



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:08 PM UTC

PDB ID : 3ES8 / pdb_00003es8
Title : Crystal structure of divergent enolase from *Oceanobacillus Iheyensis* complexed with Mg and L-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 : 2008-10-04
Resolution : 2.20 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

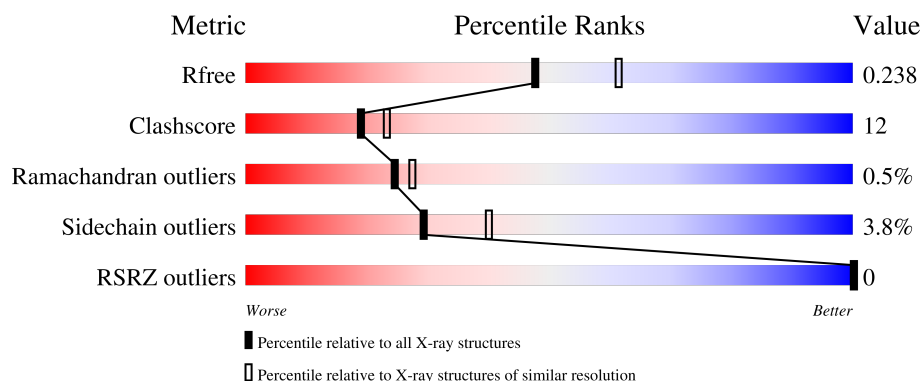
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	391	 71% 26% ..
1	B	391	 72% 24% ..
1	C	391	 72% 24% ..
1	D	391	 71% 25% ..
1	E	391	 70% 26% ..

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Mol	Chain	Length	Quality of chain
1	F	391	 70% 26% ..
1	G	391	 71% 26% ..
1	H	391	 71% 25% ..

2 Entry composition

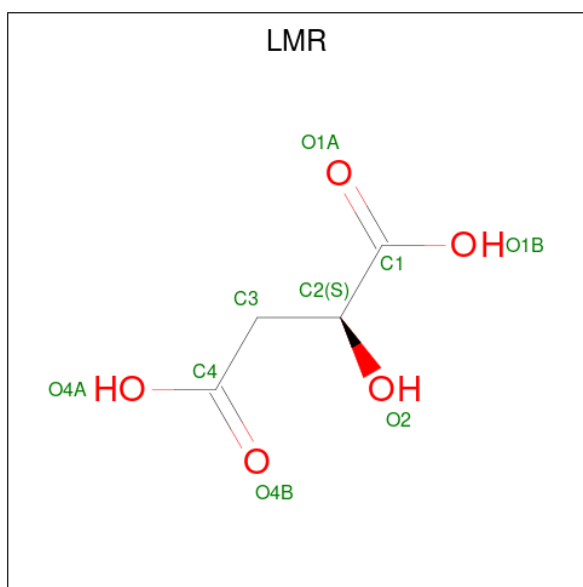
There are 4 unique types of molecules in this entry. The entry contains 25362 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Muconate cycloisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total 3097	C 1976	N 525	O 586	S 10	0	0	0
1	B	387	Total 3097	C 1976	N 525	O 586	S 10	0	0	0
1	C	387	Total 3097	C 1976	N 525	O 586	S 10	0	0	0
1	D	387	Total 3097	C 1976	N 525	O 586	S 10	0	0	0
1	E	387	Total 3097	C 1976	N 525	O 586	S 10	0	0	0
1	F	387	Total 3097	C 1976	N 525	O 586	S 10	0	0	0
1	G	387	Total 3097	C 1976	N 525	O 586	S 10	0	0	0
1	H	387	Total 3097	C 1976	N 525	O 586	S 10	0	0	0

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: C₄H₆O₅).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0
3	H	1	Total 1	Mg 1	0	0

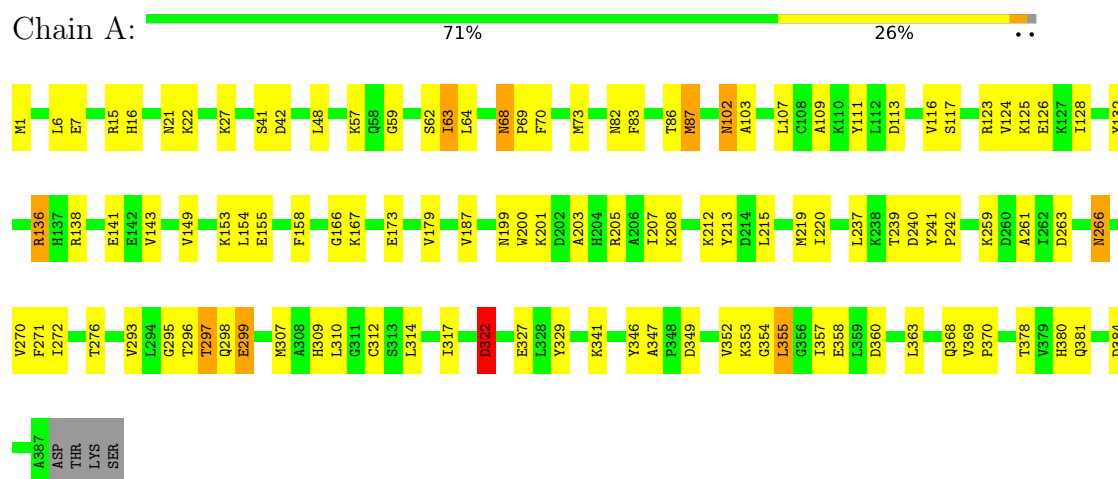
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total 79	O 79	0	0
4	B	50	Total 50	O 50	0	0
4	C	51	Total 51	O 51	0	0
4	D	64	Total 64	O 64	0	0
4	E	69	Total 69	O 69	0	0
4	F	74	Total 74	O 74	0	0
4	G	65	Total 65	O 65	0	0
4	H	54	Total 54	O 54	0	0

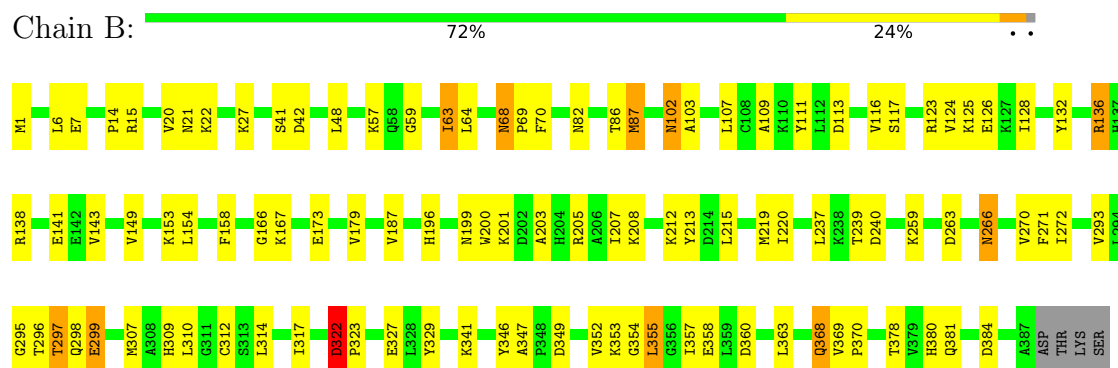
3 Residue-property plots

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.

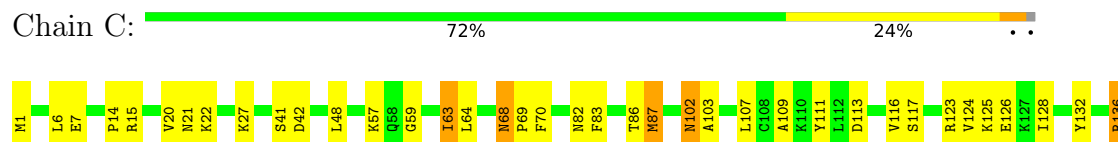
• Molecule 1: Muconate cycloisomerase

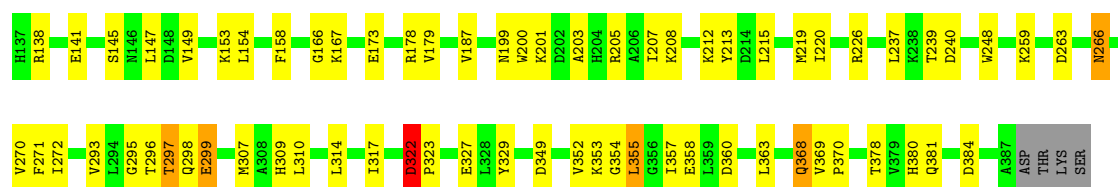


• Molecule 1: Muconate cycloisomerase



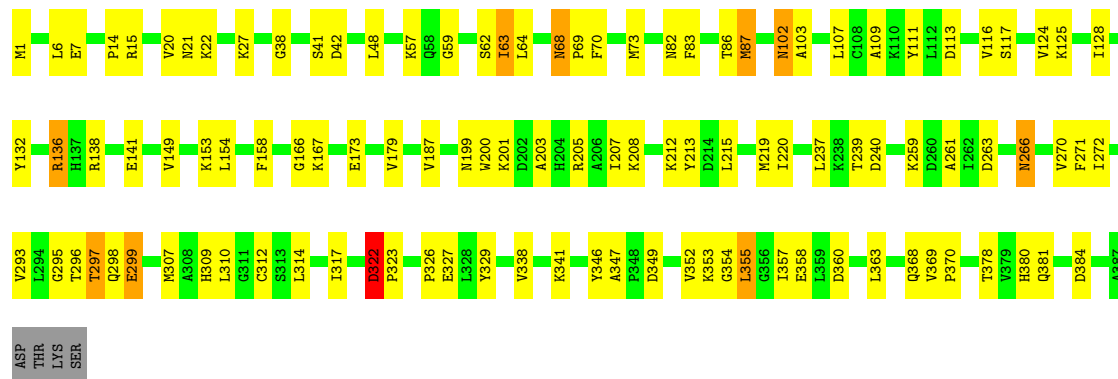
• Molecule 1: Muconate cycloisomerase





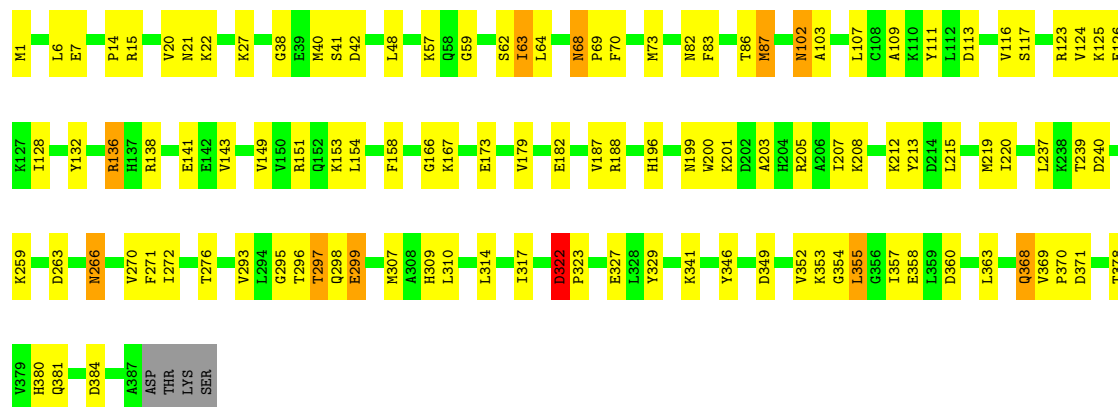
• Molecule 1: Muconate cycloisomerase

Chain D: 71% 25% ..



