



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:30 PM UTC

PDB ID : 1ZUM / pdb_00001zum
Title : Human Mitochondrial Aldehyde Dehydrogenase Asian Variant, ALDH2*2, Apo Form
Authors : Larson, H.N.; Weiner, H.; Hurley, T.D.
Deposited on : 2005-05-31
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

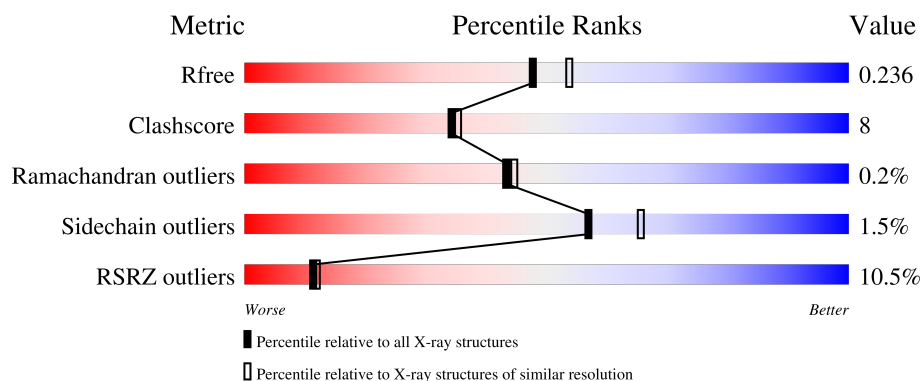
1 Overall quality at a glance

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	500	16% 77% 16% • 6%
1	B	500	3% 79% 12% • 7%
1	C	500	5% 76% 16% • 6%
1	D	500	10% 73% 20% • 6%
1	E	500	4% 77% 15% • 6%

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Mol	Chain	Length	Quality of chain
1	F	500	
1	G	500	
1	H	500	
1	I	500	
1	J	500	
1	K	500	
1	L	500	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GAI	A	3101	-	-	X	-
3	GAI	I	3107	-	-	X	-
3	GAI	L	3108	-	-	X	-
4	EDO	A	3116	-	-	X	-
4	EDO	D	3126	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 46002 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3620	2306	618	679	17			
1	B	465	Total	C	N	O	S	0	0	0
			3585	2286	610	672	17			
1	C	468	Total	C	N	O	S	0	0	0
			3612	2302	617	676	17			
1	D	468	Total	C	N	O	S	0	0	0
			3608	2301	613	677	17			
1	E	469	Total	C	N	O	S	0	0	0
			3624	2311	618	678	17			
1	F	468	Total	C	N	O	S	0	0	0
			3612	2302	617	676	17			
1	G	469	Total	C	N	O	S	0	0	0
			3624	2311	618	678	17			
1	H	469	Total	C	N	O	S	0	0	0
			3624	2311	618	678	17			
1	I	468	Total	C	N	O	S	0	0	0
			3615	2305	616	677	17			
1	J	467	Total	C	N	O	S	0	0	0
			3604	2299	612	676	17			
1	K	456	Total	C	N	O	S	0	0	0
			3526	2250	598	661	17			
1	L	462	Total	C	N	O	S	0	0	0
			3571	2279	607	668	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	487	LYS	GLU	engineered mutation	UNP P05091
B	487	LYS	GLU	engineered mutation	UNP P05091
C	487	LYS	GLU	engineered mutation	UNP P05091
D	487	LYS	GLU	engineered mutation	UNP P05091
E	487	LYS	GLU	engineered mutation	UNP P05091

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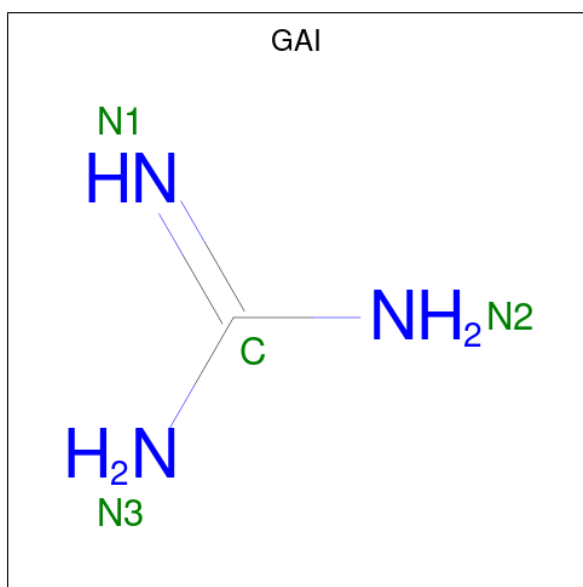
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Chain	Residue	Modelled	Actual	Comment	Reference
F	487	LYS	GLU	engineered mutation	UNP P05091
G	487	LYS	GLU	engineered mutation	UNP P05091
H	487	LYS	GLU	engineered mutation	UNP P05091
I	487	LYS	GLU	engineered mutation	UNP P05091
J	487	LYS	GLU	engineered mutation	UNP P05091
K	487	LYS	GLU	engineered mutation	UNP P05091
L	487	LYS	GLU	engineered mutation	UNP P05091

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

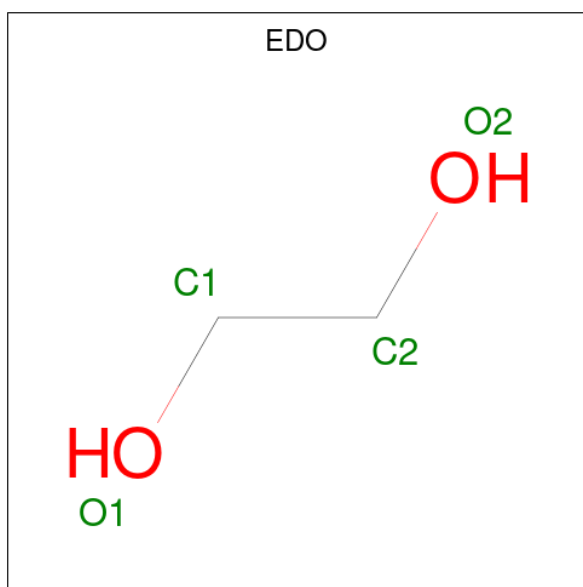
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0
2	G	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	I	1	Total Na 1 1	0	0
2	J	1	Total Na 1 1	0	0
2	K	1	Total Na 1 1	0	0
2	L	1	Total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

- Molecule 3 is GUANIDINE (CCD ID: GAI) (formula: CH₅N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			4	1	3		
3	E	1	Total	C	N	0	0
			4	1	3		
3	F	1	Total	C	N	0	0
			4	1	3		
3	F	1	Total	C	N	0	0
			4	1	3		
3	G	1	Total	C	N	0	0
			4	1	3		
3	H	1	Total	C	N	0	0
			4	1	3		
3	I	1	Total	C	N	0	0
			4	1	3		
3	L	1	Total	C	N	0	0
			4	1	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0
4	L	1	Total C O 4 2 2	0	0

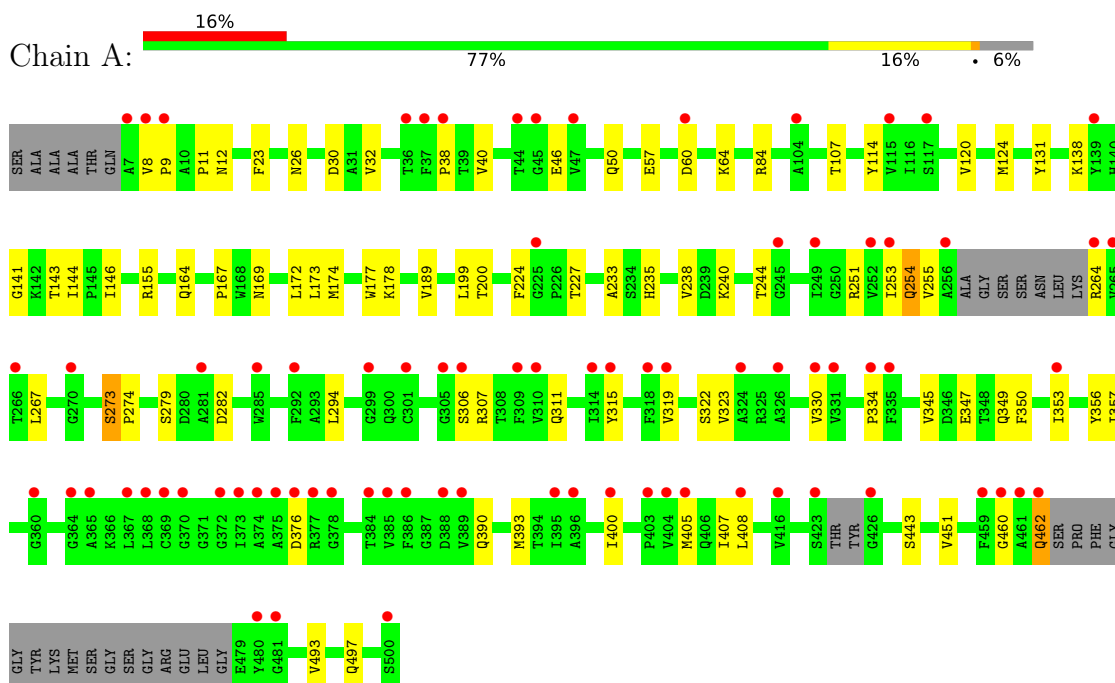
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	189	Total O 189 189	0	0
5	B	299	Total O 299 299	0	0
5	C	290	Total O 290 290	0	0
5	D	187	Total O 187 187	0	0
5	E	285	Total O 285 285	0	0
5	F	367	Total O 367 367	0	0
5	G	285	Total O 285 285	0	0
5	H	236	Total O 236 236	0	0
5	I	189	Total O 189 189	0	0
5	J	141	Total O 141 141	0	0
5	K	93	Total O 93 93	0	0
5	L	88	Total O 88 88	0	0

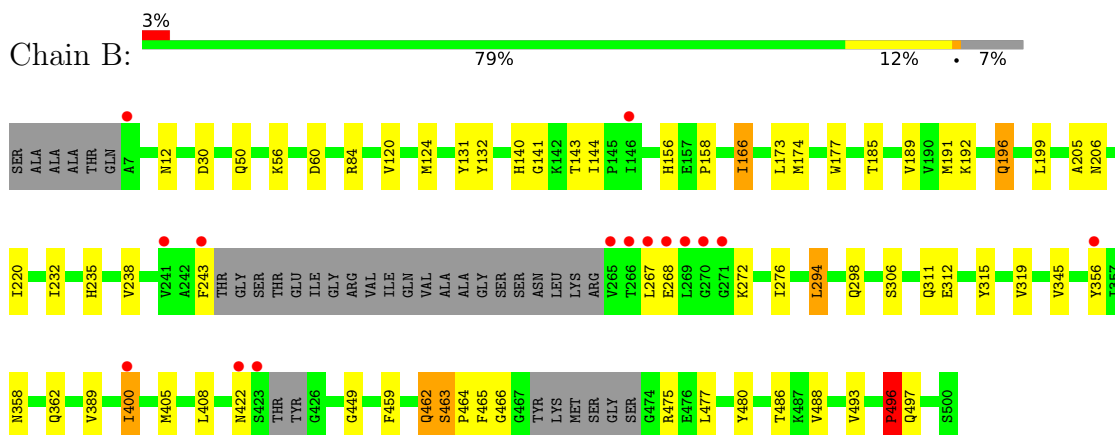
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

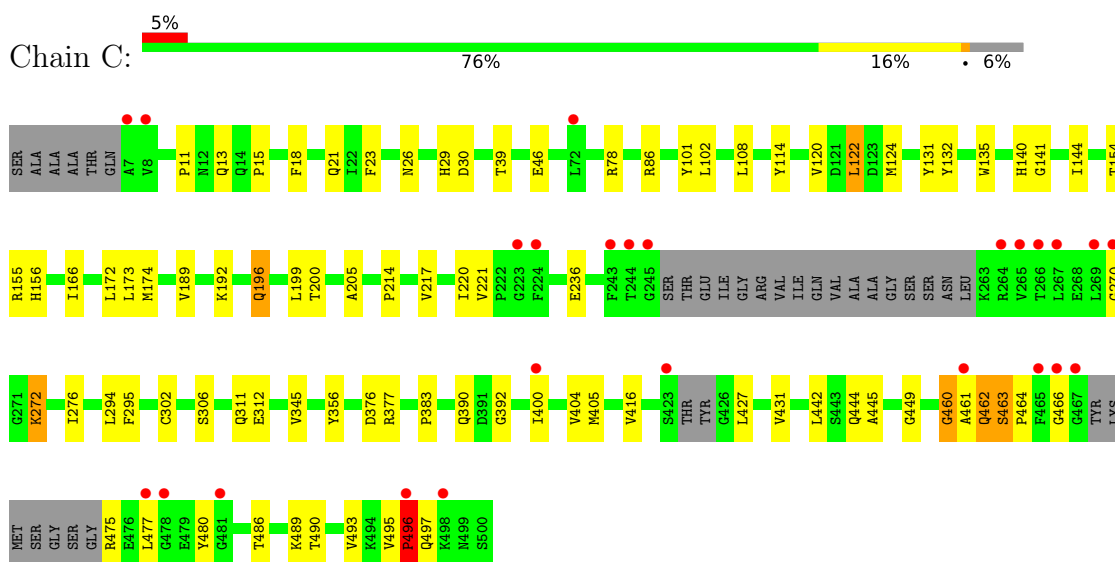
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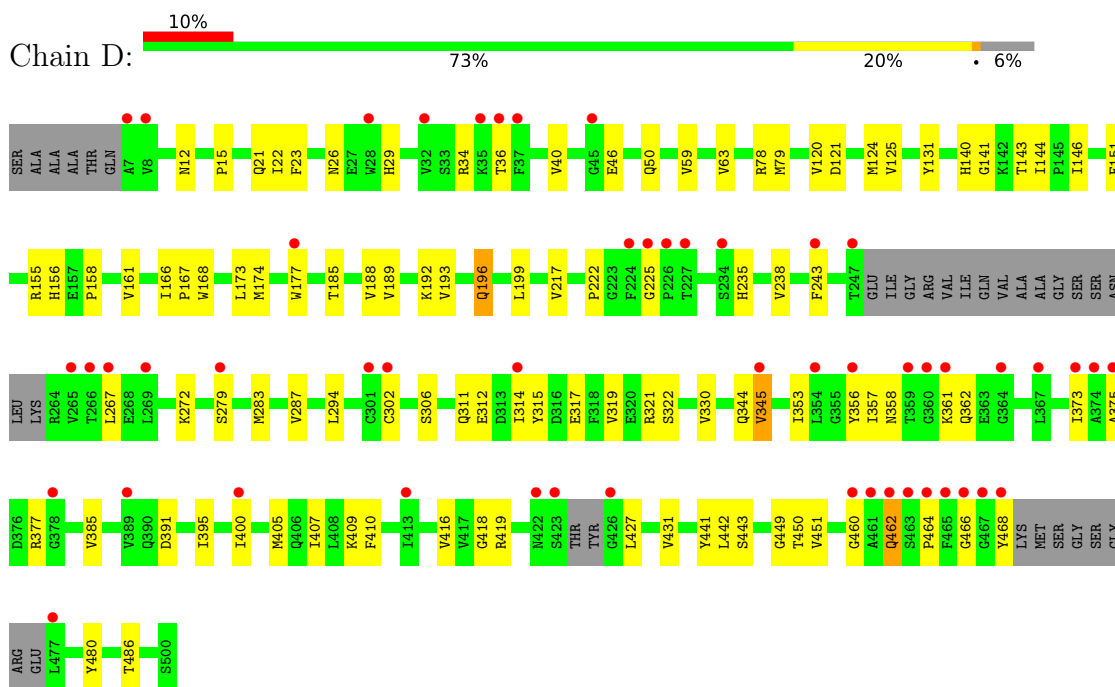
• Molecule 1: Aldehyde dehydrogenase



