



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:56 PM UTC

PDB ID : 3C0B / pdb_00003c0b
Title : Crystal structure of the conserved archaeal protein Q6M145. Northeast Structural Genomics Consortium target MrR63
Authors : Kuzin, A.P.; Su, M.; Seetharaman, J.; Wang, D.; Fang, Y.; Cunningham, K.; Ma, L.-C.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2008-01-19
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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)

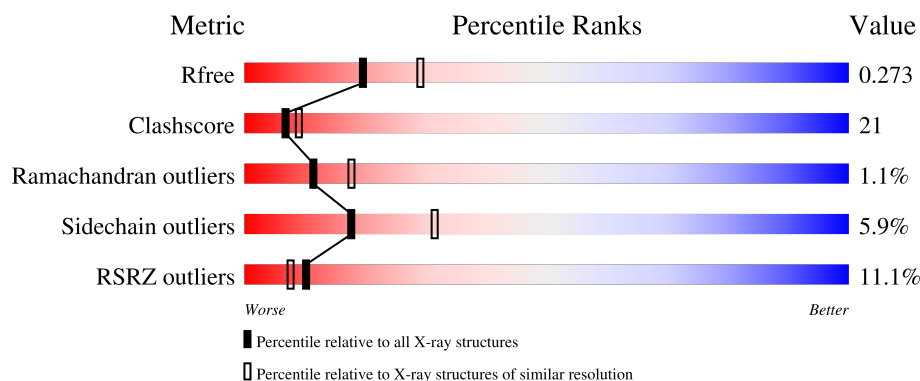
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	334	11% 59% 31% 5% 5%
1	B	334	11% 60% 30% • 5%
1	C	334	10% 63% 27% 5% 5%
1	D	334	9% 65% 26% • 6%

Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9912 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 Conserved archaeal protein Q6M145.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	Se	0	0	0
			2438	1537	397	496	4	4			
1	B	318	Total	C	N	O	S	Se	0	0	0
			2455	1544	402	501	4	4			
1	C	317	Total	C	N	O	S	Se	0	0	0
			2444	1540	397	498	4	5			
1	D	313	Total	C	N	O	S	Se	0	0	0
			2413	1522	391	491	4	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ASN	LYS	engineered mutation	UNP Q6M145
A	50	VAL	ILE	engineered mutation	UNP Q6M145
A	93	ASN	ASP	engineered mutation	UNP Q6M145
A	101	SER	GLY	engineered mutation	UNP Q6M145
A	106	ASN	TYR	engineered mutation	UNP Q6M145
A	146	GLU	ASP	engineered mutation	UNP Q6M145
A	182	SER	LEU	engineered mutation	UNP Q6M145
A	187	ASP	ASN	engineered mutation	UNP Q6M145
A	254	ASN	THR	engineered mutation	UNP Q6M145
A	268	GLU	LYS	engineered mutation	UNP Q6M145
A	269	ASN	LYS	engineered mutation	UNP Q6M145
A	284	LEU	ILE	engineered mutation	UNP Q6M145
A	294	ALA	GLY	engineered mutation	UNP Q6M145
A	327	LEU	-	expression tag	UNP Q6M145
A	328	GLU	-	expression tag	UNP Q6M145
A	329	HIS	-	expression tag	UNP Q6M145
A	330	HIS	-	expression tag	UNP Q6M145
A	331	HIS	-	expression tag	UNP Q6M145
A	332	HIS	-	expression tag	UNP Q6M145
A	333	HIS	-	expression tag	UNP Q6M145
A	334	HIS	-	expression tag	UNP Q6M145

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Chain	Residue	Modelled	Actual	Comment	Reference
B	48	ASN	LYS	engineered mutation	UNP Q6M145
B	50	VAL	ILE	engineered mutation	UNP Q6M145
B	93	ASN	ASP	engineered mutation	UNP Q6M145
B	101	SER	GLY	engineered mutation	UNP Q6M145
B	106	ASN	TYR	engineered mutation	UNP Q6M145
B	146	GLU	ASP	engineered mutation	UNP Q6M145
B	182	SER	LEU	engineered mutation	UNP Q6M145
B	187	ASP	ASN	engineered mutation	UNP Q6M145
B	254	ASN	THR	engineered mutation	UNP Q6M145
B	268	GLU	LYS	engineered mutation	UNP Q6M145
B	269	ASN	LYS	engineered mutation	UNP Q6M145
B	284	LEU	ILE	engineered mutation	UNP Q6M145
B	294	ALA	GLY	engineered mutation	UNP Q6M145
B	327	LEU	-	expression tag	UNP Q6M145
B	328	GLU	-	expression tag	UNP Q6M145
B	329	HIS	-	expression tag	UNP Q6M145
B	330	HIS	-	expression tag	UNP Q6M145
B	331	HIS	-	expression tag	UNP Q6M145
B	332	HIS	-	expression tag	UNP Q6M145
B	333	HIS	-	expression tag	UNP Q6M145
B	334	HIS	-	expression tag	UNP Q6M145
C	48	ASN	LYS	engineered mutation	UNP Q6M145
C	50	VAL	ILE	engineered mutation	UNP Q6M145
C	93	ASN	ASP	engineered mutation	UNP Q6M145
C	101	SER	GLY	engineered mutation	UNP Q6M145
C	106	ASN	TYR	engineered mutation	UNP Q6M145
C	146	GLU	ASP	engineered mutation	UNP Q6M145
C	182	SER	LEU	engineered mutation	UNP Q6M145
C	187	ASP	ASN	engineered mutation	UNP Q6M145
C	254	ASN	THR	engineered mutation	UNP Q6M145
C	268	GLU	LYS	engineered mutation	UNP Q6M145
C	269	ASN	LYS	engineered mutation	UNP Q6M145
C	284	LEU	ILE	engineered mutation	UNP Q6M145
C	294	ALA	GLY	engineered mutation	UNP Q6M145
C	327	LEU	-	expression tag	UNP Q6M145
C	328	GLU	-	expression tag	UNP Q6M145
C	329	HIS	-	expression tag	UNP Q6M145
C	330	HIS	-	expression tag	UNP Q6M145
C	331	HIS	-	expression tag	UNP Q6M145
C	332	HIS	-	expression tag	UNP Q6M145
C	333	HIS	-	expression tag	UNP Q6M145
C	334	HIS	-	expression tag	UNP Q6M145

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Chain	Residue	Modelled	Actual	Comment	Reference
D	48	ASN	LYS	engineered mutation	UNP Q6M145
D	50	VAL	ILE	engineered mutation	UNP Q6M145
D	93	ASN	ASP	engineered mutation	UNP Q6M145
D	101	SER	GLY	engineered mutation	UNP Q6M145
D	106	ASN	TYR	engineered mutation	UNP Q6M145
D	146	GLU	ASP	engineered mutation	UNP Q6M145
D	182	SER	LEU	engineered mutation	UNP Q6M145
D	187	ASP	ASN	engineered mutation	UNP Q6M145
D	254	ASN	THR	engineered mutation	UNP Q6M145
D	268	GLU	LYS	engineered mutation	UNP Q6M145
D	269	ASN	LYS	engineered mutation	UNP Q6M145
D	284	LEU	ILE	engineered mutation	UNP Q6M145
D	294	ALA	GLY	engineered mutation	UNP Q6M145
D	327	LEU	-	expression tag	UNP Q6M145
D	328	GLU	-	expression tag	UNP Q6M145
D	329	HIS	-	expression tag	UNP Q6M145
D	330	HIS	-	expression tag	UNP Q6M145
D	331	HIS	-	expression tag	UNP Q6M145
D	332	HIS	-	expression tag	UNP Q6M145
D	333	HIS	-	expression tag	UNP Q6M145
D	334	HIS	-	expression tag	UNP Q6M145

