



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:24 PM EDT

PDB ID : 3D47 / pdb_00003d47
Title : Crystal structure of L-rhamnonate dehydratase from Salmonella typhimurium complexed with Mg and D-malate
Authors : Fedorov, A.A.; Fedorov, E.V.; Sauder, J.M.; Burley, S.K.; Gerlt, J.A.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-05-14
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

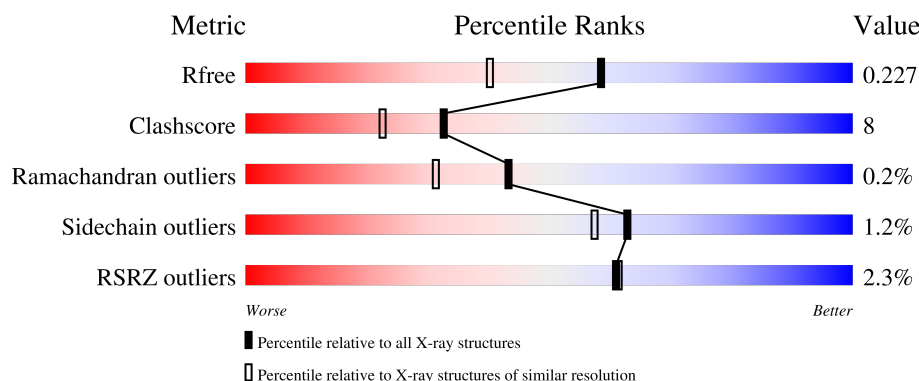
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	405	0% 83% 16% .
1	B	405	2% 81% 19% .
1	C	405	3% 80% 19% .
1	D	405	0% 82% 17% .
1	E	405	2% 82% 17% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	405	2% 81% 17%
1	G	405	2% 80% 19%
1	H	405	3% 77% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26892 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 Putative galactonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3137	1988	543	579	27			
1	B	405	Total	C	N	O	S	0	0	0
			3137	1988	543	579	27			
1	C	405	Total	C	N	O	S	0	0	0
			3137	1988	543	579	27			
1	D	405	Total	C	N	O	S	0	0	0
			3137	1988	543	579	27			
1	E	405	Total	C	N	O	S	0	0	0
			3137	1988	543	579	27			
1	F	405	Total	C	N	O	S	0	0	0
			3137	1988	543	579	27			
1	G	405	Total	C	N	O	S	0	0	0
			3137	1988	543	579	27			
1	H	405	Total	C	N	O	S	0	0	0
			3137	1988	543	579	27			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

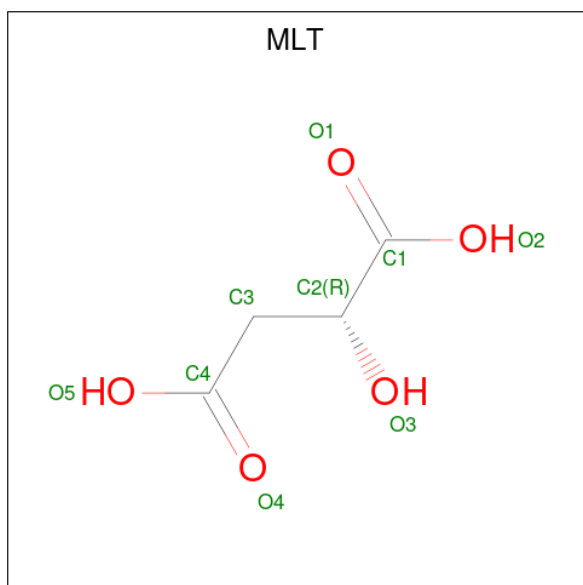
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	H	1	Total	Mg	0	0
			1	1		

- Molecule 3 is D-MALATE (CCD ID: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	4	5		
3	B	1	Total	C	O	0	0
			9	4	5		
3	C	1	Total	C	O	0	0
			9	4	5		
3	D	1	Total	C	O	0	0
			9	4	5		
3	E	1	Total	C	O	0	0
			9	4	5		
3	F	1	Total	C	O	0	0
			9	4	5		
3	G	1	Total	C	O	0	0
			9	4	5		
3	H	1	Total	C	O	0	0
			9	4	5		

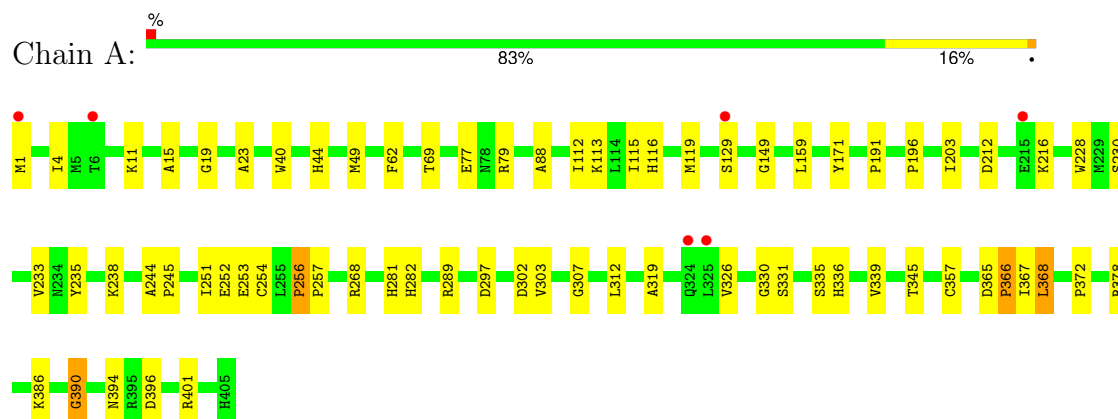
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	274	Total 274	O 274	0	0
4	B	202	Total 202	O 202	0	0
4	C	237	Total 237	O 237	0	0
4	D	165	Total 165	O 165	0	0
4	E	194	Total 194	O 194	0	0
4	F	225	Total 225	O 225	0	0
4	G	267	Total 267	O 267	0	0
4	H	152	Total 152	O 152	0	0

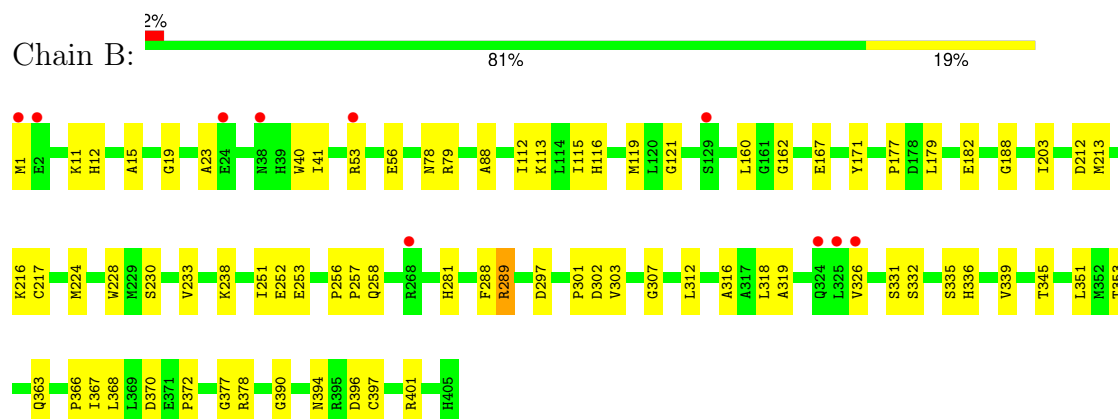
3 Residue-property plots [i](#)

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.