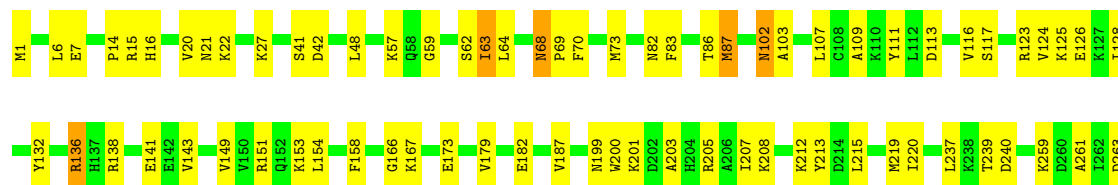
• Molecule 1: Muconate cycloisomerase

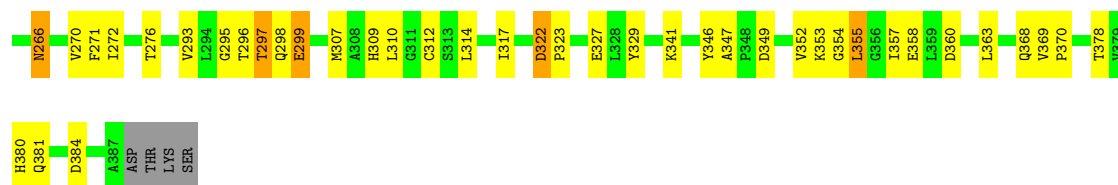
Chain E: 70% 26% ..



• Molecule 1: Muconate cycloisomerase

Chain F: 70% 26% ..





• Molecule 1: Muconate cycloisomerase

Chain G: 71% 26% ..



• Molecule 1: Muconate cycloisomerase

Chain H: 71% 25% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	105.58Å 105.69Å 105.72Å 109.31° 109.47° 109.66°	Depositor
Resolution (Å)	24.94 – 2.20 24.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.7 (24.94-2.20) 94.9 (24.94-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.241 0.221 , 0.238	Depositor DCC
R_{free} test set	8612 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage

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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.

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Property	Value	Source
Estimated twinning fraction	0.440 for $-k, h+k+1, -h$ 0.440 for $-l, -h, h+k+1$ 0.002 for $-l, h+k+1, -k$ 0.002 for $h+k+1, -l, -h$ 0.002 for $-k, -l, h+k+1$ 0.002 for $h+k+1, -h, -k$ 0.000 for $h, l, -h-k-l$ 0.000 for $h, -h-k-l, k$ 0.001 for l, h, k 0.001 for k, l, h 0.001 for $-h-k-l, k, h$ 0.001 for $l, k, -h-k-l$ 0.000 for $-h-k-l, h, l$ 0.000 for $k, -h-k-l, l$ 0.470 for $-h-k-l, l, k$ 0.023 for $h+k+1, -k, -l$ 0.024 for $k, h, -h-k-l$ 0.003 for $-k, -h, -l$ 0.024 for $l, -h-k-l, h$ 0.003 for $-h, h+k+1, -l$ 0.022 for $-h, -l, -k$ 0.002 for $-h, -k, h+k+1$ 0.002 for $-l, -k, -h$	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	25362	wwPDB-VP
Average B, all atoms ($\text{\AA}^2$)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.43	0/3163	0.97	18/4276 (0.4%)
1	B	0.40	0/3163	0.96	15/4276 (0.4%)
1	C	0.41	0/3163	0.96	16/4276 (0.4%)
1	D	0.42	0/3163	0.96	17/4276 (0.4%)
1	E	0.41	0/3163	0.96	18/4276 (0.4%)
1	F	0.41	0/3163	0.96	18/4276 (0.4%)
1	G	0.42	0/3163	0.96	17/4276 (0.4%)
1	H	0.40	0/3163	0.96	17/4276 (0.4%)
All	All	0.41	0/25304	0.96	136/34208 (0.4%)

There are no bond length outliers.

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	124	VAL	N-CA-C	-9.39	103.57	112.96
1	D	124	VAL	N-CA-C	-9.35	103.61	112.96
1	A	124	VAL	N-CA-C	-9.32	103.64	112.96
1	G	124	VAL	N-CA-C	-9.10	103.86	112.96
1	C	124	VAL	N-CA-C	-8.99	103.97	112.96
1	E	124	VAL	N-CA-C	-8.99	103.97	112.96
1	B	124	VAL	N-CA-C	-8.98	103.98	112.96
1	H	212	LYS	N-CA-C	-8.93	101.82	112.89
1	C	212	LYS	N-CA-C	-8.91	101.83	112.89
1	B	212	LYS	N-CA-C	-8.90	101.86	112.89
1	H	124	VAL	N-CA-C	-8.89	104.07	112.96
1	E	212	LYS	N-CA-C	-8.78	102.00	112.89
1	D	212	LYS	N-CA-C	-8.68	102.13	112.89
1	F	212	LYS	N-CA-C	-8.64	102.17	112.89
1	A	212	LYS	N-CA-C	-8.59	102.23	112.89
1	G	212	LYS	N-CA-C	-8.59	102.24	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ARG	N-CA-C	7.83	121.58	110.23
1	G	136	ARG	N-CA-C	7.81	121.55	110.23
1	E	136	ARG	N-CA-C	7.79	121.52	110.23
1	F	136	ARG	N-CA-C	7.78	121.52	110.23
1	D	136	ARG	N-CA-C	7.76	121.48	110.23
1	B	136	ARG	N-CA-C	7.73	121.44	110.23
1	H	136	ARG	N-CA-C	7.70	121.40	110.23
1	C	136	ARG	N-CA-C	7.63	121.29	110.23
1	E	166	GLY	N-CA-C	7.61	121.72	113.58
1	C	166	GLY	N-CA-C	7.57	121.68	113.58
1	B	166	GLY	N-CA-C	7.49	121.60	113.58
1	A	166	GLY	N-CA-C	7.43	121.53	113.58
1	A	41	SER	N-CA-C	7.13	121.46	110.20
1	H	166	GLY	N-CA-C	7.06	122.05	113.79
1	D	41	SER	N-CA-C	6.99	121.24	110.20
1	G	41	SER	N-CA-C	6.99	121.24	110.20
1	H	41	SER	N-CA-C	6.97	121.21	110.20
1	F	41	SER	N-CA-C	6.96	121.20	110.20
1	E	41	SER	N-CA-C	6.92	121.14	110.20
1	C	41	SER	N-CA-C	6.91	121.12	110.20
1	B	41	SER	N-CA-C	6.87	121.05	110.20
1	A	200	TRP	N-CA-C	6.80	119.56	111.33
1	G	166	GLY	N-CA-C	6.80	121.75	113.79
1	F	200	TRP	N-CA-C	6.75	119.50	111.33
1	F	166	GLY	N-CA-C	6.73	121.66	113.79
1	G	200	TRP	N-CA-C	6.71	119.45	111.33
1	G	64	LEU	N-CA-C	6.66	120.62	112.23
1	D	64	LEU	N-CA-C	6.65	120.61	112.23
1	F	64	LEU	N-CA-C	6.58	120.52	112.23
1	D	200	TRP	N-CA-C	6.54	119.24	111.33
1	D	166	GLY	N-CA-C	6.54	121.44	113.79
1	E	200	TRP	N-CA-C	6.52	119.22	111.33
1	B	64	LEU	N-CA-C	6.51	120.44	112.23
1	H	64	LEU	N-CA-C	6.51	120.44	112.23
1	C	64	LEU	N-CA-C	6.50	120.41	112.23
1	H	200	TRP	N-CA-C	6.48	119.17	111.33
1	A	64	LEU	N-CA-C	6.43	120.33	112.23
1	E	64	LEU	N-CA-C	6.39	120.28	112.23
1	B	200	TRP	N-CA-C	6.36	119.03	111.33
1	C	200	TRP	N-CA-C	6.36	119.02	111.33
1	H	297	THR	N-CA-C	-6.34	104.09	113.61
1	F	297	THR	N-CA-C	-6.33	104.11	113.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	322	ASP	N-CA-C	6.28	123.68	109.81
1	B	322	ASP	N-CA-C	6.26	123.64	109.81
1	H	322	ASP	N-CA-C	6.26	123.64	109.81
1	B	297	THR	N-CA-C	-6.24	104.24	113.61
1	G	297	THR	N-CA-C	-6.23	104.27	113.61
1	A	138	ARG	N-CA-C	-6.21	106.02	113.97
1	A	322	ASP	N-CA-C	6.19	123.48	109.81
1	E	322	ASP	N-CA-C	6.18	123.48	109.81
1	D	297	THR	N-CA-C	-6.17	104.36	113.61
1	F	138	ARG	N-CA-C	-6.17	106.08	113.97
1	A	297	THR	N-CA-C	-6.15	104.39	113.61
1	G	322	ASP	N-CA-C	6.13	123.36	109.81
1	D	322	ASP	N-CA-C	6.12	123.34	109.81
1	C	297	THR	N-CA-C	-6.11	104.45	113.61
1	E	297	THR	N-CA-C	-6.10	104.46	113.61
1	C	138	ARG	N-CA-C	-6.08	106.19	113.97
1	C	322	ASP	N-CA-C	6.08	123.24	109.81
1	G	220	ILE	N-CA-C	-6.01	99.70	108.11
1	H	138	ARG	N-CA-C	-5.99	106.30	113.97
1	D	138	ARG	N-CA-C	-5.97	106.33	113.97
1	B	138	ARG	N-CA-C	-5.94	106.37	113.97
1	G	138	ARG	N-CA-C	-5.93	106.38	113.97
1	E	138	ARG	N-CA-C	-5.92	106.39	113.97
1	A	220	ILE	N-CA-C	-5.79	100.00	108.11
1	H	199	ASN	N-CA-C	-5.76	102.38	110.50
1	A	261	ALA	N-CA-C	5.74	118.48	111.82
1	A	270	VAL	N-CA-C	5.74	116.48	110.62
1	F	261	ALA	N-CA-C	5.74	118.48	111.82
1	H	270	VAL	N-CA-C	5.72	116.45	110.62
1	E	199	ASN	N-CA-C	-5.68	102.49	110.50
1	B	220	ILE	N-CA-C	-5.64	100.21	108.11
1	E	220	ILE	N-CA-C	-5.64	100.27	108.17
1	H	261	ALA	N-CA-C	5.63	118.36	111.82
1	C	270	VAL	N-CA-C	5.62	116.35	110.62
1	F	220	ILE	N-CA-C	-5.59	100.28	108.11
1	D	220	ILE	N-CA-C	-5.58	100.29	108.11
1	B	199	ASN	N-CA-C	-5.57	102.64	110.50
1	C	220	ILE	N-CA-C	-5.57	100.38	108.17
1	G	270	VAL	N-CA-C	5.56	116.29	110.62
1	D	261	ALA	N-CA-C	5.55	118.26	111.82
1	A	199	ASN	N-CA-C	-5.52	102.72	110.50
1	E	270	VAL	N-CA-C	5.48	116.21	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ASN	N-CA-C	-5.48	102.77	110.50
1	G	261	ALA	N-CA-C	5.46	118.16	111.82
1	H	63	ILE	CB-CA-C	-5.46	104.92	112.24
1	H	220	ILE	N-CA-C	-5.44	100.56	108.17
1	B	63	ILE	CB-CA-C	-5.43	104.96	112.24
1	B	270	VAL	N-CA-C	5.42	116.15	110.62
1	F	270	VAL	N-CA-C	5.41	116.79	110.62
1	G	199	ASN	N-CA-C	-5.39	102.89	110.50
1	E	63	ILE	CB-CA-C	-5.39	105.02	112.24
1	C	63	ILE	CB-CA-C	-5.38	105.03	112.24
1	F	199	ASN	N-CA-C	-5.35	102.96	110.50
1	D	199	ASN	N-CA-C	-5.23	103.13	110.50
1	F	83	PHE	CA-C-N	5.22	125.22	119.89
1	F	83	PHE	C-N-CA	5.22	125.22	119.89
1	H	83	PHE	CA-C-N	5.20	125.19	119.89
1	H	83	PHE	C-N-CA	5.20	125.19	119.89
1	A	63	ILE	CB-CA-C	-5.20	105.28	112.24
1	G	63	ILE	CB-CA-C	-5.16	105.32	112.24
1	D	270	VAL	N-CA-C	5.16	116.50	110.62
1	E	83	PHE	CA-C-N	5.15	125.14	119.89
1	E	83	PHE	C-N-CA	5.15	125.14	119.89
1	B	143	VAL	N-CA-C	5.14	115.28	110.30
1	E	143	VAL	N-CA-C	5.14	115.28	110.30
1	C	83	PHE	CA-C-N	5.13	125.12	119.89
1	C	83	PHE	C-N-CA	5.13	125.12	119.89
1	D	83	PHE	CA-C-N	5.12	125.12	119.89
1	D	83	PHE	C-N-CA	5.12	125.12	119.89
1	A	83	PHE	CA-C-N	5.12	125.11	119.89
1	A	83	PHE	C-N-CA	5.12	125.11	119.89
1	D	63	ILE	CB-CA-C	-5.09	105.42	112.24
1	F	63	ILE	CB-CA-C	-5.05	105.47	112.24
1	E	40	MET	N-CA-C	-5.04	98.37	107.75
1	G	83	PHE	CA-C-N	5.03	125.02	119.89
1	G	83	PHE	C-N-CA	5.03	125.02	119.89
1	A	143	VAL	N-CA-C	5.03	115.18	110.30
1	F	143	VAL	N-CA-C	5.03	115.18	110.30

