



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:39 PM UTC

PDB ID : 3HK9 / pdb_00003hk9
Title : Crystal structure of uronate isomerase from *Bacillus halodurans* complexed with zinc and D-Glucuronate
Authors : Fedorov, A.A.; Fedorov, E.V.; Nguyen, T.T.; Raushel, F.M.; Almo, S.C.
Deposited on : 2009-05-22
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

<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

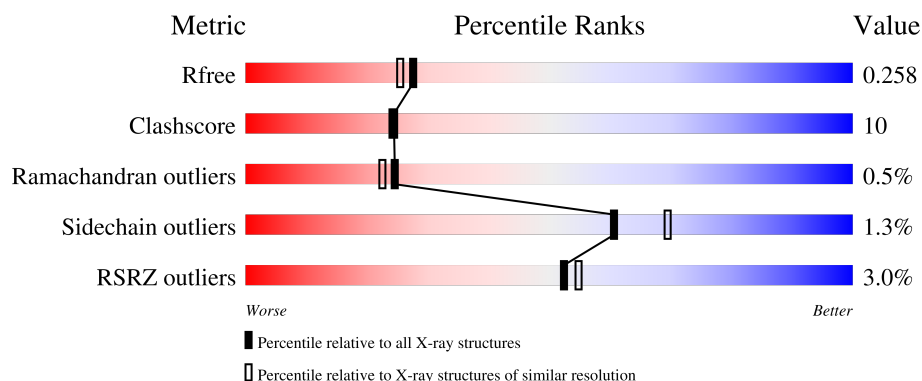
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



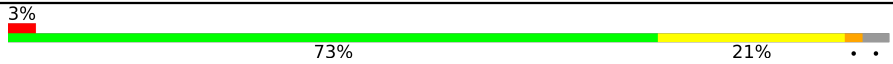
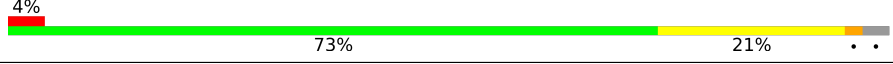
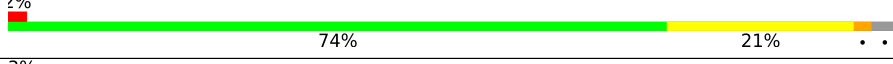
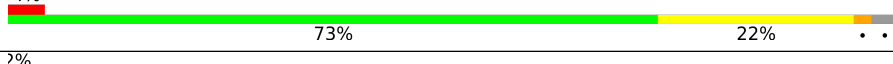
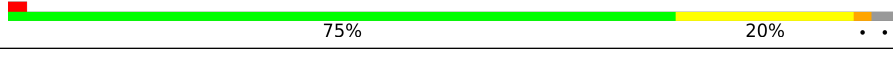
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	427	2% 73% 22% ..
1	B	427	5% 72% 21% ..
1	C	427	2% 74% 20% ..
1	D	427	0% 74% 20% ..
1	E	427	4% 68% 26% ..

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Mol	Chain	Length	Quality of chain
1	F	427	
1	G	427	
1	H	427	
1	I	427	
1	J	427	
1	K	427	
1	L	427	

2 Entry composition

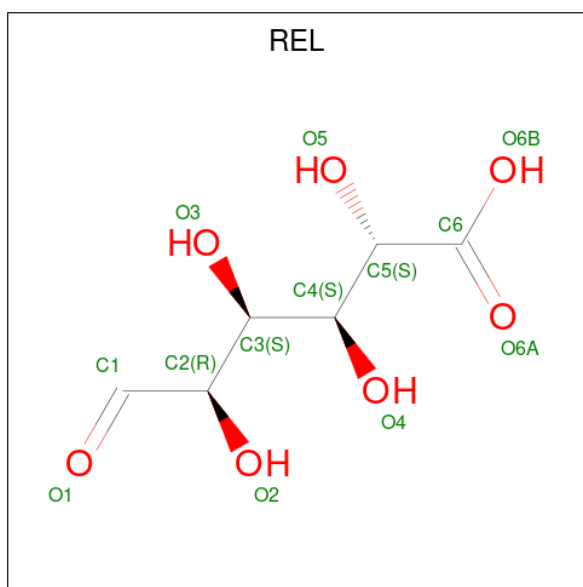
There are 6 unique types of molecules in this entry. The entry contains 42892 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uronate isomerase.

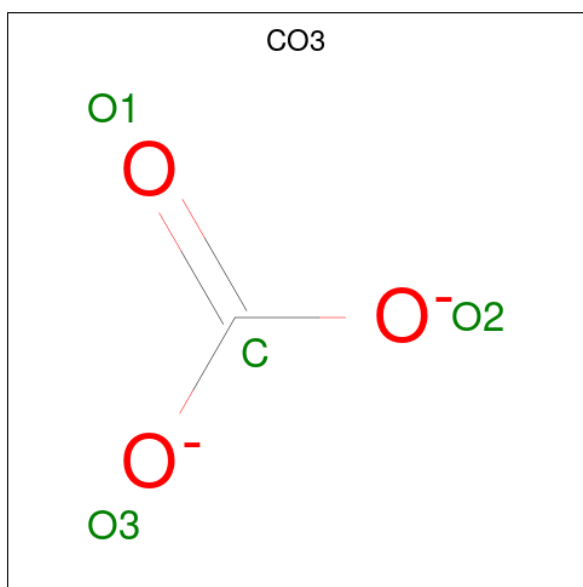
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3404	2170	588	626	20			
1	B	413	Total	C	N	O	S	0	0	0
			3404	2170	588	626	20			
1	C	413	Total	C	N	O	S	0	0	0
			3404	2170	588	626	20			
1	D	413	Total	C	N	O	S	0	0	0
			3404	2170	588	626	20			
1	E	413	Total	C	N	O	S	0	0	0
			3404	2170	588	626	20			
1	F	413	Total	C	N	O	S	0	0	0
			3404	2170	588	626	20			
1	G	413	Total	C	N	O	S	0	0	0
			3404	2170	588	626	20			
1	H	413	Total	C	N	O	S	0	0	0
			3404	2170	588	626	20			
1	I	413	Total	C	N	O	S	0	0	0
			3404	2170	588	626	20			
1	J	413	Total	C	N	O	S	0	0	0
			3404	2170	588	626	20			
1	K	413	Total	C	N	O	S	0	0	0
			3404	2170	588	626	20			
1	L	413	Total	C	N	O	S	0	0	0
			3404	2170	588	626	20			

- Molecule 2 is D-glucuronic acid (CCD ID: REL) (formula: C₆H₁₀O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		
2	G	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		
2	I	1	Total	C	O	0	0
			13	6	7		
2	J	1	Total	C	O	0	0
			13	6	7		
2	K	1	Total	C	O	0	0
			13	6	7		
2	L	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0
5	H	1	Total Cl 1 1	0	0
5	K	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	155	Total O 155 155	0	0
6	B	123	Total O 123 123	0	0

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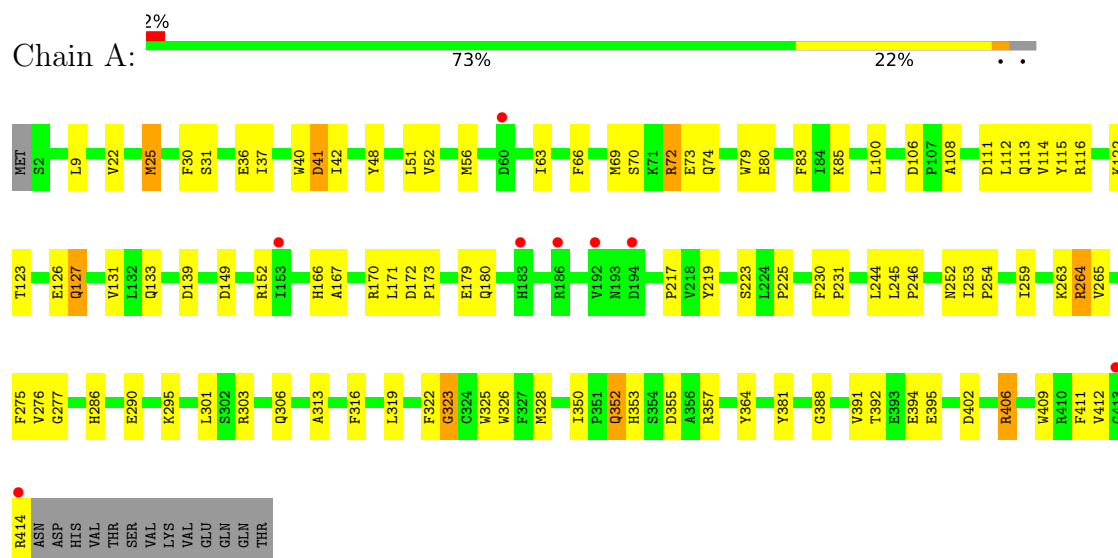
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	169	Total 169	O 169	0	0
6	D	189	Total 189	O 189	0	0
6	E	128	Total 128	O 128	0	0
6	F	163	Total 163	O 163	0	0
6	G	136	Total 136	O 136	0	0
6	H	143	Total 143	O 143	0	0
6	I	141	Total 141	O 141	0	0
6	J	160	Total 160	O 160	0	0
6	K	135	Total 135	O 135	0	0
6	L	182	Total 182	O 182	0	0

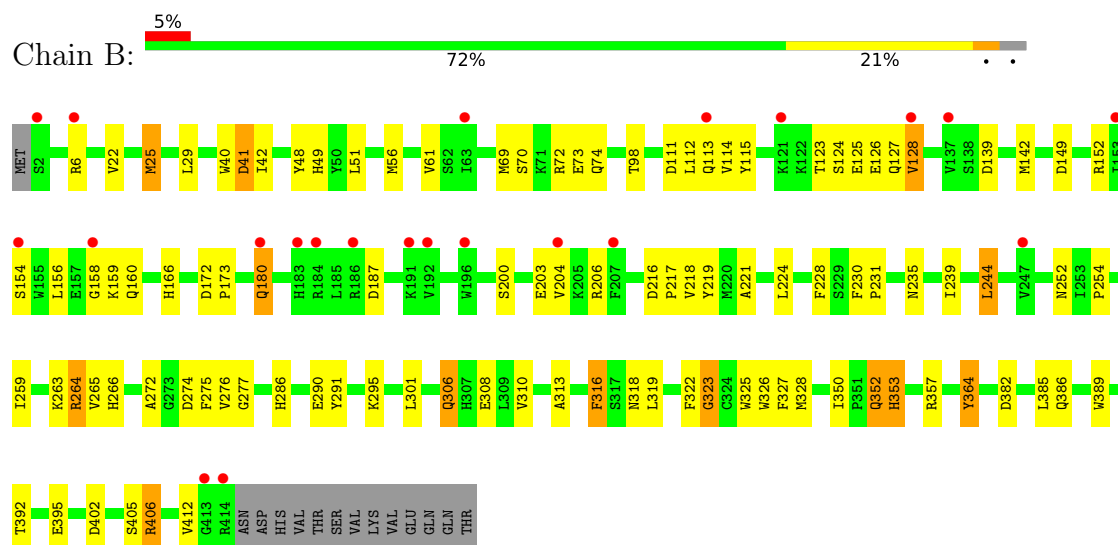
3 Residue-property plots [i](#)

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.

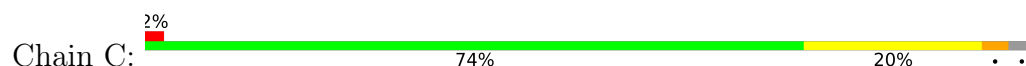
• Molecule 1: Uronate isomerase

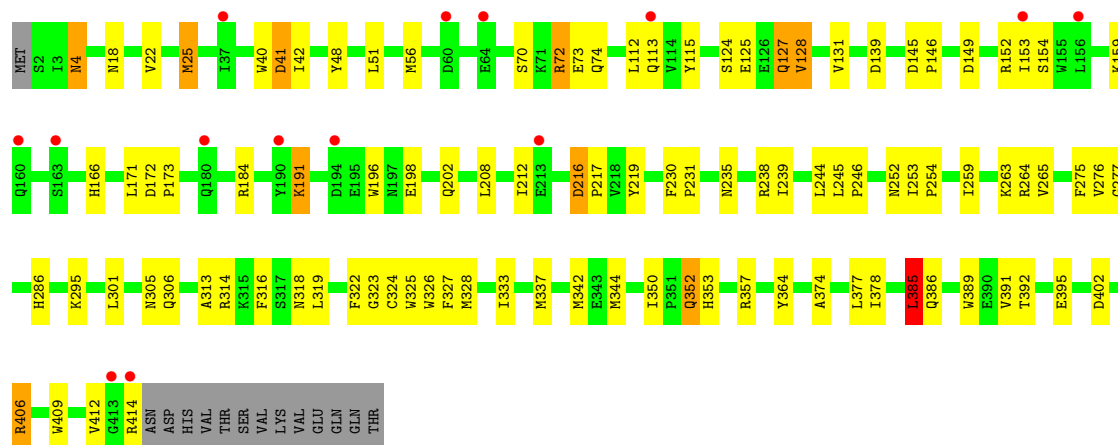


• Molecule 1: Uronate isomerase

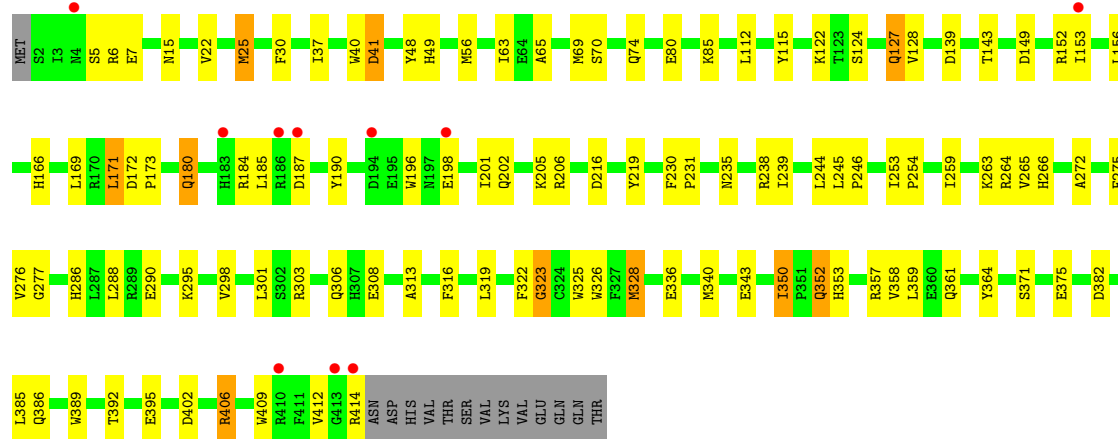
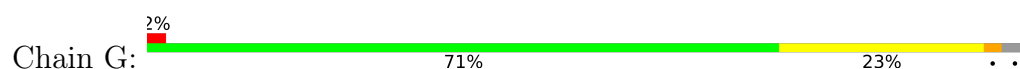