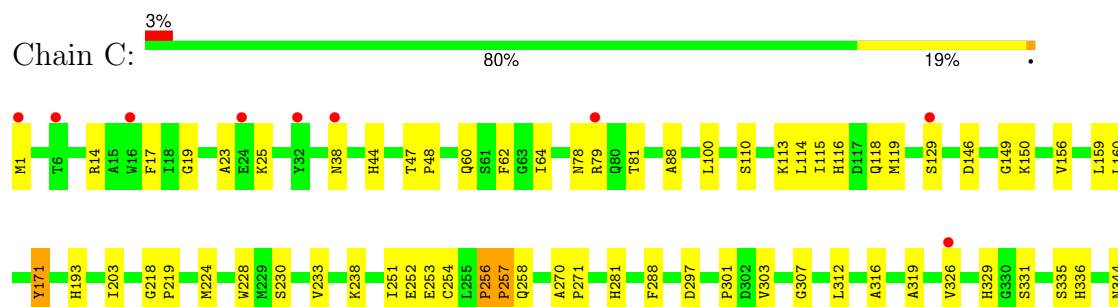
• Molecule 1: Putative galactonate dehydratase



• Molecule 1: Putative galactonate dehydratase

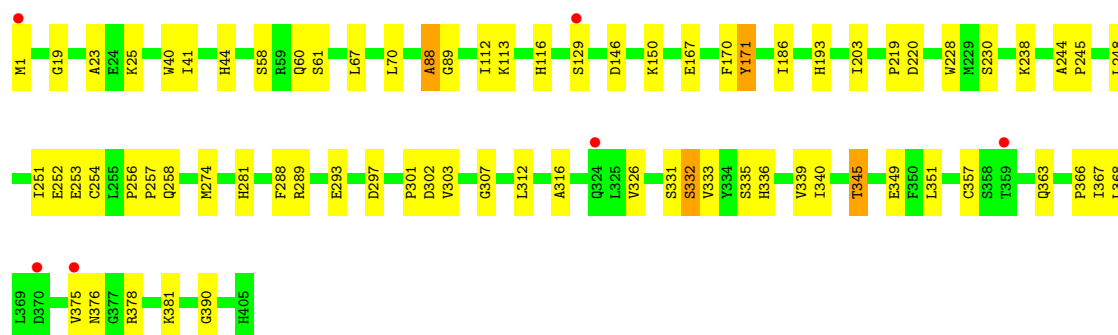
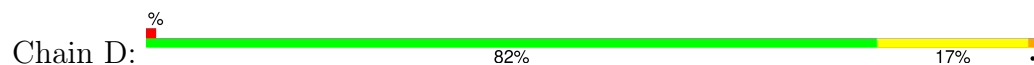


• Molecule 1: Putative galactonate dehydratase

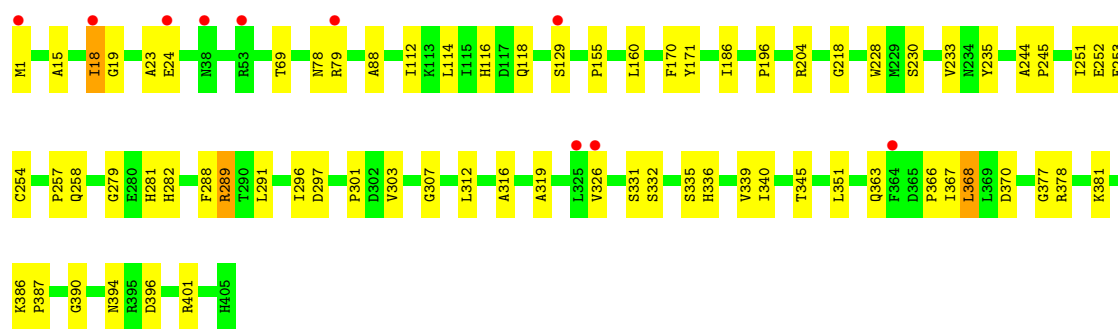
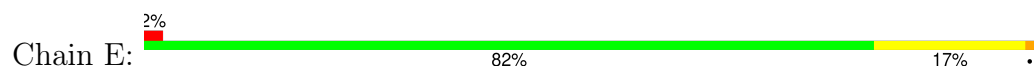




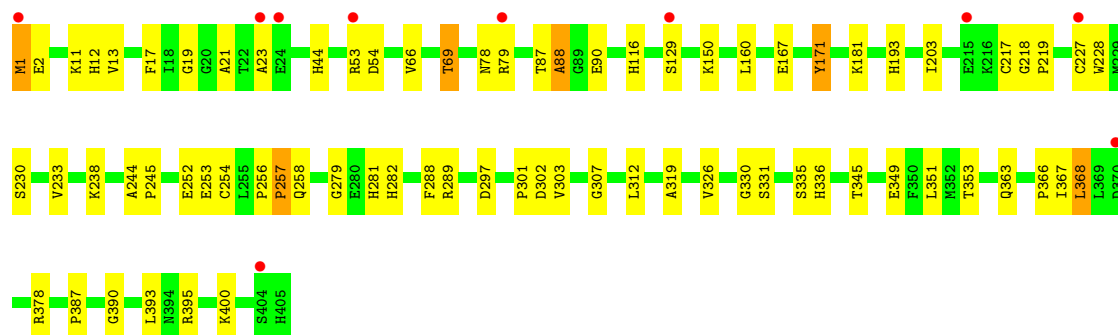
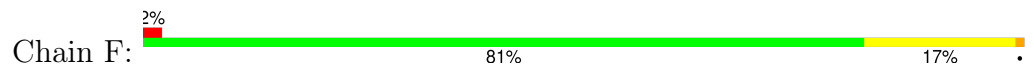
● Molecule 1: Putative galactonate dehydratase



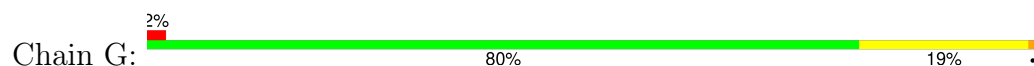
● Molecule 1: Putative galactonate dehydratase

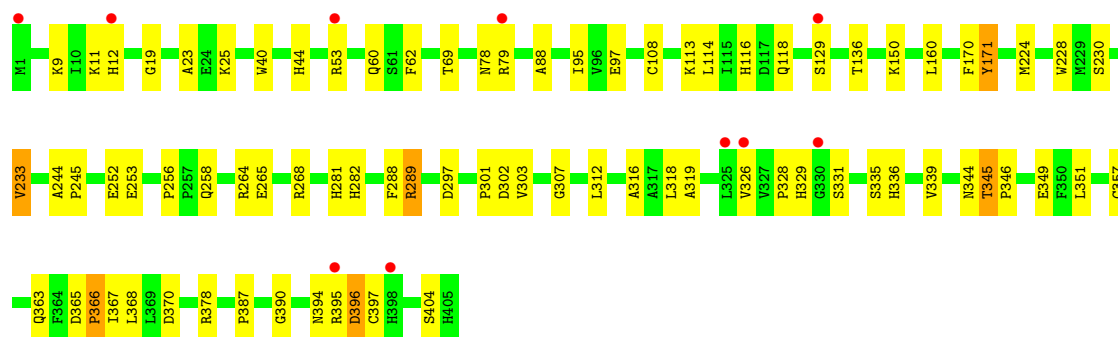


● Molecule 1: Putative galactonate dehydratase

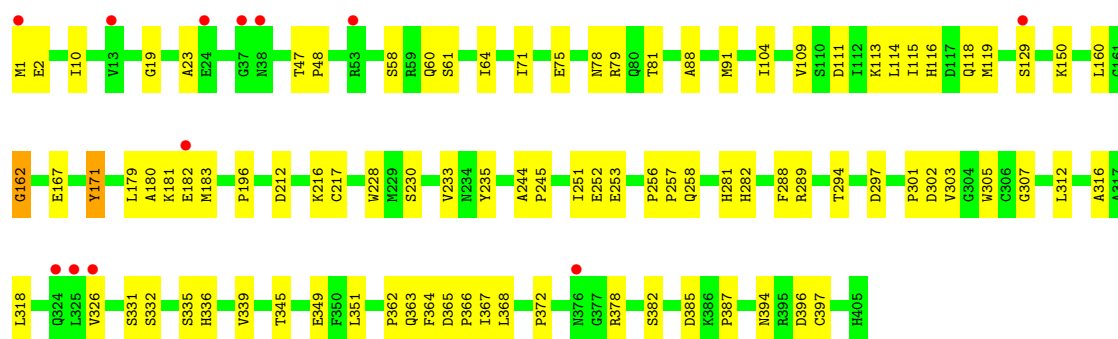
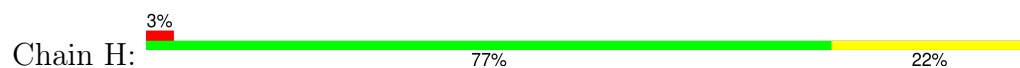


● Molecule 1: Putative galactonate dehydratase





● Molecule 1: Putative galactonate dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.22Å 122.00Å 141.35Å 90.00° 108.24° 90.00°	Depositor
Resolution (Å)	24.88 – 1.80 24.88 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (24.88-1.80) 96.8 (24.88-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.232 0.198 , 0.227	Depositor DCC
R_{free} test set	14317 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26892	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.39	1/3218 (0.0%)	0.95	12/4358 (0.3%)
1	B	0.37	0/3218	0.95	15/4358 (0.3%)
1	C	0.38	0/3218	0.94	14/4358 (0.3%)
1	D	0.36	0/3218	0.95	12/4358 (0.3%)
1	E	0.36	0/3218	0.93	10/4358 (0.2%)
1	F	0.38	0/3218	0.96	17/4358 (0.4%)
1	G	0.38	0/3218	0.94	14/4358 (0.3%)
1	H	0.37	0/3218	0.95	12/4358 (0.3%)
All	All	0.37	1/25744 (0.0%)	0.95	106/34864 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	PRO	CA-C	5.03	1.54	1.51