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

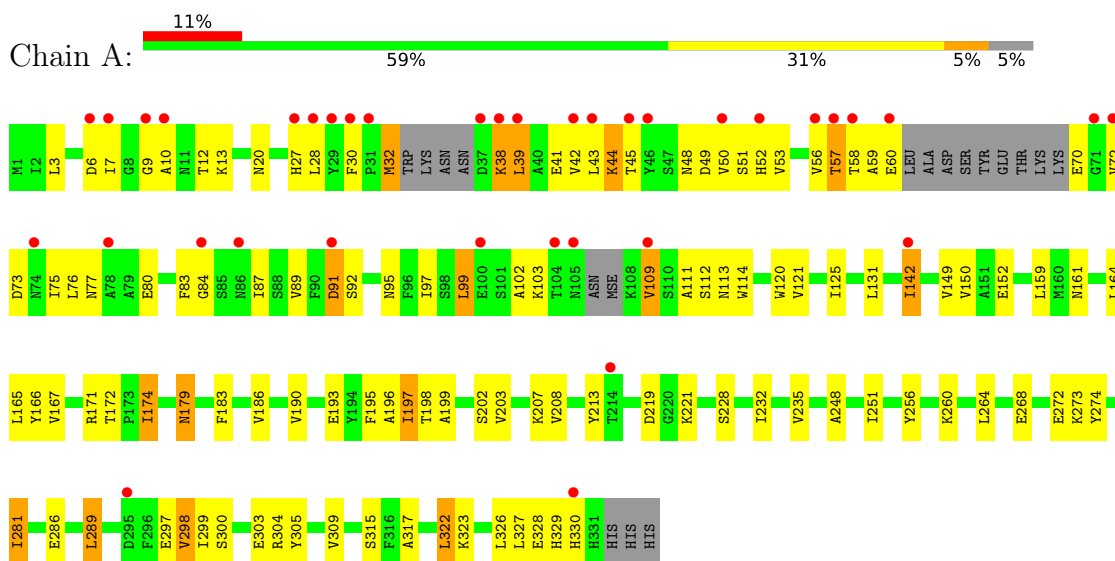
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	28	Total O 28 28	0	0
3	B	32	Total O 32 32	0	0
3	C	42	Total O 42 42	0	0
3	D	58	Total O 58 58	0	0

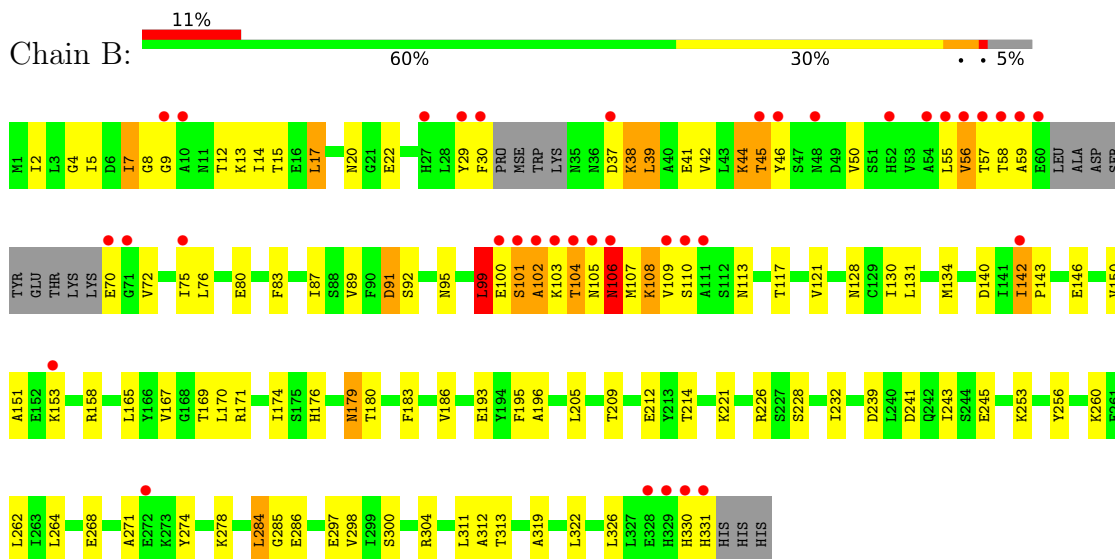
3 Residue-property plots [i](#)

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.

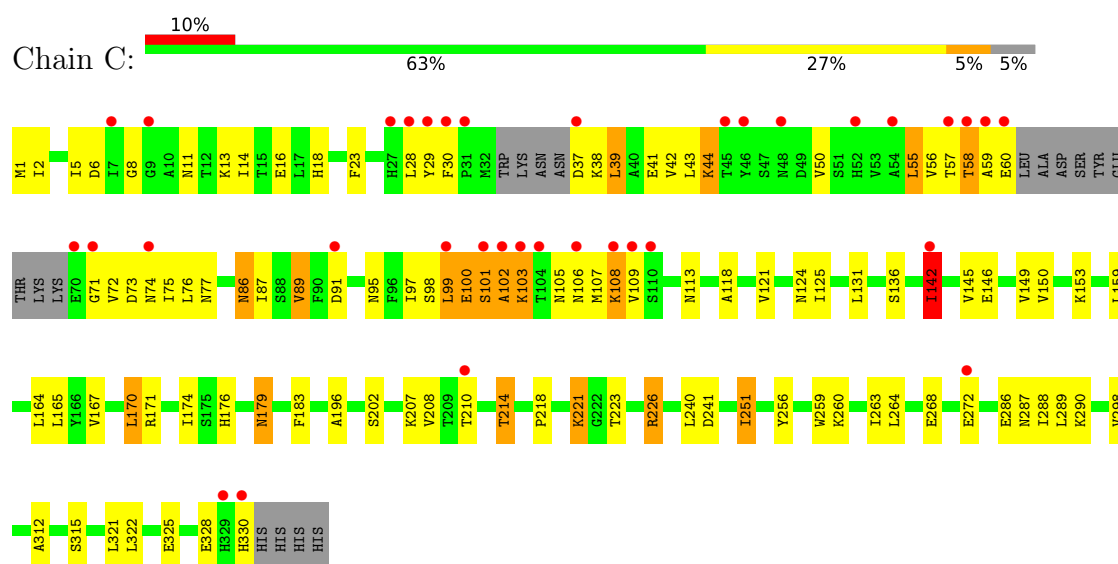
• Molecule 1: Conserved archaeal protein Q6M145



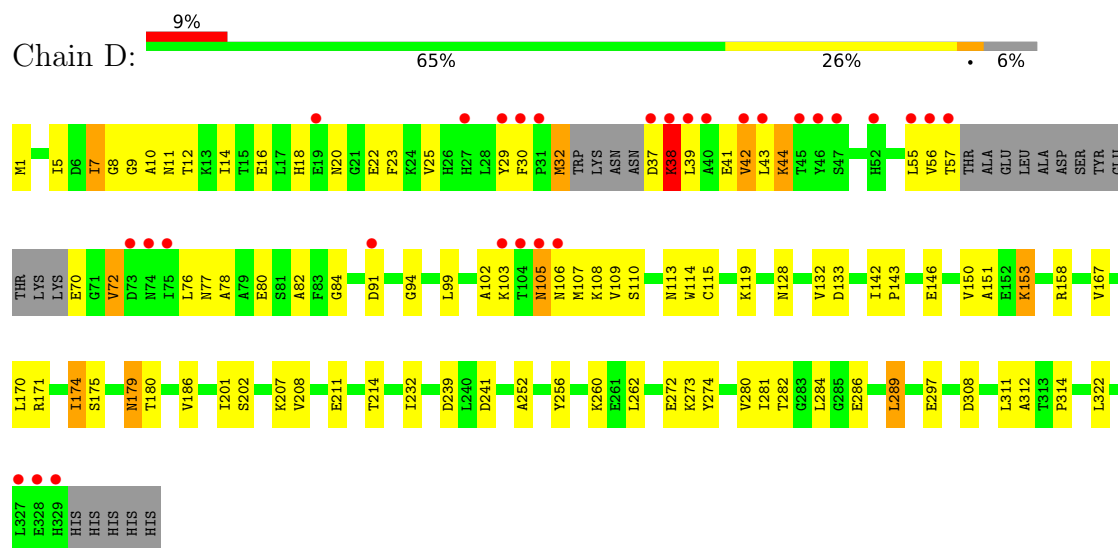
• Molecule 1: Conserved archaeal protein Q6M145