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	3097	0	3076	81	0
1	B	3097	0	3076	76	0
1	C	3097	0	3076	78	0
1	D	3097	0	3076	76	0
1	E	3097	0	3076	82	0
1	F	3097	0	3076	78	0
1	G	3097	0	3076	76	0
1	H	3097	0	3076	78	0
2	A	9	0	3	0	0
2	B	9	0	4	1	0
2	C	9	0	4	1	0
2	D	9	0	3	0	0
2	E	9	0	3	1	0
2	F	9	0	3	0	0
2	G	9	0	3	0	0
2	H	9	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	79	0	0	3	0
4	B	50	0	0	1	0
4	C	51	0	0	1	0
4	D	64	0	0	0	0
4	E	69	0	0	3	0
4	F	74	0	0	1	0
4	G	65	0	0	1	0
4	H	54	0	0	1	0
All	All	25362	0	24634	584	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 12.

All (584) 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:266:ASN:HD21	1:E:295:GLY:HA3	1.17	1.10
1:G:266:ASN:HD21	1:G:295:GLY:HA3	1.17	1.09
1:D:266:ASN:HD21	1:D:295:GLY:HA3	1.17	1.08
1:C:266:ASN:HD21	1:C:295:GLY:HA3	1.16	1.05
1:B:266:ASN:HD21	1:B:295:GLY:HA3	1.16	1.04
1:H:266:ASN:HD21	1:H:295:GLY:HA3	1.17	1.03
1:F:266:ASN:HD21	1:F:295:GLY:HA3	1.18	1.02
1:A:266:ASN:HD21	1:A:295:GLY:HA3	1.19	1.01
1:A:102:ASN:HD22	1:A:103:ALA:N	1.75	0.85
1:E:102:ASN:HD22	1:E:103:ALA:N	1.74	0.85
1:C:102:ASN:HD22	1:C:103:ALA:N	1.74	0.84
1:D:102:ASN:HD22	1:D:103:ALA:N	1.74	0.84
1:B:102:ASN:HD22	1:B:103:ALA:N	1.74	0.84
1:G:102:ASN:HD22	1:G:103:ALA:N	1.75	0.83
1:F:102:ASN:HD22	1:F:103:ALA:N	1.76	0.83
1:H:102:ASN:HD22	1:H:103:ALA:N	1.75	0.83
1:A:155:GLU:HG3	4:A:398:HOH:O	1.85	0.77
1:C:266:ASN:HD21	1:C:295:GLY:CA	1.99	0.76
1:D:266:ASN:HD22	1:D:266:ASN:C	1.95	0.75
1:H:266:ASN:HD21	1:H:295:GLY:CA	2.00	0.74
1:F:266:ASN:C	1:F:266:ASN:HD22	1.96	0.74
1:B:266:ASN:HD21	1:B:295:GLY:CA	1.99	0.74
1:A:266:ASN:C	1:A:266:ASN:HD22	1.95	0.73
1:B:266:ASN:C	1:B:266:ASN:HD22	1.96	0.73
1:D:266:ASN:HD21	1:D:295:GLY:CA	2.00	0.72
1:H:266:ASN:C	1:H:266:ASN:HD22	1.97	0.71
1:E:266:ASN:C	1:E:266:ASN:HD22	1.98	0.71
1:G:266:ASN:C	1:G:266:ASN:HD22	1.98	0.71
1:C:266:ASN:C	1:C:266:ASN:HD22	1.97	0.70
1:D:117:SER:OG	1:D:309:HIS:HD2	1.75	0.70
1:C:219:MET:HE1	1:C:293:VAL:HG11	1.74	0.70
1:A:173:GLU:HG3	1:A:213:TYR:HE2	1.57	0.69
1:G:173:GLU:HG3	1:G:213:TYR:HE2	1.58	0.69
1:B:266:ASN:ND2	1:B:295:GLY:HA3	2.01	0.69
1:F:22:LYS:HE2	1:F:369:VAL:HG11	1.75	0.69
1:E:15:ARG:NE	1:E:21:ASN:HD21	1.91	0.68
1:F:173:GLU:HG3	1:F:213:TYR:HE2	1.57	0.68
1:B:167:LYS:HZ3	1:B:380:HIS:HD2	1.42	0.68
1:G:22:LYS:HE2	1:G:369:VAL:HG11	1.76	0.68
1:H:173:GLU:HG3	1:H:213:TYR:HE2	1.59	0.68
1:E:196:HIS:HD2	4:E:445:HOH:O	1.77	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:ASN:HD21	1:G:295:GLY:CA	2.00	0.68
1:B:196:HIS:HD2	4:B:423:HOH:O	1.76	0.68
1:F:266:ASN:HD21	1:F:295:GLY:CA	2.01	0.68
1:A:167:LYS:NZ	1:A:380:HIS:HD2	1.92	0.67
1:F:314:LEU:HD12	1:F:317:ILE:HD11	1.76	0.67
1:B:173:GLU:HG3	1:B:213:TYR:HE2	1.59	0.67
1:C:314:LEU:HD12	1:C:317:ILE:HD11	1.76	0.67
1:E:173:GLU:HG3	1:E:213:TYR:HE2	1.59	0.67
1:D:22:LYS:HE2	1:D:369:VAL:HG11	1.76	0.67
1:D:219:MET:HE1	1:D:293:VAL:HG11	1.74	0.67
1:A:314:LEU:HD12	1:A:317:ILE:HD11	1.76	0.67
1:C:173:GLU:HG3	1:C:213:TYR:HE2	1.60	0.67
1:H:15:ARG:NE	1:H:21:ASN:HD21	1.92	0.67
1:B:15:ARG:NE	1:B:21:ASN:HD21	1.92	0.67
1:C:117:SER:OG	1:C:309:HIS:HD2	1.77	0.67
1:E:266:ASN:HD21	1:E:295:GLY:CA	2.01	0.67
1:G:117:SER:OG	1:G:309:HIS:HD2	1.78	0.67
1:G:167:LYS:HZ3	1:G:380:HIS:HD2	1.43	0.67
1:A:219:MET:HE1	1:A:293:VAL:HG11	1.76	0.66
1:D:314:LEU:HD12	1:D:317:ILE:HD11	1.76	0.66
1:A:117:SER:OG	1:A:309:HIS:HD2	1.77	0.66
1:B:117:SER:OG	1:B:309:HIS:HD2	1.78	0.66
1:E:167:LYS:NZ	1:E:380:HIS:HD2	1.93	0.66
1:E:219:MET:HE1	1:E:293:VAL:HG11	1.77	0.66
1:E:314:LEU:HD12	1:E:317:ILE:HD11	1.78	0.66
1:F:219:MET:HE1	1:F:293:VAL:HG11	1.77	0.66
1:D:266:ASN:ND2	1:D:295:GLY:HA3	2.01	0.66
1:E:117:SER:OG	1:E:309:HIS:HD2	1.78	0.66
1:F:117:SER:OG	1:F:309:HIS:HD2	1.77	0.66
1:G:219:MET:HE1	1:G:293:VAL:HG11	1.77	0.66
1:H:167:LYS:NZ	1:H:380:HIS:HD2	1.94	0.66
1:B:314:LEU:HD12	1:B:317:ILE:HD11	1.77	0.66
1:F:167:LYS:NZ	1:F:380:HIS:HD2	1.93	0.66
1:H:117:SER:OG	1:H:309:HIS:HD2	1.78	0.65
1:C:15:ARG:NE	1:C:21:ASN:HD21	1.94	0.65
1:C:167:LYS:NZ	1:C:380:HIS:HD2	1.95	0.65
1:D:173:GLU:HG3	1:D:213:TYR:HE2	1.59	0.65
1:A:22:LYS:HE2	1:A:369:VAL:HG11	1.78	0.65
1:G:167:LYS:NZ	1:G:380:HIS:HD2	1.95	0.65
1:A:15:ARG:NE	1:A:21:ASN:HD21	1.95	0.65
1:G:314:LEU:HD12	1:G:317:ILE:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LYS:HE2	1:B:369:VAL:HG11	1.78	0.65
1:G:15:ARG:NE	1:G:21:ASN:HD21	1.95	0.65
1:B:219:MET:HE1	1:B:293:VAL:HG11	1.79	0.64
1:H:314:LEU:HD12	1:H:317:ILE:HD11	1.77	0.64
1:B:167:LYS:NZ	1:B:380:HIS:HD2	1.95	0.64
1:C:266:ASN:ND2	1:C:295:GLY:HA3	2.01	0.64
1:F:266:ASN:ND2	1:F:295:GLY:HA3	2.03	0.64
1:H:219:MET:HE1	1:H:293:VAL:HG11	1.78	0.64
1:F:15:ARG:NE	1:F:21:ASN:HD21	1.95	0.64
1:A:266:ASN:ND2	1:A:295:GLY:HA3	2.03	0.63
1:C:22:LYS:HE2	1:C:369:VAL:HG11	1.81	0.63
1:H:196:HIS:HD2	4:H:447:HOH:O	1.81	0.62
1:D:167:LYS:NZ	1:D:380:HIS:HD2	1.97	0.62
1:C:167:LYS:HZ3	1:C:380:HIS:HD2	1.46	0.62
1:A:266:ASN:HD21	1:A:295:GLY:CA	2.03	0.62
1:D:15:ARG:NE	1:D:21:ASN:HD21	1.97	0.62
1:H:22:LYS:HE2	1:H:369:VAL:HG11	1.80	0.62
1:F:167:LYS:HZ3	1:F:380:HIS:HD2	1.47	0.62
1:E:266:ASN:ND2	1:E:295:GLY:HA3	2.01	0.62
1:E:22:LYS:HE2	1:E:369:VAL:HG11	1.82	0.61
1:G:102:ASN:HD22	1:G:103:ALA:H	1.47	0.61
1:A:1:MET:HE2	1:A:111:TYR:CD1	2.35	0.61
1:F:102:ASN:HD22	1:F:103:ALA:H	1.48	0.61
1:A:68:ASN:C	1:A:68:ASN:HD22	2.08	0.60
1:A:102:ASN:HD22	1:A:103:ALA:H	1.47	0.60
1:G:68:ASN:C	1:G:68:ASN:HD22	2.10	0.60
1:A:240:ASP:OD1	1:G:208:LYS:HE3	2.01	0.60
1:G:266:ASN:ND2	1:G:295:GLY:HA3	2.02	0.60
1:F:68:ASN:C	1:F:68:ASN:HD22	2.08	0.60
1:B:86:THR:O	1:G:86:THR:O	2.19	0.60
1:B:378:THR:OG1	1:B:381:GLN:HG3	2.02	0.60
1:C:102:ASN:HD22	1:C:103:ALA:H	1.50	0.60
1:D:86:THR:O	1:E:86:THR:O	2.19	0.60
1:D:208:LYS:HE3	1:F:240:ASP:OD1	2.02	0.60
1:H:266:ASN:ND2	1:H:295:GLY:HA3	2.02	0.60
1:A:167:LYS:HZ3	1:A:380:HIS:HD2	1.49	0.60
1:E:378:THR:OG1	1:E:381:GLN:HG3	2.02	0.60
1:H:378:THR:OG1	1:H:381:GLN:HG3	2.02	0.60
1:D:102:ASN:HD22	1:D:103:ALA:H	1.48	0.59
1:G:1:MET:HE2	1:G:111:TYR:CD1	2.37	0.59
1:E:15:ARG:HE	1:E:21:ASN:ND2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:378:THR:OG1	1:G:381:GLN:HG3	2.03	0.59
1:A:173:GLU:HG3	1:A:213:TYR:CE2	2.37	0.59
1:E:102:ASN:HD22	1:E:103:ALA:H	1.47	0.59
1:G:173:GLU:HG3	1:G:213:TYR:CE2	2.37	0.59
1:C:68:ASN:HD22	1:C:68:ASN:C	2.10	0.59
1:E:188:ARG:HD2	4:E:424:HOH:O	2.02	0.59
1:B:68:ASN:C	1:B:68:ASN:HD22	2.10	0.59
1:D:68:ASN:C	1:D:68:ASN:HD22	2.10	0.59
1:E:1:MET:HE2	1:E:111:TYR:CD1	2.38	0.59
1:B:1:MET:HE2	1:B:111:TYR:CD1	2.38	0.58
1:D:1:MET:HE2	1:D:111:TYR:CD1	2.38	0.58
1:E:167:LYS:HZ3	1:E:380:HIS:HD2	1.51	0.58
1:F:1:MET:HE2	1:F:111:TYR:CD1	2.38	0.58