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	171	TYR	N-CA-C	-8.12	96.72	109.72
1	H	171	TYR	N-CA-C	-7.95	97.29	109.85
1	A	171	TYR	N-CA-C	-7.82	97.52	109.95
1	C	252	GLU	N-CA-C	7.58	121.79	109.59
1	G	252	GLU	N-CA-C	7.53	122.11	109.76
1	A	230	SER	N-CA-C	7.44	122.20	113.20
1	C	171	TYR	N-CA-C	-7.43	98.14	109.95
1	F	230	SER	N-CA-C	7.37	122.30	113.16
1	D	230	SER	N-CA-C	7.33	122.25	113.16
1	C	230	SER	N-CA-C	7.33	122.24	113.16
1	B	171	TYR	N-CA-C	-7.28	98.07	109.72
1	E	171	TYR	N-CA-C	-7.28	98.07	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	252	GLU	N-CA-C	7.22	121.21	109.59
1	F	171	TYR	N-CA-C	-7.21	98.97	110.14
1	G	345	THR	CA-C-N	7.21	126.91	119.56
1	G	345	THR	C-N-CA	7.21	126.91	119.56
1	E	230	SER	N-CA-C	7.16	121.86	113.20
1	B	252	GLU	N-CA-C	7.08	121.37	109.76
1	C	297	ASP	N-CA-C	6.88	118.57	111.14
1	A	252	GLU	N-CA-C	6.84	120.61	109.59
1	D	252	GLU	N-CA-C	6.79	120.90	109.76
1	B	297	ASP	N-CA-C	6.78	118.75	111.36
1	F	297	ASP	N-CA-C	6.75	118.72	111.36
1	H	252	GLU	N-CA-C	6.70	120.75	109.76
1	E	252	GLU	N-CA-C	6.70	120.74	109.76
1	G	297	ASP	N-CA-C	6.68	118.64	111.36
1	A	297	ASP	N-CA-C	6.66	118.62	111.36
1	G	230	SER	N-CA-C	6.65	121.40	113.16
1	G	171	TYR	N-CA-C	-6.62	99.43	109.95
1	C	233	VAL	N-CA-C	6.47	117.16	110.36
1	D	297	ASP	N-CA-C	6.43	118.37	111.36
1	A	256	PRO	N-CA-C	-6.34	104.38	110.47
1	H	230	SER	N-CA-C	6.30	120.97	113.16
1	H	397	CYS	N-CA-C	-6.24	102.29	110.53
1	B	230	SER	N-CA-C	6.19	120.84	113.16
1	F	256	PRO	N-CA-C	-6.07	104.64	110.47
1	F	218	GLY	CA-C-N	6.07	125.62	119.19
1	F	218	GLY	C-N-CA	6.07	125.62	119.19
1	E	112	ILE	N-CA-C	6.03	116.15	110.30
1	F	233	VAL	N-CA-C	6.01	116.19	110.42
1	D	390	GLY	N-CA-C	6.00	123.54	114.61
1	F	219	PRO	N-CA-C	5.96	121.37	113.57
1	H	217	CYS	N-CA-C	5.92	120.57	113.23
1	D	112	ILE	N-CA-C	5.91	116.09	110.42
1	A	302	ASP	N-CA-C	-5.89	99.64	109.24
1	H	233	VAL	N-CA-C	5.89	116.54	110.36
1	E	289	ARG	N-CA-C	-5.87	104.81	111.14
1	D	332	SER	CB-CA-C	-5.86	109.80	116.54
1	B	353	THR	N-CA-C	-5.85	106.19	113.38
1	B	397	CYS	N-CA-C	-5.83	102.28	110.50
1	B	162	GLY	N-CA-C	5.81	120.20	112.65
1	C	256	PRO	N-CA-C	-5.80	104.90	110.47
1	C	329	HIS	N-CA-C	-5.75	101.77	110.28
1	G	256	PRO	CA-C-N	5.74	125.87	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	256	PRO	C-N-CA	5.74	125.87	119.32
1	H	297	ASP	N-CA-C	5.74	118.75	111.69
1	C	390	GLY	N-CA-C	5.73	123.15	114.61
1	E	233	VAL	N-CA-C	5.72	116.37	110.36
1	G	397	CYS	N-CA-C	-5.71	102.99	110.53
1	H	332	SER	CB-CA-C	-5.71	109.98	116.54
1	C	354	SER	N-CA-C	-5.68	102.62	109.83
1	B	332	SER	CB-CA-C	-5.62	110.07	116.54
1	E	332	SER	CB-CA-C	-5.56	110.14	116.54
1	F	390	GLY	N-CA-C	5.53	123.27	115.30
1	D	256	PRO	N-CA-C	-5.51	105.18	110.47
1	C	219	PRO	N-CA-C	5.50	120.77	113.57
1	F	345	THR	CA-C-N	5.47	125.14	119.56
1	F	345	THR	C-N-CA	5.47	125.14	119.56
1	G	289	ARG	N-CA-C	-5.47	105.40	111.36
1	A	390	GLY	N-CA-C	5.46	123.16	115.30
1	B	390	GLY	N-CA-C	5.45	123.14	115.30
1	E	297	ASP	N-CA-C	5.38	117.22	111.36
1	D	302	ASP	N-CA-C	-5.32	100.57	109.24
1	H	256	PRO	N-CA-C	-5.31	105.37	110.47
1	F	302	ASP	N-CA-C	-5.28	100.63	109.24
1	C	100	LEU	N-CA-C	5.28	117.78	111.71
1	F	257	PRO	N-CA-C	5.26	121.44	113.81
1	A	69	THR	N-CA-C	5.26	118.19	109.46
1	E	218	GLY	CA-C-N	5.25	124.58	118.85
1	E	218	GLY	C-N-CA	5.25	124.58	118.85
1	A	233	VAL	N-CA-C	5.22	115.43	110.42
1	B	256	PRO	N-CA-C	-5.21	105.47	110.47
1	C	218	GLY	CA-C-N	5.20	124.70	119.19
1	C	218	GLY	C-N-CA	5.20	124.70	119.19
1	B	217	CYS	N-CA-C	5.19	119.67	113.23
1	H	104	ILE	N-CA-C	5.18	116.27	111.45
1	F	69	THR	N-CA-C	5.14	118.00	109.46
1	B	302	ASP	N-CA-C	-5.13	100.87	109.24
1	G	69	THR	N-CA-C	5.13	117.60	109.24
1	F	353	THR	N-CA-C	-5.12	107.08	113.38
1	A	112	ILE	N-CA-C	5.12	115.33	110.42
1	D	345	THR	CA-C-N	5.11	124.78	119.56
1	D	345	THR	C-N-CA	5.11	124.78	119.56
1	G	170	PHE	N-CA-C	5.11	117.89	109.72
1	H	162	GLY	N-CA-C	5.09	120.35	112.81
1	G	302	ASP	N-CA-C	-5.09	100.94	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	257	PRO	N-CA-C	5.09	120.52	113.65
1	G	233	VAL	N-CA-C	5.08	115.81	110.62
1	F	90	GLU	N-CA-C	5.08	117.48	111.33
1	B	289	ARG	N-CA-C	-5.07	105.66	111.14
1	H	294	THR	N-CA-C	-5.06	106.62	112.89
1	A	257	PRO	N-CA-C	5.05	120.47	113.65
1	B	112	ILE	N-CA-C	5.05	115.27	110.53
1	A	289	ARG	N-CA-C	-5.03	105.71	111.14
1	D	60	GLN	N-CA-C	-5.01	105.94	111.71
1	B	233	VAL	N-CA-C	5.01	115.62	110.36

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	3137	0	3059	46	0
1	B	3137	0	3059	45	0
1	C	3137	0	3059	60	0
1	D	3137	0	3059	51	0
1	E	3137	0	3059	52	0
1	F	3137	0	3059	56	0
1	G	3137	0	3059	68	0
1	H	3137	0	3059	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	9	0	3	0	0
3	B	9	0	3	0	0
3	C	9	0	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	9	0	4	0	0
3	E	9	0	3	0	0
3	F	9	0	3	0	0
3	G	9	0	3	0	0
3	H	9	0	3	0	0
4	A	274	0	0	8	0
4	B	202	0	0	3	0
4	C	237	0	0	4	0
4	D	165	0	0	5	0
4	E	194	0	0	7	0
4	F	225	0	0	4	0
4	G	267	0	0	9	0
4	H	152	0	0	5	0
All	All	26892	0	24498	392	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 8.