• Molecule 1: Uronate isomerase

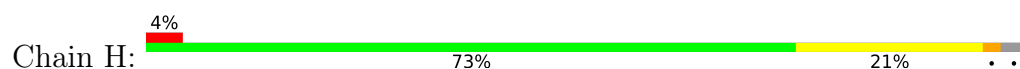




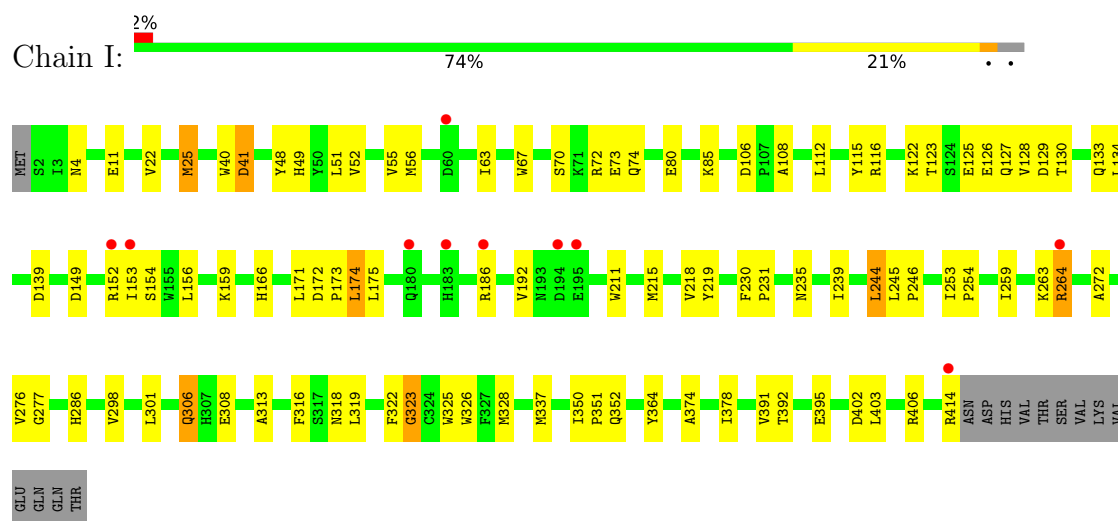
• Molecule 1: Uronate isomerase



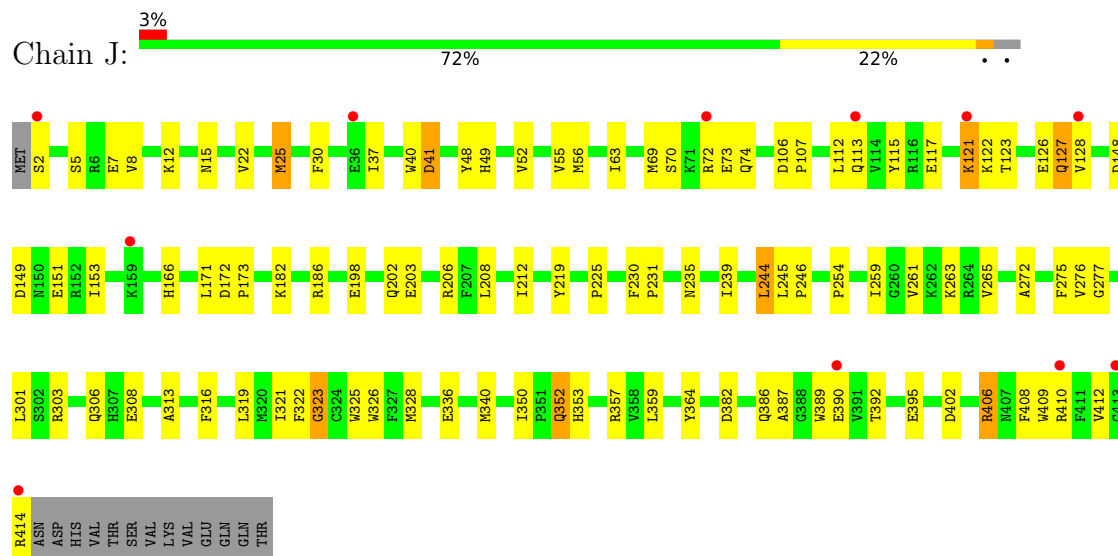
• Molecule 1: Uronate isomerase



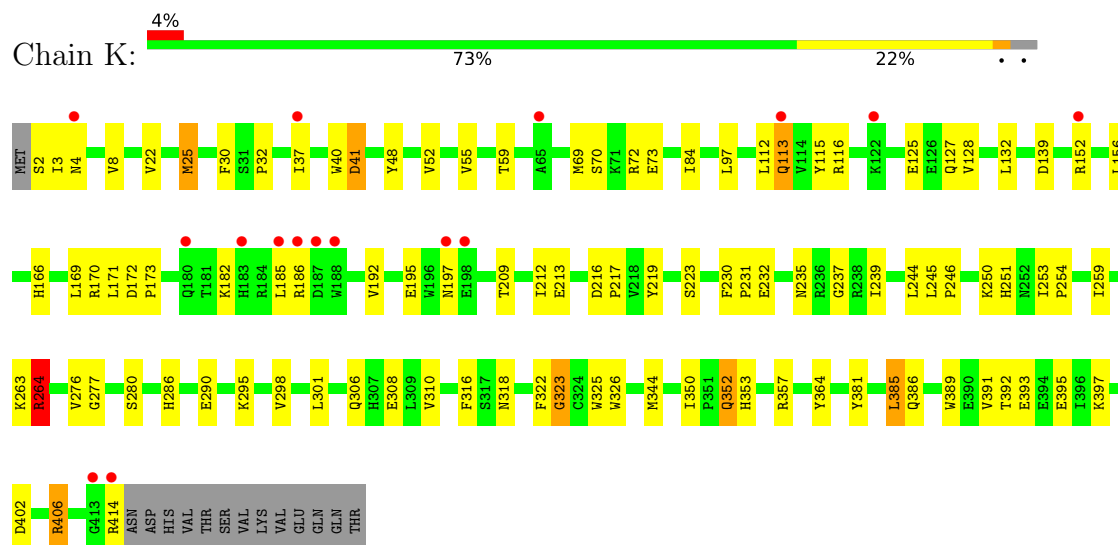
• Molecule 1: Uronate isomerase



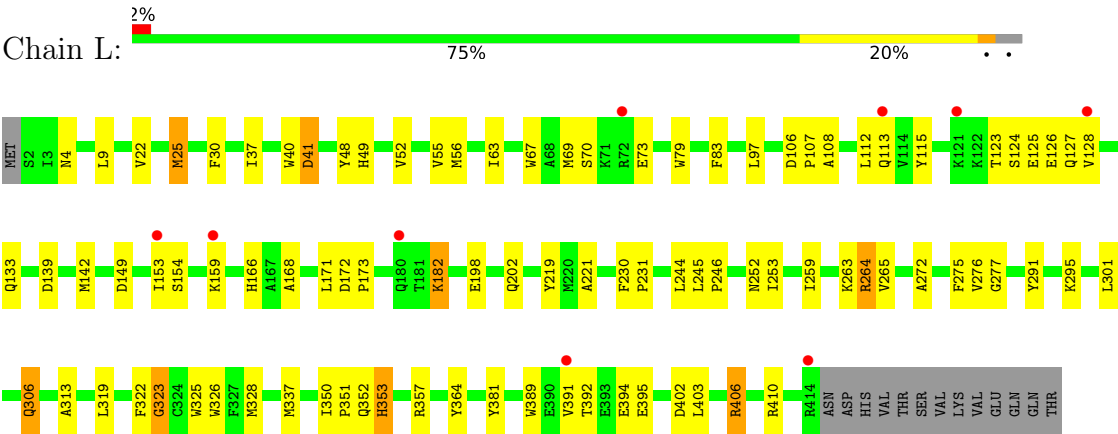
• Molecule 1: Uronate isomerase



• Molecule 1: Uronate isomerase



● Molecule 1: Uronate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	274.09Å 156.88Å 185.21Å 90.00° 115.78° 90.00°	Depositor
Resolution (Å)	24.95 – 2.10 24.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (24.95-2.10) 98.7 (24.95-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.258 0.227 , 0.258	Depositor DCC
R_{free} test set	20501 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	42892	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2942e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: REL, ZN, CL, CO3

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	0.38	0/3488	0.94	17/4726 (0.4%)
1	B	0.38	0/3488	0.95	18/4726 (0.4%)
1	C	0.39	0/3488	0.93	14/4726 (0.3%)
1	D	0.40	0/3488	0.95	16/4726 (0.3%)
1	E	0.38	0/3488	0.94	15/4726 (0.3%)
1	F	0.38	0/3488	0.93	18/4726 (0.4%)
1	G	0.39	0/3488	0.94	21/4726 (0.4%)
1	H	0.39	0/3488	0.93	17/4726 (0.4%)
1	I	0.38	0/3488	0.93	12/4726 (0.3%)
1	J	0.39	0/3488	0.92	12/4726 (0.3%)
1	K	0.39	0/3488	0.92	16/4726 (0.3%)
1	L	0.39	0/3488	0.94	17/4726 (0.4%)
All	All	0.39	0/41856	0.94	193/56712 (0.3%)

There are no bond length outliers.

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ILE	N-CA-C	8.42	121.26	108.71
1	B	325	TRP	N-CA-C	8.27	122.37	109.96
1	K	306	GLN	N-CA-C	8.05	120.06	111.28
1	B	306	GLN	N-CA-C	8.01	119.64	111.07
1	D	259	ILE	N-CA-C	7.99	120.61	108.71
1	E	25	MET	N-CA-C	7.79	122.42	113.15
1	H	325	TRP	N-CA-C	7.74	121.57	109.96
1	C	325	TRP	N-CA-C	7.72	121.54	109.96
1	L	325	TRP	N-CA-C	7.68	121.48	109.96
1	F	306	GLN	N-CA-C	7.66	119.27	111.07
1	I	259	ILE	N-CA-C	7.64	120.09	108.71
1	D	325	TRP	N-CA-C	7.62	121.88	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	325	TRP	N-CA-C	7.61	121.37	109.96
1	L	25	MET	N-CA-C	7.57	122.16	113.15
1	J	325	TRP	N-CA-C	7.51	120.74	109.25
1	H	306	GLN	N-CA-C	7.50	120.11	111.11
1	L	259	ILE	N-CA-C	7.39	119.72	108.71
1	L	306	GLN	N-CA-C	7.29	118.87	111.07
1	C	259	ILE	N-CA-C	7.21	119.45	108.71
1	D	25	MET	N-CA-C	7.19	121.90	113.20
1	G	325	TRP	N-CA-C	7.19	121.19	109.76
1	K	325	TRP	N-CA-C	7.12	120.65	109.96
1	G	259	ILE	N-CA-C	7.12	119.32	108.71
1	E	325	TRP	N-CA-C	7.08	120.58	109.96
1	B	259	ILE	N-CA-C	7.08	119.25	108.71
1	A	325	TRP	N-CA-C	7.07	121.00	109.76
1	F	25	MET	N-CA-C	7.01	121.49	113.15
1	C	306	GLN	N-CA-C	6.92	118.82	111.28
1	E	259	ILE	N-CA-C	6.84	118.91	108.71
1	K	25	MET	N-CA-C	6.84	121.33	113.19
1	J	263	LYS	N-CA-C	6.71	119.96	110.50
1	I	325	TRP	N-CA-C	6.71	120.42	109.76
1	F	385	LEU	N-CA-C	-6.67	104.09	111.36
1	D	306	GLN	N-CA-C	6.63	119.07	111.11
1	D	264	ARG	N-CA-C	6.57	120.45	111.39
1	J	171	LEU	N-CA-C	6.54	120.92	112.41
1	J	259	ILE	N-CA-C	6.49	118.39	108.71
1	G	263	LYS	N-CA-C	6.46	119.60	110.23
1	H	352	GLN	N-CA-C	6.45	118.88	109.07
1	C	263	LYS	N-CA-C	6.44	119.81	110.28
1	K	406	ARG	N-CA-C	6.38	118.23	111.28
1	E	406	ARG	N-CA-C	6.38	118.23	111.28
1	I	25	MET	N-CA-C	6.36	122.15	113.37
1	K	352	GLN	N-CA-C	6.36	118.73	109.07
1	K	59	THR	N-CA-C	6.34	118.98	110.35
1	A	306	GLN	N-CA-C	6.32	118.69	111.11
1	J	406	ARG	N-CA-C	6.31	118.16	111.28
1	E	264	ARG	N-CA-C	6.27	120.01	111.17
1	B	25	MET	N-CA-C	6.26	122.01	113.37
1	H	259	ILE	N-CA-C	6.22	118.62	108.97
1	I	306	GLN	N-CA-C	6.22	118.58	111.11
1	F	264	ARG	N-CA-C	6.18	119.77	111.24
1	B	406	ARG	N-CA-C	6.18	118.01	111.28
1	A	357	ARG	N-CA-C	-6.15	106.10	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	306	GLN	N-CA-C	6.10	117.60	111.07
1	D	22	VAL	N-CA-C	6.10	118.14	108.87
1	A	406	ARG	N-CA-C	6.09	117.92	111.28
1	K	385	LEU	N-CA-C	-6.09	104.64	111.28
1	G	352	GLN	N-CA-C	6.03	118.02	108.79
1	H	406	ARG	N-CA-C	6.02	117.84	111.28
1	H	22	VAL	N-CA-C	6.00	117.65	108.71
1	A	352	GLN	N-CA-C	5.99	117.96	108.79
1	F	259	ILE	N-CA-C	5.99	118.26	108.97
1	L	22	VAL	N-CA-C	5.98	117.62	108.71
1	H	357	ARG	N-CA-C	-5.97	106.33	113.97
1	L	406	ARG	N-CA-C	5.97	118.57	111.71
1	E	357	ARG	N-CA-C	-5.95	106.35	113.97
1	K	259	ILE	N-CA-C	5.95	118.19	108.97
1	H	385	LEU	N-CA-C	-5.93	104.90	111.36
1	G	22	VAL	N-CA-C	5.92	117.53	108.71
1	D	352	GLN	N-CA-C	5.91	117.83	108.79
1	C	25	MET	N-CA-C	5.91	121.52	113.37
1	B	352	GLN	N-CA-C	5.90	117.81	108.79
1	A	131	VAL	N-CA-C	5.89	116.08	110.42
1	E	306	GLN	N-CA-C	5.86	118.15	111.11
1	D	48	TYR	N-CA-C	-5.86	101.98	110.24
1	G	406	ARG	N-CA-C	5.84	117.65	111.28
1	B	264	ARG	N-CA-C	5.83	119.39	111.17
1	K	264	ARG	N-CA-C	5.83	119.43	111.39
1	I	263	LYS	N-CA-C	5.79	118.63	110.23
1	H	261	VAL	N-CA-C	5.79	116.53	108.89
1	A	48	TYR	N-CA-C	-5.78	101.85	110.23
1	G	25	MET	N-CA-C	5.77	120.18	113.20
1	G	264	ARG	N-CA-C	5.77	119.35	111.39
1	C	171	LEU	N-CA-C	5.76	119.90	112.41
1	G	48	TYR	N-CA-C	-5.76	102.12	110.24
1	K	263	LYS	N-CA-C	5.76	118.58	110.23
1	C	406	ARG	N-CA-C	5.75	118.29	111.33
1	F	48	TYR	N-CA-C	-5.74	102.14	110.24
1	D	266	HIS	CA-C-N	5.72	125.84	119.32
1	D	266	HIS	C-N-CA	5.72	125.84	119.32
1	F	4	ASN	N-CA-C	5.70	119.96	112.89
1	G	306	GLN	N-CA-C	5.70	117.17	111.07
1	H	25	MET	N-CA-C	5.70	121.23	113.37
1	L	351	PRO	N-CA-C	5.69	121.43	113.53
1	E	22	VAL	N-CA-C	5.67	117.16	108.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	PHE	N-CA-C	5.65	117.61	108.41
1	E	48	TYR	N-CA-C	-5.65	102.28	110.24
1	I	48	TYR	N-CA-C	-5.63	102.06	110.23
1	J	352	GLN	N-CA-C	5.62	117.39	108.79
1	L	171	LEU	N-CA-C	5.60	119.76	111.87
1	A	22	VAL	N-CA-C	5.59	117.04	108.71
1	H	266	HIS	CA-C-N	5.59	125.69	119.32
1	H	266	HIS	C-N-CA	5.59	125.69	119.32
1	E	353	HIS	N-CA-C	-5.58	100.22	108.99
1	K	22	VAL	N-CA-C	5.57	117.01	108.71
1	I	22	VAL	N-CA-C	5.57	117.00	108.71
1	K	84	ILE	N-CA-C	5.56	116.62	111.45
1	I	351	PRO	N-CA-C	5.54	121.23	113.53
1	A	52	VAL	N-CA-C	-5.54	105.33	110.53
1	L	48	TYR	N-CA-C	-5.53	102.21	110.23
1	C	352	GLN	N-CA-C	5.52	117.46	109.07
1	A	25	MET	N-CA-C	5.50	120.95	113.37
1	D	223	SER	N-CA-C	-5.49	100.76	109.76
1	L	264	ARG	N-CA-C	5.49	118.81	111.24
1	B	357	ARG	N-CA-C	-5.46	106.98	113.97
1	J	25	MET	N-CA-C	5.45	119.63	113.15
1	D	263	LYS	N-CA-C	5.44	118.21	110.10
1	B	266	HIS	CA-C-N	5.44	126.64	119.84
1	B	266	HIS	C-N-CA	5.44	126.64	119.84
1	H	264	ARG	N-CA-C	5.43	118.83	111.17
1	B	48	TYR	N-CA-C	-5.42	102.60	110.24
1	H	48	TYR	N-CA-C	-5.41	102.39	110.23
1	F	131	VAL	N-CA-C	5.40	115.60	110.42
1	J	316	PHE	N-CA-C	5.40	117.21	108.41
1	B	353	HIS	N-CA-C	-5.39	101.09	109.24
1	F	171	LEU	N-CA-C	5.38	119.46	111.87
1	E	298	VAL	N-CA-C	5.38	116.48	108.46
1	D	42	ILE	N-CA-C	5.38	116.10	110.62
1	E	280	SER	N-CA-C	-5.37	102.53	110.48
1	B	22	VAL	N-CA-C	5.36	117.01	108.87
1	F	352	GLN	N-CA-C	5.36	117.21	109.07
1	F	22	VAL	N-CA-C	5.34	116.67	108.71
1	F	406	ARG	N-CA-C	5.34	117.10	111.28
1	B	221	ALA	N-CA-C	5.34	117.79	109.52
1	D	355	ASP	N-CA-C	-5.32	106.73	113.23
1	E	263	LYS	N-CA-C	5.32	117.95	110.23
1	G	328	MET	N-CA-C	-5.32	106.79	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	216	ASP	CA-C-N	5.32	125.22	119.85
1	G	216	ASP	C-N-CA	5.32	125.22	119.85
1	L	403	LEU	N-CA-C	5.32	116.76	111.07
1	J	48	TYR	N-CA-C	-5.32	102.75	110.24
1	A	355	ASP	N-CA-C	-5.30	106.11	112.58
1	K	48	TYR	N-CA-C	-5.30	102.77	110.24
1	I	264	ARG	N-CA-C	5.30	118.64	111.17
1	A	171	LEU	N-CA-C	5.28	119.27	112.41
1	E	171	LEU	N-CA-C	5.27	119.30	111.87
1	G	171	LEU	N-CA-C	5.27	119.26	112.41
1	J	22	VAL	N-CA-C	5.26	116.56	108.71
1	L	357	ARG	N-CA-C	-5.26	107.03	113.50
1	B	42	ILE	N-CA-C	5.25	115.98	110.62
1	F	216	ASP	CA-C-N	5.25	125.15	119.85
1	F	216	ASP	C-N-CA	5.25	125.15	119.85
1	L	263	LYS	N-CA-C	5.23	118.02	110.28
1	L	291	TYR	CA-C-N	5.23	124.89	119.56
1	L	291	TYR	C-N-CA	5.23	124.89	119.56
1	L	353	HIS	N-CA-C	-5.23	101.12	109.07
1	I	171	LEU	N-CA-C	5.23	119.21	112.41
1	H	263	LYS	N-CA-C	5.21	117.79	110.23
1	K	280	SER	N-CA-C	-5.20	102.78	110.48
1	F	263	LYS	N-CA-C	5.19	117.97	110.28
1	D	406	ARG	N-CA-C	5.18	116.93	111.28
1	G	143	THR	N-CA-C	-5.18	98.95	108.02
1	F	357	ARG	N-CA-C	-5.16	107.36	113.97
1	A	225	PRO	CA-C-N	5.16	124.96	119.28
1	A	225	PRO	C-N-CA	5.16	124.96	119.28
1	G	298	VAL	N-CA-C	5.15	116.13	108.46
1	G	357	ARG	N-CA-C	-5.14	107.39	113.97
1	C	264	ARG	N-CA-C	5.14	118.48	111.39
1	I	298	VAL	N-CA-C	5.14	116.12	108.46
1	G	316	PHE	N-CA-C	5.12	116.76	108.41
1	H	316	PHE	N-CA-C	5.12	116.74	108.34
1	E	352	GLN	N-CA-C	5.12	116.63	108.79
1	D	316	PHE	N-CA-C	5.10	116.71	108.34
1	K	357	ARG	N-CA-C	-5.10	107.45	113.97
1	G	266	HIS	CA-C-N	5.09	126.21	119.84
1	G	266	HIS	C-N-CA	5.09	126.21	119.84
1	C	4	ASN	N-CA-C	5.09	119.20	112.89
1	A	31	SER	N-CA-C	-5.08	103.75	109.60
1	J	357	ARG	N-CA-C	-5.08	107.47	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	385	LEU	N-CA-C	-5.07	105.75	111.28
1	A	316	PHE	N-CA-C	5.06	116.64	108.34
1	I	403	LEU	N-CA-C	5.06	116.80	111.28
1	K	298	VAL	N-CA-C	5.05	115.99	108.46
1	L	221	ALA	N-CA-C	5.05	116.87	109.24
1	G	350	ILE	N-CA-C	-5.05	103.15	108.15
1	B	291	TYR	CA-C-N	5.04	124.65	119.56
1	B	291	TYR	C-N-CA	5.04	124.65	119.56
1	C	216	ASP	CA-C-N	5.03	124.96	119.78
1	C	216	ASP	C-N-CA	5.03	124.96	119.78
1	C	357	ARG	N-CA-C	-5.03	107.53	113.97
1	F	42	ILE	N-CA-C	5.01	115.73	110.62
1	H	171	LEU	N-CA-C	5.01	118.92	112.41

