D	204	LMZ	C5-N5	2.27	1.42	1.35
3	A	201	LMZ	C12-C11	2.30	1.58	1.52
3	C	203	LMZ	C6-N7	2.33	1.38	1.34
3	A	201	LMZ	C8-N7	2.33	1.49	1.45
3	A	201	LMZ	C6-N7	2.37	1.38	1.34
3	A	201	LMZ	C5-N5	2.39	1.43	1.35
3	I	209	LMZ	C12-C11	2.40	1.59	1.52
3	C	203	LMZ	C8-N7	2.41	1.50	1.45
3	G	207	LMZ	C5-N5	2.41	1.43	1.35
3	G	207	LMZ	C6-N7	2.41	1.38	1.34
3	F	206	LMZ	C5-N5	2.43	1.43	1.35
3	H	208	LMZ	C8-N7	2.43	1.50	1.45
3	E	205	LMZ	C5-N5	2.43	1.43	1.35
3	C	203	LMZ	C12-C11	2.45	1.59	1.52
3	E	205	LMZ	C6-N7	2.46	1.38	1.34
3	B	202	LMZ	C8-N7	2.46	1.50	1.45
3	E	205	LMZ	C8-N7	2.48	1.50	1.45
3	J	210	LMZ	C5-N5	2.49	1.43	1.35
3	I	209	LMZ	C6-N1	2.51	1.39	1.34
3	I	209	LMZ	C8-N7	2.52	1.50	1.45
3	A	201	LMZ	C6-N1	2.52	1.39	1.34
3	J	210	LMZ	C12-C11	2.57	1.59	1.52
3	I	209	LMZ	C4-N3	2.57	1.37	1.33
3	C	203	LMZ	C6-N1	2.58	1.39	1.34
3	D	204	LMZ	C12-C11	2.58	1.59	1.52
3	G	207	LMZ	C12-C11	2.58	1.59	1.52
3	E	205	LMZ	C6-N1	2.59	1.39	1.34
3	J	210	LMZ	C6-N1	2.59	1.39	1.34
3	F	206	LMZ	C6-N1	2.60	1.39	1.34
3	H	208	LMZ	C6-N1	2.61	1.39	1.34
3	D	204	LMZ	C8-N7	2.63	1.50	1.45
3	G	207	LMZ	C8-N7	2.64	1.50	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	LMZ	C12-C11	2.64	1.59	1.52
3	D	204	LMZ	C6-N1	2.67	1.39	1.34
3	E	205	LMZ	C9-C10	2.72	1.59	1.53
3	F	206	LMZ	C12-C11	2.75	1.60	1.52
3	G	207	LMZ	C6-N1	2.75	1.39	1.34
3	D	204	LMZ	C4-N3	2.76	1.38	1.33
3	E	205	LMZ	C12-C11	2.77	1.60	1.52
3	B	202	LMZ	C6-N1	2.77	1.39	1.34
3	A	201	LMZ	C9-C10	2.79	1.59	1.53
3	G	207	LMZ	C9-C10	2.80	1.59	1.53
3	I	209	LMZ	C5-N5	2.81	1.44	1.35
3	I	209	LMZ	C9-C10	2.95	1.59	1.53
3	H	208	LMZ	C4-N3	2.95	1.38	1.33
3	F	206	LMZ	C4-N3	2.95	1.38	1.33
3	D	204	LMZ	C9-C10	3.04	1.59	1.53
3	C	203	LMZ	C4-N3	3.07	1.38	1.33
3	J	210	LMZ	C4-N3	3.07	1.38	1.33
3	E	205	LMZ	C4-N3	3.11	1.38	1.33
3	A	201	LMZ	C4-N3	3.15	1.38	1.33
3	F	206	LMZ	C9-C10	3.18	1.60	1.53
3	G	207	LMZ	C4-N3	3.19	1.39	1.33
3	C	203	LMZ	C9-C10	3.28	1.60	1.53
3	J	210	LMZ	C9-C10	3.37	1.60	1.53
3	B	202	LMZ	C4-N3	3.38	1.39	1.33
3	B	202	LMZ	C9-C10	3.45	1.60	1.53
3	H	208	LMZ	C9-C10	3.66	1.60	1.53
3	A	201	LMZ	C11-C10	5.51	1.64	1.53
3	I	209	LMZ	O4-C4	5.57	1.38	1.24
3	C	203	LMZ	C11-C10	5.85	1.65	1.53
3	D	204	LMZ	O4-C4	5.88	1.38	1.24
3	G	207	LMZ	O4-C4	5.92	1.38	1.24
3	G	207	LMZ	C11-C10	5.93	1.65	1.53
3	J	210	LMZ	O4-C4	5.97	1.39	1.24
3	D	204	LMZ	C11-C10	5.98	1.65	1.53
3	F	206	LMZ	C11-C10	5.99	1.65	1.53
3	E	205	LMZ	O4-C4	6.02	1.39	1.24
3	A	201	LMZ	O4-C4	6.03	1.39	1.24
3	I	209	LMZ	C11-C10	6.03	1.65	1.53
