



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:59 AM UTC

PDB ID : 3ZDS / pdb_00003zds
Title : Structure of homogentisate 1,2-dioxygenase in complex with reaction intermediates of homogentisate with oxygen.
Authors : Jeoung, J.-H.; Bommer, M.; Lin, T.-Y.; Dobbek, H.
Deposited on : 2012-11-30
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

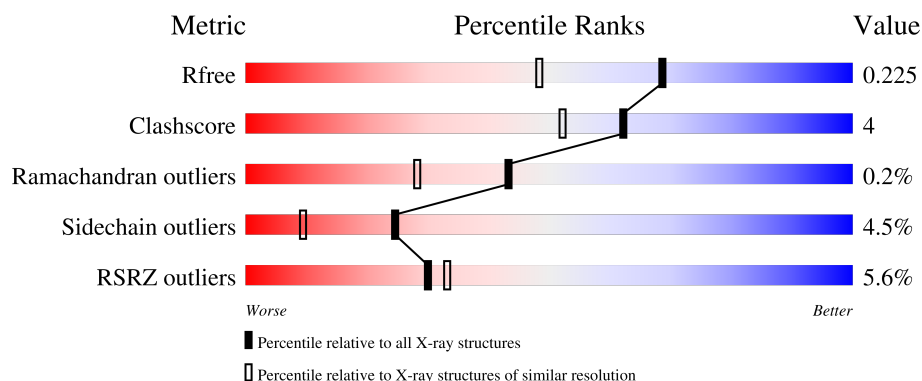
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	433	5% 85% 12% .
1	B	433	3% 89% 9% .
1	C	433	4% 85% 12% ..
1	D	433	3% 82% 15% ..
1	E	433	4% 85% 12% ..

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Mol	Chain	Length	Quality of chain
1	F	433	
1	G	433	
1	H	433	
1	I	433	
1	J	433	
1	K	433	
1	L	433	

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	M8O	A	2001	-	X	-	-
5	OXY	C	1999	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 46082 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 HOMOGENTISATE 1,2-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	16	5	0
			3365	2149	595	604	17			
1	B	426	Total	C	N	O	S	7	4	0
			3358	2145	590	606	17			
1	C	426	Total	C	N	O	S	12	3	0
			3350	2138	590	605	17			
1	D	426	Total	C	N	O	S	9	6	0
			3372	2154	596	605	17			
1	E	426	Total	C	N	O	S	5	3	0
			3351	2139	591	604	17			
1	F	426	Total	C	N	O	S	5	5	0
			3366	2151	595	603	17			
1	G	425	Total	C	N	O	S	5	3	0
			3339	2133	587	601	18			
1	H	426	Total	C	N	O	S	1	2	0
			3343	2134	588	604	17			
1	I	426	Total	C	N	O	S	8	1	0
			3335	2129	585	604	17			
1	J	426	Total	C	N	O	S	4	3	0
			3350	2141	588	603	18			
1	K	426	Total	C	N	O	S	4	3	0
			3351	2140	589	604	18			
1	L	426	Total	C	N	O	S	1	0	0
			3332	2127	585	603	17			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

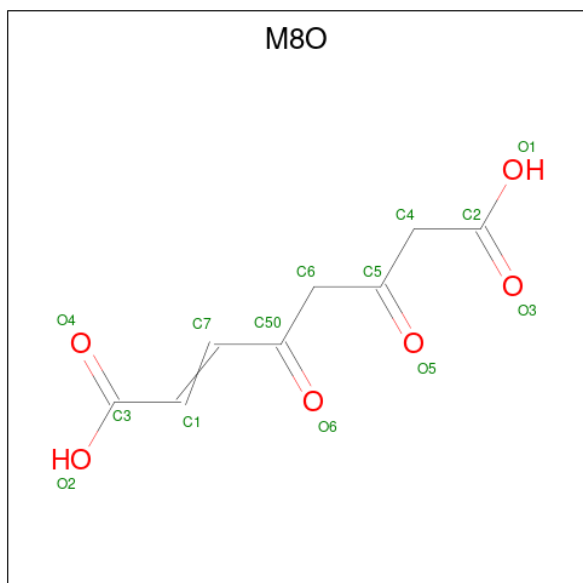
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