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	3404	0	3328	67	0
1	B	3404	0	3328	68	0
1	C	3404	0	3328	62	0
1	D	3404	0	3328	62	0
1	E	3404	0	3328	81	0
1	F	3404	0	3328	71	0
1	G	3404	0	3328	69	0
1	H	3404	0	3328	72	0
1	I	3404	0	3328	61	0
1	J	3404	0	3328	69	0
1	K	3404	0	3328	59	0
1	L	3404	0	3328	59	0
2	A	13	0	8	1	0
2	B	13	0	8	0	0
2	C	13	0	8	1	0
2	D	13	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	13	0	8	0	0
2	F	13	0	8	1	0
2	G	13	0	8	1	0
2	H	13	0	8	1	0
2	I	13	0	8	0	0
2	J	13	0	8	0	0
2	K	13	0	8	1	0
2	L	13	0	8	1	0
3	A	8	0	0	0	0
3	C	4	0	0	0	0
3	D	8	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
6	A	155	0	0	4	0
6	B	123	0	0	1	0
6	C	169	0	0	5	0
6	D	189	0	0	4	0
6	E	128	0	0	5	0
6	F	163	0	0	2	0
6	G	136	0	0	7	0
6	H	143	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	141	0	0	4	0
6	J	160	0	0	5	0
6	K	135	0	0	3	0
6	L	182	0	0	7	0
All	All	42892	0	40032	800	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (800) 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:F:333:ILE:HG22	1:F:337:MET:HE2	1.22	1.18
1:F:72:ARG:HH11	1:F:72:ARG:HB2	1.20	1.05
1:A:69:MET:HE2	1:A:73:GLU:HB3	1.45	0.98
1:G:127:GLN:HE21	1:G:127:GLN:HA	1.34	0.92
1:H:4:ASN:HB3	6:H:1604:HOH:O	1.72	0.90
1:J:127:GLN:HA	1:J:127:GLN:HE21	1.35	0.90
1:C:385:LEU:HD11	1:C:391:VAL:HG12	1.54	0.89
1:A:127:GLN:HE21	1:A:127:GLN:HA	1.37	0.88
1:B:72:ARG:HB2	1:B:72:ARG:HH11	1.40	0.86
1:D:127:GLN:HE21	1:D:127:GLN:HA	1.41	0.86
1:F:127:GLN:HE21	1:F:127:GLN:HA	1.40	0.86
1:H:220:MET:HE2	1:H:253:ILE:HD11	1.55	0.86
1:K:32:PRO:HG3	1:K:128:VAL:HG11	1.58	0.86
1:I:127:GLN:HE21	1:I:127:GLN:HA	1.42	0.85
1:L:127:GLN:HE21	1:L:127:GLN:HA	1.42	0.84
1:C:127:GLN:HA	1:C:127:GLN:HE21	1.42	0.84
1:E:72:ARG:HH11	1:E:72:ARG:HB2	1.41	0.84
1:F:72:ARG:HB2	1:F:72:ARG:NH1	1.93	0.83
1:C:36:GLU:HG2	6:C:1956:HOH:O	1.79	0.82
1:B:111:ASP:O	1:B:114:VAL:HG12	1.79	0.81
1:H:127:GLN:HE21	1:H:127:GLN:HA	1.44	0.81
1:D:72:ARG:HH11	1:D:72:ARG:HB2	1.47	0.79
1:H:40:TRP:O	1:H:41:ASP:HB3	1.81	0.78
1:D:113:GLN:HA	1:D:113:GLN:HE21	1.49	0.78
1:B:72:ARG:HB2	1:B:72:ARG:NH1	1.99	0.78
1:B:392:THR:OG1	1:B:395:GLU:HG3	1.85	0.77
1:E:72:ARG:HB2	1:E:72:ARG:NH1	1.98	0.77
1:J:2:SER:OG	1:J:390:GLU:HG3	1.85	0.77
1:K:127:GLN:HA	1:K:127:GLN:HE21	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:SER:O	1:F:128:VAL:HG12	1.86	0.76
1:E:195:GLU:HG2	6:E:453:HOH:O	1.85	0.75
1:J:72:ARG:HB2	1:J:72:ARG:HH11	1.52	0.74
1:B:127:GLN:HA	1:B:127:GLN:HE21	1.53	0.74
1:J:410:ARG:HD3	6:J:436:HOH:O	1.86	0.74
1:J:72:ARG:HB2	1:J:72:ARG:NH1	2.02	0.74
1:F:324:CYS:HB3	1:F:337:MET:HE1	1.70	0.73
1:L:410:ARG:HD3	6:L:866:HOH:O	1.87	0.73
1:C:402:ASP:HA	1:C:406:ARG:HB2	1.71	0.73
1:J:56:MET:HE2	1:J:63:ILE:HB	1.71	0.72
1:A:394:GLU:HG2	6:A:553:HOH:O	1.90	0.72
1:E:127:GLN:HA	1:E:127:GLN:HE21	1.55	0.71
1:F:252:ASN:HD21	1:F:295:LYS:HE3	1.54	0.71
1:H:32:PRO:HG3	1:H:128:VAL:HG11	1.73	0.71
1:D:72:ARG:HB2	1:D:72:ARG:NH1	2.06	0.70
1:K:381:TYR:O	1:K:385:LEU:HD23	1.91	0.70
6:G:1153:HOH:O	1:H:321:ILE:HG12	1.91	0.69
1:B:323:GLY:HA2	1:B:352:GLN:HA	1.73	0.69
1:K:264:ARG:HH11	1:K:264:ARG:HB2	1.58	0.69
1:A:127:GLN:HA	1:A:127:GLN:NE2	2.08	0.69
1:C:392:THR:OG1	1:C:395:GLU:HG3	1.93	0.69
1:C:152:ARG:HH22	1:C:184:ARG:HH22	1.42	0.68
1:F:113:GLN:HE21	1:F:113:GLN:HA	1.58	0.68
1:L:113:GLN:HE21	1:L:113:GLN:HA	1.58	0.68
1:E:25:MET:HG3	6:E:450:HOH:O	1.92	0.68
1:E:182:LYS:HB2	1:E:192:VAL:HG21	1.75	0.68
1:B:124:SER:O	1:B:128:VAL:HG12	1.93	0.68
1:F:402:ASP:HA	1:F:406:ARG:HB2	1.76	0.68
1:I:72:ARG:NH2	1:I:116:ARG:HD3	2.09	0.68
1:B:180:GLN:H	1:B:180:GLN:NE2	1.92	0.68
1:I:56:MET:HE2	1:I:63:ILE:HB	1.75	0.68
1:B:402:ASP:HA	1:B:406:ARG:HB2	1.75	0.67
1:F:333:ILE:CG2	1:F:337:MET:HE2	2.14	0.67
1:K:301:LEU:HD11	1:K:326:TRP:HB3	1.76	0.67
1:H:149:ASP:O	1:H:153:ILE:HG12	1.93	0.66
1:G:392:THR:OG1	1:G:395:GLU:HG3	1.95	0.66
1:K:70:SER:OG	1:K:73:GLU:HG3	1.95	0.66
1:E:323:GLY:HA2	1:E:352:GLN:HA	1.76	0.66
1:H:385:LEU:HD11	1:H:391:VAL:HG22	1.76	0.66
1:L:127:GLN:HA	1:L:127:GLN:NE2	2.11	0.66
1:C:323:GLY:HA2	1:C:352:GLN:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:PRO:HG3	1:D:295:LYS:HE3	1.77	0.66
1:F:392:THR:OG1	1:F:395:GLU:HG3	1.95	0.65
1:B:25:MET:HG3	6:B:434:HOH:O	1.95	0.65
1:A:80:GLU:HG3	1:A:85:LYS:NZ	2.11	0.65
1:A:263:LYS:HB3	1:A:264:ARG:HD2	1.78	0.65
1:J:392:THR:OG1	1:J:395:GLU:HG3	1.96	0.65
1:D:127:GLN:HA	1:D:127:GLN:NE2	2.12	0.65
1:G:80:GLU:O	1:G:85:LYS:HG2	1.97	0.65
1:E:70:SER:O	1:E:74:GLN:HG3	1.97	0.65
1:K:72:ARG:NH2	1:K:116:ARG:HD3	2.12	0.65
1:I:127:GLN:HA	1:I:127:GLN:NE2	2.12	0.64
1:F:323:GLY:HA2	1:F:352:GLN:HA	1.79	0.64
1:D:113:GLN:HA	1:D:113:GLN:NE2	2.12	0.64
1:D:339:ARG:O	1:D:343:GLU:HG3	1.98	0.64
1:K:323:GLY:HA2	1:K:352:GLN:HA	1.80	0.64
1:F:70:SER:O	1:F:74:GLN:HG3	1.96	0.64
6:D:1696:HOH:O	1:F:56:MET:HE3	1.98	0.63
1:E:180:GLN:H	1:E:180:GLN:NE2	1.96	0.63
1:G:198:GLU:O	1:G:202:GLN:HG2	1.99	0.63
1:A:323:GLY:HA2	1:A:352:GLN:HA	1.80	0.62
1:B:6:ARG:HH11	1:B:6:ARG:HG2	1.65	0.62
1:C:70:SER:OG	1:C:73:GLU:HG3	2.00	0.62
1:A:56:MET:HE2	1:A:63:ILE:HB	1.79	0.62
1:D:323:GLY:HA2	1:D:352:GLN:HA	1.81	0.62
1:H:323:GLY:HA2	1:H:352:GLN:HA	1.82	0.62
1:E:56:MET:HE2	1:E:63:ILE:HB	1.82	0.62
1:C:385:LEU:CD1	1:C:391:VAL:HG12	2.30	0.61
1:A:80:GLU:HG3	1:A:85:LYS:HZ1	1.64	0.61
1:H:198:GLU:O	1:H:202:GLN:HG2	2.01	0.61
1:C:149:ASP:O	1:C:153:ILE:HG13	1.99	0.61
1:G:323:GLY:HA2	1:G:352:GLN:HA	1.81	0.61
1:A:72:ARG:HH11	1:A:72:ARG:HA	1.65	0.61
1:K:170:ARG:NH2	1:K:223:SER:HB3	2.15	0.61
1:F:127:GLN:HA	1:F:127:GLN:NE2	2.14	0.61
1:J:323:GLY:HA2	1:J:352:GLN:HA	1.81	0.60
1:D:402:ASP:HA	1:D:406:ARG:HB2	1.82	0.60
1:C:412:VAL:HG23	1:C:414:ARG:HB2	1.84	0.60
1:K:125:GLU:O	1:K:128:VAL:HG22	2.01	0.60
1:J:70:SER:O	1:J:74:GLN:HG3	2.02	0.60
1:F:70:SER:OG	1:F:73:GLU:HG3	2.02	0.60
1:H:392:THR:OG1	1:H:395:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:SER:O	1:L:128:VAL:HG22	2.02	0.60
1:A:72:ARG:NH1	1:A:72:ARG:HB2	2.17	0.59
1:E:123:THR:OG1	1:E:126:GLU:HG3	2.02	0.59
1:I:123:THR:OG1	1:I:126:GLU:HG3	2.01	0.59
1:B:219:TYR:HB3	1:B:254:PRO:HG2	1.84	0.59
1:J:382:ASP:O	1:J:386:GLN:HG2	2.02	0.59
1:L:113:GLN:HA	1:L:113:GLN:NE2	2.17	0.59
1:B:230:PHE:HA	1:B:231:PRO:C	2.26	0.59
1:H:139:ASP:OD1	1:H:166:HIS:HE1	1.86	0.59
1:J:219:TYR:HB3	1:J:254:PRO:HG2	1.83	0.59
1:C:127:GLN:HA	1:C:127:GLN:NE2	2.16	0.59
1:E:402:ASP:HA	1:E:406:ARG:HB2	1.83	0.59
1:K:127:GLN:HA	1:K:127:GLN:NE2	2.17	0.59
1:G:385:LEU:HD23	1:G:385:LEU:O	2.02	0.59
1:H:48:TYR:HB3	1:H:51:LEU:HD13	1.85	0.59
1:G:402:ASP:HA	1:G:406:ARG:HB2	1.84	0.59
1:A:252:ASN:ND2	1:A:295:LYS:HE2	2.17	0.59
1:D:56:MET:HE2	1:D:63:ILE:HB	1.83	0.59
1:F:333:ILE:HG22	1:F:337:MET:CE	2.14	0.59
1:G:219:TYR:HA	1:G:253:ILE:CG2	2.32	0.59
1:C:25:MET:HG3	6:C:432:HOH:O	2.02	0.58
1:G:371:SER:O	1:G:375:GLU:HG3	2.03	0.58
1:A:402:ASP:HA	1:A:406:ARG:HB2	1.84	0.58
6:H:432:HOH:O	1:I:308:GLU:HG2	2.03	0.58
1:G:382:ASP:O	1:G:386:GLN:HG2	2.03	0.58
1:H:385:LEU:HD12	1:H:389:TRP:O	2.03	0.58
1:C:70:SER:O	1:C:74:GLN:HG3	2.04	0.58
1:K:3:ILE:HG23	1:K:8:VAL:HG23	1.86	0.58
1:E:172:ASP:HB2	1:E:173:PRO:HD3	1.86	0.58
1:I:186:ARG:NH1	1:I:192:VAL:O	2.36	0.58
1:C:264:ARG:HG2	6:C:805:HOH:O	2.04	0.58
1:I:323:GLY:HA2	1:I:352:GLN:HA	1.86	0.58
1:D:25:MET:HG3	6:D:440:HOH:O	2.04	0.57
1:D:40:TRP:O	1:D:41:ASP:CG	2.47	0.57
1:L:25:MET:HG3	6:L:453:HOH:O	2.03	0.57
1:L:323:GLY:HA2	1:L:352:GLN:HA	1.85	0.57
1:E:112:LEU:HA	1:E:115:TYR:CD2	2.39	0.57
1:E:149:ASP:O	1:E:153:ILE:HG12	2.03	0.57
1:I:25:MET:HG3	6:I:453:HOH:O	2.04	0.57
1:J:166:HIS:HD2	6:J:1185:HOH:O	1.87	0.57
1:H:402:ASP:HA	1:H:406:ARG:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASP:HB3	1:B:114:VAL:HG12	1.87	0.57
1:F:198:GLU:O	1:F:202:GLN:HG2	2.05	0.57
1:A:152:ARG:HG2	1:A:152:ARG:HH11	1.69	0.57
1:B:123:THR:OG1	1:B:126:GLU:HG3	2.05	0.57
1:D:48:TYR:HB3	1:D:51:LEU:HD13	1.87	0.57
1:I:328:MET:HE2	1:I:328:MET:HA	1.87	0.57
1:K:25:MET:HG3	6:K:609:HOH:O	2.04	0.57
1:G:56:MET:HE3	6:H:599:HOH:O	2.04	0.56
1:A:40:TRP:O	1:A:41:ASP:CG	2.48	0.56
1:B:382:ASP:O	1:B:386:GLN:HG2	2.06	0.56
1:H:146:PRO:O	1:H:152:ARG:HD3	2.05	0.56
1:L:123:THR:OG1	1:L:126:GLU:HG3	2.05	0.56
1:B:112:LEU:HA	1:B:115:TYR:CD2	2.41	0.56
1:L:276:VAL:HG22	1:L:277:GLY:N	2.20	0.56
1:B:152:ARG:NH1	1:B:152:ARG:HB3	2.20	0.56
1:E:252:ASN:ND2	1:E:295:LYS:HE2	2.21	0.56
1:B:6:ARG:HG3	1:B:382:ASP:OD1	2.06	0.56
1:H:70:SER:OG	1:H:73:GLU:HG3	2.06	0.56
1:G:56:MET:HE2	1:G:63:ILE:HB	1.88	0.56
1:I:127:GLN:HE21	1:I:127:GLN:CA	2.14	0.56
1:K:402:ASP:HA	1:K:406:ARG:HB2	1.87	0.56
1:G:166:HIS:HD2	6:G:1241:HOH:O	1.87	0.56
1:I:125:GLU:O	1:I:128:VAL:HG22	2.06	0.56
1:F:219:TYR:HB3	1:F:254:PRO:HG2	1.88	0.55
1:J:121:LYS:NZ	1:J:121:LYS:HB3	2.21	0.55
1:C:219:TYR:HA	1:C:253:ILE:CG2	2.36	0.55
1:J:122:LYS:NZ	1:J:127:GLN:NE2	2.55	0.55
1:I:219:TYR:HB3	1:I:254:PRO:HG2	1.88	0.55
1:K:245:LEU:HB2	1:K:246:PRO:HD3	1.87	0.55
1:L:106:ASP:OD2	1:L:108:ALA:HB3	2.06	0.55
2:A:428:REL:O5	2:A:428:REL:H2	2.07	0.55
1:E:113:GLN:NE2	1:E:113:GLN:HA	2.22	0.55
1:G:6:ARG:HG2	1:G:6:ARG:HH11	1.72	0.55
1:H:127:GLN:HA	1:H:127:GLN:NE2	2.20	0.55
1:H:263:LYS:CB	1:H:264:ARG:HE	2.20	0.55
1:I:301:LEU:CD1	1:I:326:TRP:HB3	2.36	0.55
1:F:113:GLN:HA	1:F:113:GLN:NE2	2.21	0.55
1:A:25:MET:HG3	6:A:452:HOH:O	2.06	0.55
1:L:402:ASP:HA	1:L:406:ARG:HB2	1.88	0.55
1:B:70:SER:O	1:B:74:GLN:HG3	2.06	0.55
1:L:328:MET:HA	1:L:328:MET:HE2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:LEU:HD11	1:E:326:TRP:HB3	1.89	0.55
1:G:254:PRO:HG3	1:G:295:LYS:HE3	1.88	0.55
1:F:25:MET:HG3	6:F:434:HOH:O	2.07	0.54
1:G:303:ARG:HB2	1:G:328:MET:HE1	1.88	0.54
1:H:245:LEU:HB2	1:H:246:PRO:HD3	1.88	0.54
1:G:149:ASP:O	1:G:153:ILE:HG13	2.07	0.54
1:H:244:LEU:HD13	1:H:244:LEU:C	2.33	0.54
1:J:149:ASP:O	1:J:153:ILE:HG13	2.08	0.54
1:A:301:LEU:HD11	1:A:326:TRP:HB3	1.89	0.54
1:K:172:ASP:HB2	1:K:173:PRO:HD3	1.89	0.54
1:J:128:VAL:CG2	6:J:1476:HOH:O	2.54	0.54
1:L:252:ASN:ND2	1:L:295:LYS:HE2	2.23	0.54
1:B:263:LYS:HB3	1:B:264:ARG:HD3	1.88	0.54
1:L:172:ASP:HB2	1:L:173:PRO:HD3	1.90	0.54
1:B:127:GLN:HA	1:B:127:GLN:NE2	2.22	0.54
1:G:343:GLU:HG2	6:G:432:HOH:O	2.08	0.54
1:J:230:PHE:HA	1:J:231:PRO:C	2.33	0.54
1:B:139:ASP:OD1	1:B:166:HIS:HE1	1.91	0.54
1:D:152:ARG:HG2	1:D:152:ARG:HH11	1.73	0.54
1:E:66:PHE:O	1:E:69:MET:HG2	2.07	0.54
1:G:230:PHE:HA	1:G:231:PRO:C	2.31	0.53
1:J:5:SER:OG	1:J:7:GLU:HG2	2.07	0.53
1:B:254:PRO:HG3	1:B:412:VAL:HG12	1.90	0.53
1:F:385:LEU:HD13	1:F:391:VAL:HG13	1.91	0.53
1:G:40:TRP:O	1:G:41:ASP:CG	2.51	0.53
1:I:80:GLU:HG3	1:I:85:LYS:HE2	1.89	0.53
1:E:156:LEU:HD21	1:E:214:ARG:NH1	2.24	0.53
1:E:244:LEU:C	1:E:244:LEU:HD13	2.34	0.53
1:C:245:LEU:HB2	1:C:246:PRO:HD3	1.90	0.53
1:G:172:ASP:HB2	1:G:173:PRO:HD3	1.90	0.53
1:J:276:VAL:HG22	1:J:277:GLY:N	2.23	0.53
1:L:202:GLN:HE21	1:L:202:GLN:HA	1.72	0.53
1:C:128:VAL:CG2	6:C:1358:HOH:O	2.55	0.53
1:C:374:ALA:O	1:C:378:ILE:HG13	2.08	0.53
1:I:276:VAL:HG22	1:I:277:GLY:N	2.23	0.53
1:G:127:GLN:HA	1:G:127:GLN:NE2	2.14	0.53
1:I:313:ALA:HA	1:I:319:LEU:HD23	1.91	0.53
1:L:392:THR:OG1	1:L:395:GLU:HG3	2.08	0.53
1:F:219:TYR:HA	1:F:253:ILE:CG2	2.38	0.53
1:K:30:PHE:CE2	1:K:37:ILE:HG12	2.44	0.53
1:K:216:ASP:OD1	1:K:414:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:428:REL:O5	2:K:428:REL:H2	2.08	0.53
1:E:245:LEU:HB2	1:E:246:PRO:HD3	1.90	0.53
1:A:111:ASP:OD1	1:A:114:VAL:HG23	2.09	0.53
1:I:154:SER:O	1:I:159:LYS:HB2	2.09	0.53
1:A:172:ASP:HB2	1:A:173:PRO:HD3	1.91	0.52
1:B:49:HIS:HB2	1:B:272:ALA:HB2	1.90	0.52
2:F:428:REL:O5	2:F:428:REL:H2	2.09	0.52
1:F:40:TRP:O	1:F:41:ASP:CG	2.52	0.52
1:G:219:TYR:HA	1:G:253:ILE:HG22	1.90	0.52
1:H:263:LYS:HB3	1:H:264:ARG:HE	1.75	0.52
1:I:230:PHE:HA	1:I:231:PRO:C	2.34	0.52
1:B:40:TRP:O	1:B:41:ASP:CG	2.51	0.52
1:D:70:SER:OG	1:D:73:GLU:HG3	2.09	0.52
1:D:78:ILE:HG23	1:D:82:LEU:HD12	1.91	0.52
1:F:385:LEU:HD12	1:F:389:TRP:O	2.09	0.52
1:I:172:ASP:HB2	1:I:173:PRO:HD3	1.91	0.52
1:B:172:ASP:HB2	1:B:173:PRO:HD3	1.91	0.52
1:D:301:LEU:HD11	1:D:326:TRP:HB3	1.92	0.52
1:E:118:TYR:HA	1:E:121:LYS:HE3	1.92	0.52
1:E:267:PRO:HG2	6:E:1783:HOH:O	2.08	0.52
1:J:198:GLU:O	1:J:202:GLN:HG2	2.10	0.52
1:K:301:LEU:CD1	1:K:326:TRP:HB3	2.39	0.52