• Molecule 1: Conserved archaeal protein Q6M145



• Molecule 1: Conserved archaeal protein Q6M145



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.40Å 87.27Å 123.99Å 90.00° 110.29° 90.00°	Depositor
Resolution (Å)	19.81 – 2.40 19.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.6 (19.81-2.40) 95.8 (19.81-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.214 , 0.259 0.227 , 0.273	Depositor DCC
R_{free} test set	5979 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9912	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: CA

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	0/2469	0.90	9/3339 (0.3%)
1	B	0.45	0/2486	0.91	6/3363 (0.2%)
1	C	0.48	0/2474	0.98	12/3345 (0.4%)
1	D	0.47	0/2442	0.99	15/3301 (0.5%)
All	All	0.45	0/9871	0.95	42/13348 (0.3%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	107	MSE	N-CA-C	-10.39	100.61	113.28
1	D	38	LYS	N-CA-C	-9.20	102.07	113.20
1	D	142	ILE	N-CA-C	9.16	118.17	107.73
1	A	113	ASN	N-CA-C	-8.04	103.49	113.38
1	D	171	ARG	N-CA-C	7.16	121.67	113.15
1	A	92	SER	N-CA-C	-7.02	104.71	113.28
1	C	298	VAL	N-CA-C	6.97	118.09	108.89
1	B	99	LEU	N-CA-C	-6.89	103.70	111.14
1	C	214	THR	N-CA-C	6.73	118.70	111.36
1	A	174	ILE	N-CA-C	6.50	117.18	110.36
1	C	171	ARG	N-CA-C	6.27	120.55	113.02
1	C	38	LYS	N-CA-C	-6.16	105.80	113.38
1	C	99	LEU	N-CA-C	-6.13	104.51	111.07
1	D	297	GLU	N-CA-C	-6.13	99.87	109.25
1	C	251	ILE	N-CA-C	-5.89	104.76	110.42
1	C	153	LYS	N-CA-C	5.87	117.47	111.14
1	D	114	TRP	N-CA-C	5.84	120.53	113.41
1	A	171	ARG	N-CA-C	5.74	120.08	111.81
1	C	142	ILE	N-CA-C	5.71	114.24	107.73
1	B	214	THR	N-CA-C	5.64	119.34	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	VAL	N-CA-C	5.54	116.29	108.36
1	C	241	ASP	N-CA-C	-5.49	107.13	113.88
1	C	170	LEU	N-CA-C	5.47	122.46	110.80
1	C	103	LYS	N-CA-C	5.42	119.95	113.23
1	B	171	ARG	N-CA-C	5.40	118.98	112.93
1	A	329	HIS	N-CA-C	-5.37	106.80	113.19
1	C	107	MSE	N-CA-C	5.36	119.44	113.01
1	D	167	VAL	N-CA-C	-5.35	100.50	108.46
1	D	207	LYS	N-CA-C	-5.33	106.94	113.50
1	D	280	VAL	N-CA-C	-5.32	100.72	108.17
1	D	214	THR	N-CA-C	5.31	117.98	111.82
1	A	297	GLU	N-CA-C	-5.29	100.55	108.96
1	B	176	HIS	N-CA-C	-5.28	105.69	111.82
1	B	298	VAL	N-CA-C	5.24	116.12	108.58
1	A	111	ALA	N-CA-C	5.18	115.08	108.24
1	D	30	PHE	CA-C-N	5.17	124.93	119.76
1	D	30	PHE	C-N-CA	5.17	124.93	119.76
1	B	92	SER	N-CA-C	-5.17	106.94	113.20
1	D	115	CYS	N-CA-C	5.15	117.30	111.11
1	D	170	LEU	N-CA-C	5.04	121.55	110.80
1	A	57	THR	CB-CA-C	-5.03	109.14	116.53
1	D	158	ARG	N-CA-C	-5.01	105.90	111.36

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	2438	0	2418	112	0
1	B	2455	0	2430	125	0
1	C	2444	0	2427	120	0
1	D	2413	0	2402	68	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	0	2	0
3	C	42	0	0	0	0
3	D	58	0	0	3	0
All	All	9912	0	9677	416	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 21.