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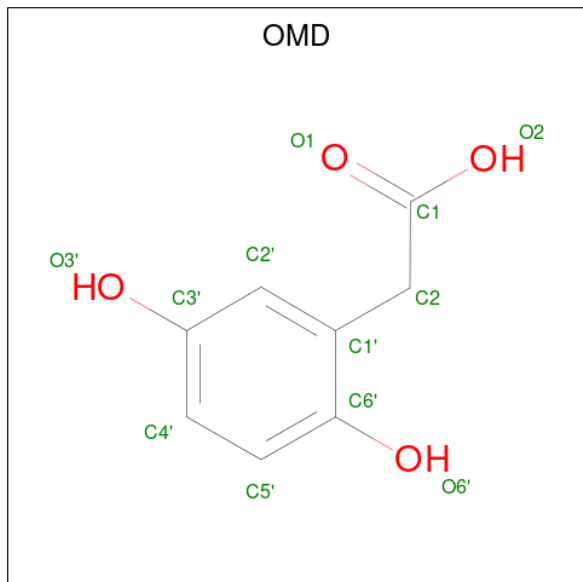
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		
2	G	1	Total	Fe	0	0
			1	1		
2	H	1	Total	Fe	0	0
			1	1		
2	I	1	Total	Fe	0	0
			1	1		
2	J	1	Total	Fe	0	0
			1	1		
2	K	1	Total	Fe	0	0
			1	1		
2	L	1	Total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

- Molecule 3 is 4-Maleylacetoacetic acid (CCD ID: M8O) (formula: $C_8H_8O_6$).



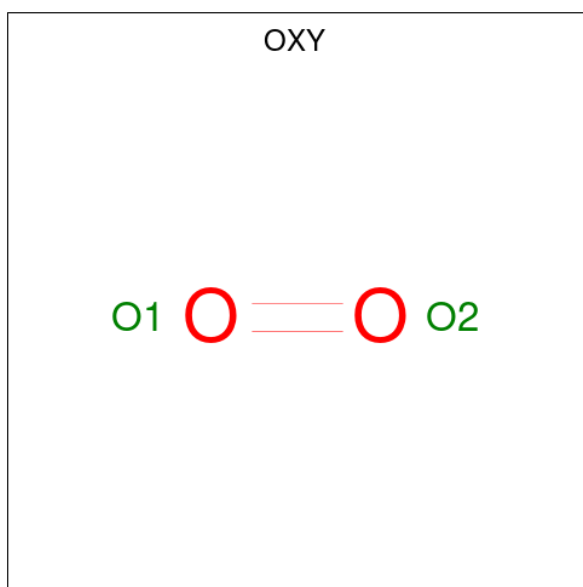
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	8	6		

- Molecule 4 is 2-(3,6-DIHYDROXYPHENYL)ACETIC ACID (CCD ID: OMD) (formula: $C_8H_8O_4$).



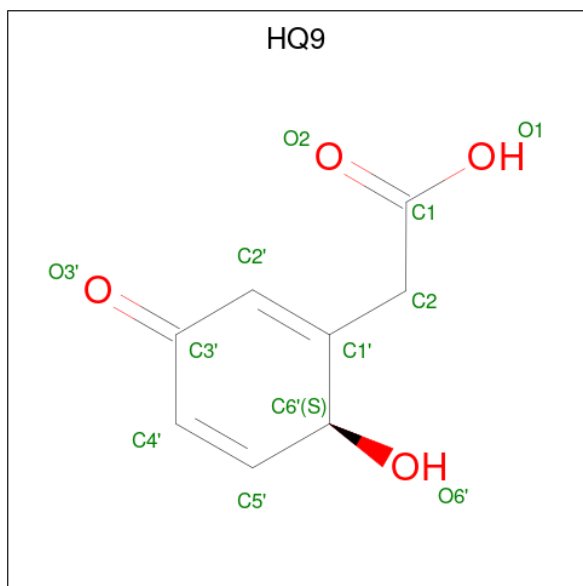
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	8	4		
4	D	1	Total	C	O	0	0
			12	8	4		
4	E	1	Total	C	O	0	0
			12	8	4		
4	G	1	Total	C	O	0	0
			12	8	4		
4	H	1	Total	C	O	0	0
			12	8	4		
4	I	1	Total	C	O	0	0
			12	8	4		
4	J	1	Total	C	O	0	0
			12	8	4		
4	K	1	Total	C	O	0	0
			12	8	4		

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	O	0	0
			2	2		

- Molecule 6 is 2-(6-oxidanyl-3-oxidanylidene-cyclohexa-1,4-dien-1-yl)ethanoic acid (CCD ID: HQ9) (formula: $C_8H_8O_4$).