1:B:265:VAL:HG21	1:B:275:PHE:HB2	1.92	0.52
1:G:124:SER:O	1:G:128:VAL:HG13	2.10	0.52
1:A:391:VAL:HG23	1:A:391:VAL:O	2.10	0.52
1:E:265:VAL:HG21	1:E:275:PHE:HB2	1.92	0.52
1:L:202:GLN:HA	1:L:202:GLN:NE2	2.24	0.52
1:C:172:ASP:HB2	1:C:173:PRO:HD3	1.91	0.52
1:E:197:ASN:HB2	6:E:1840:HOH:O	2.09	0.52
1:E:392:THR:OG1	1:E:395:GLU:HG3	2.09	0.52
1:H:172:ASP:HB2	1:H:173:PRO:HD3	1.92	0.52
1:C:123:THR:OG1	1:C:126:GLU:HG3	2.10	0.52
1:E:219:TYR:HA	1:E:253:ILE:CG2	2.40	0.52
1:F:244:LEU:HD13	1:F:244:LEU:C	2.35	0.52
1:G:180:GLN:H	1:G:180:GLN:NE2	2.08	0.52
1:K:316:PHE:HB3	1:K:318:ASN:OD1	2.09	0.52
1:A:72:ARG:HH11	1:A:72:ARG:CA	2.23	0.52
1:B:70:SER:OG	1:B:73:GLU:HG3	2.10	0.52
1:F:276:VAL:HG22	1:F:277:GLY:N	2.25	0.52
6:A:1421:HOH:O	1:C:56:MET:HE3	2.09	0.51
1:D:139:ASP:OD1	1:D:166:HIS:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:428:REL:H2	2:D:428:REL:O5	2.10	0.51
1:E:382:ASP:O	1:E:386:GLN:HG2	2.10	0.51
1:J:172:ASP:HB2	1:J:173:PRO:HD3	1.92	0.51
1:A:72:ARG:HH11	1:A:72:ARG:CB	2.23	0.51
1:C:209:THR:O	1:C:213:GLU:HG3	2.10	0.51
1:E:49:HIS:HB2	1:E:272:ALA:HB2	1.91	0.51
1:C:152:ARG:HH22	1:C:184:ARG:NH2	2.06	0.51
1:F:328:MET:HB3	1:F:337:MET:HE1	1.92	0.51
1:H:125:GLU:O	1:H:128:VAL:HG22	2.10	0.51
1:H:352:GLN:HG3	1:H:353:HIS:N	2.24	0.51
1:J:127:GLN:HA	1:J:127:GLN:NE2	2.14	0.51
1:F:196:TRP:CD1	1:F:238:ARG:HD2	2.44	0.51
1:H:181:THR:HG22	1:H:185:LEU:CD2	2.40	0.51
1:F:219:TYR:HA	1:F:253:ILE:HG22	1.91	0.51
1:G:336:GLU:O	1:G:340:MET:HG3	2.11	0.51
1:D:252:ASN:ND2	1:D:295:LYS:HE2	2.26	0.51
1:E:212:ILE:HD13	1:E:253:ILE:HD12	1.91	0.51
1:G:385:LEU:HD23	1:G:385:LEU:C	2.36	0.51
1:C:276:VAL:HG22	1:C:277:GLY:N	2.25	0.51
1:G:276:VAL:HG22	1:G:277:GLY:N	2.25	0.51
1:H:25:MET:HG3	6:H:479:HOH:O	2.10	0.51
1:H:301:LEU:HD11	1:H:326:TRP:HB3	1.91	0.51
1:J:112:LEU:HA	1:J:115:TYR:CD2	2.46	0.51
1:E:6:ARG:HG2	1:E:6:ARG:HH11	1.76	0.51
1:F:230:PHE:HA	1:F:231:PRO:C	2.35	0.51
1:A:388:GLY:HA2	1:K:4:ASN:OD1	2.11	0.51
1:I:41:ASP:OD2	1:I:41:ASP:C	2.54	0.51
1:I:218:VAL:HG23	1:I:219:TYR:CD2	2.46	0.51
1:J:128:VAL:HA	1:J:359:LEU:HD21	1.93	0.51
1:B:111:ASP:HB3	1:B:114:VAL:CG1	2.41	0.50
1:B:180:GLN:H	1:B:180:GLN:HE21	1.57	0.50
1:G:352:GLN:HG3	1:G:353:HIS:N	2.24	0.50
1:K:392:THR:OG1	1:K:395:GLU:HG3	2.11	0.50
1:I:130:THR:O	1:I:134:LEU:HG	2.12	0.50
1:I:149:ASP:O	1:I:153:ILE:HG13	2.11	0.50
1:G:245:LEU:HB2	1:G:246:PRO:HD3	1.93	0.50
1:H:235:ASN:O	1:H:239:ILE:HG13	2.11	0.50
1:I:106:ASP:OD2	1:I:108:ALA:HB3	2.11	0.50
1:A:230:PHE:HA	1:A:231:PRO:C	2.35	0.50
1:C:40:TRP:O	1:C:41:ASP:CG	2.54	0.50
1:D:286:HIS:CE1	1:D:290:GLU:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:GLN:HA	1:E:127:GLN:NE2	2.24	0.50
1:I:301:LEU:HD11	1:I:326:TRP:HB3	1.93	0.50
1:D:51:LEU:HD12	1:D:51:LEU:N	2.27	0.50
1:K:112:LEU:HA	1:K:115:TYR:CD2	2.45	0.50
1:E:230:PHE:HA	1:E:231:PRO:C	2.35	0.50
1:A:113:GLN:NE2	1:A:116:ARG:HH11	2.09	0.50
1:B:252:ASN:ND2	1:B:295:LYS:HE2	2.26	0.50
1:B:301:LEU:HD11	1:B:326:TRP:HB3	1.93	0.50
1:H:276:VAL:HG22	1:H:277:GLY:N	2.26	0.50
1:F:409:TRP:HE3	1:F:414:ARG:HB2	1.77	0.50
1:H:385:LEU:HD13	1:H:391:VAL:HG13	1.93	0.50
1:I:70:SER:OG	1:I:73:GLU:HG3	2.12	0.50
1:B:301:LEU:O	1:B:328:MET:HE3	2.12	0.49
1:D:146:PRO:O	1:D:152:ARG:HB2	2.12	0.49
1:H:286:HIS:CE1	1:H:290:GLU:HG3	2.47	0.49
1:L:230:PHE:HA	1:L:231:PRO:C	2.37	0.49
1:A:179:GLU:HB2	1:A:180:GLN:OE1	2.11	0.49
1:C:244:LEU:HD13	1:C:244:LEU:C	2.37	0.49
1:E:286:HIS:CE1	1:E:290:GLU:HG3	2.47	0.49
1:G:235:ASN:O	1:G:239:ILE:HG13	2.11	0.49
1:J:245:LEU:HB2	1:J:246:PRO:HD3	1.93	0.49
1:J:402:ASP:HA	1:J:406:ARG:HB2	1.94	0.49
1:K:389:TRP:HD1	1:K:391:VAL:HG12	1.78	0.49
1:F:51:LEU:N	1:F:51:LEU:HD12	2.27	0.49
6:G:1051:HOH:O	1:I:56:MET:HE3	2.12	0.49
1:H:70:SER:O	1:H:74:GLN:HG3	2.12	0.49
1:J:352:GLN:HG3	1:J:353:HIS:N	2.26	0.49
1:J:409:TRP:HE3	1:J:414:ARG:HB2	1.77	0.49
1:A:79:TRP:O	1:A:83:PHE:HB2	2.12	0.49
1:E:180:GLN:NE2	1:E:180:GLN:N	2.60	0.49
1:L:70:SER:OG	1:L:73:GLU:HG3	2.11	0.49
1:A:122:LYS:NZ	1:A:127:GLN:NE2	2.60	0.49
1:A:170:ARG:NH2	1:A:223:SER:HB3	2.28	0.49
1:C:14:LYS:NZ	1:C:375:GLU:OE2	2.45	0.49
1:F:172:ASP:HB2	1:F:173:PRO:HD3	1.93	0.49
1:H:408:PHE:O	1:H:412:VAL:HG22	2.12	0.49
1:I:49:HIS:HB2	1:I:272:ALA:HB2	1.94	0.49
1:K:128:VAL:O	1:K:132:LEU:HG	2.13	0.49
1:C:79:TRP:O	1:C:83:PHE:HB2	2.12	0.49
1:D:392:THR:OG1	1:D:395:GLU:HG3	2.11	0.49
1:E:235:ASN:O	1:E:239:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:181:THR:O	1:H:185:LEU:HD23	2.12	0.49
1:J:203:GLU:CD	1:J:206:ARG:NH1	2.70	0.49
1:K:352:GLN:HG3	1:K:353:HIS:N	2.26	0.49
1:B:113:GLN:HA	1:B:113:GLN:NE2	2.28	0.49
1:E:40:TRP:O	1:E:41:ASP:CG	2.55	0.49
1:F:245:LEU:HB2	1:F:246:PRO:HD3	1.95	0.49
1:K:40:TRP:O	1:K:41:ASP:CG	2.55	0.49
1:K:113:GLN:HE22	1:K:116:ARG:HH11	1.59	0.49
1:A:122:LYS:HZ3	1:A:127:GLN:HE22	1.60	0.49
1:A:219:TYR:HB3	1:A:254:PRO:HG2	1.95	0.49
1:L:301:LEU:CD1	1:L:326:TRP:HB3	2.42	0.49
1:A:245:LEU:HB2	1:A:246:PRO:HD3	1.95	0.48
1:E:128:VAL:O	1:E:132:LEU:HG	2.13	0.48
1:H:72:ARG:HH12	1:H:116:ARG:HD3	1.78	0.48
1:L:391:VAL:O	1:L:391:VAL:HG23	2.12	0.48
1:B:158:GLY:O	1:B:160:GLN:HG2	2.13	0.48
1:E:276:VAL:HG22	1:E:277:GLY:N	2.27	0.48
1:L:40:TRP:O	1:L:41:ASP:CG	2.55	0.48
1:C:198:GLU:O	1:C:202:GLN:HG2	2.13	0.48
1:E:352:GLN:HG3	1:E:353:HIS:N	2.28	0.48
1:G:5:SER:OG	1:G:7:GLU:HG2	2.13	0.48
1:B:385:LEU:HA	1:B:389:TRP:O	2.13	0.48
1:F:231:PRO:HD3	1:F:286:HIS:CD2	2.48	0.48
1:H:295:LYS:HE3	1:H:411:PHE:O	2.13	0.48
1:E:51:LEU:N	1:E:51:LEU:HD12	2.28	0.48
1:H:40:TRP:O	1:H:41:ASP:CB	2.57	0.48
1:K:254:PRO:HG3	1:K:295:LYS:HE3	1.93	0.48
1:L:139:ASP:OD1	1:L:166:HIS:HE1	1.95	0.48
1:C:252:ASN:HD21	1:C:295:LYS:HE3	1.77	0.48
1:H:301:LEU:O	1:H:328:MET:HE3	2.14	0.48
1:I:402:ASP:HA	1:I:406:ARG:HB2	1.95	0.48
1:J:122:LYS:NZ	1:J:127:GLN:HE22	2.11	0.48
1:K:69:MET:HB3	1:K:73:GLU:HB2	1.96	0.48
1:K:152:ARG:HD2	1:K:156:LEU:HD11	1.94	0.48
1:K:276:VAL:HG22	1:K:277:GLY:N	2.28	0.48
1:B:154:SER:O	1:B:159:LYS:HB2	2.14	0.48
1:C:154:SER:O	1:C:159:LYS:HB2	2.13	0.48
1:D:172:ASP:HB2	1:D:173:PRO:HD3	1.96	0.48
1:D:352:GLN:HG3	1:D:353:HIS:N	2.28	0.48
1:C:8:VAL:O	1:C:12:LYS:HG2	2.13	0.48
1:D:388:GLY:HA2	1:H:4:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:49:HIS:HB2	1:J:272:ALA:HB2	1.94	0.48
1:J:301:LEU:CD1	1:J:326:TRP:HB3	2.44	0.48
1:L:113:GLN:HG2	6:L:1347:HOH:O	2.13	0.48
1:E:316:PHE:HB3	1:E:318:ASN:OD1	2.14	0.48
1:J:30:PHE:CE2	1:J:37:ILE:HG13	2.49	0.48
1:A:244:LEU:HD13	1:A:244:LEU:C	2.38	0.47
1:A:313:ALA:HA	1:A:319:LEU:HD23	1.96	0.47
1:A:112:LEU:HA	1:A:115:TYR:CD2	2.49	0.47
1:B:244:LEU:C	1:B:244:LEU:HD13	2.39	0.47
1:D:69:MET:HB3	1:D:73:GLU:HB2	1.95	0.47
1:D:276:VAL:HG22	1:D:277:GLY:N	2.29	0.47
1:G:385:LEU:HA	1:G:389:TRP:O	2.14	0.47
1:K:209:THR:O	1:K:213:GLU:HG3	2.13	0.47
1:G:128:VAL:CG2	6:G:665:HOH:O	2.62	0.47
1:H:32:PRO:HG2	1:H:128:VAL:HG21	1.96	0.47
1:K:139:ASP:OD1	1:K:166:HIS:HE1	1.96	0.47
1:L:125:GLU:O	1:L:128:VAL:HG23	2.14	0.47
1:E:66:PHE:HA	1:E:69:MET:HE3	1.95	0.47
1:E:275:PHE:CG	1:E:276:VAL:N	2.82	0.47
1:I:219:TYR:HA	1:I:253:ILE:CG2	2.44	0.47
1:J:182:LYS:O	1:J:186:ARG:HG2	2.14	0.47
1:J:265:VAL:HG21	1:J:275:PHE:HB2	1.95	0.47
1:A:123:THR:OG1	1:A:126:GLU:HG3	2.13	0.47
6:A:445:HOH:O	1:B:308:GLU:HG2	2.14	0.47
1:B:203:GLU:OE1	1:B:206:ARG:NH1	2.47	0.47
1:G:139:ASP:OD1	1:G:166:HIS:HE1	1.97	0.47
1:H:230:PHE:HA	1:H:231:PRO:C	2.40	0.47
1:I:174:LEU:HD13	1:I:175:LEU:HD12	1.96	0.47
1:B:316:PHE:HB3	1:B:318:ASN:OD1	2.14	0.47
1:K:286:HIS:CE1	1:K:290:GLU:HG3	2.49	0.47
1:F:385:LEU:HD11	1:F:391:VAL:HG22	1.95	0.47
1:G:65:ALA:O	1:G:69:MET:HG3	2.14	0.47
1:H:322:PHE:HA	1:H:350:ILE:O	2.14	0.47
1:K:244:LEU:HD13	1:K:244:LEU:C	2.40	0.47
1:A:286:HIS:CE1	1:A:290:GLU:HG3	2.49	0.47
1:C:122:LYS:HG3	1:C:126:GLU:HB2	1.97	0.47
1:F:301:LEU:CD1	1:F:326:TRP:HB3	2.45	0.47
1:I:211:TRP:CE3	1:I:215:MET:HE3	2.49	0.47
1:L:56:MET:HE2	1:L:63:ILE:HB	1.95	0.47
2:L:428:REL:H2	2:L:428:REL:O5	2.14	0.47
1:B:56:MET:HE3	6:C:1657:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:LEU:HD12	1:C:389:TRP:O	2.15	0.47
1:F:314:ARG:HD2	1:F:344:MET:HB3	1.96	0.47
1:A:9:LEU:HD21	1:A:381:TYR:HB2	1.96	0.47
1:A:72:ARG:HH11	1:A:72:ARG:HB2	1.80	0.47
1:B:274:ASP:O	1:C:315:LYS:HD2	2.15	0.47
1:G:25:MET:HG3	6:G:445:HOH:O	2.13	0.47
1:G:198:GLU:HA	1:G:198:GLU:OE1	2.15	0.47
1:J:308:GLU:HG2	6:J:450:HOH:O	2.14	0.47
1:A:127:GLN:HE21	1:A:127:GLN:CA	2.11	0.46
1:I:40:TRP:O	1:I:41:ASP:CG	2.58	0.46
1:B:216:ASP:N	1:B:217:PRO:CD	2.78	0.46
1:F:149:ASP:O	1:F:153:ILE:HG13	2.15	0.46
1:F:324:CYS:HB3	1:F:337:MET:CE	2.43	0.46
1:J:322:PHE:HA	1:J:350:ILE:O	2.15	0.46
1:K:195:GLU:HG3	1:K:197:ASN:HD22	1.81	0.46
1:L:306:GLN:OE1	1:L:337:MET:HE3	2.14	0.46
1:A:66:PHE:CZ	1:A:74:GLN:HB3	2.50	0.46
1:A:352:GLN:HG3	1:A:353:HIS:N	2.30	0.46
1:C:30:PHE:CE2	1:C:37:ILE:HG13	2.50	0.46
1:L:9:LEU:HD21	1:L:381:TYR:CB	2.46	0.46
1:B:286:HIS:CE1	1:B:290:GLU:HG3	2.50	0.46
1:D:394:GLU:HB2	6:D:1235:HOH:O	2.14	0.46
1:H:122:LYS:HD3	6:H:1304:HOH:O	2.16	0.46
1:L:219:TYR:HA	1:L:253:ILE:CG2	2.45	0.46
1:B:218:VAL:HG23	1:B:219:TYR:CD2	2.51	0.46
1:D:230:PHE:HA	1:D:231:PRO:C	2.39	0.46
1:J:40:TRP:O	1:J:41:ASP:CG	2.58	0.46
1:L:265:VAL:HG11	1:L:275:PHE:HB3	1.97	0.46
1:B:306:GLN:O	1:B:310:VAL:HG23	2.15	0.46
1:E:139:ASP:OD1	1:E:166:HIS:HE1	1.98	0.46
1:E:244:LEU:C	1:E:244:LEU:CD1	2.88	0.46
1:G:70:SER:O	1:G:74:GLN:HG3	2.15	0.46
1:J:203:GLU:OE2	1:J:206:ARG:NH1	2.49	0.46
1:A:322:PHE:HA	1:A:350:ILE:O	2.16	0.46
1:B:125:GLU:O	1:B:128:VAL:HG13	2.15	0.46
1:B:276:VAL:HG22	1:B:277:GLY:N	2.31	0.46
1:F:191:LYS:HB3	1:F:191:LYS:NZ	2.31	0.46
1:J:303:ARG:HB2	1:J:328:MET:HE1	1.97	0.46
1:L:154:SER:O	1:L:159:LYS:HB2	2.15	0.46
1:A:51:LEU:N	1:A:51:LEU:HD12	2.31	0.46
1:B:51:LEU:HD12	1:B:51:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:GLN:HE21	1:D:127:GLN:CA	2.15	0.46
1:G:180:GLN:NE2	1:G:180:GLN:N	2.63	0.46
1:I:122:LYS:HZ3	1:I:127:GLN:HE22	1.63	0.46
1:J:113:GLN:HA	1:J:113:GLN:NE2	2.30	0.46
1:B:322:PHE:HA	1:B:350:ILE:O	2.16	0.46
1:B:352:GLN:HG3	1:B:353:HIS:N	2.30	0.46
1:H:264:ARG:HG2	1:H:264:ARG:HH11	1.80	0.46
1:J:198:GLU:HA	1:J:198:GLU:OE1	2.16	0.46
1:K:393:GLU:O	1:K:397:LYS:HG2	2.15	0.46
1:L:69:MET:HB3	1:L:73:GLU:HB2	1.98	0.46
1:L:198:GLU:O	1:L:202:GLN:HG2	2.16	0.46
1:B:235:ASN:O	1:B:239:ILE:HG13	2.16	0.46
1:C:122:LYS:CG	1:C:126:GLU:HB2	2.46	0.46
1:H:216:ASP:N	1:H:217:PRO:CD	2.79	0.46
1:H:254:PRO:HG3	1:H:295:LYS:HE2	1.97	0.46
1:J:122:LYS:HZ1	1:J:127:GLN:NE2	2.13	0.46
1:J:254:PRO:HG3	1:J:412:VAL:HG12	1.97	0.46
1:C:127:GLN:HG3	1:C:359:LEU:HD23	1.97	0.45
1:E:306:GLN:O	1:E:310:VAL:HG23	2.16	0.45
1:G:122:LYS:HZ1	1:G:127:GLN:HA	1.80	0.45
1:G:286:HIS:CE1	1:G:290:GLU:HG3	2.51	0.45
1:J:107:PRO:HA	1:J:115:TYR:OH	2.15	0.45
1:B:244:LEU:C	1:B:244:LEU:CD1	2.90	0.45
1:E:385:LEU:HA	1:E:389:TRP:O	2.16	0.45
1:I:152:ARG:O	1:I:156:LEU:HG	2.17	0.45
1:L:142:MET:O	1:L:168:ALA:HB3	2.16	0.45
1:L:322:PHE:HA	1:L:350:ILE:O	2.16	0.45
1:A:392:THR:OG1	1:A:395:GLU:HG3	2.16	0.45
1:G:409:TRP:HA	1:G:412:VAL:HG22	1.97	0.45
1:G:169:LEU:HG	1:G:171:LEU:HD21	1.98	0.45
1:H:128:VAL:O	1:H:132:LEU:HG	2.15	0.45
1:H:139:ASP:OD1	1:H:166:HIS:CE1	2.69	0.45
1:K:182:LYS:HA	1:K:185:LEU:HD12	1.98	0.45
1:A:219:TYR:HA	1:A:253:ILE:CG2	2.47	0.45
1:A:265:VAL:HG21	1:A:275:PHE:HB2	1.99	0.45
6:D:435:HOH:O	1:E:308:GLU:HG2	2.17	0.45
1:E:79:TRP:O	1:E:83:PHE:HB2	2.17	0.45
1:E:152:ARG:HH11	1:E:152:ARG:HG2	1.81	0.45
1:E:286:HIS:NE2	1:E:290:GLU:HG3	2.32	0.45
1:I:264:ARG:HG2	6:I:1147:HOH:O	2.17	0.45
1:I:391:VAL:HG23	1:I:391:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:52:VAL:O	1:K:55:VAL:HG12	2.16	0.45
1:L:301:LEU:HD11	1:L:326:TRP:HB3	1.99	0.45
1:D:382:ASP:O	1:D:386:GLN:HG2	2.17	0.45
1:D:391:VAL:O	1:D:391:VAL:HG23	2.17	0.45
1:G:128:VAL:HA	1:G:359:LEU:HD21	1.97	0.45
1:J:113:GLN:O	1:J:117:GLU:HG3	2.16	0.45
1:A:30:PHE:CE2	1:A:37:ILE:HG12	2.52	0.45
1:A:106:ASP:OD2	1:A:108:ALA:HB3	2.16	0.45
1:F:125:GLU:O	1:F:128:VAL:HG13	2.17	0.45
1:L:149:ASP:O	1:L:153:ILE:HG13	2.16	0.45
1:D:113:GLN:NE2	1:D:113:GLN:CA	2.78	0.45
1:E:122:LYS:NZ	1:E:127:GLN:NE2	2.64	0.45
1:I:70:SER:O	1:I:74:GLN:HG3	2.17	0.45
1:B:29:LEU:O	1:B:142:MET:HG2	2.17	0.45
1:C:124:SER:O	1:C:128:VAL:HG13	2.17	0.45
1:L:30:PHE:CE2	1:L:37:ILE:HG12	2.52	0.45