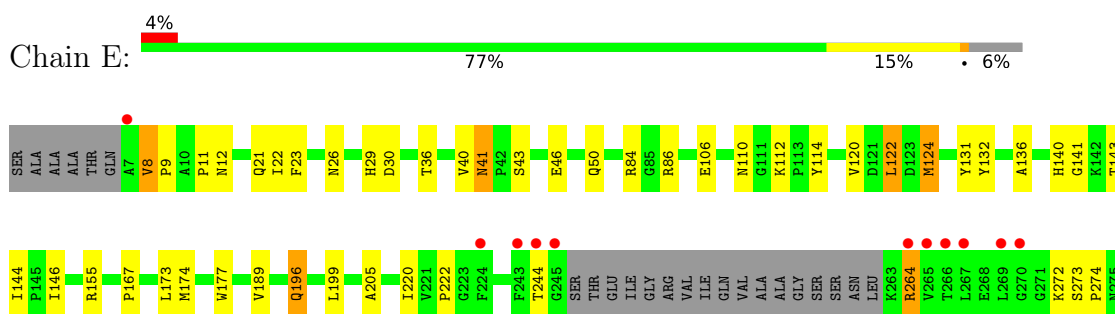
• Molecule 1: Aldehyde dehydrogenase

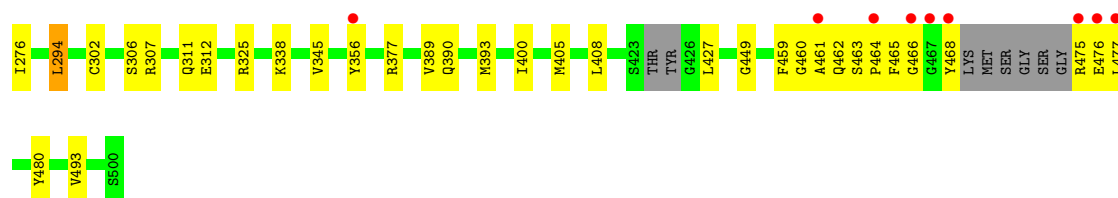


- Molecule 1: Aldehyde dehydrogenase

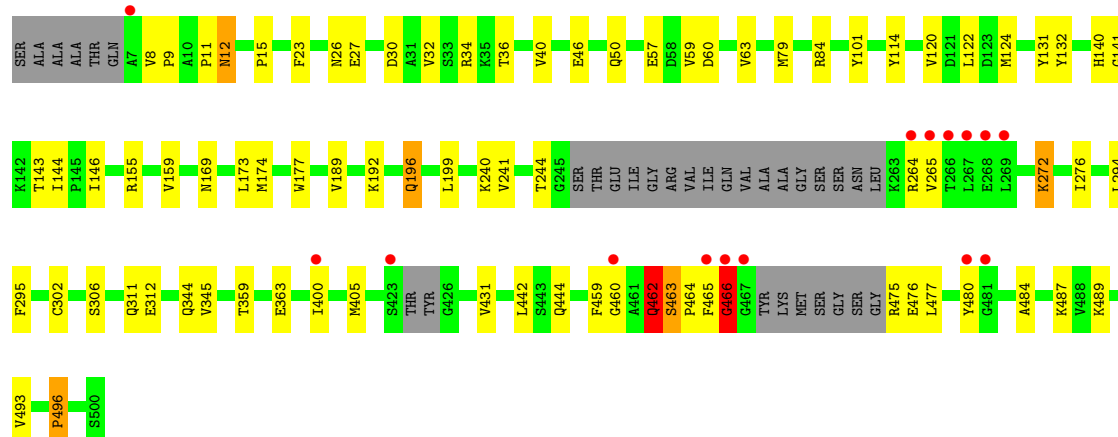
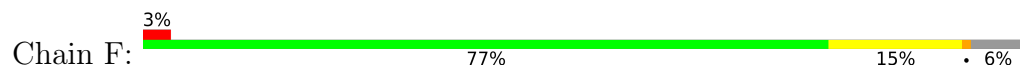


- Molecule 1: Aldehyde dehydrogenase

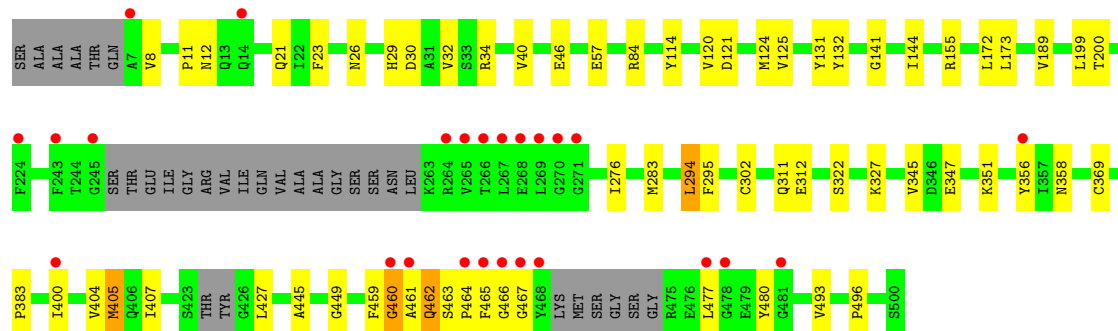
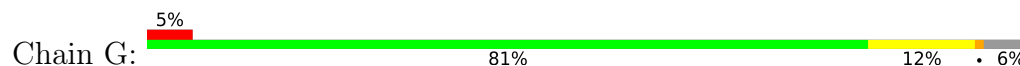




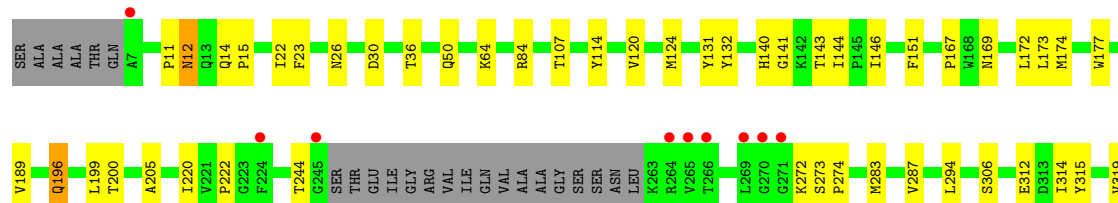
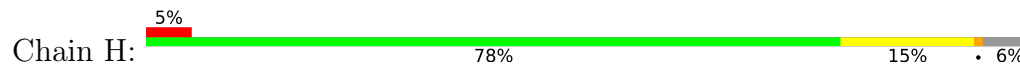
• Molecule 1: Aldehyde dehydrogenase

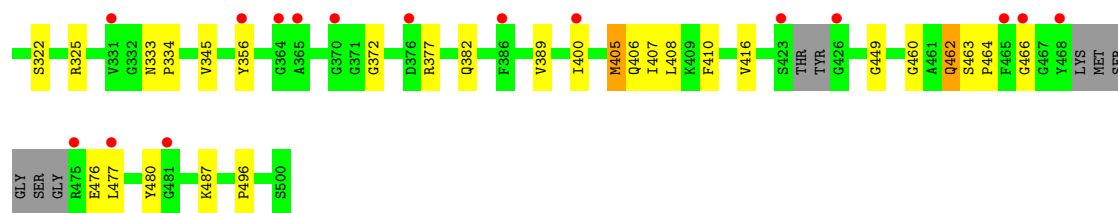


• Molecule 1: Aldehyde dehydrogenase

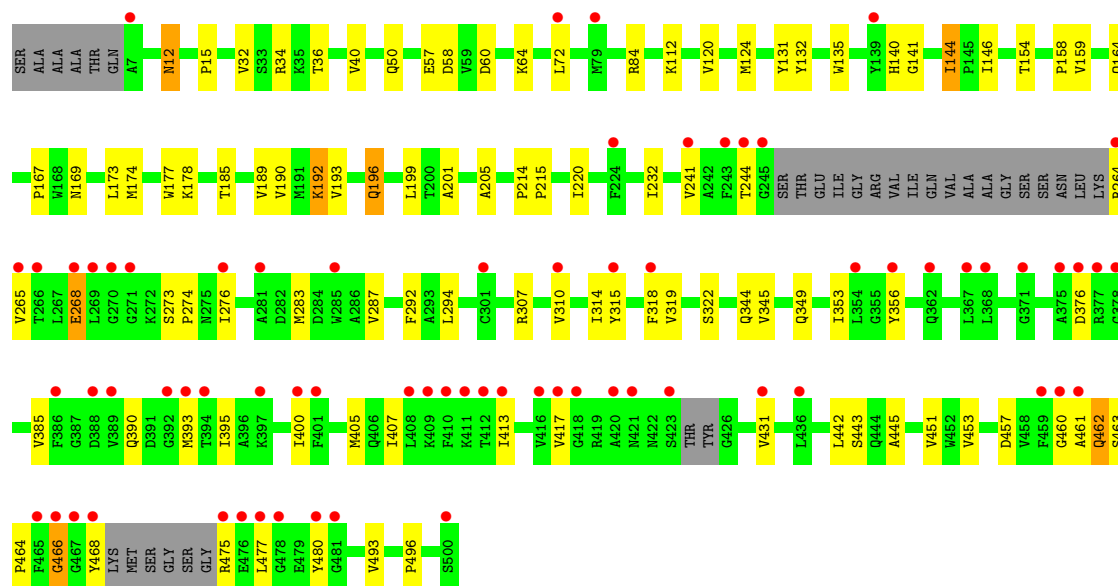
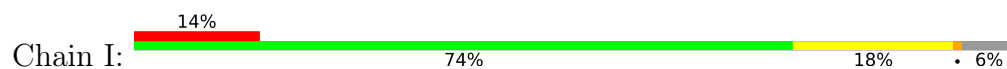


• Molecule 1: Aldehyde dehydrogenase

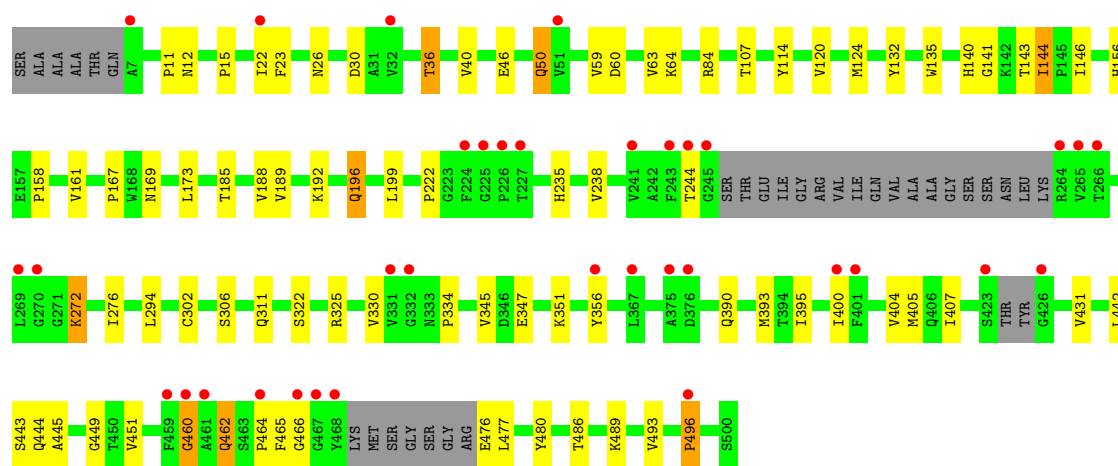
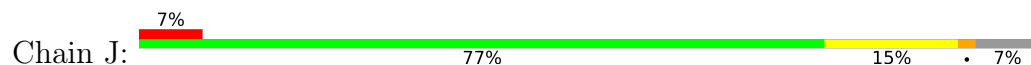




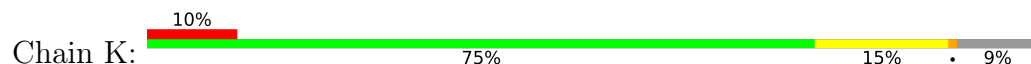
• Molecule 1: Aldehyde dehydrogenase

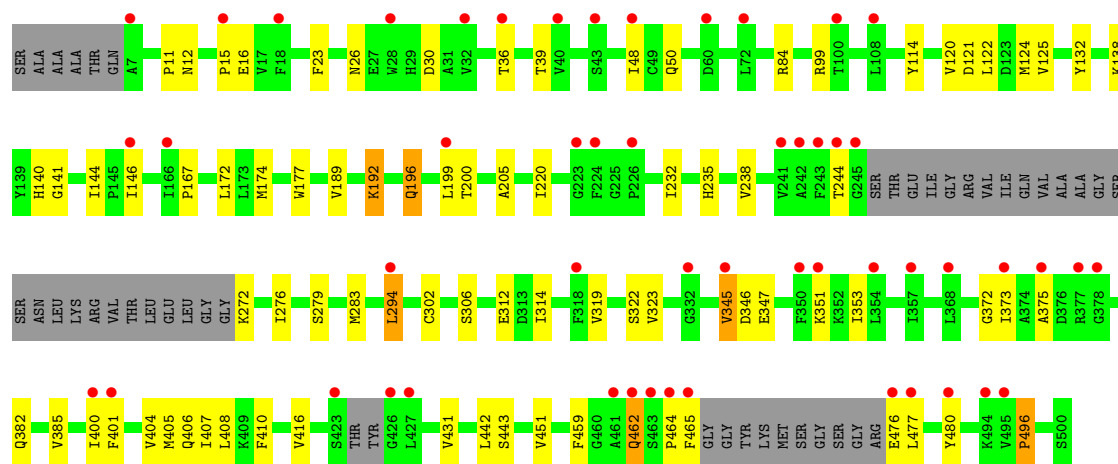


• Molecule 1: Aldehyde dehydrogenase

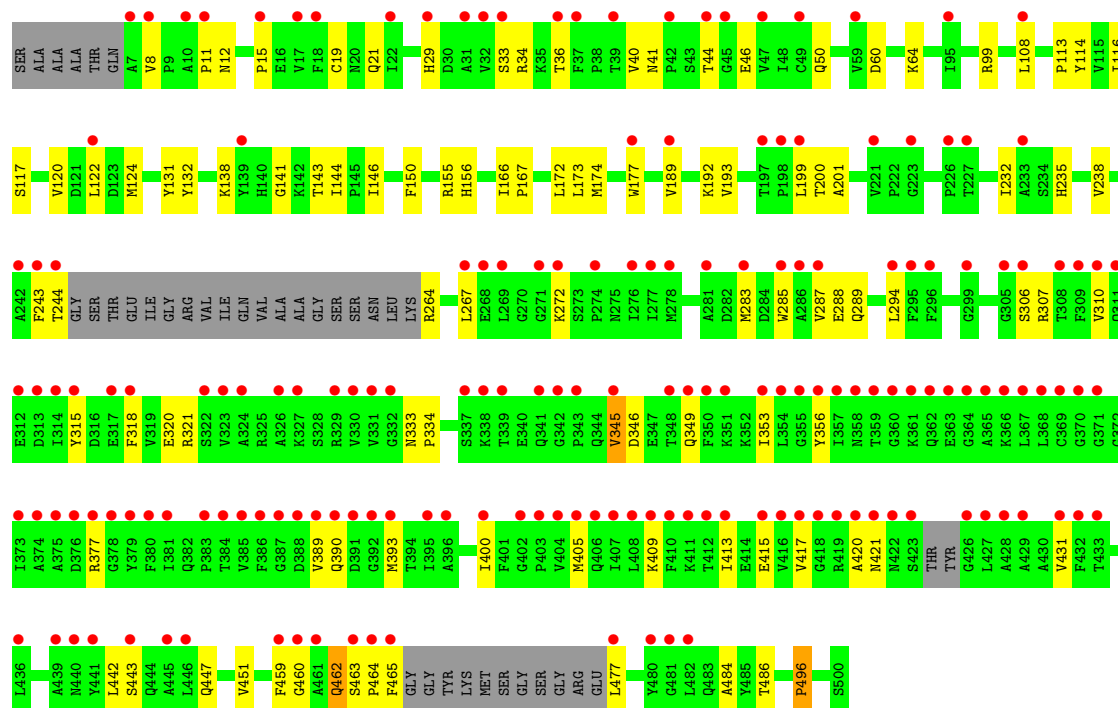


• Molecule 1: Aldehyde dehydrogenase





• Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.87Å 105.26Å 162.67Å 78.81° 81.95° 88.04°	Depositor
Resolution (Å)	42.63 – 2.10 42.63 – 2.11	Depositor EDS
% Data completeness (in resolution range)	97.7 (42.63-2.10) 97.1 (42.63-2.11)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.238 0.205 , 0.236	Depositor DCC
R_{free} test set	17348 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.5	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	0.95	EDS
Total number of atoms	46002	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: GAI, NA, EDO

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	0.50	0/3697	0.96	19/5015 (0.4%)
1	B	0.59	0/3664	0.97	17/4969 (0.3%)
1	C	0.63	0/3691	1.00	21/5004 (0.4%)
1	D	0.50	0/3688	0.94	14/5003 (0.3%)
1	E	0.59	1/3704 (0.0%)	0.96	20/5022 (0.4%)
1	F	0.67	0/3691	1.00	23/5004 (0.5%)
1	G	0.59	1/3704 (0.0%)	0.95	20/5022 (0.4%)
1	H	0.59	1/3704 (0.0%)	0.95	16/5022 (0.3%)
1	I	0.49	0/3695	0.94	15/5011 (0.3%)
1	J	0.45	0/3684	0.92	16/4997 (0.3%)
1	K	0.43	0/3605	0.91	10/4891 (0.2%)
1	L	0.43	0/3650	0.93	11/4952 (0.2%)
All	All	0.54	3/44177 (0.0%)	0.95	202/59912 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	405	MET	SD-CE	-6.88	1.62	1.79
1	E	124	MET	SD-CE	-5.72	1.65	1.79
1	H	405	MET	SD-CE	-5.60	1.65	1.79