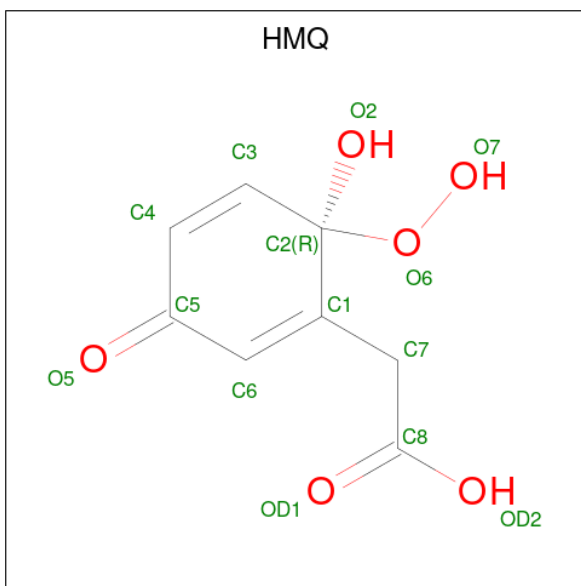
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			12	8	4		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is 2-[(6R)-6-(dioxidanyl)-6-oxidanyl-3-oxidanylidene-cyclohexa-1,4-dien-1-yl]ethanoic acid (CCD ID: HMQ) (formula: C₈H₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			14	8	6		
8	L	1	Total	C	O	0	0
			14	8	6		

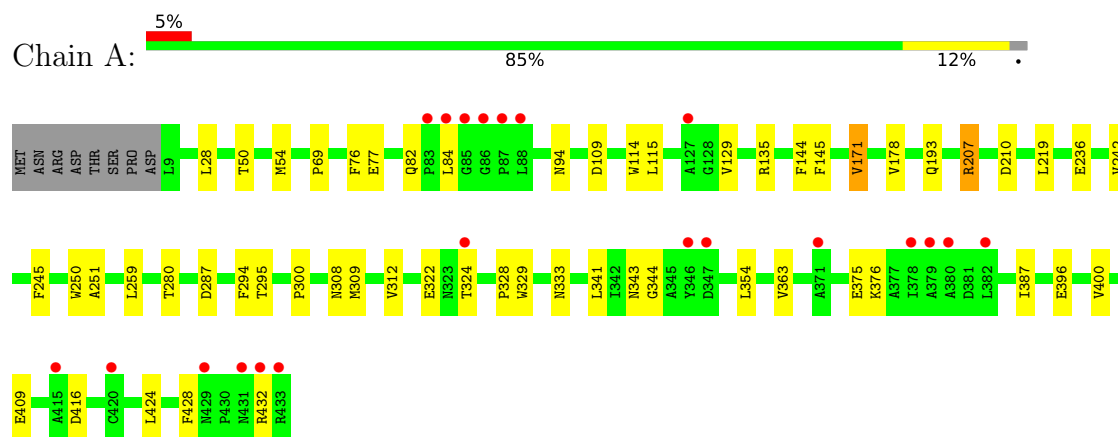
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	543	Total 543	O 543	0	0
9	B	523	Total 523	O 523	0	0
9	C	490	Total 490	O 490	0	0
9	D	547	Total 547	O 547	0	0
9	E	500	Total 500	O 500	0	0
9	F	471	Total 471	O 471	0	0
9	G	434	Total 434	O 434	0	0
9	H	475	Total 475	O 475	0	0
9	I	404	Total 404	O 404	0	0
9	J	501	Total 501	O 501	0	0
9	K	403	Total 403	O 403	0	0
9	L	410	Total 410	O 410	0	0