All (392) 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:G:303:VAL:HG23	4:G:942:HOH:O	1.59	1.01
1:C:303:VAL:HG22	1:C:312:LEU:HD22	1.44	1.00
1:A:129:SER:HB3	1:B:258:GLN:HE21	1.25	0.99
1:F:227:CYS:SG	1:F:254:CYS:HA	2.02	0.98
1:G:258:GLN:HE21	1:H:129:SER:HB3	1.27	0.98
1:C:129:SER:HB3	1:D:258:GLN:NE2	1.79	0.97
1:G:129:SER:HB3	1:H:258:GLN:HE21	1.24	0.97
1:G:258:GLN:NE2	1:H:129:SER:HB3	1.81	0.93
1:E:258:GLN:HE21	1:F:129:SER:HB3	1.32	0.92
1:C:367:ILE:HG23	1:C:368:LEU:HD13	1.53	0.91
1:E:258:GLN:NE2	1:F:129:SER:HB3	1.85	0.90
1:G:129:SER:HB3	1:H:258:GLN:NE2	1.85	0.89
1:A:129:SER:HB3	1:B:258:GLN:NE2	1.86	0.89
1:C:303:VAL:HG23	4:C:697:HOH:O	1.73	0.89
1:A:49:MET:HE3	1:B:121:GLY:HA3	1.54	0.88
1:G:303:VAL:HG22	1:G:312:LEU:HD22	1.56	0.88
1:C:129:SER:HB3	1:D:258:GLN:HE21	1.37	0.87
1:H:351:LEU:HB3	1:H:363:GLN:HE22	1.39	0.87
1:E:18:ILE:HG23	1:E:69:THR:HB	1.57	0.86
1:E:367:ILE:HG23	1:E:368:LEU:HD13	1.57	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:367:ILE:HG23	1:G:368:LEU:HD13	1.57	0.84
1:E:129:SER:HB3	1:F:258:GLN:NE2	1.93	0.83
1:A:367:ILE:HG23	1:A:368:LEU:HD13	1.62	0.82
1:C:258:GLN:NE2	1:D:129:SER:HB3	1.94	0.82
1:B:367:ILE:HG23	1:B:368:LEU:HD13	1.62	0.81
1:G:351:LEU:HB3	1:G:363:GLN:HE22	1.46	0.79
1:G:95:ILE:HD11	1:H:91:MET:HE1	1.65	0.77
1:H:367:ILE:HG23	1:H:368:LEU:HD13	1.67	0.76
1:C:316:ALA:HA	1:C:326:VAL:HG21	1.67	0.75
1:C:351:LEU:HB3	1:C:363:GLN:HE22	1.52	0.75
1:E:129:SER:HB3	1:F:258:GLN:HE21	1.53	0.73
1:H:303:VAL:HG22	1:H:312:LEU:HD22	1.69	0.73
1:G:253:GLU:OE2	1:G:281:HIS:HD2	1.72	0.72
1:H:331:SER:HB2	1:H:335:SER:HB2	1.72	0.72
1:F:253:GLU:OE2	1:F:281:HIS:HD2	1.72	0.71
1:D:253:GLU:OE2	1:D:281:HIS:HD2	1.74	0.70
1:G:336:HIS:HD2	4:G:801:HOH:O	1.75	0.69
1:H:58:SER:O	1:H:61:SER:HB3	1.92	0.69
1:D:281:HIS:HE1	4:D:517:HOH:O	1.75	0.69
1:G:316:ALA:HA	1:G:326:VAL:HG21	1.76	0.68
1:B:1:MET:HE2	1:G:387:PRO:HD2	1.76	0.68
1:A:253:GLU:OE2	1:A:281:HIS:HD2	1.77	0.67
1:D:58:SER:O	1:D:61:SER:HB3	1.95	0.67
1:A:336:HIS:HD2	4:A:531:HOH:O	1.77	0.66
1:E:253:GLU:OE2	1:E:281:HIS:HD2	1.79	0.66
1:H:180:ALA:HA	1:H:183:MET:HE3	1.77	0.66
1:C:156:VAL:O	1:C:160:LEU:HD13	1.95	0.66
1:H:167:GLU:OE2	1:H:378:ARG:HD3	1.96	0.65
1:F:11:LYS:HE3	1:F:12:HIS:NE2	2.12	0.65
1:H:316:ALA:HA	1:H:326:VAL:HG21	1.77	0.65
1:C:1:MET:HE2	1:H:387:PRO:HD2	1.79	0.65
1:B:177:PRO:HG2	1:B:213:MET:SD	2.37	0.65
1:D:146:ASP:O	1:D:150:LYS:HG2	1.96	0.64
1:A:44:HIS:HE1	4:A:533:HOH:O	1.79	0.64
1:B:1:MET:HE3	1:G:150:LYS:HE2	1.79	0.64
1:D:336:HIS:HD2	4:D:592:HOH:O	1.80	0.64
1:A:116:HIS:HE1	1:A:307:GLY:O	1.81	0.64
1:G:331:SER:HB2	1:G:335:SER:HB2	1.80	0.64
4:A:670:HOH:O	1:E:1:MET:HE2	1.97	0.64
1:H:339:VAL:HB	1:H:345:THR:HG21	1.80	0.64
1:B:116:HIS:HD2	4:G:976:HOH:O	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:GLU:OE2	1:B:281:HIS:HD2	1.81	0.63
1:B:351:LEU:HB3	1:B:363:GLN:HE22	1.64	0.63
1:G:268:ARG:HB3	1:G:268:ARG:NH1	2.13	0.63
1:A:1:MET:HE2	1:E:387:PRO:HD2	1.81	0.62
1:G:394:ASN:OD1	1:G:396:ASP:HB2	1.99	0.62
1:D:1:MET:HE3	1:F:150:LYS:HE2	1.80	0.62
1:E:303:VAL:HG22	1:E:312:LEU:HD22	1.82	0.62
1:G:11:LYS:HE3	1:G:12:HIS:NE2	2.15	0.61
1:C:253:GLU:OE2	1:C:281:HIS:HD2	1.83	0.61
1:C:319:ALA:CB	1:C:326:VAL:HG22	2.31	0.61
1:F:303:VAL:HG22	1:F:312:LEU:HD22	1.82	0.61
1:C:258:GLN:HE21	1:D:129:SER:HB3	1.64	0.60
1:C:19:GLY:O	1:C:23:ALA:HB3	2.01	0.60
1:A:49:MET:HA	1:A:49:MET:HE2	1.83	0.60
1:C:326:VAL:HG23	1:C:344:ASN:ND2	2.15	0.60
4:D:590:HOH:O	1:F:116:HIS:HD2	1.83	0.60
1:H:281:HIS:HE1	4:H:577:HOH:O	1.83	0.60
1:C:336:HIS:HD2	4:C:616:HOH:O	1.84	0.60
1:G:95:ILE:CD1	1:H:91:MET:HE1	2.32	0.60
1:F:227:CYS:HG	1:F:254:CYS:HA	1.66	0.60
1:F:351:LEU:HB3	1:F:363:GLN:HE22	1.67	0.60
1:G:233:VAL:HG11	1:G:265:GLU:HG2	1.85	0.59
1:G:78:ASN:O	1:G:79:ARG:HB2	2.01	0.59
1:A:390:GLY:HA2	1:E:1:MET:HE1	1.84	0.59
1:B:167:GLU:OE2	1:B:378:ARG:HD3	2.02	0.59
1:D:367:ILE:HG23	1:D:368:LEU:CD1	2.32	0.59
1:A:378:ARG:HG3	1:A:378:ARG:HH11	1.67	0.58
1:B:331:SER:HB2	1:B:335:SER:HB2	1.85	0.58
1:G:44:HIS:HE1	4:G:893:HOH:O	1.86	0.58
1:A:116:HIS:HD2	4:E:608:HOH:O	1.87	0.58
1:D:113:LYS:HE3	1:F:160:LEU:O	2.04	0.58
1:C:319:ALA:HB3	1:C:326:VAL:HG22	1.86	0.58
1:C:146:ASP:OD2	1:C:150:LYS:HE2	2.03	0.58
1:F:257:PRO:HG2	1:F:258:GLN:NE2	2.19	0.57
1:H:253:GLU:OE2	1:H:281:HIS:HD2	1.86	0.57
1:B:303:VAL:HG22	1:B:312:LEU:HD22	1.86	0.57
1:D:19:GLY:O	1:D:23:ALA:HB3	2.05	0.57
1:H:351:LEU:HB3	1:H:363:GLN:NE2	2.17	0.57
1:C:257:PRO:HG2	1:C:258:GLN:NE2	2.20	0.57
1:A:281:HIS:HE1	4:A:560:HOH:O	1.88	0.57
1:F:44:HIS:HE1	4:F:684:HOH:O	1.88	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ALA:HB3	1:C:326:VAL:CG2	2.35	0.56
1:D:331:SER:HB2	1:D:335:SER:HB2	1.87	0.56
1:D:367:ILE:HG23	1:D:368:LEU:HD13	1.87	0.56
1:A:339:VAL:HB	1:A:345:THR:HG21	1.87	0.56
1:E:316:ALA:HA	1:E:326:VAL:HG21	1.86	0.56
1:C:1:MET:HE3	1:H:150:LYS:HE2	1.88	0.56
1:A:331:SER:HB2	1:A:335:SER:HB2	1.87	0.55
1:A:113:LYS:HE3	1:E:160:LEU:O	2.05	0.55
1:B:11:LYS:HE3	1:B:12:HIS:NE2	2.21	0.55
1:C:129:SER:CB	1:D:258:GLN:HE21	2.13	0.55
1:F:331:SER:HB2	1:F:335:SER:HB2	1.88	0.55
1:D:1:MET:HE1	1:F:387:PRO:O	2.05	0.55
1:D:303:VAL:HG22	1:D:312:LEU:HD22	1.88	0.55
1:E:19:GLY:O	1:E:23:ALA:HB3	2.07	0.55
1:F:116:HIS:HE1	1:F:307:GLY:O	1.90	0.55
1:G:319:ALA:HB3	1:G:326:VAL:CG2	2.37	0.55
1:F:19:GLY:O	1:F:23:ALA:HB3	2.06	0.55
1:D:171:TYR:CZ	1:D:349:GLU:HB2	2.42	0.54
1:F:79:ARG:HD2	1:F:79:ARG:N	2.23	0.54
1:H:378:ARG:HG3	1:H:378:ARG:HH11	1.71	0.54
1:B:288:PHE:CZ	1:B:301:PRO:HB3	2.43	0.54
1:B:319:ALA:CB	1:B:326:VAL:HG23	2.37	0.54
1:C:303:VAL:CG2	1:C:312:LEU:HD22	2.29	0.54
1:B:1:MET:HE1	1:G:390:GLY:HA2	1.88	0.54
1:B:19:GLY:O	1:B:23:ALA:HB3	2.07	0.54
1:C:203:ILE:CD1	1:C:238:LYS:HE2	2.37	0.54
1:F:367:ILE:HG23	1:F:368:LEU:HD13	1.89	0.54
1:D:351:LEU:HB3	1:D:363:GLN:HE22	1.72	0.54
1:F:53:ARG:HG3	1:F:54:ASP:N	2.23	0.54
1:F:319:ALA:CB	1:F:326:VAL:HG23	2.38	0.54
1:B:113:LYS:HE3	1:G:160:LEU:O	2.07	0.53
1:B:116:HIS:HE1	1:B:307:GLY:O	1.91	0.53
1:E:257:PRO:HG2	1:E:258:GLN:NE2	2.23	0.53
1:B:336:HIS:HD2	4:B:533:HOH:O	1.91	0.53
1:C:79:ARG:HG2	4:C:585:HOH:O	2.08	0.53
1:G:40:TRP:CD1	1:G:357:CYS:HG	2.26	0.53
1:G:114:LEU:O	1:G:118:GLN:HG3	2.08	0.53
1:H:75:GLU:HG3	1:H:81:THR:HG22	1.90	0.53
1:B:281:HIS:HE1	4:B:517:HOH:O	1.91	0.53
1:C:25:LYS:HD3	1:C:25:LYS:C	2.34	0.53
1:E:336:HIS:HD2	4:E:509:HOH:O	1.92	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:SER:HB2	1:E:335:SER:HB2	1.90	0.52
1:C:387:PRO:HD2	1:H:1:MET:HE2	1.92	0.52
1:F:319:ALA:HB3	1:F:326:VAL:HG23	1.92	0.52
1:A:4:ILE:HG21	1:E:155:PRO:HD3	1.92	0.52
1:D:1:MET:HE2	1:F:387:PRO:HD2	1.92	0.52
1:C:251:ILE:HG12	1:C:254:CYS:SG	2.50	0.52
1:D:251:ILE:HG12	1:D:254:CYS:SG	2.50	0.51
1:D:332:SER:OG	1:D:333:VAL:N	2.44	0.51
1:E:339:VAL:HB	1:E:345:THR:HG21	1.93	0.51
1:H:336:HIS:HD2	4:H:521:HOH:O	1.92	0.51
1:D:289:ARG:C	1:D:289:ARG:HD3	2.36	0.51
1:F:336:HIS:HD2	4:F:548:HOH:O	1.93	0.51
1:D:339:VAL:HB	1:D:345:THR:HG21	1.93	0.51
1:H:335:SER:O	1:H:339:VAL:HG22	2.11	0.51
1:H:47:THR:HB	1:H:48:PRO:HD2	1.92	0.51
1:B:319:ALA:HB3	1:B:326:VAL:HG23	1.93	0.51
1:F:244:ALA:N	1:F:245:PRO:HD2	2.26	0.50
1:B:257:PRO:HG2	1:B:258:GLN:NE2	2.27	0.50
1:E:281:HIS:HE1	4:E:579:HOH:O	1.93	0.50
1:D:1:MET:CE	1:F:150:LYS:HE2	2.42	0.50
1:E:116:HIS:HE1	1:E:307:GLY:O	1.95	0.50
1:H:212:ASP:OD1	1:H:216:LYS:NZ	2.45	0.50
1:H:19:GLY:O	1:H:23:ALA:HB3	2.12	0.49
1:B:160:LEU:O	1:G:113:LYS:HE3	2.12	0.49
1:C:17:PHE:HE1	1:C:23:ALA:HB2	1.77	0.49
1:C:288:PHE:CZ	1:C:301:PRO:HB3	2.47	0.49
1:F:393:LEU:HD23	1:F:395:ARG:HH11	1.77	0.49
1:G:129:SER:CB	1:H:258:GLN:HE21	2.10	0.49
1:G:339:VAL:HB	1:G:345:THR:HG21	1.94	0.49
1:H:257:PRO:HG2	1:H:258:GLN:NE2	2.28	0.49
1:D:150:LYS:HE2	1:F:1:MET:HE3	1.95	0.49
1:E:204:ARG:HG3	4:E:590:HOH:O	2.12	0.49
1:F:258:GLN:H	1:F:258:GLN:CD	2.20	0.49
1:G:288:PHE:CZ	1:G:301:PRO:HB3	2.48	0.49
1:H:71:ILE:HD12	1:H:71:ILE:N	2.27	0.49
1:H:367:ILE:HG23	1:H:368:LEU:CD1	2.40	0.49
1:C:368:LEU:HG	1:C:391:VAL:HG21	1.95	0.49
1:F:257:PRO:HG2	1:F:258:GLN:HE22	1.78	0.49
1:G:19:GLY:O	1:G:23:ALA:HB3	2.13	0.49
1:H:111:ASP:O	1:H:115:ILE:HG13	2.13	0.49
1:B:1:MET:HE1	1:G:387:PRO:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ASN:O	1:C:79:ARG:HB2	2.12	0.48
1:C:146:ASP:O	1:C:150:LYS:HG3	2.12	0.48
1:G:395:ARG:HG2	1:G:395:ARG:HH11	1.78	0.48
1:B:339:VAL:HB	1:B:345:THR:HG21	1.95	0.48
1:C:81:THR:O	1:C:150:LYS:HD2	2.13	0.48
1:F:281:HIS:HE1	4:F:579:HOH:O	1.95	0.48
1:G:264:ARG:O	1:G:268:ARG:HG3	2.13	0.48
1:E:258:GLN:CD	1:E:258:GLN:H	2.21	0.48
1:F:167:GLU:OE2	1:F:378:ARG:HD3	2.13	0.48
1:G:19:GLY:C	1:G:23:ALA:HB3	2.39	0.48
1:D:70:LEU:HB2	1:D:88:ALA:HB3	1.96	0.48
1:A:191:PRO:HB3	4:A:688:HOH:O	2.13	0.48
1:A:203:ILE:CD1	1:A:238:LYS:HE2	2.44	0.48
1:D:316:ALA:HA	1:D:326:VAL:HG21	1.95	0.48
1:B:177:PRO:HB3	1:B:188:GLY:HA3	1.96	0.48
1:B:203:ILE:HD13	1:B:238:LYS:HB3	1.95	0.47
1:E:288:PHE:CZ	1:E:301:PRO:HB3	2.48	0.47
1:E:378:ARG:HH11	1:E:378:ARG:HG3	1.79	0.47