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	199	LEU	N-CA-C	10.46	122.27	111.07
1	E	199	LEU	N-CA-C	9.63	121.37	111.07
1	C	199	LEU	N-CA-C	9.50	121.24	111.07
1	D	345	VAL	N-CA-C	9.49	120.32	110.36
1	I	199	LEU	N-CA-C	9.30	121.03	111.07
1	B	199	LEU	N-CA-C	9.22	120.93	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	199	LEU	N-CA-C	9.21	120.92	111.07
1	G	345	VAL	N-CA-C	9.04	119.84	110.62
1	C	345	VAL	N-CA-C	8.89	119.69	110.62
1	J	199	LEU	N-CA-C	8.85	121.81	111.02
1	D	144	ILE	N-CA-C	8.83	117.52	107.89
1	L	199	LEU	N-CA-C	8.66	121.50	111.11
1	E	345	VAL	N-CA-C	8.60	119.40	110.62
1	F	199	LEU	N-CA-C	8.52	120.19	111.07
1	C	144	ILE	N-CA-C	8.35	116.99	107.89
1	B	144	ILE	N-CA-C	8.32	116.96	107.89
1	G	144	ILE	N-CA-C	8.24	116.88	107.89
1	B	345	VAL	N-CA-C	8.13	118.91	110.62
1	A	199	LEU	N-CA-C	8.10	120.82	111.11
1	K	144	ILE	N-CA-C	8.04	117.54	108.05
1	L	189	VAL	N-CA-C	7.81	119.73	108.48
1	D	199	LEU	N-CA-C	7.80	120.54	111.02
1	C	189	VAL	N-CA-C	7.77	120.03	108.46
1	K	199	LEU	N-CA-C	7.74	120.46	111.02
1	C	312	GLU	N-CA-C	7.73	120.68	111.33
1	G	312	GLU	N-CA-C	7.72	120.67	111.33
1	H	345	VAL	N-CA-C	7.70	118.47	110.62
1	I	144	ILE	N-CA-C	7.67	117.10	108.05
1	A	345	VAL	N-CA-C	7.64	118.41	110.62
1	J	144	ILE	N-CA-C	7.48	116.88	108.05
1	A	84	ARG	N-CA-C	-7.44	103.17	111.28
1	F	312	GLU	N-CA-C	7.36	120.23	111.33
1	I	345	VAL	N-CA-C	7.27	118.91	110.62
1	H	312	GLU	N-CA-C	7.26	120.12	111.33
1	F	345	VAL	N-CA-C	7.22	117.98	110.62
1	B	312	GLU	N-CA-C	7.14	119.97	111.33
1	K	345	VAL	N-CA-C	7.11	117.82	110.36
1	K	189	VAL	N-CA-C	7.09	119.02	108.46
1	I	189	VAL	N-CA-C	7.02	118.92	108.46
1	F	144	ILE	N-CA-C	6.94	115.45	107.89
1	D	312	GLU	N-CA-C	6.91	119.69	111.33
1	J	345	VAL	N-CA-C	6.86	118.44	110.62
1	G	189	VAL	N-CA-C	6.85	118.66	108.46
1	A	189	VAL	N-CA-C	6.83	118.64	108.46
1	D	141	GLY	N-CA-C	-6.83	102.16	112.41
1	L	144	ILE	N-CA-C	6.77	116.04	108.05
1	H	84	ARG	N-CA-C	-6.75	103.92	111.28
1	G	141	GLY	N-CA-C	-6.73	102.32	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	345	VAL	N-CA-C	6.72	117.42	110.36
1	D	189	VAL	N-CA-C	6.72	118.47	108.46
1	F	460	GLY	N-CA-C	-6.66	100.93	111.18
1	A	143	THR	N-CA-C	-6.65	98.37	109.07
1	A	144	ILE	N-CA-C	6.64	115.13	107.89
1	B	189	VAL	N-CA-C	6.61	118.31	108.46
1	A	141	GLY	N-CA-C	-6.56	102.56	112.41
1	B	140	HIS	N-CA-C	6.55	119.73	110.50
1	B	30	ASP	N-CA-C	-6.54	101.72	110.55
1	C	141	GLY	N-CA-C	-6.54	102.60	112.41
1	G	84	ARG	N-CA-C	-6.53	104.16	111.28
1	E	143	THR	N-CA-C	-6.52	98.58	109.07
1	B	141	GLY	N-CA-C	-6.49	102.67	112.41
1	B	166	ILE	CB-CA-C	-6.49	103.65	110.53
1	B	12	ASN	N-CA-C	-6.49	97.96	108.41
1	F	189	VAL	N-CA-C	6.43	118.04	108.46
1	K	141	GLY	N-CA-C	-6.43	102.77	112.41
1	F	30	ASP	N-CA-C	-6.42	102.24	110.53
1	E	460	GLY	N-CA-C	-6.41	100.94	111.38
1	E	189	VAL	N-CA-C	6.40	118.00	108.46
1	I	12	ASN	N-CA-C	-6.39	97.28	108.20
1	J	276	ILE	N-CA-C	6.37	116.99	107.51
1	K	312	GLU	N-CA-C	6.27	118.92	111.33
1	H	144	ILE	N-CA-C	6.21	114.65	107.89
1	H	189	VAL	N-CA-C	6.19	117.68	108.46
1	H	30	ASP	N-CA-C	-6.16	102.24	110.55
1	C	30	ASP	N-CA-C	-6.14	102.26	110.55
1	C	140	HIS	N-CA-C	6.13	119.14	110.50
1	G	295	PHE	N-CA-C	6.12	120.01	112.54
1	B	463	SER	CA-C-N	6.09	126.05	119.78
1	B	463	SER	C-N-CA	6.09	126.05	119.78
1	H	141	GLY	N-CA-C	-6.01	103.40	112.41
1	K	276	ILE	N-CA-C	5.99	117.08	107.73
1	F	141	GLY	N-CA-C	-5.95	103.49	112.41
1	E	40	VAL	N-CA-C	5.93	117.54	108.71
1	G	12	ASN	N-CA-C	-5.93	98.87	108.41
1	C	497	GLN	N-CA-C	5.91	119.16	110.30
1	H	143	THR	N-CA-C	-5.90	99.57	109.07
1	E	141	GLY	N-CA-C	-5.89	103.57	112.41
1	D	143	THR	N-CA-C	-5.89	98.92	108.52
1	H	12	ASN	N-CA-C	-5.87	98.17	108.20
1	C	493	VAL	N-CA-C	5.86	116.38	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	143	THR	N-CA-C	-5.84	99.67	109.07
1	J	141	GLY	N-CA-C	-5.83	103.66	112.41
1	L	8	VAL	N-CA-C	5.82	114.54	107.61
1	E	144	ILE	N-CA-C	5.81	114.35	107.73
1	F	295	PHE	N-CA-C	5.80	119.62	112.54
1	H	140	HIS	N-CA-C	5.79	118.66	110.50
1	I	460	GLY	N-CA-C	-5.79	102.05	110.90
1	I	141	GLY	N-CA-C	-5.77	103.76	112.41
1	J	189	VAL	N-CA-C	5.76	118.25	108.86
1	H	460	GLY	N-CA-C	-5.74	102.11	110.90
1	C	295	PHE	N-CA-C	5.72	119.52	112.54
1	G	40	VAL	N-CA-C	5.72	117.84	108.97
1	E	276	ILE	N-CA-C	5.72	116.34	107.99
1	A	30	ASP	N-CA-C	-5.71	102.84	110.55
1	E	140	HIS	N-CA-C	5.71	118.93	110.48
1	F	466	GLY	N-CA-C	5.71	126.70	113.18
1	C	460	GLY	N-CA-C	-5.70	102.09	111.38
1	B	272	LYS	N-CA-C	5.69	119.42	111.74
1	F	276	ILE	N-CA-C	5.68	116.29	107.99
1	B	84	ARG	N-CA-C	-5.63	105.14	111.28
1	A	169	ASN	N-CA-C	5.62	117.41	111.28
1	J	40	VAL	N-CA-C	5.59	117.64	108.97
1	F	272	LYS	N-CA-C	5.59	119.14	111.54
1	B	276	ILE	N-CA-C	5.58	116.13	107.99
1	D	40	VAL	N-CA-C	5.56	117.58	108.97
1	E	84	ARG	N-CA-C	-5.55	105.22	111.28
1	A	273	SER	CA-C-N	5.55	126.41	120.13
1	A	273	SER	C-N-CA	5.55	126.41	120.13
1	F	344	GLN	N-CA-C	-5.55	103.20	110.53
1	F	84	ARG	N-CA-C	-5.53	105.26	111.28
1	G	30	ASP	N-CA-C	-5.50	102.38	110.52
1	J	140	HIS	N-CA-C	5.49	118.23	110.50
1	G	445	ALA	N-CA-C	5.48	118.18	111.82
1	A	40	VAL	N-CA-C	5.48	117.46	108.97
1	C	272	LYS	N-CA-C	5.47	118.98	111.54
1	G	276	ILE	N-CA-C	5.47	115.98	107.99
1	F	140	HIS	N-CA-C	5.46	117.73	110.53
1	I	276	ILE	N-CA-C	5.45	115.95	107.99
1	E	12	ASN	N-CA-C	-5.43	98.91	108.20
1	D	272	LYS	N-CA-C	5.42	118.92	111.54
1	K	30	ASP	N-CA-C	-5.42	103.23	110.55
1	J	84	ARG	N-CA-C	-5.42	105.37	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	460	GLY	N-CA-C	-5.41	102.56	111.38
1	C	221	VAL	N-CA-C	5.41	113.50	108.15
1	D	460	GLY	N-CA-C	-5.39	102.59	111.38
1	E	122	LEU	CA-CB-CG	-5.39	97.44	116.30
1	J	30	ASP	N-CA-C	-5.38	103.28	110.55
1	K	140	HIS	N-CA-C	5.38	118.08	110.50
1	L	40	VAL	N-CA-C	5.38	117.30	108.97
1	E	8	VAL	CA-C-N	5.36	125.31	119.78
1	E	8	VAL	C-N-CA	5.36	125.31	119.78
1	A	330	VAL	N-CA-C	5.36	115.30	108.12
1	C	276	ILE	N-CA-C	5.35	115.80	107.99
1	J	169	ASN	N-CA-C	5.32	117.08	111.28
1	H	144	ILE	N-CA-CB	-5.32	105.92	111.61
1	I	84	ARG	N-CA-C	-5.31	105.49	111.28
1	L	41	ASN	CA-C-N	5.31	124.98	119.56
1	L	41	ASN	C-N-CA	5.31	124.98	119.56
1	L	141	GLY	N-CA-C	-5.31	103.21	112.55
1	F	462	GLN	N-CA-C	5.30	119.75	113.28
1	A	144	ILE	N-CA-CB	-5.29	105.95	111.61
1	A	282	ASP	N-CA-C	-5.27	101.56	109.15
1	B	493	VAL	N-CA-C	5.27	115.55	108.17
1	J	460	GLY	N-CA-C	-5.27	102.84	110.90
1	I	169	ASN	N-CA-C	5.25	117.08	111.36
1	C	445	ALA	N-CA-C	5.24	117.90	111.82
1	E	312	GLU	N-CA-C	5.23	121.94	110.80
1	F	169	ASN	N-CA-C	5.22	117.05	111.36
1	J	143	THR	N-CA-C	-5.22	100.01	108.52
1	F	463	SER	CA-C-N	5.21	125.15	119.78
1	F	463	SER	C-N-CA	5.21	125.15	119.78
1	I	493	VAL	N-CA-C	5.21	115.46	108.17
1	I	40	VAL	N-CA-C	5.20	117.04	108.97
1	C	39	THR	N-CA-C	-5.18	101.24	109.59
1	E	493	VAL	N-CA-C	5.18	115.43	108.17
1	H	169	ASN	N-CA-C	5.16	116.99	111.36
1	L	143	THR	N-CA-C	-5.16	100.10	108.52
1	A	12	ASN	N-CA-C	-5.16	98.91	107.99
1	L	12	ASN	N-CA-C	-5.16	98.16	107.75
1	C	122	LEU	CA-CB-CG	-5.14	98.31	116.30
1	F	12	ASN	N-CA-C	-5.14	100.14	108.41
1	G	463	SER	CA-C-N	5.14	125.07	119.78
1	G	463	SER	C-N-CA	5.14	125.07	119.78
1	D	344	GLN	N-CA-C	-5.14	103.61	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	344	GLN	N-CA-C	-5.13	103.62	110.55
1	E	461	ALA	N-CA-C	-5.13	106.13	112.38
1	K	84	ARG	N-CA-C	-5.12	105.82	111.71
1	C	463	SER	CA-C-N	5.12	125.02	119.85
1	C	463	SER	C-N-CA	5.12	125.02	119.85
1	E	136	ALA	N-CA-C	5.11	117.51	111.33
1	D	330	VAL	N-CA-C	5.09	115.56	108.84
1	F	493	VAL	N-CA-C	5.09	115.30	108.17
1	G	467	GLY	N-CA-C	5.08	120.92	112.89
1	J	272	LYS	N-CA-C	5.08	118.45	111.54
1	D	140	HIS	N-CA-C	5.08	117.66	110.50
1	H	487	LYS	N-CA-C	-5.07	101.42	109.59
1	A	460	GLY	N-CA-C	-5.07	102.13	110.80
1	G	461	ALA	N-CA-C	-5.06	105.89	111.71
1	D	151	PHE	N-CA-C	-5.06	100.17	108.41
1	I	190	VAL	N-CA-C	-5.06	99.24	107.28
1	B	143	THR	N-CA-C	-5.05	100.29	108.52
1	I	140	HIS	N-CA-C	5.05	117.95	110.48
1	J	330	VAL	N-CA-C	5.05	116.01	108.54
1	G	493	VAL	N-CA-C	5.04	115.22	108.17
1	F	40	VAL	N-CA-C	5.03	116.77	108.97
1	G	283	MET	N-CA-C	5.02	117.13	111.11
1	H	151	PHE	N-CA-C	-5.01	100.35	108.52
1	C	461	ALA	N-CA-C	-5.01	106.27	112.38
1	J	445	ALA	N-CA-C	5.01	117.63	111.82
1	A	493	VAL	N-CA-C	5.01	115.18	108.17
1	A	497	GLN	N-CA-C	5.01	121.47	110.80
1	E	30	ASP	N-CA-C	-5.00	103.80	110.55