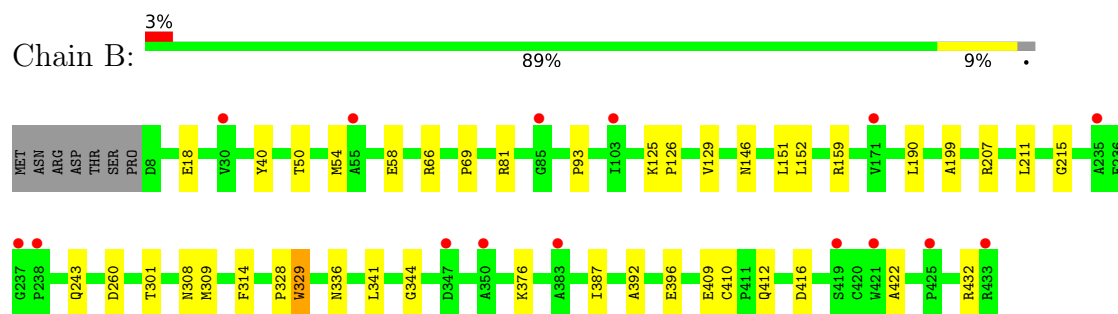
3 Residue-property plots [i](#)

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.

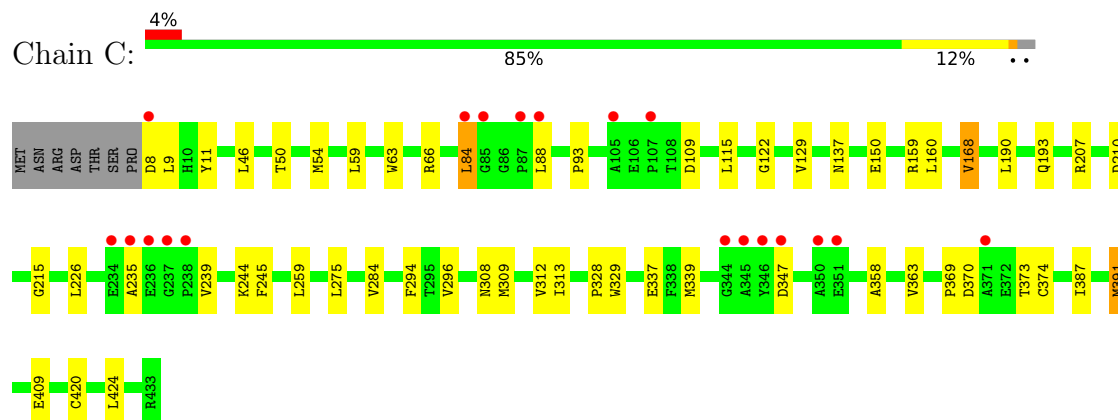
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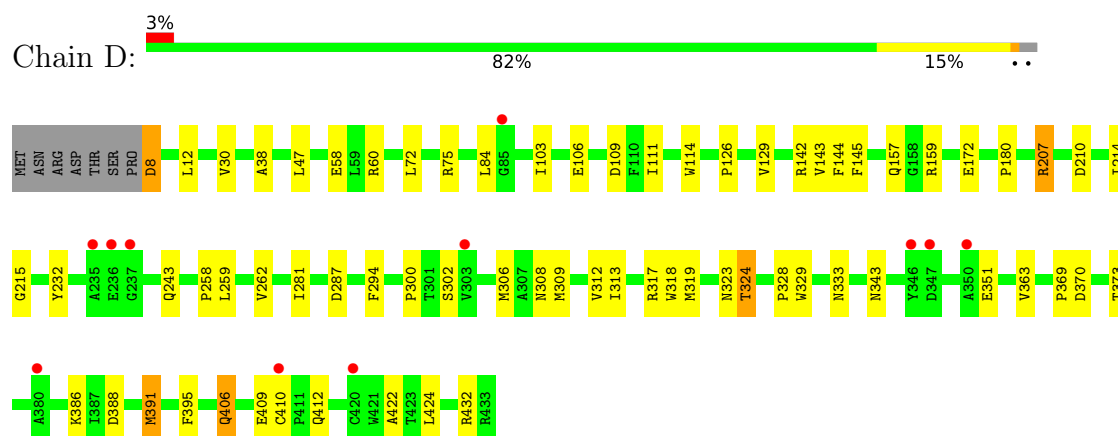
• Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