1:H:362:PRO:HB2	1:H:365:ASP:HB2	1.96	0.47
1:D:257:PRO:HG2	1:D:258:GLN:NE2	2.29	0.47
1:G:9:LYS:HE3	4:G:925:HOH:O	2.13	0.47
1:B:179:LEU:O	1:B:182:GLU:HB2	2.15	0.47
1:F:21:ALA:HB2	1:F:66:VAL:HG13	1.95	0.47
1:G:268:ARG:HB3	1:G:268:ARG:HH11	1.78	0.47
1:C:146:ASP:CG	1:C:150:LYS:HE2	2.40	0.47
1:H:116:HIS:HE1	1:H:307:GLY:O	1.98	0.47
1:C:160:LEU:O	1:H:113:LYS:HE3	2.15	0.47
1:D:25:LYS:HE2	4:D:599:HOH:O	2.14	0.47
1:F:288:PHE:CZ	1:F:301:PRO:HB3	2.50	0.47
1:C:281:HIS:HE1	4:C:512:HOH:O	1.97	0.47
1:F:279:GLY:HA2	1:F:282:HIS:HD2	1.79	0.47
1:C:110:SER:O	1:H:162:GLY:HA3	2.14	0.47
1:C:113:LYS:HE3	1:H:160:LEU:O	2.14	0.47
1:E:291:LEU:HG	1:E:296:ILE:HD11	1.97	0.47
1:D:244:ALA:N	1:D:245:PRO:CD	2.78	0.47
1:D:288:PHE:CZ	1:D:301:PRO:HB3	2.50	0.47
1:B:378:ARG:HG3	1:B:378:ARG:HH11	1.80	0.47
1:E:251:ILE:HG12	1:E:254:CYS:SG	2.55	0.47
1:A:303:VAL:HG22	1:A:312:LEU:HD22	1.96	0.46
1:C:14:ARG:HB3	1:C:401:ARG:NH1	2.30	0.46
1:C:116:HIS:HE1	1:C:307:GLY:O	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:ILE:HD13	1:F:238:LYS:HB3	1.97	0.46
1:F:253:GLU:OE2	1:F:281:HIS:CD2	2.61	0.46
1:F:171:TYR:CZ	1:F:349:GLU:HB2	2.50	0.46
1:F:279:GLY:HA2	1:F:282:HIS:CD2	2.50	0.46
1:C:115:ILE:O	1:C:119:MET:HG3	2.15	0.46
1:F:78:ASN:O	1:F:79:ARG:HB2	2.15	0.46
1:C:331:SER:HB2	1:C:335:SER:HB2	1.98	0.46
1:E:19:GLY:HA2	1:E:24:GLU:O	2.16	0.46
1:E:244:ALA:HB3	1:E:245:PRO:HD3	1.98	0.46
1:E:319:ALA:HB3	1:E:326:VAL:HG23	1.96	0.46
1:F:378:ARG:HG3	1:F:378:ARG:HH11	1.81	0.46
1:G:367:ILE:HG23	1:G:368:LEU:CD1	2.39	0.46
1:A:79:ARG:HG3	1:A:79:ARG:HH11	1.80	0.46
1:D:167:GLU:OE2	1:D:378:ARG:HD3	2.15	0.46
1:E:351:LEU:HB3	1:E:363:GLN:HE22	1.81	0.46
1:B:115:ILE:O	1:B:119:MET:HG3	2.16	0.46
1:E:282:HIS:CD2	4:E:505:HOH:O	2.68	0.46
1:E:335:SER:O	1:E:339:VAL:HG22	2.16	0.45
1:E:394:ASN:OD1	1:E:396:ASP:HB2	2.16	0.45
1:F:17:PHE:HA	1:F:69:THR:O	2.16	0.45
1:G:258:GLN:CD	1:G:258:GLN:H	2.24	0.45
1:G:378:ARG:HG3	1:G:378:ARG:HH11	1.81	0.45
1:A:378:ARG:HG3	1:A:378:ARG:NH1	2.30	0.45
1:A:11:LYS:HB2	1:A:77:GLU:HG2	1.98	0.45
1:D:150:LYS:HE2	1:F:1:MET:CE	2.46	0.45
1:F:289:ARG:HD3	1:F:289:ARG:C	2.41	0.45
1:H:378:ARG:HG3	1:H:378:ARG:NH1	2.31	0.45
1:E:244:ALA:N	1:E:245:PRO:CD	2.80	0.45
1:B:78:ASN:O	1:B:79:ARG:HB2	2.17	0.45
1:B:372:PRO:HG2	4:B:593:HOH:O	2.15	0.45
1:C:1:MET:HE1	1:H:387:PRO:O	2.17	0.45
1:D:375:VAL:O	1:D:376:ASN:HB3	2.17	0.45
1:G:116:HIS:HE1	1:G:307:GLY:O	1.99	0.45
1:A:282:HIS:HD2	4:A:532:HOH:O	2.00	0.45
1:G:303:VAL:CG2	1:G:312:LEU:HD22	2.39	0.45
1:A:1:MET:HE1	1:E:390:GLY:HA2	1.99	0.44
1:H:289:ARG:HD3	1:H:289:ARG:C	2.43	0.44
1:A:196:PRO:HA	1:A:235:TYR:CD1	2.52	0.44
1:B:15:ALA:O	1:B:401:ARG:HD2	2.16	0.44
1:H:78:ASN:O	1:H:79:ARG:HB2	2.17	0.44
1:C:14:ARG:HB3	1:C:401:ARG:HH12	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:364:PHE:O	1:H:367:ILE:HG22	2.17	0.44
1:E:289:ARG:HD3	1:E:289:ARG:C	2.43	0.44
1:D:203:ILE:HD13	1:D:238:LYS:HB3	1.99	0.44
1:E:196:PRO:HA	1:E:235:TYR:CD1	2.52	0.44
1:G:25:LYS:HE3	1:G:60:GLN:OE1	2.17	0.44
1:D:253:GLU:OE2	1:D:281:HIS:CD2	2.64	0.44
1:B:377:GLY:C	1:B:378:ARG:HG3	2.42	0.44
1:E:251:ILE:HG23	1:E:251:ILE:O	2.17	0.44
1:H:289:ARG:HA	1:H:318:LEU:HD21	2.00	0.44
1:H:382:SER:HA	1:H:385:ASP:OD2	2.18	0.44
1:G:344:ASN:C	1:G:346:PRO:HD3	2.43	0.44
1:G:395:ARG:HG2	1:G:395:ARG:NH1	2.32	0.44
1:H:171:TYR:CZ	1:H:349:GLU:HB2	2.52	0.44
1:E:282:HIS:HD2	4:E:505:HOH:O	2.00	0.43
1:F:330:GLY:O	1:F:331:SER:HB2	2.18	0.43
1:H:302:ASP:HB3	1:H:305:TRP:HB2	2.00	0.43
1:A:19:GLY:O	1:A:23:ALA:HB3	2.18	0.43
1:A:372:PRO:HG2	4:A:657:HOH:O	2.17	0.43
1:B:316:ALA:HA	1:B:326:VAL:HG21	2.00	0.43
1:C:203:ILE:HD13	1:C:238:LYS:HE2	2.00	0.43
1:D:340:ILE:HD11	1:D:381:LYS:HB3	1.99	0.43
1:G:95:ILE:HB	1:G:136:THR:HG21	2.00	0.43
1:G:171:TYR:CZ	1:G:349:GLU:HB2	2.54	0.43
1:H:179:LEU:O	1:H:182:GLU:HG2	2.19	0.43
1:A:365:ASP:HA	1:A:366:PRO:HA	1.82	0.43
1:A:394:ASN:OD1	1:A:396:ASP:HB2	2.18	0.43
1:C:171:TYR:CZ	1:C:349:GLU:HB2	2.54	0.43
1:E:114:LEU:O	1:E:118:GLN:HG3	2.18	0.43
1:G:319:ALA:CB	1:G:326:VAL:HG22	2.49	0.43
1:C:47:THR:HB	1:C:48:PRO:HD2	2.01	0.43
1:G:53:ARG:NH2	4:G:971:HOH:O	2.51	0.43
1:G:328:PRO:HG3	1:G:339:VAL:CG1	2.49	0.43
1:G:365:ASP:HA	1:G:366:PRO:HA	1.85	0.43
1:G:258:GLN:HE21	1:H:129:SER:CB	2.14	0.43
1:H:394:ASN:OD1	1:H:396:ASP:HB2	2.18	0.43
1:A:319:ALA:HB3	1:A:326:VAL:HG23	2.00	0.43
1:D:40:TRP:CD1	1:D:357:CYS:HG	2.37	0.43
1:D:378:ARG:HG3	1:D:378:ARG:HH11	1.83	0.43
1:H:251:ILE:O	1:H:251:ILE:HG23	2.18	0.43
1:A:282:HIS:CD2	4:A:532:HOH:O	2.71	0.42
1:F:203:ILE:CD1	1:F:238:LYS:HE2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:244:ALA:N	1:G:245:PRO:CD	2.82	0.42
1:H:60:GLN:HA	1:H:64:ILE:HG22	2.01	0.42
1:H:115:ILE:O	1:H:119:MET:HG3	2.19	0.42
1:B:394:ASN:OD1	1:B:396:ASP:HB2	2.19	0.42
1:D:116:HIS:HE1	1:D:307:GLY:O	2.02	0.42
1:G:9:LYS:HD3	1:G:108:CYS:HA	2.01	0.42
1:E:24:GLU:HB3	4:E:664:HOH:O	2.19	0.42
1:E:257:PRO:HG2	1:E:258:GLN:HE22	1.84	0.42
1:F:400:LYS:HE2	4:F:727:HOH:O	2.19	0.42
1:G:97:GLU:OE1	1:G:404:SER:HA	2.18	0.42
1:H:288:PHE:CZ	1:H:301:PRO:HB3	2.55	0.42
1:A:268:ARG:HB3	1:A:268:ARG:CZ	2.49	0.42
1:E:170:PHE:O	1:E:186:ILE:HG12	2.19	0.42
1:F:181:LYS:HE3	1:F:217:CYS:O	2.19	0.42
1:G:282:HIS:HD2	4:G:735:HOH:O	2.01	0.42
1:B:212:ASP:OD1	1:B:216:LYS:NZ	2.52	0.42
1:C:44:HIS:HD2	1:C:193:HIS:O	2.02	0.42
1:G:44:HIS:O	1:G:44:HIS:CD2	2.72	0.42
1:C:387:PRO:O	1:H:1:MET:HE1	2.19	0.42
1:D:40:TRP:CG	1:D:41:ILE:N	2.87	0.42
1:E:15:ALA:O	1:E:401:ARG:HD2	2.20	0.42
1:E:370:ASP:OD2	1:E:386:LYS:NZ	2.53	0.42
1:A:244:ALA:N	1:A:245:PRO:CD	2.83	0.42
1:C:60:GLN:HA	1:C:64:ILE:HG22	2.02	0.42
1:C:257:PRO:HG2	1:C:258:GLN:HE22	1.82	0.42
1:C:382:SER:HA	1:C:385:ASP:OD2	2.20	0.42
1:G:281:HIS:HE1	4:G:777:HOH:O	2.02	0.42
1:A:330:GLY:O	1:A:331:SER:HB2	2.20	0.42
1:H:244:ALA:N	1:H:245:PRO:CD	2.83	0.42
1:D:67:LEU:O	1:D:89:GLY:HA3	2.19	0.42
1:E:78:ASN:O	1:E:79:ARG:HB2	2.19	0.42
1:E:258:GLN:HE21	1:F:129:SER:CB	2.18	0.42
1:G:328:PRO:HG3	1:G:339:VAL:HG11	2.01	0.42
1:E:340:ILE:HD11	1:E:381:LYS:HB3	2.02	0.42
1:A:212:ASP:OD1	1:A:216:LYS:HE3	2.20	0.41
1:A:251:ILE:HG12	1:A:254:CYS:SG	2.59	0.41
1:F:319:ALA:CB	1:F:326:VAL:CG2	2.98	0.41
1:G:335:SER:O	1:G:339:VAL:HG22	2.20	0.41
1:G:336:HIS:CE1	4:G:823:HOH:O	2.73	0.41
1:H:196:PRO:HA	1:H:235:TYR:CD1	2.55	0.41
1:A:319:ALA:CB	1:A:326:VAL:HG23	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:HIS:HE1	4:D:653:HOH:O	2.02	0.41
1:D:289:ARG:O	1:D:293:GLU:HG3	2.19	0.41
1:G:253:GLU:OE2	1:G:281:HIS:CD2	2.63	0.41
1:A:115:ILE:O	1:A:119:MET:HG3	2.20	0.41
1:E:279:GLY:HA2	1:E:282:HIS:CD2	2.54	0.41
1:A:62:PHE:CD1	1:A:62:PHE:C	2.98	0.41
1:A:149:GLY:HA2	1:A:159:LEU:HD11	2.01	0.41
1:B:253:GLU:OE2	1:B:281:HIS:CD2	2.69	0.41
1:C:351:LEU:HB3	1:C:363:GLN:NE2	2.29	0.41
1:B:53:ARG:NH2	1:B:56:GLU:OE1	2.54	0.41
1:D:44:HIS:CD2	1:D:193:HIS:O	2.72	0.41
1:F:87:THR:O	1:F:88:ALA:HB2	2.19	0.41
1:G:289:ARG:HD3	1:G:289:ARG:C	2.46	0.41
1:H:281:HIS:CE1	4:H:577:HOH:O	2.65	0.41
1:C:149:GLY:HA2	1:C:159:LEU:HD11	2.02	0.41
1:H:282:HIS:CD2	4:H:518:HOH:O	2.73	0.41
1:A:15:ALA:O	1:A:401:ARG:HD2	2.21	0.41
1:A:40:TRP:CD1	1:A:357:CYS:HG	2.39	0.41
1:C:62:PHE:CD1	1:C:62:PHE:C	2.98	0.41
1:C:270:ALA:HA	1:C:271:PRO:HD3	1.96	0.41
1:D:219:PRO:HG2	1:D:220:ASP:OD1	2.21	0.41
1:D:258:GLN:H	1:D:258:GLN:CD	2.28	0.41
1:E:377:GLY:C	1:E:378:ARG:HG3	2.46	0.41
1:F:167:GLU:CD	1:F:378:ARG:HD3	2.46	0.41
1:H:372:PRO:HG2	4:H:641:HOH:O	2.20	0.41
1:A:268:ARG:CB	1:A:268:ARG:NH1	2.84	0.41
1:B:251:ILE:O	1:B:251:ILE:HG23	2.20	0.41
1:D:170:PHE:O	1:D:186:ILE:HG12	2.20	0.40
1:D:248:LEU:HB3	1:D:274:MET:HE2	2.03	0.40
1:H:10:ILE:HD13	1:H:109:VAL:HG12	2.03	0.40
1:G:319:ALA:CB	1:G:326:VAL:CG2	2.99	0.40
1:G:329:HIS:ND1	1:G:329:HIS:C	2.80	0.40
1:H:114:LEU:O	1:H:118:GLN:HG3	2.21	0.40
1:A:386:LYS:HB3	1:E:1:MET:HE1	2.02	0.40
1:G:62:PHE:CD1	1:G:62:PHE:C	2.98	0.40
1:B:289:ARG:HA	1:B:318:LEU:HD21	2.04	0.40
1:C:114:LEU:O	1:C:118:GLN:HG3	2.21	0.40
1:C:253:GLU:OE2	1:C:281:HIS:CD2	2.70	0.40
1:C:258:GLN:H	1:C:258:GLN:CD	2.29	0.40
1:F:13:VAL:O	1:F:13:VAL:HG13	2.21	0.40
1:G:289:ARG:HA	1:G:318:LEU:HD21	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:TRP:CG	1:B:41:ILE:N	2.90	0.40
1:B:367:ILE:HG23	1:B:368:LEU:CD1	2.44	0.40
1:F:44:HIS:HD2	1:F:193:HIS:O	2.05	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	403/405 (100%)	391 (97%)	11 (3%)	1 (0%)	43	31
1	B	403/405 (100%)	384 (95%)	18 (4%)	1 (0%)	43	31
1	C	403/405 (100%)	389 (96%)	13 (3%)	1 (0%)	43	31
1	D	403/405 (100%)	383 (95%)	19 (5%)	1 (0%)	43	31
1	E	403/405 (100%)	385 (96%)	17 (4%)	1 (0%)	43	31
1	F	403/405 (100%)	386 (96%)	16 (4%)	1 (0%)	43	31
1	G	403/405 (100%)	390 (97%)	12 (3%)	1 (0%)	43	31
1	H	403/405 (100%)	383 (95%)	19 (5%)	1 (0%)	43	31
All	All	3224/3240 (100%)	3091 (96%)	125 (4%)	8 (0%)	43	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	88	ALA
1	A	88	ALA
1	B	88	ALA
1	C	88	ALA
1	G	88	ALA
1	H	88	ALA
1	D	88	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	88	ALA