All (416) 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:B:89:VAL:HG11	1:B:103:LYS:HD3	1.25	1.08
1:C:108:LYS:HE3	1:C:108:LYS:HA	1.39	1.03
1:B:76:LEU:HD22	1:B:103:LYS:HZ2	1.24	1.02
1:C:97:ILE:HD11	1:C:103:LYS:HG3	1.42	1.00
1:A:72:VAL:HG21	1:A:109:VAL:HG21	1.46	0.94
1:A:142:ILE:HD13	1:A:149:VAL:HG13	1.49	0.93
1:B:56:VAL:HG22	1:B:57:THR:H	1.31	0.92
1:A:197:ILE:HD13	1:A:199:ALA:HB3	1.54	0.89
1:B:57:THR:HG22	1:B:58:THR:H	1.36	0.88
1:B:5:ILE:HD12	1:B:14:ILE:HD12	1.59	0.85
1:C:39:LEU:O	1:C:42:VAL:HG22	1.77	0.85
1:B:7:ILE:HD13	1:B:9:GLY:H	1.41	0.85
1:D:39:LEU:O	1:D:42:VAL:HG22	1.78	0.84
1:A:75:ILE:HD12	1:A:76:LEU:N	1.93	0.83
1:C:103:LYS:HD3	1:C:109:VAL:HG22	1.60	0.82
1:C:57:THR:HG22	1:C:58:THR:H	1.43	0.81
1:D:41:GLU:OE2	1:D:82:ALA:HA	1.81	0.81
1:C:103:LYS:NZ	1:C:109:VAL:HA	1.96	0.80
1:B:76:LEU:HD22	1:B:103:LYS:NZ	1.98	0.78
1:C:97:ILE:CD1	1:C:103:LYS:HG3	2.14	0.78
1:D:102:ALA:O	1:D:106:ASN:HB3	1.84	0.78
1:B:72:VAL:O	1:B:76:LEU:HG	1.85	0.77
1:C:102:ALA:O	1:C:106:ASN:HB2	1.84	0.77
1:A:39:LEU:O	1:A:42:VAL:HG22	1.85	0.76
1:B:20:ASN:OD1	1:B:22:GLU:HG2	1.86	0.76
1:B:131:LEU:HB3	1:B:142:ILE:HD13	1.69	0.75
1:C:142:ILE:HD13	1:C:149:VAL:HG13	1.69	0.74
1:C:56:VAL:HG22	1:C:57:THR:H	1.52	0.74
1:B:105:ASN:C	1:B:106:ASN:HD22	1.96	0.73
1:B:131:LEU:HB3	1:B:142:ILE:CD1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:ALA:HA	3:D:456:HOH:O	1.87	0.72
1:A:91:ASP:HB2	1:A:95:ASN:O	1.89	0.72
1:A:99:LEU:HD12	1:A:103:LYS:HG3	1.70	0.72
1:C:97:ILE:HD11	1:C:103:LYS:CG	2.19	0.71
1:C:98:SER:O	1:C:102:ALA:HB3	1.90	0.71
1:D:72:VAL:HG11	1:D:106:ASN:OD1	1.91	0.71
1:D:91:ASP:OD2	1:D:108:LYS:HB3	1.89	0.71
1:C:87:ILE:HB	1:C:99:LEU:HD22	1.72	0.71
1:C:89:VAL:HG21	1:C:103:LYS:HD2	1.72	0.71
1:C:268:GLU:O	1:C:272:GLU:HG2	1.89	0.71
1:A:7:ILE:HA	1:A:12:THR:HG22	1.73	0.71
1:C:72:VAL:HG21	1:C:109:VAL:HG21	1.73	0.70
1:C:91:ASP:HB2	1:C:95:ASN:O	1.90	0.70
1:A:72:VAL:CG2	1:A:109:VAL:HG21	2.19	0.70
1:B:5:ILE:CD1	1:B:14:ILE:HD12	2.21	0.70
1:B:89:VAL:CG1	1:B:103:LYS:HD3	2.12	0.70
1:B:39:LEU:O	1:B:42:VAL:HG22	1.90	0.70
1:B:99:LEU:HA	1:B:103:LYS:HE2	1.73	0.70
1:C:103:LYS:HD3	1:C:109:VAL:HG13	1.73	0.69
1:C:97:ILE:HD13	1:C:102:ALA:HB1	1.73	0.69
1:C:5:ILE:HD12	1:C:14:ILE:HG13	1.74	0.69
1:B:56:VAL:HG22	1:B:57:THR:N	2.07	0.68
1:D:8:GLY:HA2	1:D:56:VAL:N	2.09	0.68
1:A:197:ILE:CD1	1:A:199:ALA:HB3	2.23	0.68
1:C:100:GLU:O	1:C:101:SER:C	2.36	0.68
1:A:304:ARG:HE	1:C:42:VAL:CG2	2.06	0.67
1:D:273:LYS:HD2	1:D:274:TYR:CE2	2.29	0.67
1:B:91:ASP:HB2	1:B:95:ASN:O	1.95	0.67
1:A:304:ARG:HE	1:C:42:VAL:HG21	1.60	0.67
1:C:103:LYS:HZ1	1:C:109:VAL:HA	1.58	0.67
1:D:256:TYR:CE1	1:D:260:LYS:HD2	2.29	0.67
1:A:281:ILE:HD13	1:A:281:ILE:H	1.60	0.66
1:D:32:MSE:HE3	1:D:32:MSE:H	1.61	0.66
1:C:100:GLU:HG3	1:C:101:SER:H	1.61	0.66
1:C:221:LYS:HE3	1:C:221:LYS:HA	1.78	0.66
1:A:281:ILE:HD12	1:A:298:VAL:HG13	1.77	0.66
1:A:112:SER:HB3	1:A:114:TRP:CD1	2.32	0.65
1:B:142:ILE:HB	1:B:151:ALA:HB2	1.78	0.65
1:C:56:VAL:HG22	1:C:57:THR:N	2.12	0.65
1:B:256:TYR:CE2	1:B:260:LYS:HD2	2.32	0.64
1:B:89:VAL:HG21	1:B:103:LYS:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASP:HA	1:A:76:LEU:HG	1.79	0.64
1:C:89:VAL:CG2	1:C:103:LYS:HD2	2.27	0.64
1:C:226:ARG:HG3	1:C:226:ARG:HH11	1.61	0.64
1:D:106:ASN:HB2	1:D:109:VAL:HG23	1.78	0.64
1:A:179:ASN:C	1:A:179:ASN:HD22	2.05	0.64
1:B:99:LEU:HD12	1:B:103:LYS:NZ	2.13	0.64
1:A:197:ILE:HD11	1:A:213:TYR:OH	1.99	0.63
1:B:228:SER:O	1:B:232:ILE:HG12	1.98	0.63
1:D:80:GLU:CD	1:D:103:LYS:NZ	2.56	0.63
1:D:38:LYS:O	1:D:38:LYS:HG2	1.97	0.63
3:A:345:HOH:O	1:C:43:LEU:HD21	1.98	0.63
1:C:55:LEU:HD12	1:C:56:VAL:N	2.14	0.63
1:A:152:GLU:HG3	1:A:161:ASN:HD22	1.63	0.63
1:A:89:VAL:HG13	1:A:97:ILE:HG13	1.81	0.62
1:C:101:SER:HA	1:C:105:ASN:HD21	1.64	0.62
1:A:72:VAL:HG22	1:A:76:LEU:HD23	1.80	0.62
1:B:128:ASN:ND2	1:B:146:GLU:H	1.97	0.62
1:D:7:ILE:HA	1:D:12:THR:HG22	1.81	0.62
1:A:159:LEU:HG	1:A:164:LEU:HD23	1.82	0.61
1:A:228:SER:O	1:A:232:ILE:HG12	2.00	0.61
1:C:41:GLU:O	1:C:44:LYS:HD2	2.01	0.61
1:D:80:GLU:HB2	1:D:99:LEU:HD21	1.81	0.61
1:B:99:LEU:HD12	1:B:103:LYS:CE	2.30	0.61
1:C:103:LYS:HD3	1:C:109:VAL:CG2	2.30	0.61
1:B:5:ILE:HG23	1:B:14:ILE:CD1	2.31	0.61
1:A:76:LEU:HD12	1:A:77:ASN:N	2.16	0.60
1:A:305:TYR:HB3	1:A:309:VAL:HG21	1.83	0.60
1:B:106:ASN:CG	1:B:107:MSE:H	2.09	0.60
1:A:152:GLU:HG3	1:A:161:ASN:ND2	2.16	0.60
1:C:179:ASN:C	1:C:179:ASN:HD22	2.10	0.60
1:B:179:ASN:C	1:B:179:ASN:HD22	2.07	0.60
1:C:75:ILE:HD12	1:C:76:LEU:N	2.16	0.60
1:A:304:ARG:NH2	1:C:43:LEU:HG	2.16	0.60