3	F	206	LMZ	O4-C4	6.04	1.39	1.24
3	B	202	LMZ	C11-C10	6.10	1.65	1.53
3	H	208	LMZ	O4-C4	6.12	1.39	1.24
3	B	202	LMZ	O4-C4	6.12	1.39	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	203	LMZ	O4-C4	6.14	1.39	1.24
3	H	208	LMZ	C11-C10	6.29	1.66	1.53
3	E	205	LMZ	C11-C10	6.39	1.66	1.53
3	J	210	LMZ	C11-C10	6.48	1.66	1.53

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	LMZ	O11-C11-C10	-5.20	95.95	109.02
3	J	210	LMZ	O11-C11-C10	-5.14	96.09	109.02
3	D	204	LMZ	O11-C11-C10	-5.12	96.14	109.02
3	I	209	LMZ	O11-C11-C10	-5.03	96.36	109.02
3	G	207	LMZ	O11-C11-C10	-5.02	96.39	109.02
3	F	206	LMZ	O11-C11-C10	-5.00	96.44	109.02
3	B	202	LMZ	O11-C11-C10	-4.95	96.57	109.02
3	E	205	LMZ	O11-C11-C10	-4.93	96.61	109.02
3	C	203	LMZ	O11-C11-C10	-4.89	96.72	109.02
3	A	201	LMZ	C5-C4-N3	-4.75	117.09	123.59
3	H	208	LMZ	C5-C4-N3	-4.73	117.12	123.59
3	C	203	LMZ	C5-C4-N3	-4.71	117.15	123.59
3	B	202	LMZ	C5-C4-N3	-4.69	117.18	123.59
3	H	208	LMZ	O11-C11-C10	-4.68	97.25	109.02
3	I	209	LMZ	C5-C4-N3	-4.63	117.26	123.59
3	F	206	LMZ	C5-C4-N3	-4.61	117.28	123.59
3	J	210	LMZ	C5-C4-N3	-4.61	117.29	123.59
3	D	204	LMZ	C5-C4-N3	-4.59	117.31	123.59
3	G	207	LMZ	C5-C4-N3	-4.48	117.46	123.59
3	H	208	LMZ	O11-C11-C12	-4.48	98.76	109.22
3	E	205	LMZ	C5-C4-N3	-4.48	117.46	123.59
3	C	203	LMZ	O11-C11-C12	-4.33	99.12	109.22
3	J	210	LMZ	O11-C11-C12	-4.17	99.49	109.22
3	D	204	LMZ	O11-C11-C12	-4.16	99.51	109.22
3	G	207	LMZ	O11-C11-C12	-4.13	99.57	109.22
3	A	201	LMZ	O11-C11-C12	-4.13	99.58	109.22
3	E	205	LMZ	O11-C11-C12	-4.12	99.60	109.22
3	I	209	LMZ	O11-C11-C12	-4.11	99.62	109.22
3	B	202	LMZ	O11-C11-C12	-4.10	99.64	109.22
3	F	206	LMZ	O11-C11-C12	-4.02	99.85	109.22
3	D	204	LMZ	O12-C12-C11	-3.54	103.40	111.10
3	G	207	LMZ	O12-C12-C11	-3.51	103.46	111.10
3	B	202	LMZ	O12-C12-C11	-3.36	103.79	111.10
3	A	201	LMZ	O12-C12-C11	-3.36	103.79	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	210	LMZ	O12-C12-C11	-3.31	103.89	111.10
3	H	208	LMZ	O12-C12-C11	-3.27	103.99	111.10
3	I	209	LMZ	O12-C12-C11	-3.09	104.37	111.10
3	E	205	LMZ	O12-C12-C11	-3.09	104.38	111.10
3	F	206	LMZ	O12-C12-C11	-3.03	104.50	111.10
3	C	203	LMZ	O12-C12-C11	-2.91	104.77	111.10
3	A	201	LMZ	C5-C6-N7	2.37	125.56	121.69
3	E	205	LMZ	C5-C6-N7	2.38	125.58	121.69
3	B	202	LMZ	C5-C6-N7	2.39	125.59	121.69
3	G	207	LMZ	C5-C6-N7	2.42	125.64	121.69
3	D	204	LMZ	C5-C6-N7	2.49	125.76	121.69
3	J	210	LMZ	C5-C6-N7	2.52	125.80	121.69
3	I	209	LMZ	C5-C6-N7	2.52	125.81	121.69