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	333/333 (100%)	329 (99%)	4 (1%)	63	57
1	B	333/333 (100%)	329 (99%)	4 (1%)	63	57
1	C	333/333 (100%)	328 (98%)	5 (2%)	57	49
1	D	333/333 (100%)	331 (99%)	2 (1%)	78	77
1	E	333/333 (100%)	329 (99%)	4 (1%)	63	57
1	F	333/333 (100%)	328 (98%)	5 (2%)	57	49
1	G	333/333 (100%)	328 (98%)	5 (2%)	57	49
1	H	333/333 (100%)	329 (99%)	4 (1%)	63	57
All	All	2664/2664 (100%)	2631 (99%)	33 (1%)	63	57

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	TRP
1	A	256	PRO
1	A	366	PRO
1	A	368	LEU
1	B	224	MET
1	B	228	TRP
1	B	366	PRO
1	B	370	ASP
1	C	38	ASN
1	C	224	MET
1	C	228	TRP
1	C	256	PRO
1	C	366	PRO
1	D	228	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	366	PRO
1	E	18	ILE
1	E	228	TRP
1	E	366	PRO
1	E	368	LEU
1	F	1	MET
1	F	2	GLU
1	F	228	TRP
1	F	366	PRO
1	F	368	LEU
1	G	224	MET
1	G	228	TRP
1	G	366	PRO
1	G	370	ASP
1	G	396	ASP
1	H	2	GLU
1	H	181	LYS
1	H	228	TRP
1	H	366	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	116	HIS
1	A	234	ASN
1	A	281	HIS
1	A	282	HIS
1	A	336	HIS
1	B	44	HIS
1	B	116	HIS
1	B	169	GLN
1	B	193	HIS
1	B	234	ASN
1	B	258	GLN
1	B	269	ASN
1	B	281	HIS
1	B	282	HIS
1	B	336	HIS
1	C	44	HIS
1	C	116	HIS
1	C	193	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	258	GLN
1	C	281	HIS
1	C	282	HIS
1	C	336	HIS
1	D	44	HIS
1	D	116	HIS
1	D	258	GLN
1	D	281	HIS
1	D	282	HIS
1	D	336	HIS
1	E	3	ASN
1	E	44	HIS
1	E	116	HIS
1	E	135	ASN
1	E	258	GLN
1	E	281	HIS
1	E	282	HIS
1	E	336	HIS
1	F	44	HIS
1	F	116	HIS
1	F	169	GLN
1	F	234	ASN
1	F	258	GLN
1	F	281	HIS
1	F	282	HIS
1	F	336	HIS
1	G	44	HIS
1	G	116	HIS
1	G	231	GLN
1	G	234	ASN
1	G	269	ASN
1	G	281	HIS
1	G	282	HIS
1	G	336	HIS
1	H	44	HIS
1	H	116	HIS
1	H	135	ASN
1	H	258	GLN
1	H	281	HIS
1	H	282	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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	MLT	B	502	2	8,8,8	0.99	1 (12%)	10,10,10	1.49	1 (10%)
3	MLT	F	502	2	8,8,8	1.00	1 (12%)	10,10,10	1.48	1 (10%)
3	MLT	E	502	2	8,8,8	1.04	1 (12%)	10,10,10	1.46	1 (10%)
3	MLT	H	502	2	8,8,8	0.97	1 (12%)	10,10,10	1.49	1 (10%)
3	MLT	G	502	2	8,8,8	1.03	1 (12%)	10,10,10	1.41	1 (10%)
3	MLT	A	502	2	8,8,8	1.01	1 (12%)	10,10,10	1.46	1 (10%)
3	MLT	D	502	2	8,8,8	1.03	1 (12%)	10,10,10	1.50	1 (10%)
3	MLT	C	502	2	8,8,8	0.95	1 (12%)	10,10,10	1.49	1 (10%)