1:F:72:ARG:HH11	1:F:72:ARG:CB	2.09	0.45
1:F:352:GLN:HG3	1:F:353:HIS:N	2.32	0.45
1:I:122:LYS:NZ	1:I:127:GLN:NE2	2.64	0.45
1:L:40:TRP:CE3	1:L:127:GLN:HG2	2.52	0.45
1:A:113:GLN:HE22	1:A:116:ARG:HH11	1.64	0.44
1:D:9:LEU:HD21	1:D:381:TYR:HB2	1.98	0.44
1:D:245:LEU:HB2	1:D:246:PRO:HD3	1.98	0.44
1:D:409:TRP:HA	1:D:412:VAL:HG22	1.98	0.44
1:E:6:ARG:HG3	1:E:382:ASP:OD1	2.17	0.44
1:F:145:ASP:HA	1:F:146:PRO:HD2	1.91	0.44
1:F:301:LEU:HD11	1:F:326:TRP:HB3	1.99	0.44
1:J:276:VAL:CG2	1:J:277:GLY:N	2.80	0.44
1:D:106:ASP:OD2	1:D:108:ALA:HB3	2.17	0.44
1:G:244:LEU:C	1:G:244:LEU:HD13	2.42	0.44
1:G:308:GLU:HG2	6:G:443:HOH:O	2.16	0.44
1:H:301:LEU:CD1	1:H:326:TRP:HB3	2.46	0.44
1:J:25:MET:HG3	6:J:439:HOH:O	2.17	0.44
1:K:170:ARG:HH21	1:K:223:SER:HB3	1.82	0.44
1:C:41:ASP:OD1	1:C:41:ASP:C	2.61	0.44
1:D:170:ARG:NH2	1:D:223:SER:HB3	2.33	0.44
1:E:128:VAL:CG2	6:E:1666:HOH:O	2.65	0.44
1:E:313:ALA:HA	1:E:319:LEU:HD23	1.99	0.44
1:G:313:ALA:HA	1:G:319:LEU:HD23	1.98	0.44
1:I:414:ARG:HG3	1:I:414:ARG:HH11	1.82	0.44
1:K:2:SER:HA	6:K:1242:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:67:TRP:HA	1:L:67:TRP:CE3	2.52	0.44
1:A:276:VAL:HG22	1:A:277:GLY:N	2.32	0.44
1:B:113:GLN:HA	1:B:113:GLN:HE21	1.83	0.44
1:G:185:LEU:HB3	1:G:190:TYR:HB2	1.99	0.44
1:H:197:ASN:ND2	1:H:199:GLY:H	2.15	0.44
1:I:112:LEU:HA	1:I:115:TYR:CD2	2.53	0.44
1:A:42:ILE:HD13	1:A:100:LEU:HD21	1.99	0.44
1:D:219:TYR:HA	1:D:253:ILE:CG2	2.47	0.44
1:D:231:PRO:HD3	1:D:286:HIS:CG	2.52	0.44
1:G:358:VAL:HB	1:G:361:GLN:HG3	1.99	0.44
1:H:275:PHE:CG	1:H:276:VAL:N	2.82	0.44
1:C:275:PHE:CG	1:C:276:VAL:N	2.86	0.44
1:D:112:LEU:HA	1:D:115:TYR:CD2	2.53	0.44
1:F:112:LEU:HA	1:F:115:TYR:CD2	2.52	0.44
1:I:67:TRP:HA	1:I:67:TRP:CE3	2.52	0.44
1:K:250:LYS:HD3	1:K:251:HIS:CE1	2.53	0.44
1:L:182:LYS:HB2	1:L:182:LYS:NZ	2.33	0.44
1:C:69:MET:HB3	1:C:73:GLU:HB2	1.98	0.44
1:C:306:GLN:OE1	1:C:337:MET:HE3	2.18	0.44
1:C:313:ALA:HA	1:C:319:LEU:HD23	1.99	0.44
1:D:326:TRP:HB3	1:D:327:PHE:H	1.52	0.44
1:J:208:LEU:O	1:J:212:ILE:HG13	2.18	0.44
1:J:225:PRO:HA	1:J:261:VAL:O	2.17	0.44
1:L:276:VAL:CG2	1:L:277:GLY:N	2.80	0.44
1:F:139:ASP:OD1	1:F:166:HIS:HE1	2.01	0.44
1:H:113:GLN:NE2	1:H:113:GLN:HA	2.33	0.44
1:A:303:ARG:HB2	1:A:328:MET:HE1	2.00	0.44
1:C:230:PHE:HA	1:C:231:PRO:C	2.43	0.44
1:F:322:PHE:HA	1:F:350:ILE:O	2.17	0.44
1:A:286:HIS:NE2	1:A:290:GLU:HG3	2.33	0.43
1:A:328:MET:HE2	1:A:328:MET:HA	1.99	0.43
1:F:374:ALA:O	1:F:378:ILE:HG13	2.17	0.43
1:G:322:PHE:HA	1:G:350:ILE:O	2.18	0.43
1:H:123:THR:OG1	1:H:126:GLU:HG3	2.18	0.43
1:H:385:LEU:HD12	1:H:385:LEU:HA	1.92	0.43
1:J:275:PHE:CG	1:J:276:VAL:N	2.86	0.43
1:L:313:ALA:HA	1:L:319:LEU:HD23	2.00	0.43
1:L:352:GLN:HG3	1:L:353:HIS:N	2.33	0.43
1:E:30:PHE:CE2	1:E:37:ILE:HG13	2.53	0.43
1:F:4:ASN:HB2	6:I:1261:HOH:O	2.18	0.43
1:F:235:ASN:O	1:F:239:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:TRP:CE3	1:H:127:GLN:HG2	2.53	0.43
1:L:52:VAL:O	1:L:55:VAL:HG12	2.18	0.43
1:A:70:SER:O	1:A:74:GLN:HG3	2.18	0.43
1:C:182:LYS:HB2	1:C:182:LYS:NZ	2.33	0.43
1:D:80:GLU:O	1:D:85:LYS:HG3	2.18	0.43
1:I:139:ASP:OD1	1:I:166:HIS:HE1	2.01	0.43
1:I:276:VAL:CG2	1:I:277:GLY:N	2.81	0.43
1:J:235:ASN:O	1:J:239:ILE:HG13	2.18	0.43
1:C:196:TRP:CZ2	1:C:201:ILE:HG12	2.54	0.43
1:D:178:TYR:CD1	1:D:239:ILE:HD11	2.54	0.43
1:E:191:LYS:HB2	1:E:191:LYS:NZ	2.33	0.43
1:F:326:TRP:HB3	1:F:327:PHE:H	1.58	0.43
1:H:265:VAL:HG21	1:H:275:PHE:HB2	1.99	0.43
1:J:336:GLU:O	1:J:340:MET:HG3	2.19	0.43
1:K:186:ARG:NH2	1:K:192:VAL:O	2.44	0.43
1:A:139:ASP:OD1	1:A:166:HIS:HE1	2.00	0.43
1:B:231:PRO:HD3	1:B:286:HIS:CG	2.53	0.43
1:C:139:ASP:OD1	1:C:166:HIS:HE1	2.00	0.43
1:E:154:SER:O	1:E:159:LYS:HB2	2.18	0.43
1:F:152:ARG:HH22	1:F:184:ARG:HH22	1.67	0.43
1:G:112:LEU:HA	1:G:115:TYR:CD2	2.53	0.43
1:J:69:MET:HB2	1:J:73:GLU:HB2	2.00	0.43
1:J:122:LYS:HZ3	1:J:127:GLN:HE22	1.66	0.43
1:L:41:ASP:OD1	1:L:41:ASP:C	2.60	0.43
1:L:128:VAL:CG2	6:L:986:HOH:O	2.67	0.43
1:A:149:ASP:OD1	1:A:152:ARG:NH2	2.51	0.43
1:A:409:TRP:HA	1:A:412:VAL:HG22	1.99	0.43
1:F:41:ASP:C	1:F:41:ASP:OD1	2.61	0.43
1:F:342:MET:HE1	1:F:377:LEU:CD2	2.48	0.43
2:H:428:REL:H2	2:H:428:REL:O5	2.18	0.43
1:I:40:TRP:O	1:I:41:ASP:CB	2.67	0.43
1:J:128:VAL:HG12	1:J:359:LEU:HD22	2.00	0.43
1:J:321:ILE:HG12	6:L:1830:HOH:O	2.17	0.43
1:L:264:ARG:HG2	6:L:610:HOH:O	2.18	0.43
1:D:150:ASN:O	1:D:153:ILE:HG22	2.19	0.43
1:E:224:LEU:HD13	1:E:228:PHE:CD1	2.53	0.43
1:E:310:VAL:HG11	1:E:344:MET:HE3	2.01	0.43
1:F:275:PHE:CG	1:F:276:VAL:N	2.87	0.43
1:A:295:LYS:HB3	1:A:411:PHE:CZ	2.54	0.43
1:D:244:LEU:C	1:D:244:LEU:HD13	2.44	0.43
1:G:201:ILE:O	1:G:205:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:128:VAL:CG2	6:H:1281:HOH:O	2.67	0.43
1:J:389:TRP:HB2	1:L:97:LEU:HD13	2.01	0.43
1:L:112:LEU:HA	1:L:115:TYR:CD2	2.53	0.43
1:B:61:VAL:HG11	1:B:69:MET:HE3	2.01	0.42
1:E:180:GLN:H	1:E:180:GLN:HE21	1.62	0.42
1:F:216:ASP:N	1:F:217:PRO:CD	2.82	0.42
1:G:409:TRP:HE3	1:G:414:ARG:HB2	1.83	0.42
1:H:303:ARG:HB2	1:H:328:MET:HE1	2.01	0.42
1:I:128:VAL:HG23	1:I:129:ASP:N	2.33	0.42
1:C:256:ALA:HA	1:C:297:LEU:O	2.19	0.42
1:D:105:LEU:O	1:D:107:PRO:HD3	2.18	0.42
1:E:42:ILE:HD13	1:E:100:LEU:HD21	1.99	0.42
1:E:301:LEU:CD1	1:E:326:TRP:HB3	2.49	0.42
1:H:79:TRP:O	1:H:83:PHE:HB2	2.19	0.42
1:D:286:HIS:NE2	1:D:290:GLU:HG3	2.33	0.42
1:L:245:LEU:HB2	1:L:246:PRO:HD3	2.01	0.42
1:C:128:VAL:HA	1:C:359:LEU:HD21	2.01	0.42
1:C:385:LEU:HD12	1:C:385:LEU:HA	1.86	0.42
1:D:123:THR:OG1	1:D:126:GLU:HG3	2.19	0.42
1:D:149:ASP:OD1	1:D:152:ARG:NH2	2.52	0.42
1:D:154:SER:HB3	1:D:159:LYS:HG3	2.00	0.42
1:E:158:GLY:O	1:E:159:LYS:C	2.62	0.42
1:I:316:PHE:HB3	1:I:318:ASN:OD1	2.18	0.42
1:B:6:ARG:HG2	1:B:6:ARG:NH1	2.32	0.42
1:H:170:ARG:NH2	1:H:223:SER:HB3	2.34	0.42
1:J:128:VAL:HG12	1:J:359:LEU:CD2	2.49	0.42
1:C:180:GLN:NE2	1:C:180:GLN:N	2.68	0.42
1:C:216:ASP:N	1:C:217:PRO:CD	2.83	0.42
1:E:69:MET:HG3	1:E:74:GLN:HG2	2.02	0.42
1:E:326:TRP:HB3	1:E:327:PHE:H	1.61	0.42
1:H:414:ARG:HG3	1:H:414:ARG:HH11	1.85	0.42
1:J:387:ALA:O	1:L:107:PRO:HG2	2.20	0.42
1:G:275:PHE:CG	1:G:276:VAL:N	2.86	0.42
1:H:66:PHE:O	1:H:69:MET:HG2	2.19	0.42
1:H:69:MET:HB2	1:H:73:GLU:HB2	2.01	0.42
1:K:232:GLU:O	1:K:237:GLY:HA3	2.20	0.42
1:A:167:ALA:O	1:A:217:PRO:HA	2.19	0.42
1:A:252:ASN:HD21	1:A:295:LYS:HE2	1.83	0.42
1:B:152:ARG:HD2	1:B:156:LEU:HD11	2.01	0.42
1:C:358:VAL:HB	1:C:361:GLN:HG3	2.02	0.42
1:D:322:PHE:HA	1:D:350:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:GLN:O	1:E:365:LYS:HG2	2.20	0.42
1:G:180:GLN:H	1:G:180:GLN:HE21	1.66	0.42
1:K:216:ASP:N	1:K:217:PRO:CD	2.83	0.42
1:K:230:PHE:HA	1:K:231:PRO:C	2.44	0.42
1:L:79:TRP:O	1:L:83:PHE:HB2	2.20	0.42
1:C:219:TYR:HA	1:C:253:ILE:HG22	2.01	0.42
1:H:181:THR:HG22	1:H:185:LEU:HD21	2.02	0.42
1:K:97:LEU:HD13	1:L:389:TRP:HB2	2.01	0.42
1:D:139:ASP:OD1	1:D:166:HIS:CE1	2.73	0.42
1:F:301:LEU:O	1:F:328:MET:HE3	2.20	0.42
1:H:297:LEU:HD23	1:H:320:MET:HB3	2.02	0.42
1:J:8:VAL:O	1:J:12:LYS:HG2	2.19	0.42
1:A:301:LEU:CD1	1:A:326:TRP:HB3	2.49	0.41
1:D:42:ILE:HD13	1:D:100:LEU:HD21	2.01	0.41
1:E:9:LEU:O	1:E:13:VAL:HG23	2.20	0.41
1:F:389:TRP:HD1	1:F:391:VAL:HG12	1.84	0.41
1:G:152:ARG:HG2	1:G:156:LEU:HG	2.01	0.41
1:K:32:PRO:HG2	1:K:128:VAL:HG21	2.00	0.41
2:C:428:REL:H2	2:C:428:REL:O5	2.20	0.41
1:E:41:ASP:OD1	1:E:41:ASP:C	2.63	0.41
1:E:216:ASP:N	1:E:217:PRO:CD	2.83	0.41
1:J:408:PHE:O	1:J:412:VAL:HG22	2.20	0.41
1:K:219:TYR:HA	1:K:253:ILE:CG2	2.50	0.41
1:A:409:TRP:HE3	1:A:414:ARG:HB2	1.84	0.41
1:B:98:THR:HB	1:B:364:TYR:HB2	2.02	0.41
1:D:328:MET:HE2	1:D:328:MET:HA	2.02	0.41
1:E:196:TRP:CD1	1:E:238:ARG:HD2	2.54	0.41
1:G:196:TRP:CD1	1:G:238:ARG:HD2	2.55	0.41
1:I:306:GLN:OE1	1:I:337:MET:HE3	2.21	0.41
1:J:301:LEU:HD11	1:J:326:TRP:HB3	2.03	0.41
1:K:308:GLU:HG2	6:K:433:HOH:O	2.19	0.41
1:E:63:ILE:HG23	1:E:64:GLU:N	2.36	0.41
1:H:306:GLN:OE1	1:H:337:MET:HE3	2.20	0.41
1:I:392:THR:OG1	1:I:395:GLU:HG3	2.20	0.41
1:B:200:SER:O	1:B:204:VAL:HG23	2.21	0.41
1:D:40:TRP:CE3	1:D:127:GLN:HG2	2.56	0.41
1:F:18:ASN:ND2	6:F:1397:HOH:O	2.53	0.41
1:G:190:TYR:CD1	1:G:206:ARG:NH1	2.89	0.41
1:G:276:VAL:CG2	1:G:277:GLY:N	2.84	0.41
1:I:374:ALA:O	1:I:378:ILE:HG13	2.20	0.41
1:K:40:TRP:CE3	1:K:127:GLN:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ASP:OD1	1:B:152:ARG:NH2	2.53	0.41
1:B:275:PHE:CG	1:B:276:VAL:N	2.84	0.41
1:B:326:TRP:HB3	1:B:327:PHE:H	1.57	0.41
1:C:196:TRP:CD1	1:C:238:ARG:HD2	2.55	0.41
1:E:169:LEU:HG	1:E:171:LEU:HD21	2.03	0.41
1:I:231:PRO:HD3	1:I:286:HIS:CD2	2.55	0.41
1:I:244:LEU:C	1:I:244:LEU:HD13	2.45	0.41
1:I:322:PHE:HA	1:I:350:ILE:O	2.20	0.41
1:K:235:ASN:O	1:K:239:ILE:HG13	2.21	0.41
1:A:122:LYS:NZ	1:A:127:GLN:HE22	2.18	0.41
1:A:275:PHE:CG	1:A:276:VAL:N	2.88	0.41
1:C:112:LEU:HA	1:C:115:TYR:CD2	2.56	0.41
1:C:322:PHE:HA	1:C:350:ILE:O	2.20	0.41
1:E:100:LEU:O	1:E:105:LEU:HB2	2.20	0.41
1:F:386:GLN:NE2	1:I:4:ASN:OD1	2.54	0.41
1:G:49:HIS:HB2	1:G:272:ALA:HB2	2.02	0.41
1:G:152:ARG:NH2	1:G:184:ARG:HH22	2.19	0.41
1:H:125:GLU:CD	1:H:125:GLU:H	2.28	0.41
1:L:159:LYS:HD3	1:L:159:LYS:HA	1.91	0.41
1:F:316:PHE:HB3	1:F:318:ASN:OD1	2.20	0.41
2:G:428:REL:H2	2:G:428:REL:O5	2.21	0.41
1:H:326:TRP:HB3	1:H:327:PHE:H	1.65	0.41
1:C:301:LEU:CD1	1:C:326:TRP:HB3	2.51	0.41
1:D:391:VAL:O	1:D:391:VAL:CG2	2.69	0.41
1:E:322:PHE:HA	1:E:350:ILE:O	2.20	0.41
1:F:254:PRO:HG3	1:F:412:VAL:HG12	2.02	0.41
1:F:265:VAL:HG21	1:F:275:PHE:HB2	2.03	0.41
1:F:313:ALA:HA	1:F:319:LEU:HD23	2.02	0.41
1:G:254:PRO:HG2	1:G:412:VAL:HA	2.03	0.41
1:I:11:GLU:CD	6:I:984:HOH:O	2.63	0.41
1:I:51:LEU:HD12	1:I:51:LEU:N	2.36	0.41
1:I:186:ARG:HG2	1:I:186:ARG:HH11	1.85	0.41
1:I:235:ASN:O	1:I:239:ILE:HG13	2.20	0.41
1:J:244:LEU:HD13	1:J:244:LEU:C	2.46	0.41
1:K:139:ASP:OD1	1:K:166:HIS:CE1	2.73	0.41
1:B:224:LEU:HD13	1:B:228:PHE:CD1	2.55	0.41
1:D:301:LEU:CD1	1:D:326:TRP:HB3	2.50	0.41
1:J:106:ASP:HA	1:J:107:PRO:HD2	1.94	0.41
1:K:169:LEU:HG	1:K:171:LEU:HD21	2.02	0.41
1:K:212:ILE:HD13	1:K:253:ILE:HD12	2.02	0.41
1:A:80:GLU:CG	1:A:85:LYS:HZ1	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ALA:HA	1:B:319:LEU:HD23	2.03	0.40
1:E:113:GLN:HA	1:E:113:GLN:HE21	1.84	0.40
1:G:30:PHE:CE2	1:G:37:ILE:HG13	2.56	0.40
1:J:52:VAL:O	1:J:55:VAL:HG12	2.21	0.40
1:K:322:PHE:HA	1:K:350:ILE:O	2.21	0.40
1:H:342:MET:HE1	1:H:377:LEU:CD2	2.51	0.40
1:J:123:THR:OG1	1:J:126:GLU:HG3	2.21	0.40
1:K:385:LEU:HD21	1:K:391:VAL:HG22	2.04	0.40
1:D:111:ASP:OD1	1:D:114:VAL:HG23	2.21	0.40
1:D:265:VAL:HG21	1:D:275:PHE:HB2	2.02	0.40
1:G:265:VAL:HG21	1:G:275:PHE:HB2	2.04	0.40
1:G:288:LEU:CD2	1:G:319:LEU:HB2	2.51	0.40
1:I:245:LEU:HB2	1:I:246:PRO:HD3	2.04	0.40
1:J:313:ALA:HA	1:J:319:LEU:HD23	2.03	0.40
1:K:310:VAL:HG11	1:K:344:MET:HE3	2.02	0.40
1:L:49:HIS:HB2	1:L:272:ALA:HB2	2.02	0.40
1:L:394:GLU:HB2	6:L:674:HOH:O	2.20	0.40
1:C:386:GLN:NE2	1:L:4:ASN:OD1	2.55	0.40
1:E:149:ASP:OD1	1:E:152:ARG:NH2	2.54	0.40
1:E:203:GLU:OE1	1:E:206:ARG:NH1	2.54	0.40
1:F:208:LEU:O	1:F:212:ILE:HG13	2.21	0.40
1:F:276:VAL:CG2	1:F:277:GLY:N	2.83	0.40
1:G:6:ARG:HG2	1:G:6:ARG:NH1	2.37	0.40
1:G:6:ARG:HG3	1:G:382:ASP:OD1	2.22	0.40
1:G:301:LEU:HD11	1:G:326:TRP:HB3	2.04	0.40
1:I:52:VAL:O	1:I:55:VAL:HG12	2.21	0.40
1:J:148:ASP:OD2	1:J:151:GLU:HG3	2.22	0.40
1:C:170:ARG:NH2	1:C:223:SER:HB3	2.36	0.40
1:E:145:ASP:HA	1:E:146:PRO:HD2	1.92	0.40
1:F:40:TRP:O	1:F:41:ASP:CB	2.70	0.40
1:F:154:SER:O	1:F:159:LYS:HB2	2.22	0.40
1:H:204:VAL:O	1:H:207:PHE:HB3	2.22	0.40
1:H:409:TRP:HA	1:H:412:VAL:HG22	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	411/427 (96%)	398 (97%)	10 (2%)	3 (1%)	18	15
1	B	411/427 (96%)	398 (97%)	10 (2%)	3 (1%)	18	15
1	C	411/427 (96%)	399 (97%)	10 (2%)	2 (0%)	24	22
1	D	411/427 (96%)	399 (97%)	10 (2%)	2 (0%)	24	22
1	E	411/427 (96%)	396 (96%)	12 (3%)	3 (1%)	18	15
1	F	411/427 (96%)	396 (96%)	14 (3%)	1 (0%)	43	44
1	G	411/427 (96%)	401 (98%)	8 (2%)	2 (0%)	24	22
1	H	411/427 (96%)	394 (96%)	15 (4%)	2 (0%)	24	22
1	I	411/427 (96%)	396 (96%)	13 (3%)	2 (0%)	24	22
1	J	411/427 (96%)	401 (98%)	8 (2%)	2 (0%)	24	22
1	K	411/427 (96%)	399 (97%)	10 (2%)	2 (0%)	24	22
1	L	411/427 (96%)	399 (97%)	10 (2%)	2 (0%)	24	22
All	All	4932/5124 (96%)	4776 (97%)	130 (3%)	26 (0%)	24	22