3	F	206	LMZ	C5-C6-N7	2.56	125.86	121.69
3	H	208	LMZ	C5-C6-N7	2.59	125.92	121.69
3	C	203	LMZ	C5-C6-N7	2.67	126.04	121.69
3	J	210	LMZ	C4-C5-C6	4.34	117.42	114.52
3	E	205	LMZ	C4-C5-C6	4.39	117.45	114.52
3	G	207	LMZ	C4-C5-C6	4.50	117.53	114.52
3	B	202	LMZ	C4-C5-C6	4.53	117.55	114.52
3	I	209	LMZ	C4-C5-C6	4.62	117.60	114.52
3	C	203	LMZ	C4-C5-C6	4.63	117.61	114.52
3	A	201	LMZ	C4-C5-C6	4.68	117.65	114.52
3	D	204	LMZ	C4-C5-C6	4.69	117.65	114.52
3	F	206	LMZ	C4-C5-C6	4.70	117.66	114.52
3	H	208	LMZ	C4-C5-C6	4.91	117.80	114.52
3	H	208	LMZ	C12-C11-C10	6.05	126.68	112.48
3	J	210	LMZ	C12-C11-C10	6.07	126.72	112.48
3	G	207	LMZ	C12-C11-C10	6.10	126.80	112.48
3	C	203	LMZ	C12-C11-C10	6.12	126.83	112.48
3	F	206	LMZ	C12-C11-C10	6.14	126.88	112.48
3	B	202	LMZ	C12-C11-C10	6.16	126.92	112.48
3	D	204	LMZ	C12-C11-C10	6.20	127.02	112.48
3	I	209	LMZ	C12-C11-C10	6.25	127.13	112.48
3	E	205	LMZ	C12-C11-C10	6.28	127.22	112.48
3	A	201	LMZ	C12-C11-C10	6.37	127.43	112.48
3	B	202	LMZ	C4-N3-C2	11.23	124.95	115.25
3	A	201	LMZ	C4-N3-C2	11.37	125.08	115.25
3	G	207	LMZ	C4-N3-C2	11.41	125.11	115.25
3	E	205	LMZ	C4-N3-C2	11.44	125.14	115.25
3	H	208	LMZ	C4-N3-C2	11.47	125.16	115.25
3	J	210	LMZ	C4-N3-C2	11.47	125.16	115.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	204	LMZ	C4-N3-C2	11.55	125.23	115.25
3	C	203	LMZ	C4-N3-C2	11.61	125.28	115.25
3	F	206	LMZ	C4-N3-C2	11.61	125.28	115.25
3	I	209	LMZ	C4-N3-C2	11.73	125.39	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	LMZ	8	0
3	B	202	LMZ	5	0
2	B	401	SO4	2	0
3	C	203	LMZ	4	0
2	C	303	SO4	1	0
2	C	402	SO4	1	0
3	D	204	LMZ	2	0
3	E	205	LMZ	3	0
3	F	206	LMZ	4	0
2	F	306	SO4	1	0
3	G	207	LMZ	4	0
3	H	208	LMZ	3	0
3	I	209	LMZ	3	0
3	J	210	LMZ	3	0
2	J	310	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	165/200 (82%)	-0.21	2 (1%) 81 64	23, 23, 23, 23	1 (0%)
1	B	165/200 (82%)	-0.17	5 (3%) 54 29	23, 23, 23, 23	1 (0%)
1	C	165/200 (82%)	-0.04	9 (5%) 29 12	23, 23, 23, 23	1 (0%)
1	D	165/200 (82%)	-0.15	8 (4%) 34 15	23, 23, 23, 23	1 (0%)
1	E	165/200 (82%)	-0.23	1 (0%) 90 80	23, 23, 23, 23	2 (1%)
1	F	165/200 (82%)	-0.06	8 (4%) 34 15	23, 23, 23, 23	1 (0%)
1	G	165/200 (82%)	-0.14	6 (3%) 46 23	23, 23, 23, 23	2 (1%)
1	H	165/200 (82%)	-0.21	6 (3%) 46 23	23, 23, 23, 23	2 (1%)
1	I	165/200 (82%)	-0.21	3 (1%) 71 50	23, 23, 23, 23	1 (0%)
1	J	165/200 (82%)	-0.09	7 (4%) 40 19	23, 23, 23, 23	2 (1%)