1:D:174:ILE:HG12	1:D:201:ILE:HD11	1.84	0.59
1:C:97:ILE:C	1:C:97:ILE:HD12	2.28	0.59
1:A:39:LEU:HD13	1:A:42:VAL:HG11	1.83	0.59
1:B:29:TYR:O	1:B:30:PHE:HB3	2.03	0.59
1:B:130:ILE:HD11	1:B:271:ALA:HA	1.85	0.59
1:C:57:THR:HG22	1:C:58:THR:N	2.14	0.59
1:D:41:GLU:C	1:D:43:LEU:H	2.11	0.59
1:B:45:THR:O	1:B:46:TYR:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:VAL:HG22	1:A:57:THR:N	2.18	0.58
1:B:284:LEU:HD13	1:B:311:LEU:HD22	1.84	0.58
1:D:37:ASP:C	1:D:39:LEU:H	2.11	0.58
1:A:42:VAL:HG23	1:A:43:LEU:HG	1.84	0.58
1:C:100:GLU:CG	1:C:101:SER:H	2.17	0.58
1:C:86:ASN:N	1:C:86:ASN:HD22	2.02	0.58
1:A:57:THR:HG22	1:A:58:THR:H	1.68	0.58
1:A:89:VAL:HG11	1:A:102:ALA:HB2	1.84	0.58
1:A:99:LEU:CD1	1:A:103:LYS:HG3	2.33	0.58
1:B:7:ILE:HD13	1:B:7:ILE:C	2.28	0.58
1:A:30:PHE:O	1:A:32:MSE:HE2	2.03	0.58
1:D:5:ILE:HD12	1:D:14:ILE:HG12	1.84	0.58
1:A:281:ILE:HB	1:A:289:LEU:HD23	1.86	0.57
1:A:172:THR:HB	1:A:198:THR:HG23	1.86	0.57
1:C:1:MSE:HE3	1:C:18:HIS:HE1	1.69	0.57
1:B:55:LEU:HD11	1:B:113:ASN:HB2	1.87	0.57
1:B:209:THR:CG2	1:B:212:GLU:HG3	2.34	0.57
1:C:59:ALA:O	1:C:60:GLU:HG2	2.04	0.57
1:D:153:LYS:H	1:D:153:LYS:HD2	1.69	0.57
1:A:6:ASP:OD2	1:A:13:LYS:HE3	2.04	0.57
1:B:150:VAL:HG22	1:B:150:VAL:O	2.04	0.57
1:D:76:LEU:HD12	1:D:77:ASN:N	2.20	0.57
1:D:56:VAL:HG22	1:D:57:THR:N	2.20	0.57
1:B:75:ILE:HG13	1:B:76:LEU:N	2.20	0.56
1:B:80:GLU:HB2	1:B:99:LEU:HD11	1.88	0.56
1:A:197:ILE:HD13	1:A:199:ALA:CB	2.32	0.56
1:A:264:LEU:O	1:A:268:GLU:HG3	2.04	0.56
1:C:97:ILE:HD13	1:C:102:ALA:CB	2.35	0.56
1:C:103:LYS:CD	1:C:109:VAL:HG22	2.31	0.56
1:A:281:ILE:HD12	1:A:298:VAL:CG1	2.34	0.56
1:A:165:LEU:HG	1:A:167:VAL:HG22	1.88	0.56
1:A:56:VAL:HG22	1:A:57:THR:H	1.68	0.56
1:B:304:ARG:HD3	3:B:431:HOH:O	2.05	0.56
1:C:37:ASP:HB3	1:C:39:LEU:HD23	1.87	0.56
1:C:72:VAL:O	1:C:75:ILE:HG13	2.06	0.56
1:C:256:TYR:CE2	1:C:260:LYS:HD2	2.41	0.55
1:A:6:ASP:HB2	1:A:315:SER:HB3	1.89	0.55
1:B:56:VAL:CG2	1:B:57:THR:H	2.13	0.55
1:C:55:LEU:HD12	1:C:55:LEU:C	2.32	0.55
1:B:209:THR:HG22	1:B:212:GLU:OE2	2.06	0.55
1:C:29:TYR:O	1:C:30:PHE:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LYS:HA	1:C:108:LYS:CE	2.23	0.54
1:C:136:SER:HB2	1:C:170:LEU:HD12	1.90	0.54
1:A:50:VAL:HG13	1:A:87:ILE:HA	1.89	0.54
1:B:7:ILE:CD1	1:B:9:GLY:H	2.14	0.54
1:B:101:SER:O	1:B:102:ALA:C	2.49	0.54
1:D:8:GLY:HA2	1:D:56:VAL:H	1.72	0.54
1:A:87:ILE:H	1:A:87:ILE:HD12	1.73	0.54
1:D:10:ALA:O	1:D:29:TYR:HA	2.07	0.54
1:A:44:LYS:HD3	1:A:45:THR:N	2.22	0.54
1:B:239:ASP:OD1	1:B:241:ASP:HB2	2.08	0.54
1:A:20:ASN:HA	1:C:214:THR:HG23	1.90	0.54
1:A:190:VAL:HB	1:A:235:VAL:HG12	1.90	0.54
1:A:120:TRP:HB2	1:A:317:ALA:HB1	1.90	0.54
3:A:345:HOH:O	1:C:28:LEU:HD11	2.08	0.54
1:C:1:MSE:HE3	1:C:18:HIS:CE1	2.43	0.54
1:C:103:LYS:CD	1:C:109:VAL:HG13	2.36	0.54
1:A:87:ILE:HD12	1:A:87:ILE:N	2.22	0.53
1:C:97:ILE:HD12	1:C:97:ILE:O	2.08	0.53
1:B:100:GLU:HG2	1:B:101:SER:N	2.22	0.53
1:A:75:ILE:HD12	1:A:76:LEU:H	1.72	0.53
1:A:323:LYS:O	1:A:327:LEU:HD13	2.08	0.53
1:C:58:THR:O	1:C:59:ALA:HB3	2.09	0.53
1:B:103:LYS:C	1:B:105:ASN:N	2.66	0.53
1:B:274:TYR:HB2	3:B:418:HOH:O	2.09	0.53
1:D:76:LEU:HD13	1:D:103:LYS:HG2	1.91	0.53
1:A:57:THR:HG22	1:A:58:THR:N	2.23	0.52
1:A:207:LYS:HE3	1:A:256:TYR:CZ	2.45	0.52
1:B:134:MSE:HE2	1:B:285:GLY:HA3	1.92	0.52
1:B:243:ILE:HD12	1:B:243:ILE:C	2.34	0.52
1:A:80:GLU:HG3	1:A:84:GLY:O	2.10	0.52
1:A:304:ARG:HB2	1:C:42:VAL:HG21	1.92	0.52
1:C:72:VAL:HG21	1:C:109:VAL:CG2	2.39	0.52
1:C:72:VAL:HG22	1:C:76:LEU:HD11	1.91	0.52
1:C:50:VAL:HG13	1:C:87:ILE:HA	1.92	0.52
1:B:106:ASN:ND2	1:B:107:MSE:H	2.07	0.52
1:C:103:LYS:HD3	1:C:109:VAL:CG1	2.39	0.52
1:C:174:ILE:HG12	1:C:196:ALA:O	2.09	0.52
1:B:87:ILE:HD12	1:B:99:LEU:HD13	1.92	0.52
1:B:107:MSE:O	1:B:108:LYS:CB	2.58	0.52
1:B:243:ILE:HD12	1:B:243:ILE:O	2.10	0.52
1:B:103:LYS:HG3	1:B:104:THR:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LEU:HD22	1:D:311:LEU:HD22	1.91	0.51
1:A:28:LEU:N	1:A:28:LEU:HD12	2.25	0.51
1:A:38:LYS:HB2	1:A:38:LYS:NZ	2.25	0.51
1:D:55:LEU:CD1	1:D:113:ASN:HB2	2.41	0.51
1:A:172:THR:HB	1:A:198:THR:CG2	2.40	0.51
1:C:75:ILE:HD12	1:C:75:ILE:C	2.36	0.51
1:A:273:LYS:HD2	1:A:274:TYR:CE2	2.46	0.51
1:B:99:LEU:HA	1:B:103:LYS:HG2	1.93	0.51
1:C:89:VAL:HG13	1:C:97:ILE:CD1	2.41	0.51
1:D:37:ASP:C	1:D:39:LEU:N	2.69	0.51
1:B:57:THR:HG22	1:B:58:THR:N	2.16	0.51
1:B:58:THR:HG23	1:B:70:GLU:OE2	2.10	0.51
1:C:16:GLU:O	1:C:23:PHE:HA	2.11	0.51
1:D:55:LEU:HD11	1:D:113:ASN:HB2	1.93	0.51
1:D:80:GLU:HG3	1:D:84:GLY:O	2.11	0.51
1:A:48:ASN:CG	1:A:49:ASP:H	2.19	0.50
1:B:103:LYS:HB2	1:B:109:VAL:HG22	1.93	0.50