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	ASP
1	H	41	ASP
1	I	41	ASP
1	J	41	ASP
1	K	41	ASP
1	L	41	ASP
1	A	41	ASP
1	C	41	ASP
1	D	41	ASP
1	E	41	ASP
1	F	41	ASP
1	G	41	ASP

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Mol	Chain	Res	Type
1	G	323	GLY
1	H	323	GLY
1	J	323	GLY
1	K	323	GLY
1	B	323	GLY
1	E	159	LYS
1	E	323	GLY
1	A	36	GLU
1	I	323	GLY
1	L	323	GLY
1	A	323	GLY
1	B	405	SER
1	C	323	GLY
1	D	323	GLY

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	373/387 (96%)	368 (99%)	5 (1%)	61	69
1	B	373/387 (96%)	368 (99%)	5 (1%)	61	69
1	C	373/387 (96%)	368 (99%)	5 (1%)	61	69
1	D	373/387 (96%)	369 (99%)	4 (1%)	65	74
1	E	373/387 (96%)	366 (98%)	7 (2%)	50	58
1	F	373/387 (96%)	366 (98%)	7 (2%)	50	58
1	G	373/387 (96%)	368 (99%)	5 (1%)	61	69
1	H	373/387 (96%)	368 (99%)	5 (1%)	61	69
1	I	373/387 (96%)	369 (99%)	4 (1%)	65	74
1	J	373/387 (96%)	368 (99%)	5 (1%)	61	69
1	K	373/387 (96%)	369 (99%)	4 (1%)	65	74
1	L	373/387 (96%)	369 (99%)	4 (1%)	65	74
All	All	4476/4644 (96%)	4416 (99%)	60 (1%)	61	69