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	3620	0	3578	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3585	0	3531	43	0
1	C	3612	0	3564	61	0
1	D	3608	0	3553	77	0
1	E	3624	0	3573	63	0
1	F	3612	0	3564	57	0
1	G	3624	0	3573	36	0
1	H	3624	0	3573	47	0
1	I	3615	0	3560	72	0
1	J	3604	0	3547	50	0
1	K	3526	0	3469	53	0
1	L	3571	0	3523	69	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	4	0	4	2	0
3	E	4	0	5	0	0
3	F	8	0	10	0	0
3	G	4	0	4	0	0
3	H	4	0	5	0	0
3	I	4	0	4	2	0
3	L	4	0	5	4	0
4	A	16	0	24	8	0
4	B	4	0	6	0	0
4	C	12	0	18	5	0
4	D	8	0	12	6	0
4	E	4	0	6	0	0
4	F	12	0	18	4	0
4	G	12	0	18	2	0
4	I	8	0	12	0	0
4	J	4	0	6	1	0
4	L	4	0	6	1	0
5	A	189	0	0	3	0
5	B	299	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	290	0	0	5	0
5	D	187	0	0	5	0
5	E	285	0	0	6	0
5	F	367	0	0	10	0
5	G	285	0	0	6	0
5	H	236	0	0	2	0
5	I	189	0	0	4	0
5	J	141	0	0	3	0
5	K	93	0	0	1	0
5	L	88	0	0	6	0
All	All	46002	0	42771	658	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (658) 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:D:405:MET:HE3	1:D:407:ILE:HD11	1.44	1.00
1:L:390:GLN:H	1:L:393:MET:HE2	1.30	0.95
1:G:405:MET:HE3	1:G:407:ILE:HD11	1.50	0.94
1:B:120:VAL:HG12	1:B:124:MET:HE2	1.53	0.91
1:J:405:MET:HE3	1:J:407:ILE:HD11	1.55	0.89
1:C:196:GLN:HE21	1:C:196:GLN:H	1.20	0.88
1:I:466:GLY:HA3	1:I:475:ARG:HD3	1.53	0.87
1:F:120:VAL:HG12	1:F:124:MET:HE2	1.58	0.86
1:A:131:TYR:CE1	1:A:462:GLN:HG3	2.11	0.86
1:L:36:THR:OG1	1:L:50:GLN:HG3	1.75	0.86
1:K:174:MET:HE1	1:K:177:TRP:CZ3	2.11	0.85
1:H:462:GLN:H	1:H:462:GLN:NE2	1.75	0.85
1:L:421:ASN:HD21	1:L:447:GLN:HB2	1.44	0.83
1:H:405:MET:HE3	1:H:407:ILE:HD11	1.62	0.81
1:I:196:GLN:H	1:I:196:GLN:HE21	1.29	0.80
1:D:462:GLN:NE2	1:D:462:GLN:H	1.79	0.80
1:D:322:SER:HB3	1:D:405:MET:HE1	1.64	0.80
1:K:196:GLN:H	1:K:196:GLN:HE21	1.28	0.79
1:E:196:GLN:H	1:E:196:GLN:HE21	1.29	0.79
1:G:322:SER:HB3	1:G:405:MET:HE1	1.65	0.79
1:F:196:GLN:H	1:F:196:GLN:HE21	1.31	0.79
1:F:155:ARG:HD2	4:F:3120:EDO:O2	1.83	0.79
1:H:196:GLN:HE21	1:H:196:GLN:H	1.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:462:GLN:H	1:F:462:GLN:NE2	1.82	0.78
1:L:294:LEU:HD12	1:L:306:SER:HA	1.64	0.78
1:F:302:CYS:HB3	5:F:4036:HOH:O	1.84	0.77
1:A:405:MET:HE3	1:A:407:ILE:HD11	1.67	0.77
1:J:322:SER:HB3	1:J:405:MET:HE1	1.65	0.77
1:G:302:CYS:HB3	5:G:3968:HOH:O	1.85	0.77
1:G:120:VAL:HG12	1:G:124:MET:HE2	1.66	0.76
1:G:462:GLN:H	1:G:462:GLN:NE2	1.84	0.76
1:B:196:GLN:H	1:B:196:GLN:HE21	1.32	0.76
1:A:322:SER:HB3	1:A:405:MET:HE1	1.69	0.75
1:E:124:MET:HE1	5:E:3985:HOH:O	1.85	0.75
4:A:3116:EDO:H11	1:C:444:GLN:CG	2.17	0.75
1:C:302:CYS:HB3	5:C:3956:HOH:O	1.86	0.75
1:H:124:MET:HE3	1:H:173:LEU:HD22	1.69	0.75
1:K:36:THR:OG1	1:K:50:GLN:HG3	1.86	0.74
1:E:120:VAL:HG12	1:E:124:MET:HE2	1.69	0.74
1:A:279:SER:H	1:A:311:GLN:HE21	1.35	0.74
1:L:155:ARG:HD2	4:L:3129:EDO:O2	1.86	0.74
1:L:120:VAL:HG12	1:L:124:MET:HE2	1.70	0.74
1:I:159:VAL:HG21	1:I:264:ARG:NH1	2.03	0.73
1:L:421:ASN:ND2	1:L:447:GLN:HB2	2.03	0.73
1:A:279:SER:H	1:A:311:GLN:NE2	1.86	0.73
1:E:338:LYS:HD2	1:I:34:ARG:HH11	1.53	0.73
1:K:205:ALA:HB2	1:K:220:ILE:HD12	1.69	0.73
1:G:400:ILE:HD11	1:G:404:VAL:HB	1.68	0.72
1:H:322:SER:HB3	1:H:405:MET:HE1	1.72	0.71
1:I:390:GLN:H	1:I:393:MET:HE3	1.54	0.71
1:E:41:ASN:ND2	1:E:43:SER:H	1.88	0.71
1:F:466:GLY:HA3	1:F:475:ARG:HD3	1.72	0.71
1:D:120:VAL:HG12	1:D:124:MET:HE2	1.72	0.71
1:D:196:GLN:H	1:D:196:GLN:HE21	1.36	0.70
1:F:487:LYS:HD3	5:F:3915:HOH:O	1.91	0.70
1:B:497:GLN:HG3	1:C:78:ARG:NH1	2.07	0.70
1:F:60:ASP:HB2	5:F:4019:HOH:O	1.90	0.70
1:F:124:MET:HE3	1:F:173:LEU:HD22	1.72	0.70
1:A:294:LEU:HD12	1:A:306:SER:HA	1.72	0.70
1:H:120:VAL:HG12	1:H:124:MET:HE2	1.73	0.70
1:H:294:LEU:HD12	1:H:306:SER:HA	1.74	0.69
1:B:462:GLN:H	1:B:462:GLN:NE2	1.90	0.69
1:F:294:LEU:HD22	1:F:405:MET:HB2	1.72	0.69
1:E:264:ARG:HB2	1:E:264:ARG:HH11	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLN:HG2	5:B:3721:HOH:O	1.91	0.69
1:D:36:THR:OG1	1:D:50:GLN:HG3	1.93	0.69
1:J:36:THR:OG1	1:J:50:GLN:HG3	1.92	0.69
1:E:41:ASN:C	1:E:41:ASN:HD22	2.00	0.69
1:J:196:GLN:H	1:J:196:GLN:HE21	1.41	0.69
1:L:390:GLN:H	1:L:393:MET:CE	2.06	0.69
1:G:124:MET:HE3	1:G:173:LEU:HD22	1.73	0.69
1:B:464:PRO:HG3	1:B:480:TYR:CD1	2.27	0.68
1:D:311:GLN:HG2	5:D:3753:HOH:O	1.93	0.68
1:J:302:CYS:HB3	5:J:3829:HOH:O	1.92	0.68
1:F:240:LYS:HG3	1:F:264:ARG:HD2	1.74	0.68
1:L:462:GLN:H	1:L:462:GLN:NE2	1.92	0.68
1:D:124:MET:HE3	1:D:173:LEU:HD22	1.76	0.68
1:A:240:LYS:HE2	1:A:264:ARG:NH1	2.08	0.68
1:J:462:GLN:H	1:J:462:GLN:NE2	1.93	0.67
1:C:196:GLN:H	1:C:196:GLN:NE2	1.90	0.67
1:I:124:MET:HE3	1:I:173:LEU:HD22	1.76	0.67
1:G:155:ARG:HD2	4:G:3123:EDO:O2	1.95	0.66
1:K:146:ILE:HG12	3:L:3108:GAI:HN31	1.60	0.66
1:E:462:GLN:HG2	1:F:146:ILE:HG22	1.78	0.66
1:I:468:TYR:OH	1:J:489:LYS:HE3	1.96	0.66
4:A:3116:EDO:O2	1:D:155:ARG:HD2	1.95	0.66
1:J:311:GLN:HG2	5:J:3825:HOH:O	1.95	0.66
1:L:272:LYS:HG3	1:L:307:ARG:HD3	1.78	0.65
1:D:302:CYS:SG	5:D:3865:HOH:O	2.53	0.65
1:E:377:ARG:HG3	1:E:377:ARG:HH11	1.59	0.65
1:L:99:ARG:HG3	1:L:122:LEU:HD23	1.76	0.65
1:E:294:LEU:HD22	1:E:405:MET:HB2	1.77	0.65
1:D:294:LEU:HD12	1:D:306:SER:HA	1.77	0.65
1:D:302:CYS:HB3	5:D:3864:HOH:O	1.95	0.65
1:F:302:CYS:SG	5:F:4035:HOH:O	2.54	0.65
1:A:390:GLN:HG2	1:A:393:MET:HE3	1.80	0.64
1:C:294:LEU:HD22	1:C:405:MET:HB2	1.80	0.64
1:F:462:GLN:NE2	5:F:3953:HOH:O	2.30	0.64
1:I:462:GLN:NE2	1:I:462:GLN:H	1.96	0.64
1:K:405:MET:HE3	1:K:407:ILE:HD11	1.79	0.64
1:A:462:GLN:H	1:A:462:GLN:NE2	1.95	0.63
4:A:3116:EDO:H11	1:C:444:GLN:HG3	1.80	0.63
1:C:462:GLN:H	1:C:462:GLN:NE2	1.95	0.63
1:I:132:TYR:OH	1:I:477:LEU:HA	1.98	0.63
1:J:156:HIS:HB3	1:J:486:THR:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:MET:HE1	1:A:177:TRP:CZ3	2.33	0.63
1:J:124:MET:HE3	1:J:173:LEU:HD22	1.81	0.63
1:C:311:GLN:HG2	5:C:3748:HOH:O	1.98	0.62
1:C:78:ARG:HG2	1:C:78:ARG:HH11	1.64	0.62
4:A:3116:EDO:H11	1:C:444:GLN:HG2	1.81	0.62
1:E:124:MET:HE3	1:E:173:LEU:HD22	1.80	0.62
1:E:311:GLN:HG2	5:E:3756:HOH:O	1.99	0.62
1:K:294:LEU:HD22	1:K:405:MET:HB2	1.80	0.62
1:J:120:VAL:HG12	1:J:124:MET:HE2	1.79	0.62
1:K:322:SER:HB3	1:K:405:MET:HE1	1.82	0.62
1:I:322:SER:HB3	1:I:405:MET:HE1	1.82	0.62
1:K:99:ARG:HG3	1:K:122:LEU:HD23	1.82	0.61
1:D:168:TRP:CE3	1:D:345:VAL:HG21	2.36	0.61
1:H:196:GLN:H	1:H:196:GLN:NE2	1.99	0.61
1:A:46:GLU:HB2	4:A:3110:EDO:H21	1.83	0.61
1:F:196:GLN:H	1:F:196:GLN:NE2	1.98	0.61
1:D:431:VAL:HG21	1:D:442:LEU:HB3	1.83	0.60
1:A:60:ASP:O	1:A:64:LYS:HG2	2.01	0.60
1:B:235:HIS:HB3	1:B:238:VAL:HG23	1.83	0.60
1:C:156:HIS:HB3	1:C:486:THR:HG21	1.83	0.60
1:L:19:CYS:HA	5:L:3769:HOH:O	2.01	0.60
5:A:3864:HOH:O	1:C:86:ARG:HD3	2.00	0.60
1:E:464:PRO:HG3	1:E:480:TYR:CD1	2.36	0.60
1:K:462:GLN:HG2	1:L:146:ILE:HG22	1.83	0.60
1:E:338:LYS:HD2	1:I:34:ARG:NH1	2.16	0.60
1:H:22:ILE:HD13	1:H:222:PRO:HD2	1.83	0.60
1:A:155:ARG:HD2	4:A:3109:EDO:O2	1.99	0.60
1:L:272:LYS:HG3	1:L:307:ARG:CD	2.31	0.60
1:D:12:ASN:O	1:D:15:PRO:HD3	2.01	0.60
1:I:405:MET:HE3	1:I:407:ILE:HD11	1.84	0.60
1:F:36:THR:HB	1:F:50:GLN:HG3	1.83	0.59
1:I:159:VAL:HG21	1:I:264:ARG:HH12	1.66	0.59
1:J:294:LEU:HD12	1:J:306:SER:HA	1.84	0.59
1:D:317:GLU:HG2	1:D:321:ARG:HE	1.67	0.59
1:K:177:TRP:CD1	1:K:477:LEU:HD21	2.37	0.59
1:E:356:TYR:CD2	1:E:400:ILE:HG12	2.38	0.59
1:D:294:LEU:HD13	1:D:405:MET:HA	1.85	0.59
1:F:464:PRO:HG3	1:F:480:TYR:HD1	1.68	0.59
1:E:41:ASN:HD22	1:E:43:SER:H	1.50	0.58
1:G:356:TYR:CD1	1:G:400:ILE:HG22	2.38	0.58
1:C:460:GLY:HA3	1:D:146:ILE:HG13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:462:GLN:NE2	5:E:3929:HOH:O	2.36	0.58
1:J:60:ASP:O	1:J:64:LYS:HG2	2.02	0.58
1:I:390:GLN:N	1:I:393:MET:HE3	2.18	0.58
1:K:172:LEU:HD21	1:K:200:THR:HB	1.85	0.58
1:K:283:MET:HE1	1:K:314:ILE:HB	1.86	0.58
1:J:465:PHE:O	1:J:476:GLU:HB2	2.02	0.58
1:L:44:THR:OG1	1:L:46:GLU:HG2	2.04	0.58
1:C:120:VAL:HG12	1:C:124:MET:HE2	1.85	0.58
1:I:376:ASP:HA	5:I:3746:HOH:O	2.04	0.58
1:J:196:GLN:H	1:J:196:GLN:NE2	2.01	0.58
1:I:120:VAL:HG12	1:I:124:MET:HE2	1.84	0.57
1:L:172:LEU:HD21	1:L:200:THR:HB	1.86	0.57
1:D:283:MET:O	1:D:287:VAL:HG23	2.03	0.57
1:E:146:ILE:HG22	1:F:462:GLN:HG2	1.86	0.57
1:H:132:TYR:OH	1:H:477:LEU:HA	2.04	0.57
1:A:120:VAL:HG12	1:A:124:MET:HE2	1.87	0.57
1:B:124:MET:HE3	1:B:173:LEU:HD22	1.85	0.57
1:E:389:VAL:HB	1:E:408:LEU:HG	1.87	0.57
1:I:462:GLN:HG2	1:J:146:ILE:HG22	1.86	0.57
1:J:132:TYR:OH	1:J:477:LEU:HA	2.04	0.57
1:H:377:ARG:HG3	1:H:377:ARG:HH11	1.69	0.57
1:A:356:TYR:CD2	1:A:400:ILE:HG12	2.40	0.57
1:G:302:CYS:SG	1:G:427:LEU:HD21	2.45	0.57
1:G:462:GLN:H	1:G:462:GLN:HE21	1.51	0.56
1:I:36:THR:CB	1:I:50:GLN:HG3	2.35	0.56
1:I:356:TYR:CD2	1:I:400:ILE:HG12	2.40	0.56
1:K:196:GLN:H	1:K:196:GLN:NE2	2.01	0.56
1:L:389:VAL:HA	1:L:393:MET:HE1	1.86	0.56
1:C:120:VAL:CG1	1:C:124:MET:HE2	2.36	0.56
1:I:60:ASP:O	1:I:64:LYS:HG2	2.06	0.56
1:I:196:GLN:H	1:I:196:GLN:NE2	2.02	0.56
1:D:395:ILE:HG12	5:D:3886:HOH:O	2.06	0.56
1:F:359:THR:O	1:F:363:GLU:HG3	2.05	0.56
1:I:174:MET:HE1	1:I:177:TRP:CZ3	2.41	0.56
1:J:167:PRO:HD3	1:J:244:THR:HB	1.87	0.56
1:I:36:THR:HB	1:I:50:GLN:HG3	1.88	0.56
1:J:449:GLY:HA3	1:J:466:GLY:O	2.05	0.56
1:B:358:ASN:O	1:B:362:GLN:HG2	2.06	0.56
1:F:464:PRO:HG3	1:F:480:TYR:CD1	2.41	0.56
1:L:120:VAL:CG1	1:L:124:MET:HE2	2.36	0.56
1:C:462:GLN:NE2	5:C:3931:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:LYS:HE2	4:D:3126:EDO:H21	1.88	0.56
1:D:196:GLN:H	1:D:196:GLN:NE2	2.03	0.55
1:J:272:LYS:HA	1:J:306:SER:OG	2.06	0.55
1:I:356:TYR:CG	1:I:400:ILE:HG12	2.41	0.55
1:A:311:GLN:HG2	5:A:3752:HOH:O	2.07	0.55
1:I:135:TRP:CE2	1:K:138:LYS:HD3	2.42	0.55
1:J:12:ASN:O	1:J:15:PRO:HD3	2.06	0.55
1:C:489:LYS:HB2	1:D:468:TYR:OH	2.07	0.55
1:E:466:GLY:HA3	1:E:475:ARG:HD3	1.88	0.55
1:I:36:THR:OG1	1:I:50:GLN:HG3	2.07	0.55
1:H:464:PRO:HG3	1:H:480:TYR:CD1	2.41	0.55
1:F:46:GLU:HB2	4:F:3121:EDO:H21	1.89	0.54
1:A:172:LEU:HD21	1:A:200:THR:HB	1.88	0.54
1:E:167:PRO:HD3	1:E:244:THR:HB	1.87	0.54
1:K:23:PHE:CZ	1:K:26:ASN:HA	2.43	0.54
1:K:462:GLN:H	1:K:462:GLN:NE2	2.04	0.54
1:L:235:HIS:HB3	1:L:238:VAL:HG23	1.89	0.54
1:A:167:PRO:HD3	1:A:244:THR:HB	1.88	0.54
1:B:294:LEU:HD12	1:B:306:SER:HA	1.90	0.54
1:L:320:GLU:HB2	5:L:3748:HOH:O	2.08	0.54
1:E:459:PHE:HE2	1:E:465:PHE:CE1	2.26	0.54
1:L:11:PRO:HB3	1:L:114:TYR:CZ	2.42	0.54
1:L:389:VAL:HG13	1:L:393:MET:CE	2.38	0.54