1:A:86:THR:O	1:C:86:THR:O	2.21	0.58
1:H:15:ARG:HE	1:H:21:ASN:ND2	2.02	0.58
1:H:102:ASN:HD22	1:H:103:ALA:H	1.50	0.58
1:D:378:THR:OG1	1:D:381:GLN:HG3	2.02	0.58
1:H:173:GLU:HG3	1:H:213:TYR:CE2	2.39	0.58
1:H:68:ASN:HD22	1:H:68:ASN:C	2.10	0.58
1:A:378:THR:OG1	1:A:381:GLN:HG3	2.03	0.58
1:F:173:GLU:HG3	1:F:213:TYR:CE2	2.37	0.58
1:C:378:THR:OG1	1:C:381:GLN:HG3	2.04	0.58
1:F:86:THR:O	1:H:86:THR:O	2.21	0.58
1:B:102:ASN:HD22	1:B:103:ALA:H	1.49	0.58
1:C:173:GLU:HG3	1:C:213:TYR:CE2	2.39	0.58
1:E:173:GLU:HG3	1:E:213:TYR:CE2	2.39	0.57
1:E:68:ASN:C	1:E:68:ASN:HD22	2.11	0.57
1:F:378:THR:OG1	1:F:381:GLN:HG3	2.04	0.57
1:H:1:MET:HE2	1:H:111:TYR:CD1	2.39	0.57
1:C:1:MET:HE2	1:C:111:TYR:CD1	2.40	0.57
1:F:201:LYS:HD3	1:G:263:ASP:OD2	2.05	0.57
1:D:201:LYS:HD3	1:F:263:ASP:OD2	2.04	0.57
1:D:167:LYS:HZ3	1:D:380:HIS:HD2	1.52	0.57
1:C:68:ASN:HD22	1:C:69:PRO:CD	2.18	0.57
1:A:136:ARG:HD2	1:A:384:ASP:OD1	2.05	0.57
1:A:309:HIS:HE1	1:A:355:LEU:O	1.88	0.56
1:D:68:ASN:HD22	1:D:69:PRO:CD	2.19	0.56
1:D:215:LEU:HD12	1:D:215:LEU:N	2.21	0.56
1:E:369:VAL:HG13	1:E:370:PRO:HD2	1.87	0.56
1:F:68:ASN:HD22	1:F:69:PRO:CD	2.18	0.56
1:H:167:LYS:HZ3	1:H:380:HIS:HD2	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HD12	1:A:215:LEU:N	2.21	0.56
1:B:15:ARG:HE	1:B:21:ASN:ND2	2.02	0.56
1:B:136:ARG:HD2	1:B:384:ASP:OD1	2.05	0.56
1:F:208:LYS:HE3	1:G:240:ASP:OD1	2.04	0.56
1:D:173:GLU:HG3	1:D:213:TYR:CE2	2.39	0.56
1:B:173:GLU:HG3	1:B:213:TYR:CE2	2.38	0.56
1:C:136:ARG:HD2	1:C:384:ASP:OD1	2.05	0.56
1:G:309:HIS:HE1	1:G:355:LEU:O	1.88	0.56
1:H:102:ASN:HD22	1:H:102:ASN:C	2.14	0.56
1:G:15:ARG:HE	1:G:21:ASN:ND2	2.04	0.56
1:A:208:LYS:HE3	1:D:240:ASP:OD1	2.06	0.56
1:A:15:ARG:HE	1:A:21:ASN:ND2	2.04	0.56
1:F:87:MET:HB3	1:H:87:MET:HB3	1.88	0.56
1:D:102:ASN:HD22	1:D:102:ASN:C	2.13	0.55
1:H:136:ARG:HD2	1:H:384:ASP:OD1	2.05	0.55
1:E:68:ASN:HD22	1:E:69:PRO:CD	2.19	0.55
1:F:215:LEU:HD12	1:F:215:LEU:N	2.21	0.55
1:G:215:LEU:N	1:G:215:LEU:HD12	2.21	0.55
1:B:102:ASN:HD22	1:B:102:ASN:C	2.13	0.55
1:F:309:HIS:HE1	1:F:355:LEU:O	1.89	0.55
1:A:68:ASN:HD22	1:A:69:PRO:CD	2.19	0.55
1:F:15:ARG:HE	1:F:21:ASN:ND2	2.04	0.55
1:D:309:HIS:HE1	1:D:355:LEU:O	1.89	0.55
1:H:68:ASN:HD22	1:H:69:PRO:CD	2.19	0.55
1:F:136:ARG:HD2	1:F:384:ASP:OD1	2.07	0.55
1:H:309:HIS:HE1	1:H:355:LEU:O	1.89	0.55
1:B:68:ASN:HD22	1:B:69:PRO:CD	2.19	0.55
1:B:296:THR:HG22	1:B:322:ASP:HB2	1.88	0.55
1:E:309:HIS:HE1	1:E:355:LEU:O	1.90	0.54
1:A:87:MET:HB3	1:C:87:MET:HB3	1.89	0.54
1:A:102:ASN:HD22	1:A:102:ASN:C	2.15	0.54
1:A:263:ASP:OD2	1:G:201:LYS:HD3	2.07	0.54
1:B:15:ARG:HE	1:B:21:ASN:HD21	1.55	0.54
1:C:15:ARG:HE	1:C:21:ASN:ND2	2.05	0.54
1:E:136:ARG:HD2	1:E:384:ASP:OD1	2.06	0.54
1:F:205:ARG:HD3	1:G:240:ASP:O	2.07	0.54
1:A:201:LYS:HD3	1:D:263:ASP:OD2	2.07	0.54
1:G:296:THR:HG22	1:G:322:ASP:HB2	1.90	0.54
1:C:68:ASN:HD22	1:C:69:PRO:HD2	1.72	0.54
1:E:102:ASN:HD22	1:E:102:ASN:C	2.13	0.54
1:C:309:HIS:HE1	1:C:355:LEU:O	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:369:VAL:HG13	1:F:370:PRO:HD2	1.90	0.54
1:H:369:VAL:HG13	1:H:370:PRO:HD2	1.89	0.54
1:A:369:VAL:HG13	1:A:370:PRO:HD2	1.88	0.54
1:D:87:MET:HB3	1:E:87:MET:HB3	1.89	0.54
1:A:296:THR:HG22	1:A:322:ASP:HB2	1.91	0.53
1:B:309:HIS:HE1	1:B:355:LEU:O	1.91	0.53
1:D:68:ASN:HD22	1:D:69:PRO:HD2	1.72	0.53
1:G:369:VAL:HG13	1:G:370:PRO:HD2	1.90	0.53
1:B:68:ASN:HD22	1:B:69:PRO:HD2	1.73	0.53
1:E:15:ARG:HE	1:E:21:ASN:HD21	1.53	0.53
1:F:132:TYR:CE2	1:F:153:LYS:HE2	2.43	0.53
1:H:215:LEU:HD12	1:H:215:LEU:N	2.24	0.53
1:B:87:MET:HB3	1:G:87:MET:HB3	1.89	0.53
1:G:136:ARG:HD2	1:G:384:ASP:OD1	2.08	0.53
1:B:215:LEU:N	1:B:215:LEU:HD12	2.23	0.53
1:A:349:ASP:HB3	1:A:352:VAL:HG23	1.91	0.53
1:C:215:LEU:N	1:C:215:LEU:HD12	2.23	0.53
1:D:132:TYR:CE2	1:D:153:LYS:HE2	2.43	0.53
1:H:68:ASN:HD22	1:H:69:PRO:HD2	1.73	0.53
1:H:349:ASP:HB3	1:H:352:VAL:HG23	1.91	0.53
1:C:296:THR:HG22	1:C:322:ASP:HB2	1.91	0.53
1:C:369:VAL:HG13	1:C:370:PRO:HD2	1.91	0.53
1:D:136:ARG:HD2	1:D:384:ASP:OD1	2.09	0.53
1:D:369:VAL:HG13	1:D:370:PRO:HD2	1.89	0.53
1:F:68:ASN:HD22	1:F:69:PRO:HD2	1.73	0.53
1:G:68:ASN:HD22	1:G:69:PRO:CD	2.21	0.53
1:E:349:ASP:HB3	1:E:352:VAL:HG23	1.91	0.53
1:G:102:ASN:HD22	1:G:102:ASN:C	2.15	0.53
1:A:68:ASN:HD22	1:A:69:PRO:HD2	1.74	0.52
1:E:68:ASN:HD22	1:E:69:PRO:HD2	1.73	0.52
1:F:296:THR:HG22	1:F:322:ASP:HB2	1.89	0.52
1:B:349:ASP:HB3	1:B:352:VAL:HG23	1.92	0.52
1:B:369:VAL:HG13	1:B:370:PRO:HD2	1.91	0.52
1:C:102:ASN:HD22	1:C:102:ASN:C	2.13	0.52
1:D:15:ARG:HE	1:D:21:ASN:ND2	2.08	0.52
1:F:15:ARG:HE	1:F:21:ASN:HD21	1.58	0.52
1:D:296:THR:HG22	1:D:322:ASP:HB2	1.91	0.51
1:F:349:ASP:HB3	1:F:352:VAL:HG23	1.92	0.51
1:G:349:ASP:HB3	1:G:352:VAL:HG23	1.91	0.51
1:E:215:LEU:N	1:E:215:LEU:HD12	2.24	0.51
1:G:7:GLU:HB2	1:G:27:LYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:TYR:CE2	1:G:153:LYS:HE2	2.45	0.51
1:H:15:ARG:HE	1:H:21:ASN:HD21	1.54	0.51
1:C:132:TYR:CE2	1:C:153:LYS:HE2	2.45	0.51
1:G:68:ASN:HD22	1:G:69:PRO:HD2	1.76	0.51
1:A:109:ALA:HB3	1:A:354:GLY:HA2	1.93	0.51
1:A:132:TYR:CE2	1:A:153:LYS:HE2	2.45	0.51
1:H:132:TYR:CE2	1:H:153:LYS:HE2	2.46	0.51
1:H:296:THR:HG22	1:H:322:ASP:HB2	1.92	0.51
1:D:7:GLU:HB2	1:D:27:LYS:HB2	1.92	0.51
1:A:68:ASN:HD22	1:A:69:PRO:N	2.09	0.51
1:A:158:PHE:HZ	1:A:327:GLU:HG3	1.76	0.51
1:B:132:TYR:CE2	1:B:153:LYS:HE2	2.46	0.51
1:B:240:ASP:OD1	1:C:208:LYS:HE3	2.12	0.50
1:C:7:GLU:HB2	1:C:27:LYS:HB2	1.93	0.50
1:E:109:ALA:HB3	1:E:354:GLY:HA2	1.93	0.50
1:E:296:THR:HG22	1:E:322:ASP:HB2	1.91	0.50
1:B:7:GLU:HB2	1:B:27:LYS:HB2	1.91	0.50
1:C:349:ASP:HB3	1:C:352:VAL:HG23	1.93	0.50
1:E:7:GLU:HB2	1:E:27:LYS:HB2	1.92	0.50
1:F:7:GLU:HB2	1:F:27:LYS:HB2	1.93	0.50
1:A:7:GLU:HB2	1:A:27:LYS:HB2	1.93	0.50
1:D:349:ASP:HB3	1:D:352:VAL:HG23	1.93	0.50
1:F:102:ASN:HD22	1:F:102:ASN:C	2.17	0.50
1:A:15:ARG:HE	1:A:21:ASN:HD21	1.59	0.50
1:F:109:ALA:HB3	1:F:354:GLY:HA2	1.93	0.50
1:H:271:PHE:CZ	1:H:297:THR:HB	2.47	0.50
1:C:158:PHE:HZ	1:C:327:GLU:HG3	1.76	0.50
1:E:21:ASN:HD22	1:E:329:TYR:HE1	1.59	0.50
1:E:298:GLN:OE1	1:E:298:GLN:HA	2.11	0.50
1:B:109:ALA:HB3	1:B:354:GLY:HA2	1.94	0.49
1:F:158:PHE:HZ	1:F:327:GLU:HG3	1.76	0.49
1:A:205:ARG:HD3	1:D:240:ASP:O	2.11	0.49
1:G:271:PHE:CZ	1:G:297:THR:HB	2.47	0.49
1:E:158:PHE:HZ	1:E:327:GLU:HG3	1.77	0.49
1:F:271:PHE:CZ	1:F:297:THR:HB	2.47	0.49
1:A:271:PHE:CZ	1:A:297:THR:HB	2.47	0.49
1:C:68:ASN:HD22	1:C:69:PRO:N	2.11	0.49
1:G:109:ALA:HB3	1:G:354:GLY:HA2	1.93	0.49
1:H:7:GLU:HB2	1:H:27:LYS:HB2	1.93	0.49
1:E:132:TYR:CE2	1:E:153:LYS:HE2	2.48	0.49
1:F:68:ASN:HD22	1:F:69:PRO:N	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:PHE:HZ	1:G:327:GLU:HG3	1.78	0.49