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	127	GLN
1	A	133	GLN
1	A	264	ARG
1	A	364	TYR
1	B	128	VAL
1	B	180	GLN
1	B	187	ASP
1	B	244	LEU
1	B	364	TYR
1	C	127	GLN
1	C	182	LYS
1	C	244	LEU
1	C	364	TYR
1	C	385	LEU
1	D	127	GLN
1	D	133	GLN
1	D	206	ARG
1	D	364	TYR
1	E	15	ASN
1	E	175	LEU
1	E	180	GLN
1	E	185	LEU
1	E	191	LYS
1	E	244	LEU
1	E	364	TYR
1	F	72	ARG
1	F	127	GLN
1	F	128	VAL
1	F	191	LYS
1	F	305	ASN
1	F	364	TYR
1	F	385	LEU
1	G	15	ASN
1	G	127	GLN
1	G	180	GLN
1	G	187	ASP
1	G	364	TYR
1	H	41	ASP
1	H	127	GLN
1	H	364	TYR
1	H	385	LEU

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Mol	Chain	Res	Type
1	H	386	GLN
1	I	133	GLN
1	I	174	LEU
1	I	244	LEU
1	I	364	TYR
1	J	15	ASN
1	J	121	LYS
1	J	127	GLN
1	J	244	LEU
1	J	364	TYR
1	K	113	GLN
1	K	264	ARG
1	K	364	TYR
1	K	386	GLN
1	L	133	GLN
1	L	182	LYS
1	L	244	LEU
1	L	364	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	20	GLN
1	A	113	GLN
1	A	127	GLN
1	A	166	HIS
1	A	252	ASN
1	A	293	ASN
1	B	4	ASN
1	B	18	ASN
1	B	113	GLN
1	B	127	GLN
1	B	166	HIS
1	B	180	GLN
1	B	202	GLN
1	B	252	ASN
1	B	293	ASN
1	C	4	ASN
1	C	18	ASN
1	C	20	GLN
1	C	127	GLN

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Mol	Chain	Res	Type
1	C	166	HIS
1	C	180	GLN
1	C	202	GLN
1	C	252	ASN
1	C	293	ASN
1	C	386	GLN
1	D	18	ASN
1	D	74	GLN
1	D	113	GLN
1	D	127	GLN
1	D	166	HIS
1	D	183	HIS
1	D	193	ASN
1	D	202	GLN
1	D	252	ASN
1	D	293	ASN
1	D	367	HIS
1	E	18	ASN
1	E	74	GLN
1	E	113	GLN
1	E	127	GLN
1	E	166	HIS
1	E	180	GLN
1	E	202	GLN
1	E	251	HIS
1	E	252	ASN
1	E	293	ASN
1	F	4	ASN
1	F	18	ASN
1	F	20	GLN
1	F	113	GLN
1	F	127	GLN
1	F	166	HIS
1	F	180	GLN
1	F	202	GLN
1	F	235	ASN
1	F	252	ASN
1	F	293	ASN
1	F	386	GLN
1	G	18	ASN
1	G	127	GLN
1	G	166	HIS

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Mol	Chain	Res	Type
1	G	180	GLN
1	G	193	ASN
1	H	18	ASN
1	H	20	GLN
1	H	127	GLN
1	H	166	HIS
1	H	180	GLN
1	H	193	ASN
1	H	197	ASN
1	H	330	ASN
1	H	386	GLN
1	I	18	ASN
1	I	101	GLN
1	I	127	GLN
1	I	166	HIS
1	I	293	ASN
1	J	18	ASN
1	J	20	GLN
1	J	113	GLN
1	J	127	GLN
1	J	166	HIS
1	J	235	ASN
1	J	252	ASN
1	K	18	ASN
1	K	20	GLN
1	K	113	GLN
1	K	127	GLN
1	K	166	HIS
1	K	252	ASN
1	K	286	HIS
1	K	330	ASN
1	K	386	GLN
1	L	18	ASN
1	L	113	GLN
1	L	127	GLN
1	L	166	HIS
1	L	183	HIS
1	L	202	GLN
1	L	252	ASN
1	L	293	ASN
1	L	367	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 40 ligands modelled in this entry, 16 are monoatomic - leaving 24 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	REL	F	428	4	11,12,12	0.99	0	14,16,16	1.22	1 (7%)
2	REL	I	428	4	11,12,12	1.00	0	14,16,16	1.11	1 (7%)
2	REL	C	428	4	11,12,12	1.07	0	14,16,16	1.16	1 (7%)
2	REL	H	428	4	11,12,12	0.98	0	14,16,16	1.13	2 (14%)
3	CO3	D	430	-	3,3,3	0.79	0	2,3,3	0.13	0
2	REL	B	428	4	11,12,12	1.07	0	14,16,16	1.08	2 (14%)
2	REL	G	428	4	11,12,12	0.99	0	14,16,16	1.16	1 (7%)
3	CO3	C	429	-	3,3,3	0.78	0	2,3,3	0.06	0
3	CO3	G	429	-	3,3,3	0.85	0	2,3,3	0.17	0
3	CO3	L	429	-	3,3,3	0.80	0	2,3,3	0.04	0
3	CO3	F	429	-	3,3,3	0.87	0	2,3,3	0.06	0
2	REL	D	428	4	11,12,12	1.00	0	14,16,16	1.15	1 (7%)
3	CO3	J	429	-	3,3,3	0.99	0	2,3,3	0.20	0
3	CO3	A	429	-	3,3,3	1.06	0	2,3,3	0.18	0
2	REL	L	428	4	11,12,12	1.01	0	14,16,16	1.13	1 (7%)
3	CO3	D	429	-	3,3,3	0.93	0	2,3,3	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CO3	K	429	-	3,3,3	0.84	0	2,3,3	0.26	0
2	REL	J	428	4	11,12,12	1.04	0	14,16,16	1.13	2 (14%)
2	REL	A	428	4	11,12,12	1.15	0	14,16,16	1.13	1 (7%)
2	REL	K	428	4	11,12,12	0.96	0	14,16,16	1.17	2 (14%)
2	REL	E	428	4	11,12,12	1.14	1 (9%)	14,16,16	1.15	2 (14%)
3	CO3	I	429	-	3,3,3	0.72	0	2,3,3	0.09	0
3	CO3	A	430	-	3,3,3	0.74	0	2,3,3	0.11	0
3	CO3	H	429	-	3,3,3	0.77	0	2,3,3	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	REL	L	428	4	-	10/17/18/18	-
2	REL	F	428	4	-	9/17/18/18	-
2	REL	K	428	4	-	10/17/18/18	-
2	REL	I	428	4	-	10/17/18/18	-
2	REL	C	428	4	-	11/17/18/18	-
2	REL	H	428	4	-	10/17/18/18	-
2	REL	J	428	4	-	11/17/18/18	-
2	REL	A	428	4	-	9/17/18/18	-
2	REL	D	428	4	-	9/17/18/18	-
2	REL	E	428	4	-	8/17/18/18	-
2	REL	B	428	4	-	9/17/18/18	-
2	REL	G	428	4	-	11/17/18/18	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	428	REL	C3-C2	2.02	1.56	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	428	REL	O6A-C6-C5	-2.38	115.28	121.62
2	J	428	REL	O6A-C6-C5	-2.37	115.30	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	428	REL	O6A-C6-C5	-2.37	115.32	121.62
2	E	428	REL	O6A-C6-C5	-2.34	115.39	121.62
2	H	428	REL	O6A-C6-C5	-2.32	115.43	121.62
2	G	428	REL	O6A-C6-C5	-2.32	115.44	121.62
2	B	428	REL	O6A-C6-C5	-2.27	115.56	121.62
2	I	428	REL	O6A-C6-C5	-2.27	115.57	121.62
2	C	428	REL	O6A-C6-C5	-2.26	115.61	121.62
2	L	428	REL	O6A-C6-C5	-2.23	115.67	121.62
2	D	428	REL	O6A-C6-C5	-2.21	115.73	121.62
2	B	428	REL	O6B-C6-C5	2.17	119.33	113.31
2	A	428	REL	O6A-C6-C5	-2.10	116.02	121.62
2	K	428	REL	O6B-C6-C5	2.09	119.12	113.31
2	E	428	REL	O6B-C6-C5	2.06	119.03	113.31
2	H	428	REL	O6B-C6-C5	2.03	118.97	113.31
2	J	428	REL	O6B-C6-C5	2.03	118.95	113.31