1:A:248:ALA:HA	1:A:251:ILE:HD12	1.93	0.50
1:C:150:VAL:O	1:C:150:VAL:HG22	2.10	0.50
1:C:322:LEU:HD13	1:C:322:LEU:C	2.37	0.50
1:A:7:ILE:CD1	1:A:75:ILE:HG21	2.42	0.50
1:D:1:MSE:HE2	1:D:18:HIS:CE1	2.46	0.50
1:B:99:LEU:CA	1:B:103:LYS:HE2	2.39	0.50
1:B:103:LYS:C	1:B:105:ASN:H	2.19	0.50
1:B:102:ALA:O	1:B:108:LYS:HD3	2.12	0.50
1:B:106:ASN:O	1:B:109:VAL:HG23	2.11	0.50
1:A:281:ILE:CD1	1:A:300:SER:HA	2.42	0.50
3:A:345:HOH:O	1:C:28:LEU:HD21	2.11	0.49
1:C:101:SER:HA	1:C:105:ASN:ND2	2.27	0.49
1:C:124:ASN:C	1:C:125:ILE:HD12	2.36	0.49
1:C:87:ILE:N	1:C:87:ILE:HD12	2.27	0.49
1:A:256:TYR:CE2	1:A:260:LYS:HD2	2.47	0.49
1:A:303:GLU:O	1:C:39:LEU:HD13	2.13	0.49
1:B:106:ASN:O	1:B:107:MSE:C	2.56	0.49
1:C:287:ASN:O	1:C:290:LYS:HG2	2.12	0.49
1:D:80:GLU:CD	1:D:103:LYS:HZ1	2.18	0.49
1:D:150:VAL:O	1:D:150:VAL:HG13	2.12	0.49
1:B:106:ASN:HD22	1:B:106:ASN:N	2.05	0.49
1:B:17:LEU:HD22	1:B:319:ALA:HB1	1.95	0.49
1:B:50:VAL:CG1	1:B:87:ILE:HG12	2.43	0.49
1:B:100:GLU:O	1:B:102:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:ARG:O	1:C:226:ARG:HD3	2.12	0.49
1:B:72:VAL:HG11	1:B:106:ASN:HB2	1.95	0.49
1:B:103:LYS:O	1:B:105:ASN:N	2.46	0.49
1:D:106:ASN:HB2	1:D:109:VAL:CG2	2.43	0.49
1:C:226:ARG:HD3	1:C:226:ARG:C	2.38	0.48
1:A:142:ILE:CD1	1:A:149:VAL:HG13	2.34	0.48
1:B:38:LYS:HB2	1:B:38:LYS:NZ	2.29	0.48
1:B:55:LEU:CD1	1:B:113:ASN:HB2	2.42	0.48
1:B:100:GLU:O	1:B:101:SER:C	2.55	0.48
1:B:7:ILE:HD13	1:B:8:GLY:N	2.28	0.48
1:B:107:MSE:O	1:B:108:LYS:HB3	2.13	0.48
1:A:6:ASP:CB	1:A:315:SER:HB3	2.44	0.48
1:A:202:SER:HB3	1:A:208:VAL:HG22	1.94	0.48
1:A:150:VAL:O	1:A:150:VAL:HG22	2.14	0.48
1:B:322:LEU:HD13	1:B:322:LEU:C	2.38	0.48
1:C:57:THR:CG2	1:C:58:THR:H	2.22	0.48
1:B:57:THR:CG2	1:B:58:THR:H	2.15	0.48
1:C:101:SER:O	1:C:102:ALA:C	2.57	0.48
1:D:56:VAL:HG22	1:D:57:THR:H	1.78	0.48
1:C:145:VAL:HG12	1:C:146:GLU:HG2	1.96	0.48
1:D:202:SER:HB3	1:D:208:VAL:HG13	1.95	0.48
1:A:328:GLU:C	1:A:330:HIS:H	2.22	0.48
1:B:284:LEU:CD1	1:B:311:LEU:HD22	2.44	0.48
1:C:207:LYS:HE3	1:C:256:TYR:CZ	2.49	0.48
1:B:2:ILE:HG23	1:B:322:LEU:HD12	1.96	0.47
1:B:72:VAL:HG11	1:B:106:ASN:CB	2.43	0.47
1:B:169:THR:O	1:B:170:LEU:HD23	2.14	0.47
1:A:3:LEU:O	1:A:50:VAL:HG23	2.14	0.47
1:C:264:LEU:O	1:C:268:GLU:HG3	2.13	0.47
1:C:118:ALA:HB1	1:C:142:ILE:HD11	1.96	0.47
1:A:76:LEU:HD13	1:A:99:LEU:HD11	1.97	0.47
1:A:76:LEU:HD12	1:A:76:LEU:C	2.40	0.47
1:B:205:LEU:HD21	1:B:253:LYS:HG2	1.96	0.47
1:A:83:PHE:HB2	1:A:87:ILE:HD11	1.97	0.47
1:C:259:TRP:CH2	1:C:288:ILE:HD13	2.50	0.47
1:A:142:ILE:HD12	1:A:142:ILE:C	2.40	0.47
1:B:107:MSE:HE3	1:B:107:MSE:HA	1.95	0.47
1:C:86:ASN:N	1:C:86:ASN:ND2	2.59	0.47
1:B:99:LEU:HD12	1:B:103:LYS:HE2	1.97	0.47
1:D:44:LYS:HB2	1:D:82:ALA:O	2.15	0.47
1:A:27:HIS:C	1:A:28:LEU:HD12	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ALA:O	1:A:60:GLU:C	2.58	0.46
1:B:76:LEU:HD13	1:B:103:LYS:HD2	1.96	0.46
1:A:183:PHE:O	1:A:186:VAL:HG22	2.14	0.46
1:B:44:LYS:HB2	1:B:83:PHE:CD1	2.50	0.46
1:B:167:VAL:HG11	1:B:262:LEU:HD23	1.96	0.46
1:C:142:ILE:HD12	1:C:142:ILE:C	2.39	0.46
1:C:72:VAL:HG22	1:C:76:LEU:CD1	2.45	0.46
1:C:165:LEU:HG	1:C:167:VAL:HG22	1.97	0.46
1:C:202:SER:HB3	1:C:208:VAL:HG22	1.98	0.46
1:A:89:VAL:CG1	1:A:97:ILE:HG13	2.45	0.46
1:A:219:ASP:O	1:A:221:LYS:HG3	2.16	0.46
1:C:39:LEU:N	1:C:39:LEU:HD22	2.31	0.46
1:D:80:GLU:CD	1:D:103:LYS:HZ3	2.24	0.46
1:B:70:GLU:HA	1:B:70:GLU:OE1	2.15	0.46
1:B:193:GLU:HB2	1:B:195:PHE:CE2	2.50	0.46
1:C:226:ARG:HG3	1:C:226:ARG:NH1	2.30	0.46
1:A:196:ALA:HB1	1:A:232:ILE:HD13	1.97	0.45
1:B:2:ILE:HD12	1:B:2:ILE:N	2.31	0.45
1:B:167:VAL:HG23	1:B:167:VAL:O	2.15	0.45
1:D:232:ILE:HD13	1:D:252:ALA:HB2	1.98	0.45
1:B:89:VAL:HG21	1:B:103:LYS:CB	2.46	0.45
1:B:264:LEU:O	1:B:268:GLU:HG3	2.16	0.45
1:D:41:GLU:C	1:D:43:LEU:N	2.74	0.45
1:A:193:GLU:HB2	1:A:195:PHE:CE2	2.51	0.45
1:B:46:TYR:CG	1:B:46:TYR:O	2.68	0.45
1:B:143:PRO:HG2	1:B:150:VAL:HG13	1.98	0.45
1:D:314:PRO:HD2	3:D:438:HOH:O	2.16	0.45
1:A:281:ILE:HD13	1:A:299:ILE:O	2.15	0.45
1:B:183:PHE:O	1:B:186:VAL:HG22	2.16	0.45
1:A:41:GLU:C	1:A:43:LEU:H	2.23	0.45
1:C:73:ASP:O	1:C:77:ASN:ND2	2.49	0.45
1:D:103:LYS:O	1:D:105:ASN:N	2.50	0.45
1:A:51:SER:HB3	1:A:322:LEU:HD12	1.98	0.45
1:B:2:ILE:CG2	1:B:322:LEU:HD12	2.47	0.45
1:B:58:THR:HG22	1:B:58:THR:O	2.17	0.45
1:C:5:ILE:HD12	1:C:14:ILE:CG1	2.46	0.45
1:C:121:VAL:HA	1:C:125:ILE:HD13	1.99	0.45
1:B:179:ASN:C	1:B:179:ASN:ND2	2.75	0.44
1:D:8:GLY:C	1:D:56:VAL:HB	2.42	0.44
1:A:53:VAL:HG13	1:A:53:VAL:O	2.15	0.44