1:H:158:PHE:HZ	1:H:327:GLU:HG3	1.77	0.49
1:H:21:ASN:HD22	1:H:329:TYR:HE1	1.60	0.49
1:C:271:PHE:CZ	1:C:297:THR:HB	2.48	0.49
1:E:116:VAL:HG21	1:E:355:LEU:CD1	2.43	0.49
1:H:68:ASN:HD22	1:H:69:PRO:N	2.10	0.49
1:B:21:ASN:HD22	1:B:329:TYR:HE1	1.60	0.49
1:D:205:ARG:HD3	1:F:240:ASP:O	2.13	0.49
1:D:158:PHE:HZ	1:D:327:GLU:HG3	1.77	0.48
1:D:179:VAL:CG1	1:D:187:VAL:HG21	2.43	0.48
1:G:68:ASN:HD22	1:G:69:PRO:N	2.10	0.48
1:H:109:ALA:HB3	1:H:354:GLY:HA2	1.95	0.48
1:B:158:PHE:HZ	1:B:327:GLU:HG3	1.77	0.48
1:B:201:LYS:HD3	1:H:263:ASP:OD2	2.13	0.48
1:D:271:PHE:CZ	1:D:297:THR:HB	2.49	0.48
1:H:298:GLN:HA	1:H:298:GLN:OE1	2.13	0.48
1:C:109:ALA:HB3	1:C:354:GLY:HA2	1.94	0.48
1:G:266:ASN:C	1:G:266:ASN:ND2	2.70	0.48
1:A:298:GLN:HA	1:A:298:GLN:OE1	2.13	0.48
1:B:116:VAL:HG21	1:B:355:LEU:CD1	2.42	0.48
1:D:109:ALA:HB3	1:D:354:GLY:HA2	1.94	0.48
1:F:16:HIS:HE1	4:F:406:HOH:O	1.95	0.48
1:C:59:GLY:O	1:C:63:ILE:HG12	2.14	0.48
1:E:240:ASP:OD1	1:H:208:LYS:HE3	2.14	0.48
1:G:16:HIS:HE1	4:G:426:HOH:O	1.95	0.48
1:D:68:ASN:HD22	1:D:69:PRO:N	2.10	0.48
1:A:68:ASN:C	1:A:68:ASN:ND2	2.72	0.48
1:B:266:ASN:C	1:B:266:ASN:ND2	2.69	0.48
1:B:271:PHE:CZ	1:B:297:THR:HB	2.48	0.48
1:E:68:ASN:HD22	1:E:69:PRO:N	2.11	0.48
1:F:266:ASN:C	1:F:266:ASN:ND2	2.68	0.47
1:G:179:VAL:CG1	1:G:187:VAL:HG21	2.44	0.47
1:B:208:LYS:HE3	1:H:240:ASP:OD1	2.14	0.47
1:D:266:ASN:C	1:D:266:ASN:ND2	2.67	0.47
1:H:116:VAL:HG21	1:H:355:LEU:CD1	2.44	0.47
1:A:125:LYS:HD2	1:A:128:ILE:HG22	1.97	0.47
1:A:299:GLU:OE2	1:A:307:MET:SD	2.73	0.47
1:G:151:ARG:NH1	1:G:182:GLU:OE2	2.39	0.47
1:A:266:ASN:C	1:A:266:ASN:ND2	2.68	0.47
1:B:59:GLY:O	1:B:63:ILE:HG12	2.14	0.47
1:B:240:ASP:O	1:C:205:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:ASN:C	1:F:68:ASN:ND2	2.73	0.47
1:F:59:GLY:O	1:F:63:ILE:HG12	2.15	0.47
1:G:59:GLY:O	1:G:63:ILE:HG12	2.14	0.47
1:B:68:ASN:HD22	1:B:69:PRO:N	2.12	0.47
1:D:59:GLY:O	1:D:63:ILE:HG12	2.15	0.47
1:A:240:ASP:O	1:G:205:ARG:HD3	2.15	0.47
1:C:116:VAL:HG21	1:C:355:LEU:CD1	2.45	0.47
1:C:298:GLN:HA	1:C:298:GLN:OE1	2.15	0.47
1:D:116:VAL:HG21	1:D:355:LEU:CD1	2.45	0.47
1:E:271:PHE:CZ	1:E:297:THR:HB	2.49	0.47
1:E:357:ILE:CG2	1:E:358:GLU:N	2.78	0.47
1:A:59:GLY:O	1:A:63:ILE:HG12	2.15	0.47
1:A:179:VAL:CG1	1:A:187:VAL:HG21	2.44	0.47
1:A:82:ASN:ND2	1:C:48:LEU:HD22	2.29	0.47
1:C:21:ASN:HD22	1:C:329:TYR:HE1	1.63	0.47
1:D:82:ASN:ND2	1:E:48:LEU:HD22	2.30	0.47
1:F:179:VAL:CG1	1:F:187:VAL:HG21	2.45	0.47
1:G:21:ASN:HD22	1:G:329:TYR:HE1	1.62	0.47
1:C:240:ASP:OD1	1:E:208:LYS:HE3	2.16	0.47
1:D:299:GLU:OE2	1:D:307:MET:SD	2.73	0.47
1:B:263:ASP:OD2	1:C:201:LYS:HD3	2.15	0.46
1:B:298:GLN:OE1	1:B:298:GLN:HA	2.14	0.46
1:G:299:GLU:OE2	1:G:307:MET:SD	2.73	0.46
1:B:179:VAL:CG1	1:B:187:VAL:HG21	2.45	0.46
1:C:357:ILE:CG2	1:C:358:GLU:N	2.78	0.46
1:D:149:VAL:O	1:D:153:LYS:HG2	2.16	0.46
1:H:357:ILE:CG2	1:H:358:GLU:N	2.78	0.46
1:H:179:VAL:CG1	1:H:187:VAL:HG21	2.45	0.46
1:B:68:ASN:C	1:B:68:ASN:ND2	2.74	0.46
1:F:298:GLN:HA	1:F:298:GLN:OE1	2.15	0.46
1:G:298:GLN:OE1	1:G:298:GLN:HA	2.14	0.46
1:E:59:GLY:O	1:E:63:ILE:HG12	2.15	0.46
1:F:82:ASN:ND2	1:H:48:LEU:HD22	2.31	0.46
1:F:299:GLU:OE2	1:F:307:MET:SD	2.73	0.46
1:C:179:VAL:HG13	1:C:187:VAL:HG21	1.98	0.46
1:G:22:LYS:CE	1:G:369:VAL:HG11	2.45	0.46
1:B:357:ILE:CG2	1:B:358:GLU:N	2.78	0.46
1:C:179:VAL:CG1	1:C:187:VAL:HG21	2.46	0.46
1:E:263:ASP:OD2	1:H:201:LYS:HD3	2.15	0.46
1:A:149:VAL:O	1:A:153:LYS:HG2	2.16	0.46
1:F:21:ASN:HD22	1:F:329:TYR:HE1	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:VAL:HG21	1:F:355:LEU:CD1	2.45	0.46
1:A:155:GLU:CG	4:A:398:HOH:O	2.54	0.45
1:A:179:VAL:HG13	1:A:187:VAL:HG21	1.98	0.45
1:E:240:ASP:O	1:H:205:ARG:HD3	2.16	0.45
1:C:299:GLU:OE2	1:C:307:MET:SD	2.74	0.45
1:E:68:ASN:C	1:E:68:ASN:ND2	2.75	0.45
1:F:22:LYS:CE	1:F:369:VAL:HG11	2.44	0.45
1:G:116:VAL:HG21	1:G:355:LEU:CD1	2.46	0.45
1:G:149:VAL:O	1:G:153:LYS:HG2	2.16	0.45
1:A:116:VAL:HG21	1:A:355:LEU:CD1	2.46	0.45
1:B:48:LEU:HD22	1:G:82:ASN:ND2	2.32	0.45
1:B:125:LYS:HD2	1:B:128:ILE:HG22	1.98	0.45
1:B:299:GLU:OE2	1:B:307:MET:SD	2.75	0.45
1:C:266:ASN:C	1:C:266:ASN:ND2	2.69	0.45
1:D:360:ASP:HB3	1:D:363:LEU:HD12	1.99	0.45
1:G:360:ASP:HB3	1:G:363:LEU:HD12	1.99	0.45
1:A:21:ASN:HD22	1:A:329:TYR:HE1	1.65	0.45
1:A:357:ILE:CG2	1:A:358:GLU:N	2.79	0.45
1:E:113:ASP:OD1	1:E:353:LYS:HE2	2.17	0.45
1:G:357:ILE:CG2	1:G:358:GLU:N	2.79	0.45
1:H:68:ASN:C	1:H:68:ASN:ND2	2.74	0.45
1:H:113:ASP:OD1	1:H:353:LYS:HE2	2.17	0.45
1:A:272:ILE:HG13	1:A:272:ILE:O	2.17	0.45
1:E:21:ASN:ND2	1:E:329:TYR:HE1	2.15	0.45
1:E:179:VAL:CG1	1:E:187:VAL:HG21	2.46	0.45
1:F:179:VAL:HG13	1:F:187:VAL:HG21	1.99	0.45
1:H:360:ASP:HB3	1:H:363:LEU:HD12	1.99	0.45
1:D:272:ILE:HG13	1:D:272:ILE:O	2.17	0.45
1:E:179:VAL:HG13	1:E:187:VAL:HG21	1.99	0.45
1:C:68:ASN:C	1:C:68:ASN:ND2	2.74	0.45
1:E:360:ASP:HB3	1:E:363:LEU:HD12	1.98	0.45
1:D:68:ASN:C	1:D:68:ASN:ND2	2.74	0.45
1:E:299:GLU:OE2	1:E:307:MET:SD	2.75	0.45
1:G:125:LYS:HD2	1:G:128:ILE:HG22	1.99	0.45
1:H:59:GLY:O	1:H:63:ILE:HG12	2.16	0.45
1:A:68:ASN:ND2	1:A:70:PHE:H	2.14	0.44
1:B:297:THR:HA	2:B:392:LMR:O2	2.17	0.44
1:C:125:LYS:HD2	1:C:128:ILE:HG22	1.99	0.44
1:C:263:ASP:OD2	1:E:201:LYS:HD3	2.16	0.44
1:E:125:LYS:HD2	1:E:128:ILE:HG22	1.99	0.44
1:E:272:ILE:O	1:E:272:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:ASN:ND2	1:F:70:PHE:H	2.15	0.44
1:F:357:ILE:CG2	1:F:358:GLU:N	2.81	0.44
1:C:360:ASP:HB3	1:C:363:LEU:HD12	1.99	0.44
1:E:68:ASN:ND2	1:E:70:PHE:H	2.16	0.44
1:H:68:ASN:ND2	1:H:70:PHE:H	2.15	0.44
1:A:360:ASP:HB3	1:A:363:LEU:HD12	1.98	0.44
1:B:179:VAL:HG13	1:B:187:VAL:HG21	1.99	0.44
1:C:158:PHE:CZ	1:C:327:GLU:HG3	2.51	0.44
1:D:113:ASP:OD1	1:D:353:LYS:HE2	2.17	0.44
1:D:298:GLN:OE1	1:D:298:GLN:HA	2.17	0.44
1:G:179:VAL:HG13	1:G:187:VAL:HG21	2.00	0.44
1:B:21:ASN:ND2	1:B:329:TYR:HE1	2.15	0.44
1:B:158:PHE:CZ	1:B:327:GLU:HG3	2.52	0.44
1:F:312:CYS:SG	1:F:347:ALA:HB2	2.58	0.44
1:A:22:LYS:CE	1:A:369:VAL:HG11	2.45	0.44
1:D:21:ASN:HD22	1:D:329:TYR:HE1	1.64	0.44
1:D:357:ILE:CG2	1:D:358:GLU:N	2.80	0.44
1:E:203:ALA:O	1:E:207:ILE:HG13	2.18	0.44
1:G:68:ASN:ND2	1:G:70:PHE:H	2.15	0.44
1:A:167:LYS:NZ	1:A:380:HIS:CD2	2.81	0.44
1:C:6:LEU:O	1:C:57:LYS:HE3	2.18	0.44
1:D:179:VAL:HG13	1:D:187:VAL:HG21	1.99	0.44
1:F:149:VAL:O	1:F:153:LYS:HG2	2.17	0.44
1:F:360:ASP:HB3	1:F:363:LEU:HD12	2.00	0.44
1:G:14:PRO:HB3	1:G:20:VAL:HG22	2.00	0.44
1:H:6:LEU:O	1:H:57:LYS:HE3	2.17	0.44
1:A:158:PHE:CZ	1:A:327:GLU:HG3	2.53	0.44
1:B:113:ASP:OD1	1:B:353:LYS:HE2	2.17	0.44
1:B:360:ASP:HB3	1:B:363:LEU:HD12	2.00	0.44
1:C:145:SER:HB3	4:C:410:HOH:O	2.17	0.44
1:D:125:LYS:HD2	1:D:128:ILE:HG22	1.99	0.44
1:D:154:LEU:HA	1:D:158:PHE:O	2.18	0.44