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.43	0.54
1:H:462:GLN:H	1:H:462:GLN:CD	2.16	0.54
1:B:449:GLY:HA3	1:B:466:GLY:O	2.08	0.54
1:G:131:TYR:CE1	1:G:462:GLN:HB3	2.43	0.54
1:G:449:GLY:HA3	1:G:466:GLY:O	2.06	0.54
1:C:400:ILE:HD11	1:C:404:VAL:HB	1.90	0.54
1:A:254:GLN:HB2	1:A:267:LEU:HD11	1.90	0.54
1:I:283:MET:O	1:I:287:VAL:HG23	2.08	0.54
1:E:390:GLN:HG2	1:E:393:MET:HE3	1.89	0.54
1:G:464:PRO:HG3	1:G:480:TYR:CD1	2.42	0.54
1:E:377:ARG:HG3	1:E:377:ARG:NH1	2.23	0.53
1:H:356:TYR:CD2	1:H:400:ILE:HG12	2.42	0.53
1:B:464:PRO:HG3	1:B:480:TYR:HD1	1.73	0.53
1:L:288:GLU:HG2	5:L:3744:HOH:O	2.07	0.53
1:C:155:ARG:HD2	4:C:3113:EDO:O2	2.09	0.53
1:E:196:GLN:H	1:E:196:GLN:NE2	2.02	0.53
1:D:78:ARG:HH11	1:D:78:ARG:HG2	1.73	0.53
1:H:167:PRO:HD3	1:H:244:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:HG3	5:A:3762:HOH:O	2.09	0.53
1:G:172:LEU:HD21	1:G:200:THR:HB	1.91	0.53
1:G:294:LEU:HD22	1:G:405:MET:HB2	1.90	0.53
1:E:22:ILE:HD13	1:E:222:PRO:HD2	1.90	0.53
1:E:120:VAL:CG1	1:E:124:MET:HE2	2.38	0.53
1:F:264:ARG:HH12	1:F:484:ALA:HA	1.73	0.53
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.44	0.53
1:G:347:GLU:HG2	1:G:351:LYS:HE2	1.90	0.53
1:G:459:PHE:HE2	1:G:465:PHE:CE1	2.27	0.53
1:B:120:VAL:CG1	1:B:124:MET:HE2	2.33	0.53
1:B:196:GLN:H	1:B:196:GLN:NE2	2.05	0.53
1:L:356:TYR:CD2	1:L:400:ILE:HG12	2.43	0.52
1:A:279:SER:N	1:A:311:GLN:HE21	2.06	0.52
1:F:174:MET:HE1	1:F:244:THR:HG21	1.92	0.52
1:A:274:PRO:HG3	1:A:307:ARG:NH2	2.24	0.52
1:E:86:ARG:HG3	5:E:3791:HOH:O	2.08	0.52
1:G:462:GLN:NE2	5:G:3944:HOH:O	2.42	0.52
1:H:294:LEU:HD13	1:H:405:MET:HA	1.91	0.52
1:L:132:TYR:OH	1:L:477:LEU:HA	2.09	0.52
1:J:22:ILE:HD13	1:J:222:PRO:HD2	1.91	0.52
1:K:443:SER:HA	1:K:451:VAL:HG11	1.92	0.52
1:L:283:MET:O	1:L:287:VAL:HG23	2.09	0.52
1:F:462:GLN:H	1:F:462:GLN:CD	2.18	0.52
1:A:124:MET:HE3	1:A:173:LEU:HD22	1.91	0.51
1:C:205:ALA:HB2	1:C:220:ILE:HD12	1.92	0.51
1:D:120:VAL:CG1	1:D:124:MET:HE2	2.40	0.51
1:G:358:ASN:HB2	5:G:3991:HOH:O	2.11	0.51
1:I:294:LEU:HD13	1:I:294:LEU:C	2.36	0.51
1:L:459:PHE:HE2	1:L:465:PHE:CE1	2.28	0.51
1:E:132:TYR:OH	1:E:477:LEU:HA	2.11	0.51
1:I:395:ILE:HG23	5:I:3843:HOH:O	2.11	0.51
1:C:356:TYR:CE1	1:C:400:ILE:HG22	2.45	0.51
1:F:459:PHE:HE2	1:F:465:PHE:CE1	2.29	0.51
1:I:174:MET:HE1	1:I:177:TRP:CE3	2.45	0.51
1:I:413:ILE:O	1:I:417:VAL:HG23	2.10	0.51
1:K:459:PHE:HE2	1:K:465:PHE:CD1	2.29	0.51
1:A:405:MET:CE	1:A:407:ILE:HD11	2.40	0.51
1:A:224:PHE:HB2	1:A:227:THR:OG1	2.11	0.51
1:D:462:GLN:H	1:D:462:GLN:HE21	1.59	0.51
1:C:464:PRO:HG3	1:C:480:TYR:CD1	2.46	0.51
1:K:459:PHE:HE2	1:K:465:PHE:CE1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:131:TYR:CE1	1:H:462:GLN:HB3	2.46	0.50
1:C:18:PHE:HE1	4:C:3115:EDO:H22	1.76	0.50
1:F:264:ARG:NH1	1:F:484:ALA:HA	2.26	0.50
1:G:11:PRO:HB3	1:G:114:TYR:CZ	2.46	0.50
1:I:192:LYS:HB2	1:I:232:ILE:HD12	1.94	0.50
1:I:443:SER:HA	1:I:451:VAL:HG11	1.92	0.50
1:L:443:SER:HA	1:L:451:VAL:HG11	1.93	0.50
1:L:413:ILE:O	1:L:417:VAL:HG23	2.11	0.50
1:G:311:GLN:HG2	5:G:3715:HOH:O	2.11	0.50
1:L:307:ARG:NH2	1:L:420:ALA:HA	2.27	0.50
1:E:449:GLY:HA3	1:E:466:GLY:O	2.12	0.50
1:H:36:THR:HB	1:H:50:GLN:HG3	1.93	0.50
1:E:21:GLN:HB3	1:E:29:HIS:O	2.11	0.50
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.46	0.50
1:H:172:LEU:HD21	1:H:200:THR:HB	1.93	0.50
1:K:462:GLN:NE2	5:K:3787:HOH:O	2.45	0.50
1:K:12:ASN:O	1:K:15:PRO:HD3	2.12	0.50
1:C:356:TYR:CD1	1:C:400:ILE:HG22	2.47	0.50
1:G:302:CYS:SG	5:G:3970:HOH:O	2.59	0.50
1:L:113:PRO:HB2	1:L:116:ILE:HG12	1.94	0.50
1:L:496:PRO:HB2	5:L:3787:HOH:O	2.12	0.50
1:A:251:ARG:O	1:A:255:VAL:HG23	2.12	0.49
1:I:32:VAL:HG23	1:I:58:ASP:OD1	2.12	0.49
1:B:298:GLN:HA	5:B:3954:HOH:O	2.12	0.49
1:D:361:LYS:NZ	4:D:3126:EDO:H22	2.27	0.49
1:G:34:ARG:HG2	5:G:3948:HOH:O	2.12	0.49
1:G:356:TYR:CG	1:G:400:ILE:HG22	2.47	0.49
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.47	0.49
1:D:22:ILE:HD13	1:D:222:PRO:HD2	1.94	0.49
1:D:356:TYR:CD2	1:D:400:ILE:HG12	2.47	0.49
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.47	0.49
1:A:38:PRO:HB3	1:A:50:GLN:HE22	1.76	0.49
1:C:124:MET:HE3	1:C:173:LEU:HD22	1.95	0.49
1:I:464:PRO:HD3	1:J:144:ILE:CD1	2.43	0.49
1:C:18:PHE:CE1	4:C:3115:EDO:H22	2.48	0.49
1:C:131:TYR:CE1	1:C:462:GLN:HB3	2.48	0.49
1:E:476:GLU:HA	5:E:3839:HOH:O	2.13	0.49
1:B:356:TYR:CD2	1:B:400:ILE:HG12	2.48	0.49
1:D:279:SER:HA	1:D:314:ILE:HD13	1.93	0.49
1:I:146:ILE:HG12	3:I:3107:GAI:HN31	1.78	0.49
1:K:196:GLN:HE21	1:K:196:GLN:N	2.05	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:HG12	3:A:3101:GAI:N3	2.28	0.49
1:A:294:LEU:HD13	1:A:405:MET:HA	1.95	0.49
1:C:15:PRO:HD2	1:C:108:LEU:HD22	1.95	0.49
1:F:131:TYR:CE1	1:F:462:GLN:HB3	2.48	0.49
1:D:356:TYR:CG	1:D:400:ILE:HG12	2.48	0.49
1:F:132:TYR:OH	1:F:477:LEU:HA	2.12	0.49
1:I:268:GLU:HA	5:I:3747:HOH:O	2.13	0.49
1:B:206:ASN:ND2	5:B:3986:HOH:O	2.45	0.49
1:D:391:ASP:OD2	1:D:419:ARG:HD2	2.13	0.48
1:E:41:ASN:HD21	1:E:43:SER:HB2	1.78	0.48
1:H:36:THR:CB	1:H:50:GLN:HG3	2.43	0.48
1:B:356:TYR:CE2	1:B:400:ILE:HG12	2.48	0.48
1:I:196:GLN:HE21	1:I:196:GLN:N	2.06	0.48
1:G:11:PRO:HB3	1:G:114:TYR:CE1	2.48	0.48
1:H:174:MET:HE1	1:H:177:TRP:CZ3	2.48	0.48
1:L:156:HIS:HB3	1:L:486:THR:HG21	1.95	0.48
1:C:196:GLN:HE21	1:C:196:GLN:N	1.99	0.48
1:F:36:THR:CB	1:F:50:GLN:HG3	2.43	0.48
1:A:107:THR:HG23	1:A:334:PRO:HB2	1.96	0.48
1:A:315:TYR:O	1:A:319:VAL:HG23	2.14	0.48
1:H:283:MET:HE1	1:H:314:ILE:HB	1.94	0.48
1:D:361:LYS:CE	4:D:3126:EDO:H21	2.44	0.48
1:E:356:TYR:CG	1:E:400:ILE:HG12	2.48	0.48
1:F:32:VAL:HG11	1:F:57:GLU:OE2	2.14	0.48
1:G:464:PRO:HG3	1:G:480:TYR:HD1	1.79	0.48
1:K:120:VAL:HG12	1:K:124:MET:HE2	1.94	0.48
1:C:11:PRO:HB3	1:C:114:TYR:CE1	2.49	0.47
1:C:302:CYS:SG	1:C:427:LEU:HD21	2.54	0.47
1:D:174:MET:HE1	1:D:177:TRP:CE3	2.48	0.47
1:I:274:PRO:HG3	1:I:307:ARG:NH2	2.29	0.47
1:C:390:GLN:NE2	1:C:392:GLY:H	2.12	0.47
1:C:21:GLN:HB3	1:C:29:HIS:O	2.15	0.47
1:D:302:CYS:SG	1:D:427:LEU:HD21	2.55	0.47
1:D:462:GLN:H	1:D:462:GLN:CD	2.22	0.47
1:D:464:PRO:HG3	1:D:480:TYR:HD1	1.79	0.47
1:E:464:PRO:HG3	1:E:480:TYR:HD1	1.80	0.47
1:H:408:LEU:HD12	1:H:408:LEU:N	2.29	0.47
1:I:146:ILE:HG13	1:J:460:GLY:HA3	1.97	0.47
1:K:353:ILE:HG23	1:K:400:ILE:HD12	1.96	0.47
1:B:294:LEU:HD22	1:B:405:MET:HB2	1.97	0.47
1:C:270:GLY:HA3	1:C:302:CYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:LYS:HA	1:E:306:SER:OG	2.14	0.47
1:E:462:GLN:NE2	1:E:462:GLN:H	2.12	0.47
1:F:120:VAL:CG1	1:F:124:MET:HE2	2.37	0.47
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.97	0.47
1:H:356:TYR:CE2	1:H:400:ILE:HG12	2.48	0.47
1:K:385:VAL:HG22	1:K:405:MET:HE2	1.97	0.47
1:L:192:LYS:HB2	1:L:232:ILE:HD12	1.97	0.47
1:L:294:LEU:CD1	1:L:306:SER:HA	2.41	0.47
1:I:431:VAL:HG21	1:I:442:LEU:HB3	1.96	0.47
1:K:410:PHE:CD1	1:K:416:VAL:HB	2.50	0.47
1:C:495:VAL:C	1:C:496:PRO:O	2.57	0.47
1:E:155:ARG:HD2	5:F:4007:HOH:O	2.15	0.47
1:F:174:MET:CE	1:F:244:THR:HG21	2.45	0.47
1:I:241:VAL:CG1	1:I:265:VAL:HG22	2.45	0.47
1:J:135:TRP:CE2	1:L:138:LYS:HD3	2.50	0.47
1:J:444:GLN:HB3	5:J:3751:HOH:O	2.15	0.47
1:E:131:TYR:CE1	1:E:462:GLN:HB3	2.51	0.46
1:J:356:TYR:CD2	1:J:400:ILE:HG12	2.50	0.46
1:A:356:TYR:CG	1:A:400:ILE:HG12	2.50	0.46
1:J:431:VAL:HG21	1:J:442:LEU:HB3	1.97	0.46
1:A:164:GLN:CD	1:A:178:LYS:HB3	2.39	0.46
1:B:463:SER:HA	1:B:464:PRO:HD3	1.80	0.46
1:D:166:ILE:HD11	1:D:193:VAL:HG12	1.98	0.46
1:E:36:THR:OG1	1:E:50:GLN:HG3	2.14	0.46
1:E:468:TYR:OH	1:F:489:LYS:HB2	2.15	0.46
1:I:12:ASN:O	1:I:15:PRO:HD3	2.15	0.46
1:C:101:TYR:CG	4:C:3115:EDO:H11	2.50	0.46
1:D:156:HIS:HB3	1:D:486:THR:HG21	1.97	0.46
1:E:11:PRO:HB3	1:E:114:TYR:CZ	2.50	0.46
1:G:32:VAL:HG21	1:G:57:GLU:HG3	1.97	0.46
1:G:132:TYR:OH	1:G:477:LEU:HA	2.15	0.46
1:J:462:GLN:H	1:J:462:GLN:CD	2.22	0.46
1:J:464:PRO:HG3	1:J:480:TYR:CD1	2.50	0.46
1:K:464:PRO:HG3	1:K:480:TYR:CD1	2.51	0.46
1:C:466:GLY:HA3	1:C:475:ARG:HD3	1.98	0.46
1:I:57:GLU:H	1:I:57:GLU:CD	2.24	0.46
1:K:146:ILE:HD11	3:L:3108:GAI:N3	2.30	0.46
1:L:415:GLU:HB2	5:L:3799:HOH:O	2.16	0.46
1:A:233:ALA:HB2	1:A:253:ILE:HG23	1.96	0.46
1:C:356:TYR:CD1	1:C:400:ILE:CG2	2.99	0.46
1:F:431:VAL:HG21	1:F:442:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD22	1:A:405:MET:HB2	1.98	0.46
1:B:462:GLN:NE2	5:B:3957:HOH:O	2.49	0.46
1:I:468:TYR:OH	1:J:489:LYS:HB2	2.16	0.46
1:L:390:GLN:N	1:L:393:MET:HE2	2.13	0.46
1:D:464:PRO:CG	1:D:480:TYR:CD1	2.99	0.45
1:E:294:LEU:O	1:E:294:LEU:HG	2.15	0.45
1:G:460:GLY:HA3	1:H:146:ILE:HG13	1.98	0.45
1:J:23:PHE:CZ	1:J:26:ASN:HA	2.51	0.45
1:K:11:PRO:HB3	1:K:114:TYR:CZ	2.51	0.45
1:A:38:PRO:HB3	1:A:50:GLN:NE2	2.30	0.45
1:B:131:TYR:CE1	1:B:462:GLN:HB3	2.51	0.45
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.98	0.45
1:E:205:ALA:HB2	1:E:220:ILE:HD12	1.99	0.45
1:A:174:MET:HE1	1:A:177:TRP:CE3	2.50	0.45
1:H:449:GLY:HA3	1:H:466:GLY:O	2.16	0.45
1:H:476:GLU:O	1:H:477:LEU:HB2	2.17	0.45
1:J:443:SER:HA	1:J:451:VAL:HG11	1.98	0.45
1:K:120:VAL:CG1	1:K:124:MET:HE2	2.46	0.45
1:E:174:MET:HE1	1:E:177:TRP:CZ3	2.51	0.45
1:K:121:ASP:O	1:K:125:VAL:HG23	2.16	0.45
1:K:465:PHE:O	1:K:476:GLU:HB3	2.15	0.45
1:L:283:MET:HG3	1:L:321:ARG:NH1	2.32	0.45
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.52	0.45
1:A:46:GLU:CB	4:A:3110:EDO:H21	2.46	0.45
1:F:101:TYR:CG	4:F:3122:EDO:H11	2.52	0.45
1:D:405:MET:HE3	1:D:407:ILE:CD1	2.32	0.45
1:J:356:TYR:CG	1:J:400:ILE:HG12	2.52	0.45
1:C:272:LYS:HA	1:C:306:SER:OG	2.16	0.45
1:C:356:TYR:CG	1:C:400:ILE:HG21	2.51	0.45
1:D:353:ILE:O	1:D:357:ILE:HG13	2.16	0.45
1:D:449:GLY:HA3	1:D:466:GLY:O	2.17	0.45
1:H:36:THR:OG1	1:H:50:GLN:HG3	2.16	0.45
1:I:445:ALA:HB2	5:I:3756:HOH:O	2.17	0.45
1:D:46:GLU:HB2	4:D:3117:EDO:H21	1.99	0.45
1:D:409:LYS:O	1:D:419:ARG:NH2	2.50	0.45
1:A:131:TYR:CZ	1:A:462:GLN:HA	2.52	0.45
1:A:273:SER:HA	1:A:274:PRO:HD3	1.74	0.45
1:I:283:MET:HE1	1:I:314:ILE:HB	1.99	0.45
1:K:167:PRO:HD3	1:K:244:THR:O	2.16	0.45
1:B:464:PRO:CG	1:B:480:TYR:CD1	2.98	0.44
1:C:214:PRO:HD2	1:C:217:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:CYS:HB3	5:E:3850:HOH:O	2.17	0.44
1:H:389:VAL:HB	1:H:408:LEU:HG	1.98	0.44
1:I:463:SER:HA	1:I:464:PRO:HD3	1.85	0.44
1:J:46:GLU:HB2	4:J:3128:EDO:H21	1.98	0.44
1:L:15:PRO:HD2	1:L:108:LEU:HD22	1.99	0.44
1:A:32:VAL:HG11	1:A:57:GLU:OE2	2.17	0.44
1:A:138:LYS:HD3	1:C:135:TRP:CE2	2.52	0.44
1:D:443:SER:HA	1:D:451:VAL:HG11	1.99	0.44