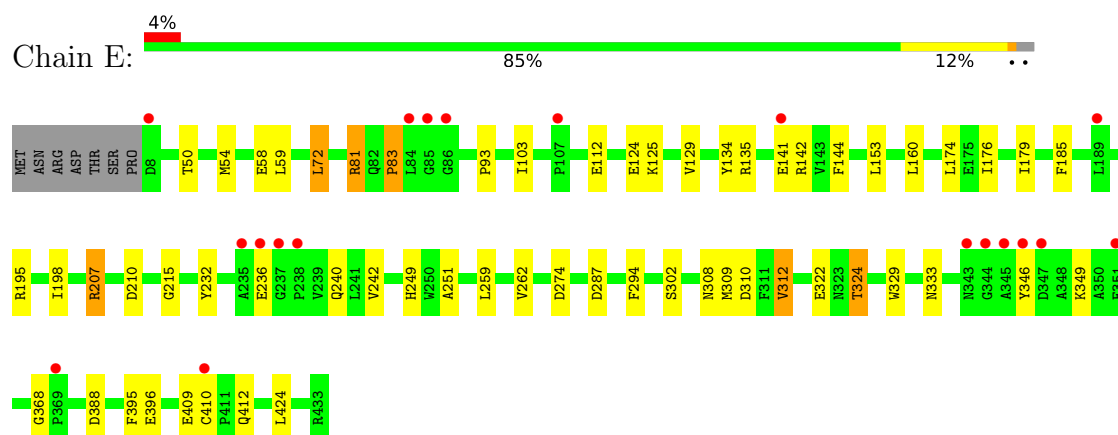
• Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



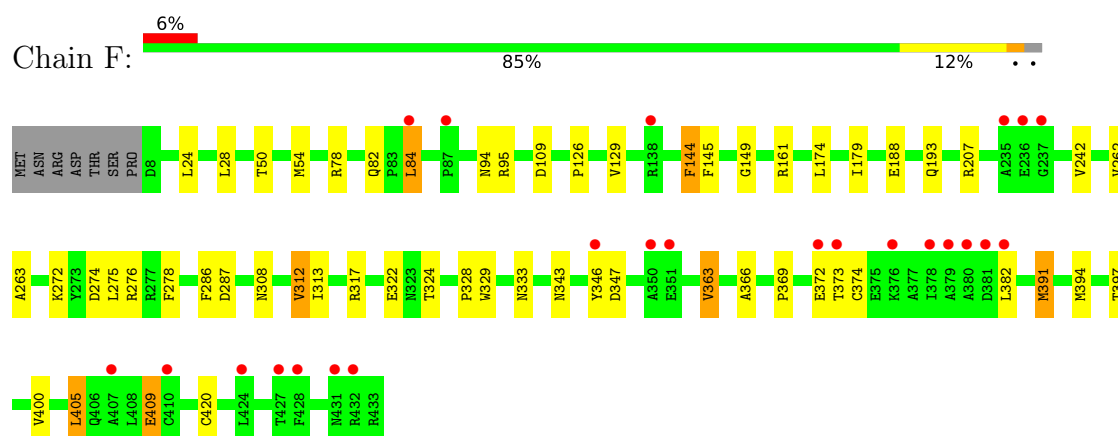
- Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



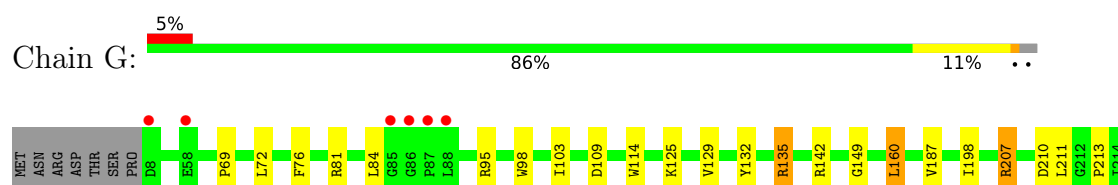
- Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



- Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE

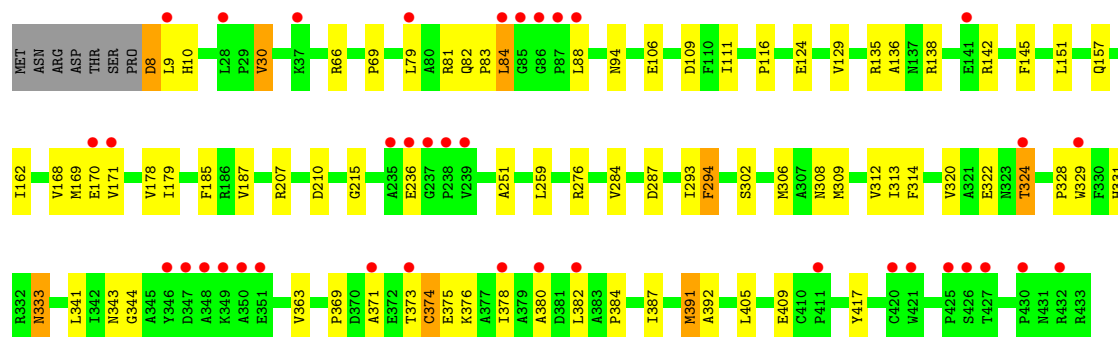
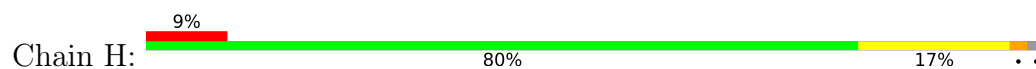


- Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE

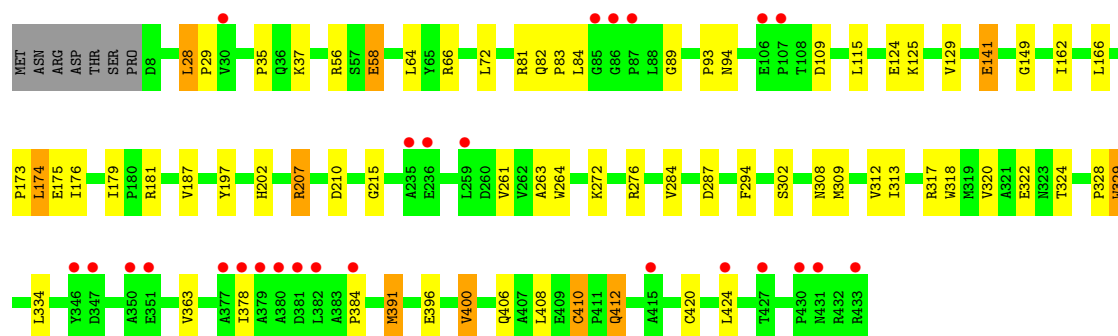
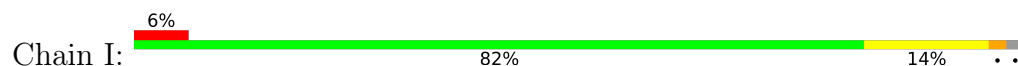




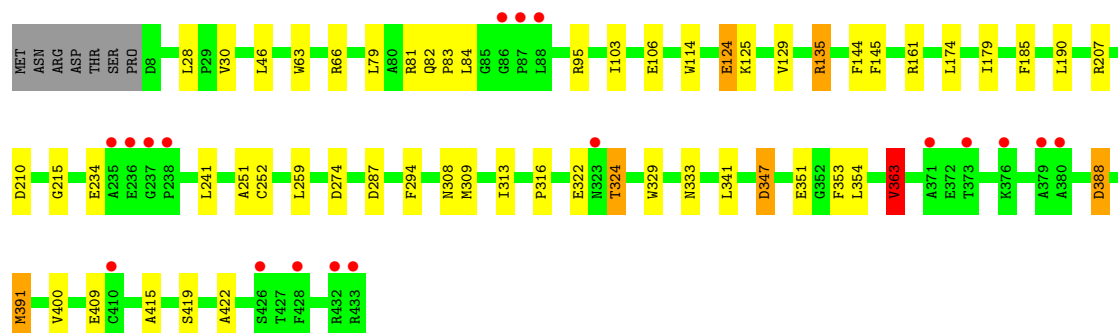
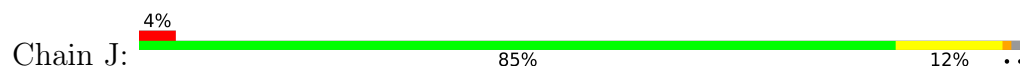
● Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