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	MLT	B	502	2	-	0/8/8/8	-
3	MLT	F	502	2	-	0/8/8/8	-
3	MLT	E	502	2	-	2/8/8/8	-
3	MLT	H	502	2	-	1/8/8/8	-
3	MLT	G	502	2	-	0/8/8/8	-
3	MLT	A	502	2	-	1/8/8/8	-
3	MLT	D	502	2	-	1/8/8/8	-
3	MLT	C	502	2	-	0/8/8/8	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	MLT	O2-C1	-2.57	1.22	1.30
3	E	502	MLT	O2-C1	-2.50	1.22	1.30
3	G	502	MLT	O2-C1	-2.48	1.22	1.30
3	D	502	MLT	O2-C1	-2.46	1.22	1.30
3	F	502	MLT	O2-C1	-2.45	1.22	1.30
3	B	502	MLT	O2-C1	-2.44	1.22	1.30
3	C	502	MLT	O2-C1	-2.36	1.23	1.30
3	H	502	MLT	O2-C1	-2.28	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	MLT	O2-C1-C2	3.41	119.95	112.74
3	D	502	MLT	O2-C1-C2	3.41	119.95	112.74
3	B	502	MLT	O2-C1-C2	3.35	119.83	112.74
3	H	502	MLT	O2-C1-C2	3.35	119.83	112.74
3	F	502	MLT	O2-C1-C2	3.35	119.82	112.74
3	E	502	MLT	O2-C1-C2	3.32	119.77	112.74
3	A	502	MLT	O2-C1-C2	3.28	119.68	112.74
3	G	502	MLT	O2-C1-C2	3.13	119.37	112.74