1:F:311:GLN:HG2	5:F:3780:HOH:O	2.17	0.44
1:G:21:GLN:HB3	1:G:29:HIS:O	2.17	0.44
1:J:161:VAL:HA	1:J:188:VAL:HG23	1.99	0.44
1:B:192:LYS:HB2	1:B:232:ILE:HD12	1.99	0.44
1:G:327:LYS:HE3	1:G:369:CYS:HB3	1.99	0.44
1:K:319:VAL:O	1:K:323:VAL:HG23	2.17	0.44
1:L:243:PHE:HB3	1:L:267:LEU:HD23	1.98	0.44
1:B:294:LEU:CD1	1:B:306:SER:HA	2.47	0.44
1:B:459:PHE:HE2	1:B:465:PHE:CD1	2.35	0.44
1:E:36:THR:CB	1:E:50:GLN:HG3	2.47	0.44
1:L:33:SER:O	1:L:34:ARG:HB2	2.17	0.44
1:C:46:GLU:HB2	4:C:3114:EDO:H21	2.00	0.44
1:D:243:PHE:HB3	1:D:267:LEU:HD23	1.98	0.44
1:D:361:LYS:HZ3	4:D:3126:EDO:H22	1.82	0.44
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.53	0.44
1:L:310:VAL:HG21	1:L:318:PHE:CD2	2.52	0.44
1:E:106:GLU:O	1:E:110:ASN:HB3	2.18	0.44
1:E:273:SER:HA	1:E:274:PRO:HD3	1.78	0.44
1:I:453:VAL:HB	1:J:493:VAL:HG13	2.00	0.44
1:K:192:LYS:HB2	1:K:232:ILE:HD12	2.00	0.44
1:H:64:LYS:HE2	5:H:3932:HOH:O	2.18	0.44
1:H:272:LYS:HA	1:H:306:SER:OG	2.18	0.44
1:K:39:THR:HG23	1:K:48:ILE:HB	1.99	0.44
1:K:294:LEU:HD12	1:K:306:SER:HA	2.00	0.44
1:A:349:GLN:O	1:A:353:ILE:HG13	2.18	0.44
1:B:243:PHE:HB3	1:B:267:LEU:HD23	2.00	0.44
1:D:391:ASP:CG	1:D:419:ARG:HH11	2.26	0.44
1:I:193:VAL:HG11	1:I:201:ALA:CB	2.48	0.44
1:I:310:VAL:HG21	1:I:318:PHE:CD2	2.53	0.44
1:L:459:PHE:O	3:L:3108:GAI:N2	2.49	0.44
1:B:400:ILE:H	1:B:400:ILE:HG13	1.71	0.44
1:C:172:LEU:HD21	1:C:200:THR:HB	1.99	0.44
1:D:188:VAL:HG12	1:D:217:VAL:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:TYR:O	1:D:319:VAL:HG23	2.18	0.44
1:H:333:ASN:HA	1:H:334:PRO:HD2	1.85	0.44
1:L:431:VAL:HG21	1:L:442:LEU:HB3	1.99	0.44
1:D:161:VAL:HA	1:D:188:VAL:HG23	1.99	0.43
1:F:159:VAL:HG21	1:F:264:ARG:HH21	1.83	0.43
1:I:146:ILE:HG12	3:I:3107:GAI:N3	2.33	0.43
1:I:158:PRO:HG3	1:I:185:THR:O	2.18	0.43
1:L:315:TYR:CE2	1:L:409:LYS:HB2	2.53	0.43
1:B:166:ILE:HD11	1:B:191:MET:HE2	2.00	0.43
1:B:496:PRO:HG2	1:D:441:TYR:HB2	2.00	0.43
1:F:174:MET:HE3	5:F:3862:HOH:O	2.19	0.43
1:I:292:PHE:HE1	1:I:457:ASP:HB2	1.82	0.43
1:L:131:TYR:CE1	1:L:462:GLN:HB3	2.52	0.43
1:D:131:TYR:CE1	1:D:462:GLN:HB3	2.53	0.43
1:A:319:VAL:O	1:A:323:VAL:HG23	2.19	0.43
1:H:283:MET:O	1:H:287:VAL:HG23	2.17	0.43
1:H:462:GLN:NE2	5:H:3866:HOH:O	2.52	0.43
1:J:235:HIS:HB3	1:J:238:VAL:HG23	2.00	0.43
1:L:21:GLN:HB3	1:L:29:HIS:O	2.17	0.43
1:L:356:TYR:CE2	1:L:400:ILE:HG12	2.54	0.43
1:A:443:SER:HA	1:A:451:VAL:HG11	2.00	0.43
1:B:158:PRO:HG3	1:B:185:THR:O	2.19	0.43
1:D:59:VAL:O	1:D:63:VAL:HG23	2.18	0.43
1:E:356:TYR:CE2	1:E:400:ILE:HG12	2.54	0.43
1:J:464:PRO:HA	1:J:476:GLU:O	2.18	0.43
1:K:272:LYS:HA	1:K:306:SER:OG	2.18	0.43
1:C:449:GLY:HA3	1:C:466:GLY:O	2.18	0.43
1:F:59:VAL:O	1:F:63:VAL:HG23	2.18	0.43
1:H:464:PRO:CG	1:H:480:TYR:CD1	3.01	0.43
1:I:205:ALA:HB2	1:I:220:ILE:HD12	2.00	0.43
1:I:385:VAL:HG22	1:I:405:MET:HE2	2.01	0.43
1:C:13:GLN:NE2	5:C:3894:HOH:O	2.51	0.43
1:F:27:GLU:HG3	5:F:3816:HOH:O	2.18	0.43
1:F:272:LYS:HA	1:F:306:SER:OG	2.18	0.43
1:I:131:TYR:CE1	1:I:462:GLN:HB3	2.54	0.43
1:I:167:PRO:HD3	1:I:244:THR:HB	2.00	0.43
1:B:156:HIS:CD2	1:B:488:VAL:HG22	2.54	0.43
1:D:377:ARG:HG3	1:D:377:ARG:HH11	1.83	0.43
1:E:36:THR:HB	1:E:50:GLN:HG3	2.00	0.43
1:J:11:PRO:HB3	1:J:114:TYR:CZ	2.54	0.43
1:K:146:ILE:HG12	3:L:3108:GAI:N3	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:CD1	1:A:306:SER:HA	2.46	0.43
1:C:462:GLN:H	1:C:462:GLN:CD	2.27	0.43
1:D:192:LYS:HD3	1:D:193:VAL:O	2.19	0.43
1:E:302:CYS:SG	1:E:427:LEU:HD21	2.59	0.43
1:F:464:PRO:CG	1:F:480:TYR:CD1	3.01	0.43
1:H:315:TYR:CE1	1:H:319:VAL:HG21	2.54	0.43
1:I:154:THR:HG21	1:J:464:PRO:HG2	2.00	0.43
1:K:404:VAL:HG12	1:K:406:GLN:OE1	2.19	0.43
1:C:294:LEU:O	1:C:294:LEU:HG	2.10	0.43
1:C:431:VAL:HG21	1:C:442:LEU:HB3	2.00	0.43
1:E:8:VAL:HA	1:E:9:PRO:HD3	1.80	0.43
1:I:464:PRO:HG3	1:I:480:TYR:CD1	2.54	0.43
1:A:235:HIS:HB3	1:A:238:VAL:HG23	2.00	0.42
1:D:294:LEU:CD1	1:D:405:MET:HA	2.47	0.42
1:F:192:LYS:NZ	5:F:3778:HOH:O	2.52	0.42
1:K:146:ILE:HG13	1:L:460:GLY:HA3	2.01	0.42
1:L:349:GLN:O	1:L:353:ILE:HG13	2.19	0.42
1:D:34:ARG:HH11	1:D:34:ARG:HB3	1.84	0.42
1:E:356:TYR:HB2	1:E:400:ILE:HG21	2.01	0.42
1:J:390:GLN:HG2	1:J:393:MET:HE3	2.01	0.42
1:K:373:ILE:HG22	1:K:375:ALA:H	1.84	0.42
1:B:174:MET:HE1	1:B:177:TRP:CE3	2.55	0.42
1:B:462:GLN:H	1:B:462:GLN:HE21	1.64	0.42
1:B:466:GLY:HA3	1:B:475:ARG:HD3	2.02	0.42
1:D:373:ILE:HG22	1:D:375:ALA:H	1.85	0.42
1:D:410:PHE:CD1	1:D:416:VAL:HB	2.54	0.42
1:F:241:VAL:CG1	1:F:265:VAL:HG22	2.49	0.42
1:H:377:ARG:HG3	1:H:377:ARG:NH1	2.34	0.42
1:I:349:GLN:O	1:I:353:ILE:HG13	2.18	0.42
1:K:132:TYR:OH	1:K:477:LEU:HA	2.19	0.42
1:D:158:PRO:HG3	1:D:185:THR:O	2.19	0.42
1:J:347:GLU:HG2	1:J:351:LYS:HE2	2.00	0.42
1:D:79:MET:HE3	1:D:79:MET:HB2	1.91	0.42
1:K:345:VAL:HG13	1:K:346:ASP:N	2.35	0.42
1:L:124:MET:HE3	1:L:173:LEU:HD22	2.01	0.42
1:L:174:MET:HE1	1:L:177:TRP:CZ3	2.54	0.42
1:H:107:THR:HG23	1:H:334:PRO:HB2	2.02	0.42
1:L:264:ARG:NH1	1:L:484:ALA:O	2.52	0.42
1:A:8:VAL:HA	1:A:9:PRO:HD3	1.93	0.42
1:E:468:TYR:HE1	1:E:475:ARG:HH21	1.67	0.42
1:H:372:GLY:O	1:H:382:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:59:VAL:O	1:J:63:VAL:HG23	2.20	0.42
1:C:400:ILE:HG21	1:C:400:ILE:HD13	1.78	0.42
1:D:21:GLN:HB3	1:D:29:HIS:O	2.19	0.42
1:J:464:PRO:HG3	1:J:480:TYR:HD1	1.85	0.42
1:I:214:PRO:HA	1:I:215:PRO:HD3	1.94	0.42
1:I:315:TYR:CE1	1:I:319:VAL:HG21	2.55	0.42
1:J:158:PRO:HG3	1:J:185:THR:O	2.20	0.42
1:D:192:LYS:HD3	1:D:192:LYS:C	2.44	0.42
1:D:361:LYS:CE	4:D:3126:EDO:C2	2.98	0.42
1:E:46:GLU:CD	1:E:377:ARG:HH22	2.28	0.42
1:F:476:GLU:O	1:F:477:LEU:HB2	2.19	0.42
1:G:46:GLU:HB2	4:G:3124:EDO:H21	2.01	0.42
1:I:461:ALA:N	1:I:462:GLN:NE2	2.68	0.42
1:L:294:LEU:CD1	1:L:405:MET:HA	2.50	0.42
1:A:353:ILE:O	1:A:357:ILE:HG13	2.20	0.41
1:B:132:TYR:OH	1:B:477:LEU:HA	2.19	0.41
1:D:121:ASP:O	1:D:125:VAL:HG23	2.21	0.41
1:F:12:ASN:O	1:F:15:PRO:HD3	2.19	0.41
1:F:463:SER:HA	1:F:464:PRO:HD3	1.79	0.41
1:L:60:ASP:O	1:L:64:LYS:HG2	2.19	0.41
1:L:463:SER:HA	1:L:464:PRO:HD3	1.87	0.41
1:B:422:ASN:HB3	5:B:3794:HOH:O	2.20	0.41
1:C:174:MET:HA	1:C:174:MET:HE2	2.02	0.41
1:E:464:PRO:CG	1:E:480:TYR:CD1	3.02	0.41
1:J:107:THR:HG23	1:J:334:PRO:HB2	2.01	0.41
1:J:356:TYR:HE2	1:J:404:VAL:HG11	1.84	0.41
1:K:431:VAL:HG21	1:K:442:LEU:HB3	2.02	0.41
1:B:174:MET:HE1	1:B:177:TRP:CZ3	2.55	0.41
1:B:389:VAL:HB	1:B:408:LEU:HG	2.02	0.41
1:D:235:HIS:HB3	1:D:238:VAL:HG23	2.02	0.41
1:I:273:SER:HA	1:I:274:PRO:HD3	1.80	0.41
1:B:315:TYR:O	1:B:319:VAL:HG23	2.20	0.41
1:B:459:PHE:HE2	1:B:465:PHE:CE1	2.39	0.41
1:C:154:THR:HA	1:C:489:LYS:O	2.20	0.41
1:E:112:LYS:HB3	1:E:112:LYS:HE2	1.92	0.41
1:F:8:VAL:HA	1:F:9:PRO:HD3	1.94	0.41
1:I:164:GLN:CD	1:I:178:LYS:HB3	2.45	0.41
1:K:302:CYS:HA	1:K:401:PHE:HE2	1.85	0.41
1:K:347:GLU:HG2	1:K:351:LYS:HE2	2.03	0.41
1:D:192:LYS:HZ3	1:D:225:GLY:HA2	1.85	0.41
1:F:196:GLN:HE21	1:F:196:GLN:N	2.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:12:ASN:O	1:H:15:PRO:HD3	2.21	0.41
1:I:144:ILE:CD1	1:J:464:PRO:HD3	2.51	0.41
1:A:167:PRO:HG2	1:A:174:MET:HG3	2.02	0.41
1:A:408:LEU:HD12	1:A:408:LEU:N	2.35	0.41
1:D:192:LYS:NZ	1:D:225:GLY:HA2	2.35	0.41
1:E:463:SER:HA	1:E:464:PRO:HD3	1.85	0.41
1:H:273:SER:HA	1:H:274:PRO:HD3	1.83	0.41
1:J:356:TYR:CE1	1:J:395:ILE:HG22	2.55	0.41
1:L:462:GLN:H	1:L:462:GLN:HE21	1.64	0.41
1:A:131:TYR:HE1	1:A:462:GLN:HG3	1.79	0.41
1:A:347:GLU:O	1:A:350:PHE:HB3	2.20	0.41
1:D:418:GLY:HA3	5:D:3775:HOH:O	2.20	0.41
1:L:146:ILE:HD11	1:L:150:PHE:HB2	2.02	0.41
1:L:345:VAL:HG13	1:L:346:ASP:N	2.35	0.41
1:F:46:GLU:CB	4:F:3121:EDO:H21	2.50	0.41
1:K:408:LEU:HD12	1:K:408:LEU:N	2.36	0.41
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.56	0.41
1:B:356:TYR:CG	1:B:400:ILE:HG12	2.56	0.41
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.56	0.41
1:C:490:THR:O	1:D:450:THR:HA	2.21	0.41
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.56	0.41
1:E:155:ARG:NH2	1:F:444:GLN:HG3	2.36	0.41
1:F:177:TRP:CD1	1:F:477:LEU:HD21	2.56	0.41
1:F:294:LEU:O	1:F:294:LEU:HG	2.18	0.41
1:H:356:TYR:CG	1:H:400:ILE:HG12	2.55	0.41
1:I:466:GLY:HA3	1:I:475:ARG:CD	2.38	0.41
1:K:235:HIS:HB3	1:K:238:VAL:HG23	2.01	0.41
1:L:166:ILE:HD11	5:L:3726:HOH:O	2.21	0.41
1:L:167:PRO:HD3	1:L:244:THR:HB	2.02	0.41
1:L:462:GLN:H	1:L:462:GLN:CD	2.29	0.41
4:A:3116:EDO:C1	1:C:444:GLN:HG3	2.51	0.41
1:K:372:GLY:O	1:K:382:GLN:HG3	2.21	0.41
1:L:294:LEU:HD13	1:L:405:MET:HA	2.03	0.41
1:C:132:TYR:OH	1:C:477:LEU:HA	2.21	0.40
1:D:34:ARG:HB3	1:D:34:ARG:NH1	2.37	0.40
1:L:285:TRP:CH2	1:L:289:GLN:NE2	2.90	0.40
1:L:377:ARG:HG3	1:L:377:ARG:HH11	1.86	0.40
1:C:102:LEU:HD23	1:C:102:LEU:HA	1.91	0.40
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.57	0.40
1:F:79:MET:HE3	1:F:79:MET:HB2	1.96	0.40
1:L:333:ASN:HA	1:L:334:PRO:HD2	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:HG12	3:A:3101:GAI:HN31	1.87	0.40
1:C:166:ILE:HD11	5:C:3707:HOH:O	2.20	0.40
1:D:167:PRO:HG2	1:D:174:MET:HG3	2.01	0.40
1:G:121:ASP:O	1:G:125:VAL:HG23	2.20	0.40
1:H:406:GLN:N	1:H:406:GLN:NE2	2.69	0.40
1:H:410:PHE:CD1	1:H:416:VAL:HB	2.57	0.40
1:I:112:LYS:HB3	1:I:112:LYS:HE2	1.96	0.40
1:I:462:GLN:H	1:I:462:GLN:CD	2.30	0.40
1:K:279:SER:HA	1:K:314:ILE:HD13	2.04	0.40
1:L:193:VAL:HG11	1:L:201:ALA:CB	2.51	0.40
1:C:463:SER:HA	1:C:464:PRO:HD3	1.79	0.40
1:D:385:VAL:HG22	1:D:405:MET:HE2	2.03	0.40
1:F:459:PHE:HE2	1:F:465:PHE:CD1	2.40	0.40
1:G:34:ARG:HD2	1:K:16:GLU:OE2	2.21	0.40
1:I:462:GLN:H	1:I:462:GLN:HE21	1.67	0.40
1:L:192:LYS:HB2	1:L:232:ILE:CD1	2.51	0.40
1:D:464:PRO:HG3	1:D:480:TYR:CD1	2.56	0.40
1:E:274:PRO:HG3	1:E:307:ARG:NH2	2.36	0.40
1:E:462:GLN:H	1:E:462:GLN:CD	2.30	0.40
1:I:72:LEU:HD12	1:I:72:LEU:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	461/500 (92%)	451 (98%)	10 (2%)	0	100	100
1	B	457/500 (91%)	449 (98%)	7 (2%)	1 (0%)	43	44
1	C	460/500 (92%)	451 (98%)	8 (2%)	1 (0%)	43	44
1	D	460/500 (92%)	448 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	461/500 (92%)	449 (97%)	12 (3%)	0	100	100
1	F	460/500 (92%)	451 (98%)	7 (2%)	2 (0%)	30	28
1	G	461/500 (92%)	452 (98%)	8 (2%)	1 (0%)	43	44
1	H	461/500 (92%)	452 (98%)	8 (2%)	1 (0%)	43	44
1	I	460/500 (92%)	448 (97%)	10 (2%)	2 (0%)	30	28
1	J	459/500 (92%)	448 (98%)	10 (2%)	1 (0%)	43	44
1	K	448/500 (90%)	437 (98%)	10 (2%)	1 (0%)	43	44
1	L	454/500 (91%)	443 (98%)	10 (2%)	1 (0%)	43	44
All	All	5502/6000 (92%)	5379 (98%)	112 (2%)	11 (0%)	43	44