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	428	REL	O2-C2-C3-C4
2	A	428	REL	C1-C2-C3-C4
2	A	428	REL	O2-C2-C3-O3
2	A	428	REL	C1-C2-C3-O3
2	B	428	REL	O2-C2-C3-C4
2	B	428	REL	C1-C2-C3-C4
2	B	428	REL	O2-C2-C3-O3
2	B	428	REL	C1-C2-C3-O3
2	B	428	REL	O1-C1-C2-C3
2	C	428	REL	O2-C2-C3-C4
2	C	428	REL	C1-C2-C3-C4
2	C	428	REL	O2-C2-C3-O3
2	C	428	REL	C1-C2-C3-O3
2	C	428	REL	O1-C1-C2-C3
2	D	428	REL	O2-C2-C3-C4
2	D	428	REL	C1-C2-C3-C4
2	D	428	REL	O2-C2-C3-O3
2	D	428	REL	C1-C2-C3-O3
2	E	428	REL	O2-C2-C3-C4
2	E	428	REL	C1-C2-C3-C4
2	E	428	REL	O2-C2-C3-O3
2	E	428	REL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	F	428	REL	O2-C2-C3-C4
2	F	428	REL	C1-C2-C3-C4
2	F	428	REL	O2-C2-C3-O3
2	G	428	REL	O2-C2-C3-C4
2	G	428	REL	C1-C2-C3-C4
2	G	428	REL	O2-C2-C3-O3
2	G	428	REL	C1-C2-C3-O3
2	G	428	REL	O1-C1-C2-C3
2	H	428	REL	O2-C2-C3-C4
2	H	428	REL	C1-C2-C3-C4
2	H	428	REL	O2-C2-C3-O3
2	H	428	REL	C1-C2-C3-O3
2	I	428	REL	O2-C2-C3-C4
2	I	428	REL	C1-C2-C3-C4
2	I	428	REL	O2-C2-C3-O3
2	I	428	REL	C1-C2-C3-O3
2	J	428	REL	O2-C2-C3-C4
2	J	428	REL	C1-C2-C3-C4
2	J	428	REL	O2-C2-C3-O3
2	J	428	REL	C1-C2-C3-O3
2	J	428	REL	O1-C1-C2-C3
2	K	428	REL	O2-C2-C3-C4
2	K	428	REL	C1-C2-C3-C4
2	K	428	REL	O2-C2-C3-O3
2	K	428	REL	O1-C1-C2-C3
2	L	428	REL	O2-C2-C3-C4
2	L	428	REL	C1-C2-C3-C4
2	L	428	REL	O2-C2-C3-O3
2	L	428	REL	C1-C2-C3-O3
2	L	428	REL	O1-C1-C2-C3
2	B	428	REL	O5-C5-C6-O6A
2	B	428	REL	O5-C5-C6-O6B
2	E	428	REL	O5-C5-C6-O6A
2	E	428	REL	O5-C5-C6-O6B
2	C	428	REL	O5-C5-C6-O6A
2	G	428	REL	O5-C5-C6-O6A
2	L	428	REL	O5-C5-C6-O6A
2	D	428	REL	O5-C5-C6-O6A
2	F	428	REL	O5-C5-C6-O6A
2	I	428	REL	O5-C5-C6-O6A
2	J	428	REL	O5-C5-C6-O6A
2	K	428	REL	O5-C5-C6-O6A

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Mol	Chain	Res	Type	Atoms
2	C	428	REL	O5-C5-C6-O6B
2	D	428	REL	O5-C5-C6-O6B
2	F	428	REL	O5-C5-C6-O6B
2	G	428	REL	O5-C5-C6-O6B
2	I	428	REL	O5-C5-C6-O6B
2	J	428	REL	O5-C5-C6-O6B
2	L	428	REL	O5-C5-C6-O6B
2	A	428	REL	O5-C5-C6-O6A
2	K	428	REL	O5-C5-C6-O6B
2	A	428	REL	O5-C5-C6-O6B
2	H	428	REL	O5-C5-C6-O6B
2	H	428	REL	O5-C5-C6-O6A
2	E	428	REL	C2-C3-C4-C5
2	G	428	REL	C2-C3-C4-C5
2	B	428	REL	C2-C3-C4-C5
2	A	428	REL	C4-C5-C6-O6A
2	F	428	REL	C1-C2-C3-O3
2	K	428	REL	C1-C2-C3-O3
2	H	428	REL	C4-C5-C6-O6B
2	C	428	REL	C2-C3-C4-C5
2	H	428	REL	C2-C3-C4-C5
2	I	428	REL	C2-C3-C4-C5
2	J	428	REL	C2-C3-C4-C5
2	H	428	REL	C4-C5-C6-O6A
2	K	428	REL	C4-C5-C6-O6A
2	E	428	REL	O3-C3-C4-C5
2	A	428	REL	C4-C5-C6-O6B
2	D	428	REL	C4-C5-C6-O6A
2	I	428	REL	C4-C5-C6-O6A
2	G	428	REL	O3-C3-C4-C5
2	K	428	REL	C4-C5-C6-O6B
2	D	428	REL	C4-C5-C6-O6B
2	J	428	REL	C4-C5-C6-O6B
2	B	428	REL	O3-C3-C4-C5
2	I	428	REL	C4-C5-C6-O6B
2	J	428	REL	C4-C5-C6-O6A
2	F	428	REL	C4-C5-C6-O6A
2	F	428	REL	C4-C5-C6-O6B
2	C	428	REL	C4-C5-C6-O6B
2	L	428	REL	C4-C5-C6-O6B
2	D	428	REL	C2-C3-C4-C5
2	F	428	REL	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	G	428	REL	C4-C5-C6-O6B
2	C	428	REL	C4-C5-C6-O6A
2	K	428	REL	C2-C3-C4-C5
2	L	428	REL	C2-C3-C4-C5
2	C	428	REL	O3-C3-C4-C5
2	I	428	REL	O3-C3-C4-C5
2	G	428	REL	C4-C5-C6-O6A
2	L	428	REL	C4-C5-C6-O6A
2	H	428	REL	O3-C3-C4-C5
2	A	428	REL	C2-C3-C4-C5
2	J	428	REL	O3-C3-C4-C5

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	428	REL	1	0
2	C	428	REL	1	0
2	H	428	REL	1	0
2	G	428	REL	1	0
2	D	428	REL	1	0
2	L	428	REL	1	0
2	A	428	REL	1	0
2	K	428	REL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	413/427 (96%)	0.14	8 (1%) 66 69	18, 28, 47, 64	0
1	B	413/427 (96%)	0.37	22 (5%) 32 34	19, 30, 50, 65	0
1	C	413/427 (96%)	0.09	9 (2%) 62 65	17, 27, 43, 63	0
1	D	413/427 (96%)	-0.01	4 (0%) 79 81	15, 25, 42, 62	0
1	E	413/427 (96%)	0.34	19 (4%) 37 39	18, 29, 47, 65	0
1	F	413/427 (96%)	0.15	14 (3%) 48 50	18, 28, 46, 65	0
1	G	413/427 (96%)	0.12	10 (2%) 59 62	18, 28, 46, 64	0
1	H	413/427 (96%)	0.14	15 (3%) 46 48	17, 28, 47, 65	0
1	I	413/427 (96%)	0.17	10 (2%) 59 62	18, 28, 48, 64	0
1	J	413/427 (96%)	0.07	11 (2%) 56 59	16, 27, 43, 64	0
1	K	413/427 (96%)	0.16	16 (3%) 43 45	17, 27, 47, 62	0
1	L	413/427 (96%)	-0.06	9 (2%) 62 65	16, 25, 44, 62	0
All	All	4956/5124 (96%)	0.14	147 (2%) 52 55	15, 28, 46, 65	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	414	ARG	4.9
1	H	414	ARG	4.4
1	E	413	GLY	4.3
1	F	413	GLY	4.3
1	B	153	ILE	4.0
1	F	414	ARG	3.9
1	E	128	VAL	3.8
1	D	60	ASP	3.8
1	E	414	ARG	3.7
1	C	413	GLY	3.7
1	L	414	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	414	ARG	3.5
1	B	414	ARG	3.4
1	B	204	VAL	3.4
1	J	390	GLU	3.4
1	A	153	ILE	3.4
1	I	414	ARG	3.3
1	B	191	LYS	3.3
1	H	60	ASP	3.2
1	A	414	ARG	3.2
1	D	414	ARG	3.1
1	E	153	ILE	3.1
1	F	180	GLN	3.1
1	H	185	LEU	3.0
1	F	153	ILE	3.0
1	B	413	GLY	3.0
1	E	195	GLU	3.0
1	L	180	GLN	3.0
1	G	414	ARG	2.9
1	A	60	ASP	2.9
1	B	192	VAL	2.9
1	C	414	ARG	2.9
1	I	186	ARG	2.9
1	H	4	ASN	2.9
1	F	37	ILE	2.9
1	K	186	ARG	2.9
1	J	2	SER	2.8
1	H	186	ARG	2.8
1	H	113	GLN	2.8
1	E	158	GLY	2.8
1	D	153	ILE	2.8
1	B	186	ARG	2.8
1	F	113	GLN	2.8
1	K	113	GLN	2.7
1	B	158	GLY	2.7
1	E	18	ASN	2.7
1	I	183	HIS	2.7
1	H	195	GLU	2.7
1	K	4	ASN	2.7
1	H	183	HIS	2.7
1	C	194	ASP	2.7
1	I	153	ILE	2.7
1	G	413	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	194	ASP	2.6
1	E	121	LYS	2.6
1	A	183	HIS	2.6
1	K	197	ASN	2.6
1	G	186	ARG	2.6
1	I	180	GLN	2.6
1	A	413	GLY	2.6
1	H	187	ASP	2.6
1	B	183	HIS	2.5
1	K	183	HIS	2.5
1	D	121	LYS	2.5
1	E	37	ILE	2.5
1	C	153	ILE	2.5
1	L	121	LYS	2.5
1	C	37	ILE	2.5
1	B	2	SER	2.4
1	L	113	GLN	2.4
1	E	113	GLN	2.4
1	G	198	GLU	2.4
1	C	60	ASP	2.4
1	E	61	VAL	2.4
1	I	264	ARG	2.4
1	J	413	GLY	2.4
1	K	413	GLY	2.4
1	J	128	VAL	2.4
1	C	121	LYS	2.4
1	G	183	HIS	2.4
1	K	185	LEU	2.3
1	A	186	ARG	2.3
1	K	37	ILE	2.3
1	B	128	VAL	2.3
1	A	194	ASP	2.3
1	H	61	VAL	2.3
1	G	4	ASN	2.3
1	H	413	GLY	2.3
1	C	195	GLU	2.3
1	L	128	VAL	2.3
1	I	152	ARG	2.3
1	H	194	ASP	2.3
1	K	122	LYS	2.3
1	K	188	TRP	2.3
1	C	113	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	113	GLN	2.2
1	K	180	GLN	2.2
1	B	63	ILE	2.2
1	B	196	TRP	2.2
1	G	410	ARG	2.2
1	E	253	ILE	2.2
1	G	194	ASP	2.2
1	I	60	ASP	2.2
1	K	198	GLU	2.2
1	B	180	GLN	2.2
1	B	207	PHE	2.2
1	J	36	GLU	2.2
1	G	187	ASP	2.2
1	G	153	ILE	2.1
1	B	247	VAL	2.1
1	E	192	VAL	2.1
1	L	391	VAL	2.1
1	L	72	ARG	2.1
1	B	121	LYS	2.1
1	B	113	GLN	2.1
1	E	152	ARG	2.1
1	J	410	ARG	2.1
1	F	156	LEU	2.1
1	J	159	LYS	2.1
1	F	60	ASP	2.1
1	K	187	ASP	2.1
1	E	183	HIS	2.1
1	E	72	ARG	2.1
1	H	72	ARG	2.1
1	L	153	ILE	2.1
1	B	137	VAL	2.1
1	B	154	SER	2.1
1	E	2	SER	2.1
1	F	64	GLU	2.1
1	I	195	GLU	2.1
1	F	160	GLN	2.1
1	B	6	ARG	2.1
1	H	122	LYS	2.1
1	H	153	ILE	2.1
1	A	192	VAL	2.1
1	E	198	GLU	2.0
1	B	184	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	72	ARG	2.0
1	K	152	ARG	2.0
1	F	190	TYR	2.0
1	F	213	GLU	2.0
1	F	163	SER	2.0
1	E	68	ALA	2.0
1	K	65	ALA	2.0
1	F	194	ASP	2.0
1	J	121	LYS	2.0
1	L	159	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	REL	I	428	13/13	0.88	0.10	27,31,32,32	0
2	REL	B	428	13/13	0.89	0.10	29,31,34,34	0
2	REL	L	428	13/13	0.89	0.10	24,27,29,29	0
2	REL	A	428	13/13	0.90	0.09	28,31,32,32	0
2	REL	E	428	13/13	0.90	0.09	27,30,34,34	0
2	REL	J	428	13/13	0.91	0.09	25,28,31,31	0
2	REL	D	428	13/13	0.92	0.08	25,27,28,29	0
2	REL	F	428	13/13	0.92	0.08	25,28,31,31	0
2	REL	K	428	13/13	0.92	0.08	26,30,31,31	0
2	REL	H	428	13/13	0.92	0.07	25,31,33,33	0
2	REL	C	428	13/13	0.93	0.08	26,29,30,30	0
2	REL	G	428	13/13	0.94	0.07	25,27,29,29	0
3	CO3	A	429	4/4	0.94	0.07	23,24,25,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CO3	C	429	4/4	0.94	0.07	22,22,23,24	0
3	CO3	F	429	4/4	0.94	0.07	24,25,26,29	0
3	CO3	I	429	4/4	0.96	0.07	23,24,26,26	0
3	CO3	A	430	4/4	0.97	0.05	21,22,23,25	0
3	CO3	H	429	4/4	0.97	0.05	24,25,25,25	0
3	CO3	D	429	4/4	0.97	0.05	18,20,21,21	0
3	CO3	K	429	4/4	0.97	0.04	20,22,22,23	0
3	CO3	L	429	4/4	0.97	0.05	19,20,23,25	0
3	CO3	D	430	4/4	0.98	0.04	20,20,21,24	0
4	ZN	E	429	1/1	0.98	0.03	27,27,27,27	0
3	CO3	J	429	4/4	0.99	0.04	18,18,20,22	0
4	ZN	A	431	1/1	0.99	0.02	27,27,27,27	0
4	ZN	B	429	1/1	0.99	0.05	36,36,36,36	0
4	ZN	C	430	1/1	0.99	0.02	26,26,26,26	0
4	ZN	D	431	1/1	0.99	0.03	21,21,21,21	0
3	CO3	G	429	4/4	0.99	0.04	19,21,22,22	0
4	ZN	F	430	1/1	0.99	0.04	30,30,30,30	0
4	ZN	I	430	1/1	0.99	0.04	32,32,32,32	0
4	ZN	K	430	1/1	0.99	0.02	29,29,29,29	0
4	ZN	L	430	1/1	0.99	0.02	24,24,24,24	0
5	CL	H	431	1/1	0.99	0.03	21,21,21,21	0
4	ZN	H	430	1/1	1.00	0.05	33,33,33,33	0
4	ZN	G	430	1/1	1.00	0.02	27,27,27,27	0
5	CL	A	432	1/1	1.00	0.03	23,23,23,23	0
5	CL	F	431	1/1	1.00	0.01	20,20,20,20	0
4	ZN	J	430	1/1	1.00	0.02	25,25,25,25	0
5	CL	K	431	1/1	1.00	0.02	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.