1:A:121:VAL:HG13	1:A:125:ILE:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ARG:NH1	1:B:245:GLU:OE2	2.50	0.44
1:C:1:MSE:HG2	1:C:2:ILE:N	2.32	0.44
1:C:125:ILE:HD12	1:C:125:ILE:N	2.32	0.44
1:C:142:ILE:CD1	1:C:149:VAL:HG13	2.44	0.44
1:D:239:ASP:OD1	1:D:241:ASP:HB2	2.17	0.44
1:B:7:ILE:HG12	1:B:12:THR:CG2	2.47	0.44
1:B:41:GLU:O	1:B:44:LYS:HB3	2.18	0.44
1:C:226:ARG:HE	1:C:240:LEU:HD12	1.81	0.44
1:D:133:ASP:OD2	1:D:133:ASP:C	2.60	0.44
1:D:179:ASN:ND2	1:D:180:THR:HG23	2.32	0.44
1:A:112:SER:HB3	1:A:114:TRP:NE1	2.32	0.44
1:A:174:ILE:HG12	1:A:196:ALA:O	2.17	0.44
1:A:57:THR:CG2	1:A:58:THR:H	2.28	0.44
1:C:5:ILE:CD1	1:C:14:ILE:HG13	2.45	0.44
1:A:9:GLY:N	1:A:56:VAL:HG11	2.32	0.44
1:A:72:VAL:HG13	1:A:73:ASP:N	2.33	0.44
1:B:13:LYS:HD3	1:B:312:ALA:HB2	2.00	0.44
1:B:209:THR:HG23	1:B:212:GLU:HG3	2.00	0.44
1:C:287:ASN:HA	1:C:290:LYS:HE3	2.00	0.44
1:D:128:ASN:ND2	1:D:146:GLU:H	2.16	0.44
1:D:72:VAL:O	1:D:76:LEU:HG	2.18	0.43
1:A:73:ASP:HB3	1:A:77:ASN:ND2	2.33	0.43
1:A:281:ILE:HD11	1:A:300:SER:HA	2.00	0.43
1:B:4:GLY:HA3	1:B:319:ALA:HB2	2.00	0.43
1:B:106:ASN:ND2	1:B:107:MSE:N	2.67	0.43
1:D:281:ILE:HB	1:D:289:LEU:HD23	2.00	0.43
1:A:87:ILE:HB	1:A:99:LEU:HD23	1.99	0.43
1:D:5:ILE:CD1	1:D:14:ILE:HG12	2.49	0.43
1:D:37:ASP:CB	1:D:78:ALA:HB1	2.48	0.43
1:A:179:ASN:C	1:A:179:ASN:ND2	2.76	0.43
1:B:117:THR:O	1:B:121:VAL:HG23	2.18	0.43
1:A:39:LEU:HA	1:A:42:VAL:HG13	2.01	0.43
1:A:328:GLU:C	1:A:330:HIS:N	2.75	0.43
1:B:179:ASN:HD22	1:B:180:THR:N	2.17	0.43
1:C:8:GLY:C	1:C:56:VAL:HB	2.43	0.43
1:C:259:TRP:O	1:C:263:ILE:HG12	2.19	0.43
1:A:10:ALA:CB	1:A:32:MSE:HE1	2.49	0.43
1:A:199:ALA:O	1:A:203:VAL:HG23	2.19	0.43
1:A:281:ILE:HD13	1:A:281:ILE:N	2.32	0.43
1:C:321:LEU:O	1:C:325:GLU:HG3	2.18	0.43
1:C:58:THR:HG22	1:C:60:GLU:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LEU:HD23	3:D:420:HOH:O	2.18	0.42
1:B:44:LYS:O	1:B:44:LYS:HG2	2.19	0.42
1:B:140:ASP:OD1	1:B:158:ARG:NH2	2.39	0.42
1:C:176:HIS:CD2	1:D:175:SER:HB2	2.54	0.42
1:D:102:ALA:O	1:D:106:ASN:ND2	2.47	0.42
1:D:132:VAL:HG12	1:D:289:LEU:HD21	2.02	0.42
1:C:87:ILE:HD13	1:C:99:LEU:HD22	2.02	0.42
1:C:183:PHE:CD1	1:C:251:ILE:HD11	2.54	0.42
1:C:210:THR:HG23	1:C:223:THR:OG1	2.19	0.42
1:B:29:TYR:CD1	1:B:29:TYR:C	2.98	0.42
1:B:165:LEU:HG	1:B:167:VAL:HG22	2.01	0.42
1:D:55:LEU:O	1:D:55:LEU:HD12	2.19	0.42
1:D:70:GLU:CB	1:D:72:VAL:HG12	2.49	0.42
1:D:179:ASN:HD22	1:D:180:THR:HG23	1.83	0.42
1:A:207:LYS:HE3	1:A:256:TYR:OH	2.19	0.42
1:D:41:GLU:O	1:D:43:LEU:N	2.52	0.42
1:A:281:ILE:H	1:A:281:ILE:CD1	2.30	0.42
1:A:327:LEU:N	1:A:327:LEU:HD12	2.34	0.42
1:B:106:ASN:CG	1:B:107:MSE:N	2.77	0.42
1:D:143:PRO:HD2	1:D:151:ALA:HB2	2.02	0.42
1:A:131:LEU:HB3	1:A:142:ILE:HG13	2.01	0.42
1:A:326:LEU:C	1:A:328:GLU:H	2.28	0.42
1:B:15:THR:HG22	1:B:17:LEU:HD13	2.02	0.42
1:D:9:GLY:C	1:D:11:ASN:N	2.77	0.42
1:B:50:VAL:HG11	1:B:87:ILE:HG12	2.02	0.42
1:C:103:LYS:CE	1:C:109:VAL:HA	2.50	0.42
1:D:16:GLU:O	1:D:23:PHE:HA	2.20	0.42
1:D:20:ASN:HD21	1:D:22:GLU:CD	2.27	0.42
1:C:100:GLU:CG	1:C:101:SER:N	2.82	0.41
1:A:41:GLU:C	1:A:43:LEU:N	2.78	0.41
1:B:209:THR:HG22	1:B:212:GLU:HG3	2.00	0.41
1:B:109:VAL:O	1:B:110:SER:C	2.62	0.41
1:B:330:HIS:O	1:B:331:HIS:C	2.63	0.41
1:C:71:GLY:HA2	1:C:74:ASN:OD1	2.20	0.41
1:D:94:GLY:O	1:D:119:LYS:HE3	2.19	0.41
1:D:282:THR:HA	1:D:286:GLU:OE1	2.21	0.41
1:D:25:VAL:HB	1:D:308:ASP:HB3	2.02	0.41
1:A:7:ILE:HD11	1:A:75:ILE:HG21	2.02	0.41
1:A:20:ASN:CB	1:C:214:THR:HG23	2.51	0.41
1:B:322:LEU:O	1:B:326:LEU:HG	2.20	0.41
1:C:6:ASP:HB3	1:C:315:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LYS:HE3	1:C:108:LYS:CA	2.29	0.41
1:C:131:LEU:HB3	1:C:142:ILE:HG13	2.01	0.41
1:A:304:ARG:HE	1:C:42:VAL:HG23	1.82	0.41
1:B:7:ILE:HD13	1:B:9:GLY:N	2.22	0.41
1:B:174:ILE:HD12	1:B:196:ALA:HB3	2.01	0.41
1:B:284:LEU:HD12	1:B:284:LEU:HA	1.95	0.41
1:B:286:GLU:OE1	1:B:300:SER:OG	2.39	0.41
1:B:131:LEU:HB3	1:B:142:ILE:HD11	2.00	0.40
1:B:134:MSE:CE	1:B:285:GLY:HA3	2.52	0.40
1:C:13:LYS:C	1:C:14:ILE:HD12	2.47	0.40
1:C:13:LYS:HD2	1:C:312:ALA:CB	2.51	0.40
1:C:59:ALA:C	1:C:60:GLU:HG2	2.46	0.40
1:A:44:LYS:HD3	1:A:45:THR:HG23	2.03	0.40
1:B:278:LYS:HE2	1:B:297:GLU:OE2	2.22	0.40
1:D:9:GLY:C	1:D:11:ASN:H	2.30	0.40
1:D:179:ASN:HD22	1:D:179:ASN:C	2.30	0.40
1:C:159:LEU:HG	1:C:164:LEU:HD23	2.03	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	308/334 (92%)	279 (91%)	29 (9%)	0	100	100
1	B	312/334 (93%)	286 (92%)	19 (6%)	7 (2%)	5	6
1	C	311/334 (93%)	292 (94%)	15 (5%)	4 (1%)	9	14
1	D	307/334 (92%)	291 (95%)	13 (4%)	3 (1%)	12	20
All	All	1238/1336 (93%)	1148 (93%)	76 (6%)	14 (1%)	11	18