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	496	PRO
1	F	466	GLY
1	I	466	GLY
1	J	496	PRO
1	C	496	PRO
1	K	496	PRO
1	L	496	PRO
1	F	496	PRO
1	I	496	PRO
1	G	496	PRO
1	H	496	PRO

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	381/402 (95%)	378 (99%)	3 (1%)	73	81
1	B	376/402 (94%)	366 (97%)	10 (3%)	39	45
1	C	379/402 (94%)	369 (97%)	10 (3%)	40	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	379/402 (94%)	375 (99%)	4 (1%)	65	74
1	E	380/402 (94%)	374 (98%)	6 (2%)	55	64
1	F	379/402 (94%)	373 (98%)	6 (2%)	55	64
1	G	380/402 (94%)	376 (99%)	4 (1%)	65	74
1	H	380/402 (94%)	375 (99%)	5 (1%)	61	69
1	I	379/402 (94%)	375 (99%)	4 (1%)	65	74
1	J	378/402 (94%)	371 (98%)	7 (2%)	50	58
1	K	371/402 (92%)	366 (99%)	5 (1%)	61	69
1	L	376/402 (94%)	374 (100%)	2 (0%)	81	88
All	All	4538/4824 (94%)	4472 (98%)	66 (2%)	57	65

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	376	ASP
1	A	462	GLN
1	B	50	GLN
1	B	56	LYS
1	B	60	ASP
1	B	196	GLN
1	B	268	GLU
1	B	294	LEU
1	B	400	ILE
1	B	462	GLN
1	B	486	THR
1	B	496	PRO
1	C	122	LEU
1	C	192	LYS
1	C	196	GLN
1	C	236	GLU
1	C	376	ASP
1	C	377	ARG
1	C	383	PRO
1	C	416	VAL
1	C	462	GLN
1	C	496	PRO
1	D	196	GLN
1	D	358	ASN

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Mol	Chain	Res	Type
1	D	362	GLN
1	D	462	GLN
1	E	41	ASN
1	E	122	LEU
1	E	196	GLN
1	E	264	ARG
1	E	294	LEU
1	E	325	ARG
1	F	34	ARG
1	F	122	LEU
1	F	196	GLN
1	F	400	ILE
1	F	462	GLN
1	F	496	PRO
1	G	8	VAL
1	G	294	LEU
1	G	383	PRO
1	G	462	GLN
1	H	14	GLN
1	H	196	GLN
1	H	325	ARG
1	H	462	GLN
1	H	463	SER
1	I	192	LYS
1	I	196	GLN
1	I	268	GLU
1	I	462	GLN
1	J	36	THR
1	J	50	GLN
1	J	192	LYS
1	J	196	GLN
1	J	325	ARG
1	J	462	GLN
1	J	496	PRO
1	K	192	LYS
1	K	196	GLN
1	K	294	LEU
1	K	462	GLN
1	K	496	PRO
1	L	117	SER
1	L	462	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	26	ASN
1	A	50	GLN
1	A	175	GLN
1	A	254	GLN
1	A	275	ASN
1	A	311	GLN
1	A	358	ASN
1	A	406	GLN
1	A	444	GLN
1	A	462	GLN
1	A	483	GLN
1	B	14	GLN
1	B	26	ASN
1	B	29	HIS
1	B	71	GLN
1	B	83	HIS
1	B	156	HIS
1	B	175	GLN
1	B	196	GLN
1	B	462	GLN
1	C	13	GLN
1	C	26	ASN
1	C	29	HIS
1	C	50	GLN
1	C	175	GLN
1	C	196	GLN
1	C	275	ASN
1	C	362	GLN
1	C	390	GLN
1	C	422	ASN
1	C	444	GLN
1	C	462	GLN
1	C	497	GLN
1	D	13	GLN
1	D	26	ASN
1	D	164	GLN
1	D	175	GLN
1	D	196	GLN
1	D	275	ASN
1	D	358	ASN
1	D	362	GLN

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Mol	Chain	Res	Type
1	D	462	GLN
1	E	13	GLN
1	E	41	ASN
1	E	196	GLN
1	E	362	GLN
1	E	422	ASN
1	E	462	GLN
1	F	26	ASN
1	F	175	GLN
1	F	196	GLN
1	F	275	ASN
1	F	390	GLN
1	F	462	GLN
1	F	483	GLN
1	G	13	GLN
1	G	21	GLN
1	G	26	ASN
1	G	175	GLN
1	G	275	ASN
1	G	462	GLN
1	H	13	GLN
1	H	25	ASN
1	H	50	GLN
1	H	89	ASN
1	H	164	GLN
1	H	196	GLN
1	H	275	ASN
1	H	362	GLN
1	H	390	GLN
1	H	462	GLN
1	I	13	GLN
1	I	26	ASN
1	I	83	HIS
1	I	175	GLN
1	I	196	GLN
1	I	275	ASN
1	I	444	GLN
1	I	462	GLN
1	J	13	GLN
1	J	26	ASN
1	J	29	HIS
1	J	175	GLN

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Mol	Chain	Res	Type
1	J	196	GLN
1	J	275	ASN
1	J	444	GLN
1	J	462	GLN
1	J	483	GLN
1	K	13	GLN
1	K	14	GLN
1	K	26	ASN
1	K	83	HIS
1	K	196	GLN
1	K	462	GLN
1	L	13	GLN
1	L	14	GLN
1	L	26	ASN
1	L	83	HIS
1	L	175	GLN
1	L	275	ASN
1	L	462	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 12 are monoatomic - leaving 29 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GAI	F	3104	-	3,3,3	1.23	0	3,3,3	1.25	0
4	EDO	I	3119	-	3,3,3	0.29	0	2,2,2	0.59	0
4	EDO	I	3127	-	3,3,3	0.36	0	2,2,2	0.54	0
4	EDO	C	3115	-	3,3,3	0.36	0	2,2,2	0.50	0
4	EDO	C	3113	-	3,3,3	0.64	0	2,2,2	0.13	0
4	EDO	D	3126	-	3,3,3	0.38	0	2,2,2	0.44	0
3	GAI	I	3107	-	3,3,3	1.09	0	3,3,3	1.28	0
4	EDO	G	3123	-	3,3,3	0.40	0	2,2,2	0.42	0
4	EDO	D	3117	-	3,3,3	0.45	0	2,2,2	0.27	0
4	EDO	C	3114	-	3,3,3	0.25	0	2,2,2	0.45	0
4	EDO	G	3124	-	3,3,3	0.44	0	2,2,2	0.28	0
3	GAI	G	3105	-	3,3,3	1.04	0	3,3,3	1.29	0
4	EDO	F	3120	-	3,3,3	0.36	0	2,2,2	0.37	0
4	EDO	A	3111	-	3,3,3	0.54	0	2,2,2	0.35	0
3	GAI	F	3103	-	3,3,3	1.14	0	3,3,3	1.26	0
4	EDO	B	3112	-	3,3,3	0.39	0	2,2,2	0.35	0
4	EDO	J	3128	-	3,3,3	0.44	0	2,2,2	0.25	0
4	EDO	A	3109	-	3,3,3	0.39	0	2,2,2	0.33	0
4	EDO	F	3121	-	3,3,3	0.40	0	2,2,2	0.43	0
3	GAI	L	3108	-	3,3,3	1.28	1 (33%)	3,3,3	1.25	0
4	EDO	A	3110	-	3,3,3	0.39	0	2,2,2	0.34	0
4	EDO	G	3125	-	3,3,3	0.45	0	2,2,2	0.44	0
4	EDO	L	3129	-	3,3,3	0.47	0	2,2,2	0.31	0
3	GAI	E	3102	-	3,3,3	1.21	0	3,3,3	1.11	0
4	EDO	A	3116	-	3,3,3	0.59	0	2,2,2	0.12	0
4	EDO	E	3118	-	3,3,3	0.42	0	2,2,2	0.32	0
4	EDO	F	3122	-	3,3,3	0.32	0	2,2,2	0.55	0
3	GAI	A	3101	-	3,3,3	0.87	0	3,3,3	1.35	1 (33%)
3	GAI	H	3106	-	3,3,3	1.18	1 (33%)	3,3,3	1.24	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
4	EDO	I	3119	-	-	1/1/1/1	-
4	EDO	I	3127	-	-	1/1/1/1	-
4	EDO	C	3115	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	3113	-	-	0/1/1/1	-
4	EDO	D	3126	-	-	1/1/1/1	-
4	EDO	G	3123	-	-	0/1/1/1	-
4	EDO	D	3117	-	-	0/1/1/1	-
4	EDO	C	3114	-	-	0/1/1/1	-
4	EDO	G	3124	-	-	0/1/1/1	-
4	EDO	F	3120	-	-	0/1/1/1	-
4	EDO	A	3111	-	-	1/1/1/1	-
4	EDO	B	3112	-	-	0/1/1/1	-
4	EDO	J	3128	-	-	0/1/1/1	-
4	EDO	A	3109	-	-	0/1/1/1	-
4	EDO	F	3121	-	-	0/1/1/1	-
4	EDO	A	3110	-	-	0/1/1/1	-
4	EDO	G	3125	-	-	1/1/1/1	-
4	EDO	L	3129	-	-	0/1/1/1	-
4	EDO	E	3118	-	-	0/1/1/1	-
4	EDO	A	3116	-	-	0/1/1/1	-
4	EDO	F	3122	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	3108	GAI	C-N1	2.16	1.36	1.30
3	H	3106	GAI	C-N1	2.05	1.35	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3101	GAI	N3-C-N2	2.01	120.88	116.18

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3111	EDO	O1-C1-C2-O2
4	C	3115	EDO	O1-C1-C2-O2
4	D	3126	EDO	O1-C1-C2-O2
4	F	3122	EDO	O1-C1-C2-O2
4	G	3125	EDO	O1-C1-C2-O2
4	I	3127	EDO	O1-C1-C2-O2
4	I	3119	EDO	O1-C1-C2-O2

There are no ring outliers.

18 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3115	EDO	3	0
4	C	3113	EDO	1	0
4	D	3126	EDO	5	0
3	I	3107	GAI	2	0
4	G	3123	EDO	1	0
4	D	3117	EDO	1	0
4	C	3114	EDO	1	0
4	G	3124	EDO	1	0
4	F	3120	EDO	1	0
4	J	3128	EDO	1	0
4	A	3109	EDO	1	0
4	F	3121	EDO	2	0
3	L	3108	GAI	4	0
4	A	3110	EDO	2	0
4	L	3129	EDO	1	0
4	A	3116	EDO	5	0
4	F	3122	EDO	1	0
3	A	3101	GAI	2	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	469/500 (93%)	0.97	80 (17%) 4 4	13, 49, 74, 82	0
1	B	465/500 (93%)	-0.10	15 (3%) 50 53	15, 28, 50, 92	0
1	C	468/500 (93%)	-0.04	25 (5%) 32 34	14, 27, 56, 83	0
1	D	468/500 (93%)	0.81	52 (11%) 10 10	15, 45, 71, 83	0
1	E	469/500 (93%)	-0.01	20 (4%) 40 41	12, 29, 53, 83	0
1	F	468/500 (93%)	-0.29	15 (3%) 50 53	13, 24, 48, 83	0
1	G	469/500 (93%)	-0.01	25 (5%) 32 34	15, 30, 56, 79	0
1	H	469/500 (93%)	0.22	25 (5%) 32 34	13, 33, 62, 78	0
1	I	468/500 (93%)	0.84	70 (14%) 5 5	25, 43, 74, 86	0
1	J	467/500 (93%)	0.78	35 (7%) 20 21	26, 47, 70, 87	0
1	K	456/500 (91%)	1.07	52 (11%) 10 10	34, 53, 73, 92	0
1	L	462/500 (92%)	1.72	175 (37%) 1 1	32, 64, 88, 95	0
All	All	5598/6000 (93%)	0.49	589 (10%) 11 12	12, 39, 74, 95	0