All	All	1650/2000 (82%)	-0.15	55 (3%) 50 26	23, 23, 23, 23	14 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	8	PRO	5.6
1	C	8	PRO	5.1
1	J	7	THR	5.0
1	C	107	SER	4.4
1	D	6	PRO	4.4
1	C	7	THR	4.2
1	D	7	THR	4.2
1	C	108	THR	4.0
1	I	7	THR	4.0
1	C	10	GLN	3.9
1	F	7	THR	3.8
1	F	108	THR	3.7
1	D	107	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	7	THR	3.7
1	F	8	PRO	3.6
1	H	7	THR	3.6
1	F	107	SER	3.3
1	D	8	PRO	3.2
1	C	9	GLN	3.2
1	D	10	GLN	3.1
1	I	108	THR	3.0
1	J	108	THR	3.0
1	H	108	THR	2.9
1	H	10	GLN	2.9
1	H	8	PRO	2.9
1	B	107	SER	2.8
1	F	9	GLN	2.8
1	J	10	GLN	2.7
1	I	107	SER	2.7
1	D	108	THR	2.7
1	G	6	PRO	2.6
1	G	172	GLY	2.6
1	G	12	ASP	2.5
1	H	173	SER	2.5
1	A	8	PRO	2.5
1	G	10	GLN	2.5
1	F	10	GLN	2.4
1	C	172	GLY	2.4
1	C	5	GLY	2.3
1	B	8	PRO	2.3
1	D	173	SER	2.3
1	J	9	GLN	2.3
1	E	172	GLY	2.2
1	J	6	PRO	2.2
1	J	107	SER	2.2
1	C	6	PRO	2.2
1	D	9	GLN	2.1
1	G	160	ASP	2.1
1	B	172	GLY	2.1
1	A	5	GLY	2.1
1	F	197	GLY	2.0
1	B	108	THR	2.0
1	H	107	SER	2.0
1	F	6	PRO	2.0
1	G	8	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	404	5/5	0.84	0.65	3.05	20,20,20,20	0
2	SO4	J	408	5/5	0.90	0.56	2.87	20,20,20,20	0
3	LMZ	I	209	20/20	0.89	0.24	2.17	23,23,23,23	0
3	LMZ	A	201	20/20	0.92	0.24	1.43	23,23,23,23	0
3	LMZ	J	210	20/20	0.91	0.22	1.35	23,23,23,23	0
3	LMZ	H	208	20/20	0.91	0.20	1.05	23,23,23,23	0
3	LMZ	G	207	20/20	0.91	0.21	1.04	23,23,23,23	0
3	LMZ	F	206	20/20	0.92	0.20	0.93	23,23,23,23	0
3	LMZ	B	202	20/20	0.93	0.19	0.55	23,23,23,23	0
3	LMZ	D	204	20/20	0.93	0.20	0.55	23,23,23,23	0
3	LMZ	C	203	20/20	0.90	0.21	0.53	23,23,23,23	0
2	SO4	B	401	5/5	0.92	0.31	0.47	20,20,20,20	0
3	LMZ	E	205	20/20	0.94	0.18	0.12	23,23,23,23	0
2	SO4	A	301	5/5	0.96	0.13	-1.13	23,23,23,23	0
2	SO4	H	308	5/5	0.96	0.14	-1.21	23,23,23,23	0
2	SO4	G	307	5/5	0.98	0.10	-1.75	23,23,23,23	0
2	SO4	E	305	5/5	0.98	0.11	-1.82	23,23,23,23	0
2	SO4	C	303	5/5	0.98	0.10	-1.90	23,23,23,23	0
2	SO4	D	304	5/5	0.98	0.10	-2.13	23,23,23,23	0
2	SO4	I	309	5/5	0.98	0.12	-2.13	23,23,23,23	0
2	SO4	J	310	5/5	0.98	0.11	-2.27	23,23,23,23	0
2	SO4	F	306	5/5	0.98	0.10	-2.32	23,23,23,23	0
2	SO4	B	302	5/5	0.99	0.12	-3.85	23,23,23,23	0
2	SO4	I	407	5/5	0.94	0.32	-	20,20,20,20	0
2	SO4	C	402	5/5	0.95	0.33	-	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	F	405	5/5	0.93	0.34	-	20,20,20,20	0
2	SO4	C	410	5/5	0.86	0.50	-	20,20,20,20	0
2	SO4	E	403	5/5	0.95	0.39	-	20,20,20,20	0
2	SO4	H	406	5/5	0.94	0.39	-	20,20,20,20	0
2	SO4	I	409	5/5	0.91	0.49	-	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.