1:H:125:LYS:HD2	1:H:128:ILE:HG22	1.99	0.44
1:H:272:ILE:HG13	1:H:272:ILE:O	2.18	0.44
1:B:203:ALA:O	1:B:207:ILE:HG13	2.17	0.44
1:E:158:PHE:CZ	1:E:327:GLU:HG3	2.52	0.44
1:F:125:LYS:HD2	1:F:128:ILE:HG22	1.98	0.44
1:G:113:ASP:OD1	1:G:353:LYS:HE2	2.17	0.44
1:H:149:VAL:O	1:H:153:LYS:HG2	2.18	0.44
1:H:179:VAL:HG13	1:H:187:VAL:HG21	1.98	0.44
1:A:113:ASP:OD1	1:A:353:LYS:HE2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ARG:NH1	1:C:126:GLU:OE2	2.51	0.43
1:F:113:ASP:OD1	1:F:353:LYS:HE2	2.18	0.43
1:E:14:PRO:HB3	1:E:20:VAL:HG22	2.00	0.43
1:F:6:LEU:O	1:F:57:LYS:HE3	2.19	0.43
1:F:158:PHE:CZ	1:F:327:GLU:HG3	2.52	0.43
1:G:123:ARG:NH1	1:G:126:GLU:OE2	2.51	0.43
1:H:21:ASN:ND2	1:H:329:TYR:HE1	2.15	0.43
1:A:16:HIS:HE1	4:A:412:HOH:O	2.02	0.43
1:B:272:ILE:HG13	1:B:272:ILE:O	2.18	0.43
1:C:113:ASP:OD1	1:C:353:LYS:HE2	2.18	0.43
1:G:68:ASN:C	1:G:68:ASN:ND2	2.74	0.43
1:B:68:ASN:ND2	1:B:70:PHE:H	2.16	0.43
1:C:149:VAL:O	1:C:153:LYS:HG2	2.17	0.43
1:D:22:LYS:CE	1:D:369:VAL:HG11	2.46	0.43
1:G:6:LEU:O	1:G:57:LYS:HE3	2.18	0.43
1:A:341:LYS:HB3	1:A:346:TYR:HE2	1.84	0.43
1:B:6:LEU:O	1:B:57:LYS:HE3	2.17	0.43
1:B:14:PRO:HB3	1:B:20:VAL:HG22	2.00	0.43
1:E:6:LEU:O	1:E:57:LYS:HE3	2.19	0.43
1:F:341:LYS:HB3	1:F:346:TYR:HE2	1.84	0.43
1:H:14:PRO:HB3	1:H:20:VAL:HG22	2.01	0.43
1:E:149:VAL:O	1:E:153:LYS:HG2	2.18	0.43
1:H:158:PHE:CZ	1:H:327:GLU:HG3	2.53	0.43
1:G:203:ALA:O	1:G:207:ILE:HG13	2.18	0.43
1:C:357:ILE:HD13	1:C:357:ILE:HA	1.90	0.43
1:D:68:ASN:ND2	1:D:70:PHE:H	2.16	0.43
1:B:357:ILE:HD13	1:B:357:ILE:HA	1.90	0.42
1:C:203:ALA:O	1:C:207:ILE:HG13	2.19	0.42
1:F:167:LYS:NZ	1:F:380:HIS:CD2	2.82	0.42
1:A:6:LEU:O	1:A:57:LYS:HE3	2.19	0.42
1:B:205:ARG:HD3	1:H:240:ASP:O	2.19	0.42
1:C:68:ASN:ND2	1:C:70:PHE:H	2.17	0.42
1:G:158:PHE:CZ	1:G:327:GLU:HG3	2.54	0.42
1:G:272:ILE:O	1:G:272:ILE:HG13	2.19	0.42
1:H:123:ARG:NH1	1:H:126:GLU:OE2	2.51	0.42
1:B:123:ARG:NH1	1:B:126:GLU:OE2	2.51	0.42
1:B:149:VAL:O	1:B:153:LYS:HG2	2.19	0.42
1:E:123:ARG:NH1	1:E:126:GLU:OE2	2.51	0.42
1:E:371:ASP:HB2	4:E:429:HOH:O	2.20	0.42
1:F:123:ARG:NH1	1:F:126:GLU:OE2	2.52	0.42
1:A:59:GLY:O	1:A:62:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:LYS:CE	1:E:369:VAL:HG11	2.47	0.42
1:A:123:ARG:NH1	1:A:126:GLU:OE2	2.51	0.42
1:C:21:ASN:ND2	1:C:329:TYR:HE1	2.16	0.42
1:D:73:MET:HA	1:D:73:MET:HE2	2.02	0.42
1:F:117:SER:OG	1:F:309:HIS:CD2	2.66	0.42
1:F:151:ARG:NH1	1:F:182:GLU:OE2	2.41	0.42
1:C:14:PRO:HB3	1:C:20:VAL:HG22	2.00	0.42
1:D:203:ALA:O	1:D:207:ILE:HG13	2.19	0.42
1:H:154:LEU:HA	1:H:158:PHE:O	2.20	0.42
1:H:203:ALA:O	1:H:207:ILE:HG13	2.20	0.42
1:H:368:GLN:HE21	1:H:368:GLN:C	2.28	0.42
1:C:154:LEU:HA	1:C:158:PHE:O	2.20	0.42
1:A:369:VAL:CG1	1:A:370:PRO:HD2	2.50	0.42
1:D:341:LYS:HB3	1:D:346:TYR:HE2	1.85	0.42
1:E:297:THR:HA	2:E:392:LMR:O2	2.20	0.42
1:G:326:PRO:HG2	1:G:338:VAL:HG22	2.02	0.42
1:B:22:LYS:CE	1:B:369:VAL:HG11	2.47	0.42
1:C:272:ILE:HG13	1:C:272:ILE:O	2.19	0.42
1:G:21:ASN:ND2	1:G:329:TYR:HE1	2.18	0.42
1:G:357:ILE:HD13	1:G:357:ILE:HA	1.88	0.42
1:H:299:GLU:OE2	1:H:307:MET:SD	2.78	0.42
1:A:73:MET:HE2	1:A:73:MET:HA	2.01	0.41
1:B:154:LEU:HA	1:B:158:PHE:O	2.19	0.41
1:D:158:PHE:CZ	1:D:327:GLU:HG3	2.53	0.41
1:F:154:LEU:HA	1:F:158:PHE:O	2.20	0.41
1:A:312:CYS:SG	1:A:347:ALA:HB2	2.60	0.41
1:D:14:PRO:HB3	1:D:20:VAL:HG22	2.02	0.41
1:E:369:VAL:CG1	1:E:370:PRO:HD2	2.49	0.41
1:F:203:ALA:O	1:F:207:ILE:HG13	2.20	0.41
1:H:59:GLY:O	1:H:62:SER:HB3	2.20	0.41
1:A:203:ALA:O	1:A:207:ILE:HG13	2.20	0.41
1:D:21:ASN:ND2	1:D:329:TYR:HE1	2.18	0.41
1:E:151:ARG:NH1	1:E:182:GLU:OE2	2.44	0.41
1:F:21:ASN:ND2	1:F:329:TYR:HE1	2.19	0.41
1:G:86:THR:O	1:G:87:MET:CB	2.69	0.41
1:G:341:LYS:HB3	1:G:346:TYR:HE2	1.86	0.41
1:H:86:THR:O	1:H:87:MET:CB	2.67	0.41
1:C:226:ARG:HG2	1:C:248:TRP:CH2	2.56	0.41
1:A:21:ASN:ND2	1:A:329:TYR:HE1	2.19	0.41
1:A:86:THR:O	1:A:87:MET:CB	2.68	0.41
1:C:322:ASP:N	1:C:323:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:GLY:O	1:D:62:SER:HB3	2.20	0.41
1:F:48:LEU:HD22	1:H:82:ASN:ND2	2.36	0.41
1:G:73:MET:HE1	1:G:276:THR:HG23	2.03	0.41
1:C:297:THR:HA	2:C:392:LMR:O2	2.20	0.41
1:C:368:GLN:HE21	1:C:368:GLN:C	2.29	0.41
1:D:117:SER:OG	1:D:309:HIS:CD2	2.65	0.41
1:D:326:PRO:HG2	1:D:338:VAL:HG22	2.03	0.41
1:E:38:GLY:HA3	1:E:103:ALA:HB2	2.03	0.41
1:E:322:ASP:N	1:E:323:PRO:CD	2.84	0.41
1:F:59:GLY:O	1:F:62:SER:HB3	2.21	0.41
1:F:73:MET:HE1	1:F:276:THR:HG23	2.03	0.41
1:H:210:LEU:C	1:H:212:LYS:H	2.29	0.41
1:A:82:ASN:HD22	1:C:48:LEU:HD22	1.86	0.41
1:A:154:LEU:HA	1:A:158:PHE:O	2.20	0.41
1:A:241:TYR:HA	1:A:242:PRO:HD3	1.93	0.41
1:B:312:CYS:SG	1:B:347:ALA:HB2	2.61	0.41
1:C:86:THR:O	1:C:87:MET:CB	2.68	0.41
1:E:59:GLY:O	1:E:62:SER:HB3	2.21	0.41
1:E:154:LEU:HA	1:E:158:PHE:O	2.20	0.41
1:E:368:GLN:C	1:E:368:GLN:HE21	2.29	0.41
1:C:22:LYS:CE	1:C:369:VAL:HG11	2.48	0.41
1:C:147:LEU:HD11	1:C:178:ARG:HB3	2.03	0.41
1:D:322:ASP:N	1:D:323:PRO:HD2	2.35	0.41
1:F:14:PRO:HB3	1:F:20:VAL:HG22	2.02	0.41
1:F:272:ILE:HG13	1:F:272:ILE:O	2.21	0.41
1:H:22:LYS:CE	1:H:369:VAL:HG11	2.48	0.41
1:A:73:MET:HE1	1:A:276:THR:HG23	2.03	0.40
1:B:82:ASN:ND2	1:G:48:LEU:HD22	2.37	0.40
1:B:322:ASP:N	1:B:323:PRO:CD	2.85	0.40
1:E:73:MET:HE1	1:E:276:THR:HG23	2.03	0.40
1:E:86:THR:O	1:E:87:MET:CB	2.68	0.40
1:E:341:LYS:HB3	1:E:346:TYR:HE2	1.86	0.40
1:D:6:LEU:O	1:D:57:LYS:HE3	2.20	0.40
1:D:38:GLY:HA3	1:D:103:ALA:HB2	2.03	0.40
1:G:154:LEU:HA	1:G:158:PHE:O	2.21	0.40
1:H:38:GLY:HA3	1:H:103:ALA:HB2	2.03	0.40
1:E:167:LYS:NZ	1:E:380:HIS:CD2	2.82	0.40
1:F:322:ASP:N	1:F:323:PRO:CD	2.85	0.40
1:A:48:LEU:HD22	1:C:82:ASN:ND2	2.37	0.40
1:B:341:LYS:HB3	1:B:346:TYR:HE2	1.87	0.40
1:B:368:GLN:C	1:B:368:GLN:HE21	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:ASP:O	1:E:205:ARG:HD3	2.22	0.40
1:H:226:ARG:HG2	1:H:248:TRP:CH2	2.57	0.40
1:H:304:THR:HA	1:H:307:MET:HG2	2.04	0.40
1:C:322:ASP:N	1:C:323:PRO:HD2	2.36	0.40
1:D:48:LEU:HD22	1:E:82:ASN:ND2	2.36	0.40
1:D:312:CYS:SG	1:D:347:ALA:HB2	2.62	0.40
1:D:322:ASP:N	1:D:323:PRO:CD	2.84	0.40
1:G:322:ASP:N	1:G:323:PRO:HD2	2.37	0.40
1:H:73:MET:HE1	1:H:276:THR:HG23	2.04	0.40
1:H:382:LEU:HD23	1:H:382:LEU:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	385/391 (98%)	374 (97%)	9 (2%)	2 (0%)	24	27
1	B	385/391 (98%)	374 (97%)	9 (2%)	2 (0%)	24	27
1	C	385/391 (98%)	373 (97%)	10 (3%)	2 (0%)	24	27
1	D	385/391 (98%)	373 (97%)	10 (3%)	2 (0%)	24	27
1	E	385/391 (98%)	372 (97%)	11 (3%)	2 (0%)	24	27
1	F	385/391 (98%)	373 (97%)	11 (3%)	1 (0%)	36	42
1	G	385/391 (98%)	373 (97%)	10 (3%)	2 (0%)	24	27
1	H	385/391 (98%)	371 (96%)	13 (3%)	1 (0%)	36	42
All	All	3080/3128 (98%)	2983 (97%)	83 (3%)	14 (0%)	24	27