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	SER
1	B	102	ALA
1	B	106	ASN
1	C	101	SER
1	C	102	ALA
1	B	108	LYS
1	C	58	THR
1	D	42	VAL
1	D	105	ASN
1	D	110	SER
1	B	56	VAL
1	B	59	ALA
1	B	104	THR
1	C	100	GLU

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	275/287 (96%)	257 (94%)	18 (6%)	15	27
1	B	277/287 (96%)	261 (94%)	16 (6%)	18	32
1	C	276/287 (96%)	259 (94%)	17 (6%)	16	29
1	D	273/287 (95%)	259 (95%)	14 (5%)	21	37
All	All	1101/1148 (96%)	1036 (94%)	65 (6%)	18	31

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MSE
1	A	38	LYS
1	A	39	LEU
1	A	44	LYS
1	A	52	HIS
1	A	70	GLU
1	A	91	ASP
1	A	99	LEU

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Mol	Chain	Res	Type
1	A	109	VAL
1	A	142	ILE
1	A	166	TYR
1	A	179	ASN
1	A	197	ILE
1	A	272	GLU
1	A	281	ILE
1	A	286	GLU
1	A	289	LEU
1	A	322	LEU
1	B	7	ILE
1	B	17	LEU
1	B	37	ASP
1	B	38	LYS
1	B	39	LEU
1	B	44	LYS
1	B	45	THR
1	B	91	ASP
1	B	99	LEU
1	B	106	ASN
1	B	142	ILE
1	B	153	LYS
1	B	179	ASN
1	B	221	LYS
1	B	284	LEU
1	B	313	THR
1	C	11	ASN
1	C	39	LEU
1	C	44	LYS
1	C	55	LEU
1	C	86	ASN
1	C	89	VAL
1	C	108	LYS
1	C	113	ASN
1	C	142	ILE
1	C	179	ASN
1	C	218	PRO
1	C	221	LYS
1	C	226	ARG
1	C	286	GLU
1	C	289	LEU
1	C	328	GLU

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Mol	Chain	Res	Type
1	C	330	HIS
1	D	7	ILE
1	D	32	MSE
1	D	38	LYS
1	D	44	LYS
1	D	72	VAL
1	D	153	LYS
1	D	174	ILE
1	D	179	ASN
1	D	186	VAL
1	D	211	GLU
1	D	262	LEU
1	D	272	GLU
1	D	289	LEU
1	D	322	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	86	ASN
1	A	124	ASN
1	A	128	ASN
1	A	161	ASN
1	A	179	ASN
1	A	254	ASN
1	A	287	ASN
1	B	11	ASN
1	B	77	ASN
1	B	86	ASN
1	B	93	ASN
1	B	95	ASN
1	B	106	ASN
1	B	128	ASN
1	B	161	ASN
1	B	176	HIS
1	B	179	ASN
1	B	242	GLN
1	B	254	ASN
1	B	287	ASN
1	B	324	ASN
1	B	329	HIS

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Mol	Chain	Res	Type
1	C	18	HIS
1	C	77	ASN
1	C	86	ASN
1	C	105	ASN
1	C	128	ASN
1	C	176	HIS
1	C	179	ASN
1	C	254	ASN
1	C	266	ASN
1	C	330	HIS
1	D	11	ASN
1	D	18	HIS
1	D	20	ASN
1	D	77	ASN
1	D	105	ASN
1	D	128	ASN
1	D	162	HIS
1	D	176	HIS
1	D	179	ASN
1	D	189	ASN
1	D	242	GLN
1	D	254	ASN
1	D	269	ASN
1	D	287	ASN

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	312/334 (93%)	0.70	37 (11%) 9 6	21, 46, 105, 128	0
1	B	314/334 (94%)	0.46	37 (11%) 9 6	16, 38, 81, 121	0
1	C	312/334 (93%)	0.31	35 (11%) 10 7	13, 31, 82, 125	0
1	D	308/334 (92%)	0.21	29 (9%) 14 11	12, 31, 85, 116	0
All	All	1246/1336 (93%)	0.42	138 (11%) 10 7	12, 37, 96, 128	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	103	LYS	6.2
1	B	101	SER	5.6
1	B	106	ASN	5.1
1	B	71	GLY	4.9
1	D	37	ASP	4.7
1	B	55	LEU	4.5
1	B	30	PHE	4.5
1	C	30	PHE	4.3
1	A	43	LEU	4.2
1	B	103	LYS	4.2
1	C	58	THR	4.2
1	C	31	PRO	4.1
1	D	30	PHE	4.1
1	C	91	ASP	4.1
1	A	46	TYR	4.1
1	C	59	ALA	4.0
1	C	101	SER	4.0
1	B	59	ALA	3.9
1	C	104	THR	3.9
1	A	52	HIS	3.9
1	B	56	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	30	PHE	3.9
1	C	27	HIS	3.9
1	B	105	ASN	3.8
1	A	330	HIS	3.7
1	D	40	ALA	3.7
1	B	58	THR	3.6
1	D	105	ASN	3.6
1	B	111	ALA	3.5
1	B	110	SER	3.5
1	C	102	ALA	3.5
1	B	9	GLY	3.4
1	C	37	ASP	3.4
1	A	31	PRO	3.4
1	C	28	LEU	3.3
1	D	31	PRO	3.3
1	C	330	HIS	3.3
1	C	108	LYS	3.3
1	B	37	ASP	3.3
1	D	329	HIS	3.3
1	C	329	HIS	3.3
1	B	102	ALA	3.2
1	A	38	LYS	3.2
1	B	60	GLU	3.1
1	B	100	GLU	3.1
1	C	60	GLU	3.1
1	B	27	HIS	3.1
1	A	56	VAL	3.1
1	A	91	ASP	3.1
1	A	109	VAL	3.1
1	C	70	GLU	3.0
1	A	71	GLY	3.0
1	C	45	THR	3.0
1	D	19	GLU	3.0
1	A	105	ASN	3.0
1	C	109	VAL	3.0
1	B	57	THR	3.0
1	A	39	LEU	3.0
1	C	29	TYR	2.9
1	D	91	ASP	2.9
1	A	7	ILE	2.8
1	D	55	LEU	2.8
1	B	329	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	42	VAL	2.8
1	D	328	GLU	2.8
1	C	48	ASN	2.7
1	D	43	LEU	2.7
1	A	104	THR	2.7
1	B	75	ILE	2.7
1	D	75	ILE	2.7
1	A	57	THR	2.7
1	B	331	HIS	2.7
1	C	74	ASN	2.7
1	D	46	TYR	2.7
1	C	57	THR	2.7
1	A	9	GLY	2.6
1	D	57	THR	2.6
1	A	27	HIS	2.6
1	C	46	TYR	2.6
1	A	78	ALA	2.6
1	D	29	TYR	2.6
1	B	48	ASN	2.6
1	D	106	ASN	2.6
1	C	52	HIS	2.6
1	C	71	GLY	2.5
1	A	28	LEU	2.5
1	B	46	TYR	2.5
1	A	74	ASN	2.5
1	D	27	HIS	2.5
1	A	10	ALA	2.5
1	A	84	GLY	2.5
1	C	9	GLY	2.5
1	B	272	GLU	2.5
1	D	103	LYS	2.5
1	B	54	ALA	2.5
1	D	56	VAL	2.5
1	D	74	ASN	2.5
1	A	214	THR	2.5
1	B	104	THR	2.5
1	B	330	HIS	2.4
1	A	58	THR	2.4
1	B	45	THR	2.4
1	B	328	GLU	2.4
1	B	142	ILE	2.4
1	A	37	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	45	THR	2.3
1	D	104	THR	2.3
1	C	142	ILE	2.3
1	A	86	ASN	2.3
1	D	52	HIS	2.3
1	A	72	VAL	2.3
1	C	110	SER	2.3
1	A	6	ASP	2.3
1	C	99	LEU	2.2
1	D	47	SER	2.2
1	D	327	LEU	2.2
1	A	50	VAL	2.2
1	B	10	ALA	2.2
1	A	45	THR	2.2
1	B	52	HIS	2.2
1	C	7	ILE	2.2
1	A	29	TYR	2.2
1	A	100	GLU	2.2
1	D	39	LEU	2.1
1	A	60	GLU	2.1
1	B	29	TYR	2.1
1	B	109	VAL	2.1
1	C	272	GLU	2.1
1	B	153	LYS	2.1
1	B	70	GLU	2.1
1	A	142	ILE	2.1
1	D	38	LYS	2.0
1	D	42	VAL	2.0
1	C	54	ALA	2.0
1	C	106	ASN	2.0
1	C	210	THR	2.0
1	A	295	ASP	2.0
1	D	73	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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	CA	D	401	1/1	0.79	0.15	57,57,57,57	0
2	CA	B	402	1/1	0.82	0.14	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.