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	502	MLT	C1-C2-C3-C4
3	E	502	MLT	O3-C2-C3-C4
3	A	502	MLT	C1-C2-C3-C4
3	D	502	MLT	C1-C2-C3-C4
3	H	502	MLT	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	405/405 (100%)	-0.21	6 (1%) 72 72	9, 16, 30, 45	0
1	B	405/405 (100%)	0.07	10 (2%) 58 58	10, 20, 32, 45	0
1	C	405/405 (100%)	0.04	11 (2%) 56 56	10, 19, 32, 44	0
1	D	405/405 (100%)	0.25	6 (1%) 72 72	14, 22, 33, 44	0
1	E	405/405 (100%)	0.34	10 (2%) 58 58	12, 21, 32, 42	0
1	F	405/405 (100%)	0.03	10 (2%) 58 58	9, 19, 32, 45	0
1	G	405/405 (100%)	0.03	10 (2%) 58 58	9, 19, 32, 44	0
1	H	405/405 (100%)	0.43	12 (2%) 52 52	14, 23, 34, 44	0
All	All	3240/3240 (100%)	0.12	75 (2%) 61 61	9, 20, 32, 45	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	38	ASN	4.9
1	B	1	MET	4.5
1	H	38	ASN	4.4
1	C	1	MET	4.3
1	D	1	MET	4.3
1	E	1	MET	4.3
1	H	1	MET	4.1
1	A	129	SER	4.0
1	F	1	MET	3.9
1	E	129	SER	3.8
1	G	12	HIS	3.7
1	C	32	TYR	3.7
1	E	53	ARG	3.6
1	C	129	SER	3.4
1	H	129	SER	3.4
1	G	79	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	129	SER	3.2
1	F	227	CYS	3.2
1	G	1	MET	3.2
1	H	324	GLN	3.2
1	E	18	ILE	3.1
1	A	1	MET	3.0
1	F	129	SER	2.9
1	B	2	GLU	2.9
1	H	37	GLY	2.9
1	B	53	ARG	2.9
1	D	129	SER	2.8
1	G	326	VAL	2.8
1	D	370	ASP	2.8
1	F	404	SER	2.8
1	F	53	ARG	2.8
1	B	324	GLN	2.7
1	H	24	GLU	2.7
1	C	79	ARG	2.7
1	H	325	LEU	2.7
1	C	24	GLU	2.6
1	C	326	VAL	2.6
1	G	53	ARG	2.6
1	C	401	ARG	2.6
1	F	370	ASP	2.6
1	H	376	ASN	2.6
1	H	326	VAL	2.5
1	A	324	GLN	2.5
1	B	325	LEU	2.5
1	B	326	VAL	2.5
1	D	324	GLN	2.5
1	H	53	ARG	2.5
1	F	215	GLU	2.5
1	F	24	GLU	2.4
1	A	215	GLU	2.4
1	B	268	ARG	2.3
1	E	325	LEU	2.3
1	F	79	ARG	2.3
1	E	24	GLU	2.3
1	B	24	GLU	2.2
1	E	326	VAL	2.2
1	E	38	ASN	2.2
1	A	6	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	325	LEU	2.2
1	G	325	LEU	2.2
1	G	398	HIS	2.2
1	D	375	VAL	2.2
1	C	6	THR	2.2
1	G	129	SER	2.2
1	E	364	PHE	2.1
1	G	330	GLY	2.1
1	B	38	ASN	2.1
1	C	16	TRP	2.1
1	H	13	VAL	2.1
1	H	182	GLU	2.1
1	C	395	ARG	2.1
1	E	79	ARG	2.0
1	F	23	ALA	2.0
1	G	395	ARG	2.0
1	D	359	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	MG	D	501	1/1	0.78	0.09	18,18,18,18	0
2	MG	F	501	1/1	0.86	0.06	14,14,14,14	0
3	MLT	E	502	9/9	0.89	0.10	26,27,29,30	0
2	MG	C	501	1/1	0.90	0.07	15,15,15,15	0
3	MLT	D	502	9/9	0.91	0.09	26,28,32,33	0
3	MLT	H	502	9/9	0.91	0.09	26,27,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MLT	B	502	9/9	0.92	0.08	21,24,28,28	0
3	MLT	F	502	9/9	0.92	0.08	18,21,26,28	0
3	MLT	G	502	9/9	0.92	0.09	16,21,28,30	0
2	MG	E	501	1/1	0.92	0.04	20,20,20,20	0
2	MG	H	501	1/1	0.93	0.04	22,22,22,22	0
3	MLT	C	502	9/9	0.95	0.07	16,19,25,26	0
2	MG	G	501	1/1	0.95	0.05	15,15,15,15	0
3	MLT	A	502	9/9	0.97	0.06	12,16,22,23	0
2	MG	B	501	1/1	0.98	0.03	17,17,17,17	0
2	MG	A	501	1/1	0.99	0.02	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.