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	B	42	ASP
1	C	42	ASP
1	D	42	ASP
1	E	42	ASP
1	F	42	ASP
1	G	42	ASP
1	H	42	ASP
1	A	322	ASP
1	B	322	ASP
1	C	322	ASP
1	D	322	ASP
1	E	322	ASP
1	G	322	ASP

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	341/345 (99%)	328 (96%)	13 (4%)	29	40
1	B	341/345 (99%)	328 (96%)	13 (4%)	29	40
1	C	341/345 (99%)	328 (96%)	13 (4%)	29	40
1	D	341/345 (99%)	328 (96%)	13 (4%)	29	40
1	E	341/345 (99%)	328 (96%)	13 (4%)	29	40
1	F	341/345 (99%)	328 (96%)	13 (4%)	29	40
1	G	341/345 (99%)	328 (96%)	13 (4%)	29	40
1	H	341/345 (99%)	328 (96%)	13 (4%)	29	40
All	All	2728/2760 (99%)	2624 (96%)	104 (4%)	29	40

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	87	MET

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Mol	Chain	Res	Type
1	A	102	ASN
1	A	107	LEU
1	A	141	GLU
1	A	237	LEU
1	A	239	THR
1	A	259	LYS
1	A	266	ASN
1	A	299	GLU
1	A	310	LEU
1	A	355	LEU
1	A	368	GLN
1	B	68	ASN
1	B	87	MET
1	B	102	ASN
1	B	107	LEU
1	B	141	GLU
1	B	237	LEU
1	B	239	THR
1	B	259	LYS
1	B	266	ASN
1	B	299	GLU
1	B	310	LEU
1	B	355	LEU
1	B	368	GLN
1	C	68	ASN
1	C	87	MET
1	C	102	ASN
1	C	107	LEU
1	C	141	GLU
1	C	237	LEU
1	C	239	THR
1	C	259	LYS
1	C	266	ASN
1	C	299	GLU
1	C	310	LEU
1	C	355	LEU
1	C	368	GLN
1	D	68	ASN
1	D	87	MET
1	D	102	ASN
1	D	107	LEU
1	D	141	GLU