All (589) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	356	TYR	6.9
1	L	378	GLY	6.8
1	A	481	GLY	6.4
1	L	386	PHE	6.0
1	L	7	ALA	5.9
1	K	461	ALA	5.7
1	L	367	LEU	5.6
1	J	468	TYR	5.6
1	I	375	ALA	5.4
1	D	463	SER	5.3
1	G	468	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	480	TYR	5.2
1	C	265	VAL	5.1
1	J	270	GLY	5.1
1	A	256	ALA	5.0
1	A	375	ALA	5.0
1	A	461	ALA	4.8
1	L	421	ASN	4.8
1	E	468	TYR	4.8
1	A	373	ILE	4.7
1	J	467	GLY	4.7
1	A	7	ALA	4.7
1	I	413	ILE	4.5
1	B	267	LEU	4.5
1	G	400	ILE	4.5
1	D	465	PHE	4.5
1	I	245	GLY	4.5
1	K	245	GLY	4.5
1	E	265	VAL	4.5
1	I	461	ALA	4.5
1	D	269	LEU	4.5
1	J	269	LEU	4.5
1	D	466	GLY	4.4
1	E	466	GLY	4.4
1	L	420	ALA	4.4
1	D	374	ALA	4.4
1	A	265	VAL	4.3
1	L	385	VAL	4.3
1	L	387	GLY	4.3
1	L	465	PHE	4.3
1	I	266	THR	4.2
1	I	389	VAL	4.2
1	L	364	GLY	4.2
1	B	266	THR	4.2
1	L	400	ILE	4.2
1	L	322	SER	4.2
1	I	468	TYR	4.2
1	J	265	VAL	4.1
1	L	287	VAL	4.1
1	K	463	SER	4.1
1	D	461	ALA	4.0
1	L	403	PRO	4.0
1	G	478	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	269	LEU	4.0
1	J	7	ALA	4.0
1	D	267	LEU	4.0
1	L	243	PHE	4.0
1	H	270	GLY	4.0
1	I	265	VAL	3.9
1	I	244	THR	3.9
1	A	252	VAL	3.9
1	G	270	GLY	3.9
1	L	269	LEU	3.9
1	L	244	THR	3.9
1	H	265	VAL	3.9
1	I	393	MET	3.9
1	B	243	PHE	3.9
1	K	400	ILE	3.9
1	C	270	GLY	3.9
1	C	267	LEU	3.9
1	D	423	SER	3.8
1	L	354	LEU	3.8
1	L	391	ASP	3.8
1	L	384	THR	3.8
1	L	379	TYR	3.7
1	D	468	TYR	3.7
1	H	468	TYR	3.7
1	L	446	LEU	3.7
1	L	407	ILE	3.7
1	F	264	ARG	3.7
1	L	368	LEU	3.7
1	E	467	GLY	3.7
1	J	245	GLY	3.7
1	L	417	VAL	3.7
1	L	318	PHE	3.7
1	L	310	VAL	3.6
1	L	416	VAL	3.6
1	L	463	SER	3.6
1	L	361	LYS	3.6
1	K	465	PHE	3.6
1	L	309	PHE	3.6
1	L	405	MET	3.6
1	L	375	ALA	3.6
1	L	357	ILE	3.6
1	L	381	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	464	PRO	3.6
1	K	464	PRO	3.6
1	H	264	ARG	3.6
1	A	372	GLY	3.6
1	C	243	PHE	3.5
1	J	266	THR	3.5
1	F	269	LEU	3.5
1	B	271	GLY	3.5
1	A	462	GLN	3.5
1	H	7	ALA	3.5
1	L	461	ALA	3.5
1	L	377	ARG	3.5
1	L	29	HIS	3.5
1	L	358	ASN	3.5
1	G	269	LEU	3.5
1	H	269	LEU	3.5
1	I	269	LEU	3.4
1	L	281	ALA	3.4
1	I	477	LEU	3.4
1	L	314	ILE	3.4
1	L	360	GLY	3.4
1	L	327	LYS	3.4
1	L	350	PHE	3.4
1	L	419	ARG	3.4
1	L	389	VAL	3.4
1	I	481	GLY	3.4
1	A	374	ALA	3.4
1	A	460	GLY	3.3
1	B	265	VAL	3.3
1	K	48	ILE	3.3
1	L	408	LEU	3.3
1	J	244	THR	3.3
1	L	433	THR	3.3
1	L	359	THR	3.3
1	H	423	SER	3.3
1	L	276	ILE	3.3
1	L	413	ILE	3.3
1	D	477	LEU	3.3
1	L	44	THR	3.2
1	H	245	GLY	3.2
1	C	7	ALA	3.2
1	G	461	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	36	THR	3.2
1	L	402	GLY	3.2
1	L	404	VAL	3.2
1	L	267	LEU	3.2
1	L	366	LYS	3.2
1	A	331	VAL	3.2
1	I	356	TYR	3.2
1	J	400	ILE	3.2
1	K	477	LEU	3.2
1	L	315	TYR	3.2
1	H	224	PHE	3.2
1	I	224	PHE	3.2
1	K	401	PHE	3.2
1	D	226	PRO	3.2
1	C	8	VAL	3.1
1	L	330	VAL	3.1
1	D	413	ILE	3.1
1	I	315	TYR	3.1
1	A	423	SER	3.1
1	K	243	PHE	3.1
1	L	380	PHE	3.1
1	L	355	GLY	3.1
1	L	242	ALA	3.1
1	L	396	ALA	3.1
1	D	373	ILE	3.1
1	A	44	THR	3.1
1	C	245	GLY	3.1
1	D	378	GLY	3.1
1	I	271	GLY	3.1
1	K	318	PHE	3.1
1	K	426	GLY	3.1
1	L	42	PRO	3.1
1	L	268	GLU	3.1
1	C	269	LEU	3.1
1	A	139	TYR	3.1
1	B	270	GLY	3.1
1	H	481	GLY	3.1
1	G	7	ALA	3.1
1	L	365	ALA	3.1
1	K	108	LEU	3.1
1	I	362	GLN	3.1
1	F	466	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	317	GLU	3.0
1	D	462	GLN	3.0
1	G	245	GLY	3.0
1	G	467	GLY	3.0
1	L	294	LEU	3.0
1	I	400	ILE	3.0
1	H	364	GLY	3.0
1	H	466	GLY	3.0
1	J	225	GLY	3.0
1	L	285	TRP	3.0
1	F	465	PHE	3.0
1	L	306	SER	3.0
1	H	477	LEU	3.0
1	I	310	VAL	3.0
1	I	436	LEU	3.0
1	A	360	GLY	3.0
1	L	308	THR	3.0
1	G	264	ARG	2.9
1	D	375	ALA	2.9
1	L	445	ALA	2.9
1	G	267	LEU	2.9
1	G	477	LEU	2.9
1	I	301	CYS	2.9
1	G	265	VAL	2.9
1	L	47	VAL	2.9
1	A	426	GLY	2.9
1	J	466	GLY	2.9
1	L	481	GLY	2.9
1	F	400	ILE	2.9
1	B	7	ALA	2.9
1	J	461	ALA	2.9
1	L	326	ALA	2.9
1	F	467	GLY	2.9
1	A	389	VAL	2.9
1	K	32	VAL	2.9
1	K	226	PRO	2.9
1	A	335	PHE	2.9
1	L	33	SER	2.9
1	L	15	PRO	2.9
1	A	326	ALA	2.9
1	E	7	ALA	2.9
1	I	371	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	460	GLY	2.9
1	F	266	THR	2.8
1	L	277	ILE	2.8
1	L	226	PRO	2.8
1	B	423	SER	2.8
1	B	356	TYR	2.8
1	D	467	GLY	2.8
1	H	266	THR	2.8
1	C	400	ILE	2.8
1	L	464	PRO	2.8
1	I	423	SER	2.8
1	J	423	SER	2.8
1	A	459	PHE	2.8
1	E	356	TYR	2.8
1	L	371	GLY	2.8
1	I	367	LEU	2.8
1	E	266	THR	2.8
1	C	496	PRO	2.8
1	L	189	VAL	2.8
1	K	351	LYS	2.8
1	K	357	ILE	2.8
1	A	225	GLY	2.8
1	I	460	GLY	2.8
1	D	356	TYR	2.8
1	D	266	THR	2.8
1	K	36	THR	2.8
1	A	47	VAL	2.8
1	L	406	GLN	2.7
1	A	364	GLY	2.7
1	E	245	GLY	2.7
1	L	426	GLY	2.7
1	E	243	PHE	2.7
1	J	375	ALA	2.7
1	I	139	TYR	2.7
1	K	72	LEU	2.7
1	L	477	LEU	2.7
1	I	431	VAL	2.7
1	L	17	VAL	2.7
1	H	400	ILE	2.7
1	K	146	ILE	2.7
1	F	423	SER	2.7
1	L	278	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	28	TRP	2.7
1	L	392	GLY	2.7
1	E	224	PHE	2.7
1	E	461	ALA	2.7
1	I	243	PHE	2.7
1	L	18	PHE	2.7
1	C	264	ARG	2.7
1	I	264	ARG	2.7
1	L	480	TYR	2.7
1	F	265	VAL	2.7
1	L	373	ILE	2.7
1	I	281	ALA	2.7
1	I	465	PHE	2.7
1	J	224	PHE	2.7
1	K	224	PHE	2.7
1	L	286	ALA	2.7
1	L	374	ALA	2.7
1	L	429	ALA	2.7
1	D	32	VAL	2.7
1	K	166	ILE	2.7
1	L	331	VAL	2.7
1	L	351	LYS	2.7
1	I	466	GLY	2.7
1	L	418	GLY	2.7
1	H	465	PHE	2.6
1	K	244	THR	2.6
1	L	393	MET	2.6
1	L	343	PRO	2.6
1	K	494	LYS	2.6
1	L	323	VAL	2.6
1	L	369	CYS	2.6
1	I	7	ALA	2.6
1	G	266	THR	2.6
1	I	412	THR	2.6
1	L	339	THR	2.6
1	L	410	PHE	2.6
1	E	264	ARG	2.6
1	A	115	VAL	2.6
1	I	276	ILE	2.6
1	K	241	VAL	2.6
1	D	45	GLY	2.6
1	D	422	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	384	THR	2.6
1	K	427	LEU	2.6
1	L	409	LYS	2.6
1	H	376	ASP	2.6
1	A	8	VAL	2.6
1	L	345	VAL	2.6
1	A	378	GLY	2.6
1	I	478	GLY	2.6
1	B	422	ASN	2.6
1	D	227	THR	2.6
1	H	475	ARG	2.6
1	D	234	SER	2.6
1	I	72	LEU	2.6
1	L	177	TRP	2.6
1	J	459	PHE	2.5
1	L	296	PHE	2.5
1	A	400	ILE	2.5
1	B	400	ILE	2.5
1	K	332	GLY	2.5
1	L	441	TYR	2.5
1	I	500	SER	2.5
1	D	224	PHE	2.5
1	A	330	VAL	2.5
1	I	270	GLY	2.5
1	G	356	TYR	2.5
1	A	264	ARG	2.5
1	A	334	PRO	2.5
1	C	423	SER	2.5
1	F	7	ALA	2.5
1	J	226	PRO	2.5
1	K	462	GLN	2.5
1	G	268	GLU	2.5
1	I	268	GLU	2.5
1	L	324	ALA	2.5
1	A	368	LEU	2.5
1	E	267	LEU	2.5
1	E	269	LEU	2.5
1	F	267	LEU	2.5
1	A	386	PHE	2.5
1	K	18	PHE	2.5
1	L	295	PHE	2.5
1	H	356	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	268	GLU	2.5
1	L	415	GLU	2.5
1	D	247	THR	2.5
1	I	368	LEU	2.5
1	A	37	PHE	2.5
1	L	329	ARG	2.5
1	A	245	GLY	2.5
1	A	370	GLY	2.5
1	H	271	GLY	2.5
1	L	59	VAL	2.4
1	F	268	GLU	2.4
1	I	394	THR	2.4
1	C	467	GLY	2.4
1	D	243	PHE	2.4
1	H	370	GLY	2.4
1	A	395	ILE	2.4
1	B	146	ILE	2.4
1	D	8	VAL	2.4
1	L	32	VAL	2.4
1	L	221	VAL	2.4
1	A	369	CYS	2.4
1	L	197	THR	2.4
1	K	15	PRO	2.4
1	L	283	MET	2.4
1	A	104	ALA	2.4
1	G	466	GLY	2.4
1	J	426	GLY	2.4
1	G	465	PHE	2.4
1	L	37	PHE	2.4
1	L	353	ILE	2.4
1	A	405	MET	2.4
1	L	423	SER	2.4
1	A	36	THR	2.4
1	J	264	ARG	2.4
1	A	365	ALA	2.4
1	D	7	ALA	2.4
1	I	420	ALA	2.4
1	L	439	ALA	2.4
1	K	354	LEU	2.4
1	D	460	GLY	2.4
1	L	45	GLY	2.4
1	I	376	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	313	ASP	2.4
1	A	318	PHE	2.4
1	G	243	PHE	2.4
1	J	243	PHE	2.4
1	A	253	ILE	2.4
1	A	416	VAL	2.4
1	H	331	VAL	2.4
1	I	416	VAL	2.4
1	L	10	ALA	2.3
1	L	363	GLU	2.3
1	J	367	LEU	2.3
1	L	390	GLN	2.3
1	L	482	LEU	2.3
1	D	426	GLY	2.3
1	L	332	GLY	2.3
1	D	279	SER	2.3
1	L	443	SER	2.3
1	C	266	THR	2.3
1	J	464	PRO	2.3
1	L	440	ASN	2.3
1	A	367	LEU	2.3
1	A	408	LEU	2.3
1	F	481	GLY	2.3
1	I	378	GLY	2.3
1	I	388	ASP	2.3
1	A	377	ARG	2.3
1	K	377	ARG	2.3
1	A	314	ILE	2.3
1	L	22	ILE	2.3
1	D	265	VAL	2.3
1	J	32	VAL	2.3
1	L	431	VAL	2.3
1	L	39	THR	2.3
1	L	227	THR	2.3
1	L	348	THR	2.3
1	L	412	THR	2.3
1	A	285	TRP	2.3
1	D	225	GLY	2.3
1	D	364	GLY	2.3
1	J	332	GLY	2.3
1	L	337	SER	2.3
1	I	459	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	249	ILE	2.3
1	A	353	ILE	2.3
1	D	389	VAL	2.3
1	J	51	VAL	2.3
1	K	495	VAL	2.3
1	L	274	PRO	2.3
1	I	377	ARG	2.3
1	L	49	CYS	2.3
1	A	396	ALA	2.3
1	C	461	ALA	2.3
1	L	376	ASP	2.3
1	L	388	ASP	2.3
1	C	223	GLY	2.3
1	L	223	GLY	2.3
1	L	299	GLY	2.3
1	C	477	LEU	2.3
1	K	480	TYR	2.3
1	L	139	TYR	2.3
1	L	312	GLU	2.2
1	I	401	PHE	2.2
1	L	432	PHE	2.2
1	A	404	VAL	2.2
1	L	198	PRO	2.2
1	D	301	CYS	2.2
1	H	365	ALA	2.2
1	I	79	MET	2.2
1	L	342	GLY	2.2
1	K	476	GLU	2.2
1	G	14	GLN	2.2
1	A	309	PHE	2.2
1	C	224	PHE	2.2
1	J	401	PHE	2.2
1	L	459	PHE	2.2
1	A	38	PRO	2.2
1	J	227	THR	2.2
1	K	373	ILE	2.2
1	L	95	ILE	2.2
1	A	319	VAL	2.2
1	L	8	VAL	2.2
1	A	376	ASP	2.2
1	A	305	GLY	2.2
1	I	392	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	467	GLY	2.2
1	K	7	ALA	2.2
1	L	31	ALA	2.2
1	E	477	LEU	2.2
1	L	199	LEU	2.2
1	A	117	SER	2.2
1	L	338	LYS	2.2
1	L	383	PRO	2.2
1	A	388	ASP	2.2
1	K	60	ASP	2.2
1	A	310	VAL	2.2
1	I	241	VAL	2.2
1	J	241	VAL	2.2
1	L	370	GLY	2.2
1	L	341	GLN	2.2
1	L	436	LEU	2.2
1	E	475	ARG	2.2
1	I	480	TYR	2.2
1	I	409	LYS	2.2
1	I	411	LYS	2.2
1	I	421	ASN	2.2
1	E	244	THR	2.2
1	J	496	PRO	2.1
1	L	36	THR	2.2
1	D	314	ILE	2.1
1	I	476	GLU	2.1
1	K	350	PHE	2.1
1	L	395	ILE	2.1
1	B	241	VAL	2.1
1	J	331	VAL	2.1
1	C	466	GLY	2.1
1	I	418	GLY	2.1
1	J	460	GLY	2.1
1	A	324	ALA	2.1
1	I	475	ARG	2.1
1	L	108	LEU	2.1
1	A	60	ASP	2.1
1	J	376	ASP	2.1
1	E	464	PRO	2.1
1	L	362	GLN	2.1
1	C	465	PHE	2.1
1	D	37	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	270	GLY	2.1
1	A	299	GLY	2.1
1	C	481	GLY	2.1
1	D	345	VAL	2.1
1	H	426	GLY	2.1
1	I	417	VAL	2.1
1	K	40	VAL	2.1
1	K	223	GLY	2.1
1	K	345	VAL	2.1
1	D	367	LEU	2.1
1	I	397	LYS	2.1
1	I	408	LEU	2.1
1	K	294	LEU	2.1
1	K	368	LEU	2.1
1	L	122	LEU	2.1
1	L	411	LYS	2.1
1	D	302	CYS	2.1
1	E	476	GLU	2.1
1	J	356	TYR	2.1
1	A	403	PRO	2.1
1	D	359	THR	2.1
1	G	464	PRO	2.1
1	K	100	THR	2.1
1	A	45	GLY	2.1
1	D	360	GLY	2.1
1	G	224	PHE	2.1
1	H	386	PHE	2.1
1	I	285	TRP	2.1
1	I	318	PHE	2.1
1	K	28	TRP	2.1
1	A	385	VAL	2.1
1	D	35	LYS	2.1
1	K	242	ALA	2.1
1	A	306	SER	2.1
1	D	354	LEU	2.1
1	K	423	SER	2.1
1	A	9	PRO	2.1
1	A	266	THR	2.1
1	F	480	TYR	2.1
1	L	11	PRO	2.1
1	E	270	GLY	2.1
1	L	271	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	292	PHE	2.1
1	K	43	SER	2.1
1	K	375	ALA	2.1
1	C	72	LEU	2.0
1	I	354	LEU	2.0
1	K	199	LEU	2.0
1	L	427	LEU	2.0
1	L	422	ASN	2.0
1	A	301	CYS	2.0
1	L	311	GLN	2.0
1	C	244	THR	2.0
1	C	498	LYS	2.0
1	L	272	LYS	2.0
1	G	481	GLY	2.0
1	L	305	GLY	2.0
1	D	400	ILE	2.0
1	J	22	ILE	2.0
1	I	386	PHE	2.0
1	I	410	PHE	2.0
1	A	500	SER	2.0
1	A	281	ALA	2.0
1	D	177	TRP	2.0
1	L	233	ALA	2.0
1	L	428	ALA	2.0
1	L	349	GLN	2.0
1	D	361	LYS	2.0
1	C	478	GLY	2.0
1	F	460	GLY	2.0
1	G	271	GLY	2.0
1	G	460	GLY	2.0
1	K	378	GLY	2.0
1	A	315	TYR	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

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
4	EDO	I	3127	4/4	0.65	0.25	52,52,57,58	0
3	GAI	L	3108	4/4	0.71	0.23	52,53,55,57	0
4	EDO	A	3116	4/4	0.72	0.22	47,49,53,54	0
4	EDO	D	3117	4/4	0.76	0.16	50,54,56,56	0
4	EDO	I	3119	4/4	0.77	0.21	53,53,57,61	0
4	EDO	A	3111	4/4	0.77	0.14	55,57,57,58	0
4	EDO	G	3125	4/4	0.78	0.17	56,56,58,59	0
3	GAI	F	3103	4/4	0.79	0.15	52,55,55,58	0
4	EDO	D	3126	4/4	0.80	0.17	55,58,59,59	0
4	EDO	A	3110	4/4	0.81	0.18	55,57,57,58	0
4	EDO	C	3115	4/4	0.82	0.17	53,53,57,59	0
4	EDO	C	3113	4/4	0.82	0.14	53,54,57,57	0
4	EDO	G	3123	4/4	0.84	0.16	51,55,55,56	0
4	EDO	F	3122	4/4	0.84	0.21	47,50,54,56	0
4	EDO	J	3128	4/4	0.84	0.13	51,52,54,56	0
2	NA	J	3710	1/1	0.86	0.10	48,48,48,48	0
2	NA	D	3704	1/1	0.86	0.09	55,55,55,55	0
4	EDO	L	3129	4/4	0.86	0.12	55,55,56,57	0
4	EDO	A	3109	4/4	0.87	0.12	47,51,51,56	0
3	GAI	I	3107	4/4	0.87	0.15	48,50,53,54	0
2	NA	K	3711	1/1	0.87	0.11	73,73,73,73	0
2	NA	L	3712	1/1	0.88	0.09	60,60,60,60	0
4	EDO	E	3118	4/4	0.89	0.12	39,49,51,53	0
4	EDO	G	3124	4/4	0.90	0.11	41,48,51,52	0
3	GAI	H	3106	4/4	0.90	0.19	48,48,49,50	0
2	NA	A	3701	1/1	0.91	0.12	57,57,57,57	0
4	EDO	F	3120	4/4	0.91	0.14	50,52,55,55	0
3	GAI	F	3104	4/4	0.91	0.12	46,46,46,47	0
3	GAI	E	3102	4/4	0.91	0.11	34,38,40,44	0
4	EDO	B	3112	4/4	0.91	0.12	38,44,48,50	0
3	GAI	A	3101	4/4	0.92	0.10	40,43,45,45	0
4	EDO	C	3114	4/4	0.93	0.14	43,45,46,50	0
2	NA	C	3703	1/1	0.94	0.07	34,34,34,34	0
3	GAI	G	3105	4/4	0.95	0.07	40,45,46,47	0
2	NA	H	3708	1/1	0.95	0.04	36,36,36,36	0
2	NA	I	3709	1/1	0.95	0.06	36,36,36,36	0
2	NA	B	3702	1/1	0.95	0.06	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	F	3121	4/4	0.96	0.09	27,42,45,46	0
2	NA	E	3705	1/1	0.97	0.04	28,28,28,28	0
2	NA	F	3706	1/1	0.98	0.03	25,25,25,25	0
2	NA	G	3707	1/1	0.98	0.04	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.