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Mol	Chain	Res	Type
1	D	237	LEU
1	D	239	THR
1	D	259	LYS
1	D	266	ASN
1	D	299	GLU
1	D	310	LEU
1	D	355	LEU
1	D	368	GLN
1	E	68	ASN
1	E	87	MET
1	E	102	ASN
1	E	107	LEU
1	E	141	GLU
1	E	237	LEU
1	E	239	THR
1	E	259	LYS
1	E	266	ASN
1	E	299	GLU
1	E	310	LEU
1	E	355	LEU
1	E	368	GLN
1	F	68	ASN
1	F	87	MET
1	F	102	ASN
1	F	107	LEU
1	F	141	GLU
1	F	237	LEU
1	F	239	THR
1	F	259	LYS
1	F	266	ASN
1	F	299	GLU
1	F	310	LEU
1	F	355	LEU
1	F	368	GLN
1	G	68	ASN
1	G	87	MET
1	G	102	ASN
1	G	107	LEU
1	G	141	GLU
1	G	237	LEU
1	G	239	THR
1	G	259	LYS

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Mol	Chain	Res	Type
1	G	266	ASN
1	G	299	GLU
1	G	310	LEU
1	G	355	LEU
1	G	368	GLN
1	H	68	ASN
1	H	87	MET
1	H	102	ASN
1	H	107	LEU
1	H	141	GLU
1	H	237	LEU
1	H	239	THR
1	H	259	LYS
1	H	266	ASN
1	H	299	GLU
1	H	310	LEU
1	H	355	LEU
1	H	368	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	21	ASN
1	A	68	ASN
1	A	102	ASN
1	A	146	ASN
1	A	152	GLN
1	A	196	HIS
1	A	199	ASN
1	A	246	HIS
1	A	254	GLN
1	A	266	ASN
1	A	309	HIS
1	A	368	GLN
1	A	376	ASN
1	A	380	HIS
1	B	9	HIS
1	B	16	HIS
1	B	21	ASN
1	B	45	HIS
1	B	68	ASN

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Mol	Chain	Res	Type
1	B	102	ASN
1	B	152	GLN
1	B	196	HIS
1	B	199	ASN
1	B	254	GLN
1	B	266	ASN
1	B	309	HIS
1	B	368	GLN
1	B	376	ASN
1	B	380	HIS
1	C	9	HIS
1	C	16	HIS
1	C	21	ASN
1	C	68	ASN
1	C	102	ASN
1	C	146	ASN
1	C	152	GLN
1	C	196	HIS
1	C	199	ASN
1	C	246	HIS
1	C	254	GLN
1	C	266	ASN
1	C	309	HIS
1	C	368	GLN
1	C	376	ASN
1	C	380	HIS
1	D	9	HIS
1	D	16	HIS
1	D	21	ASN
1	D	68	ASN
1	D	102	ASN
1	D	146	ASN
1	D	152	GLN
1	D	196	HIS
1	D	199	ASN
1	D	254	GLN
1	D	266	ASN
1	D	309	HIS
1	D	336	ASN
1	D	368	GLN
1	D	376	ASN
1	D	380	HIS

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Mol	Chain	Res	Type
1	E	9	HIS
1	E	16	HIS
1	E	21	ASN
1	E	68	ASN
1	E	102	ASN
1	E	152	GLN
1	E	196	HIS
1	E	199	ASN
1	E	254	GLN
1	E	266	ASN
1	E	309	HIS
1	E	368	GLN
1	E	376	ASN
1	E	380	HIS
1	F	16	HIS
1	F	21	ASN
1	F	68	ASN
1	F	102	ASN
1	F	146	ASN
1	F	152	GLN
1	F	196	HIS
1	F	199	ASN
1	F	254	GLN
1	F	266	ASN
1	F	309	HIS
1	F	368	GLN
1	F	376	ASN
1	F	380	HIS
1	G	9	HIS
1	G	16	HIS
1	G	21	ASN
1	G	68	ASN
1	G	102	ASN
1	G	146	ASN
1	G	152	GLN
1	G	196	HIS
1	G	199	ASN
1	G	254	GLN
1	G	266	ASN
1	G	309	HIS
1	G	368	GLN
1	G	376	ASN

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Mol	Chain	Res	Type
1	G	380	HIS
1	H	9	HIS
1	H	16	HIS
1	H	21	ASN
1	H	68	ASN
1	H	102	ASN
1	H	146	ASN
1	H	152	GLN
1	H	196	HIS
1	H	199	ASN
1	H	254	GLN
1	H	266	ASN
1	H	309	HIS
1	H	368	GLN
1	H	376	ASN
1	H	380	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	LMR	C	392	3	8,8,8	1.31	0	10,10,10	2.17	3 (30%)
2	LMR	D	392	3	8,8,8	1.21	0	10,10,10	2.11	3 (30%)
2	LMR	F	392	3	8,8,8	1.21	0	10,10,10	2.07	3 (30%)
2	LMR	G	392	3	8,8,8	1.15	0	10,10,10	2.04	2 (20%)
2	LMR	H	392	3	8,8,8	1.27	1 (12%)	10,10,10	2.07	2 (20%)
2	LMR	A	392	3	8,8,8	1.20	0	10,10,10	1.97	2 (20%)
2	LMR	B	392	3	8,8,8	1.32	0	10,10,10	2.14	2 (20%)
2	LMR	E	392	3	8,8,8	1.23	0	10,10,10	2.11	2 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMR	C	392	3	-	2/8/8/8	-
2	LMR	D	392	3	-	4/8/8/8	-
2	LMR	F	392	3	-	3/8/8/8	-
2	LMR	G	392	3	-	3/8/8/8	-
2	LMR	H	392	3	-	2/8/8/8	-
2	LMR	A	392	3	-	3/8/8/8	-
2	LMR	B	392	3	-	2/8/8/8	-
2	LMR	E	392	3	-	2/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	392	LMR	O4B-C4	2.02	1.28	1.22

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	392	LMR	O1B-C1-C2	4.87	123.03	112.74
2	B	392	LMR	O1B-C1-C2	4.80	122.89	112.74
2	E	392	LMR	O1B-C1-C2	4.75	122.78	112.74
2	H	392	LMR	O1B-C1-C2	4.71	122.70	112.74
2	G	392	LMR	O1B-C1-C2	4.58	122.43	112.74
2	F	392	LMR	O1B-C1-C2	4.57	122.41	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	392	LMR	O1B-C1-C2	4.56	122.38	112.74
2	A	392	LMR	O1B-C1-C2	4.39	122.01	112.74
2	B	392	LMR	O1B-C1-O1A	-2.63	118.12	124.08
2	D	392	LMR	O1B-C1-O1A	-2.59	118.21	124.08
2	G	392	LMR	O1B-C1-O1A	-2.50	118.41	124.08
2	C	392	LMR	O1B-C1-O1A	-2.49	118.43	124.08
2	F	392	LMR	O1B-C1-O1A	-2.49	118.44	124.08
2	E	392	LMR	O1B-C1-O1A	-2.48	118.45	124.08
2	H	392	LMR	O1B-C1-O1A	-2.43	118.56	124.08
2	A	392	LMR	O1B-C1-O1A	-2.32	118.83	124.08
2	D	392	LMR	O4A-C4-C3	2.09	120.49	114.00
2	C	392	LMR	O1A-C1-C2	-2.03	118.55	122.60
2	F	392	LMR	O4A-C4-C3	2.00	120.22	114.00

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	392	LMR	O1A-C1-C2-O2
2	D	392	LMR	O1A-C1-C2-C3
2	D	392	LMR	O1B-C1-C2-C3
2	A	392	LMR	O1A-C1-C2-O2
2	A	392	LMR	O1B-C1-C2-O2
2	B	392	LMR	O1A-C1-C2-O2
2	B	392	LMR	O1B-C1-C2-O2
2	C	392	LMR	O1A-C1-C2-O2
2	C	392	LMR	O1B-C1-C2-O2
2	D	392	LMR	O1B-C1-C2-O2
2	E	392	LMR	O1A-C1-C2-O2
2	E	392	LMR	O1B-C1-C2-O2
2	F	392	LMR	O1B-C1-C2-O2
2	G	392	LMR	O1A-C1-C2-O2
2	G	392	LMR	O1B-C1-C2-O2
2	H	392	LMR	O1A-C1-C2-O2
2	H	392	LMR	O1B-C1-C2-O2
2	A	392	LMR	O1A-C1-C2-C3
2	F	392	LMR	O1A-C1-C2-C3
2	G	392	LMR	O1A-C1-C2-C3
2	F	392	LMR	O1A-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	392	LMR	1	0
2	B	392	LMR	1	0
2	E	392	LMR	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	387/391 (98%)	-1.25	0 100 100	28, 42, 54, 67	0
1	B	387/391 (98%)	-1.25	0 100 100	30, 43, 57, 71	0
1	C	387/391 (98%)	-1.22	0 100 100	31, 44, 59, 71	0
1	D	387/391 (98%)	-1.25	0 100 100	30, 42, 54, 62	0
1	E	387/391 (98%)	-1.21	0 100 100	29, 43, 57, 70	0
1	F	387/391 (98%)	-1.22	0 100 100	28, 41, 53, 64	0
1	G	387/391 (98%)	-1.27	0 100 100	30, 42, 54, 67	0
1	H	387/391 (98%)	-1.18	0 100 100	31, 44, 58, 68	0
All	All	3096/3128 (98%)	-1.23	0 100 100	28, 43, 57, 71	0

There are no RSRZ outliers to report.

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	LMR	A	392	9/9	0.98	0.05	34,38,39,41	0
2	LMR	C	392	9/9	0.98	0.05	51,54,56,57	0
2	LMR	F	392	9/9	0.98	0.04	40,42,45,46	0
2	LMR	H	392	9/9	0.98	0.05	55,56,57,57	0
2	LMR	E	392	9/9	0.99	0.04	47,50,52,53	0
2	LMR	B	392	9/9	0.99	0.04	44,46,52,53	0
2	LMR	G	392	9/9	0.99	0.04	41,45,47,47	0
2	LMR	D	392	9/9	0.99	0.04	42,43,44,45	0
3	MG	A	393	1/1	1.00	0.01	19,19,19,19	0
3	MG	B	393	1/1	1.00	0.02	20,20,20,20	0
3	MG	C	393	1/1	1.00	0.03	24,24,24,24	0
3	MG	D	393	1/1	1.00	0.01	18,18,18,18	0
3	MG	E	393	1/1	1.00	0.01	20,20,20,20	0
3	MG	F	393	1/1	1.00	0.01	18,18,18,18	0
3	MG	G	393	1/1	1.00	0.01	22,22,22,22	0
3	MG	H	393	1/1	1.00	0.01	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.