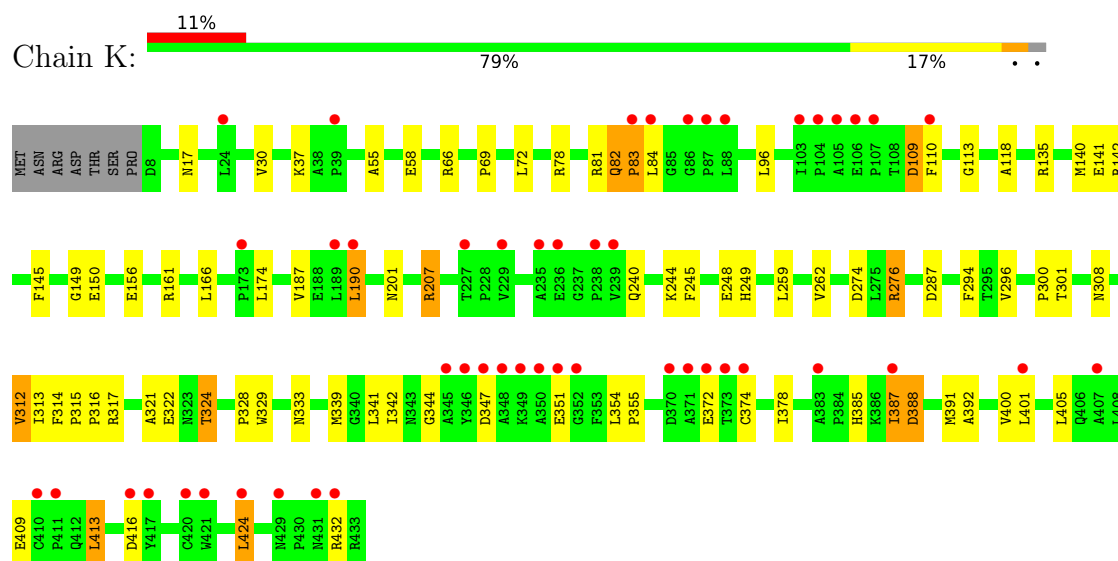
● Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



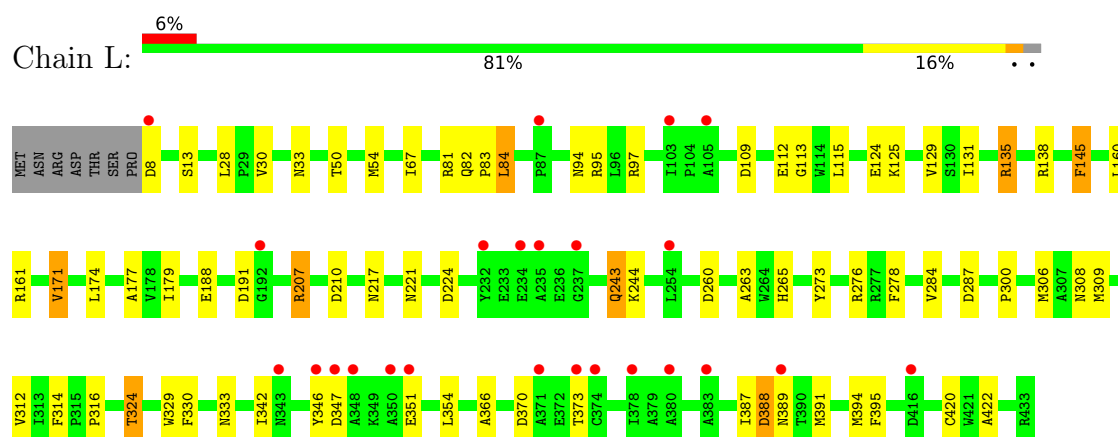
● Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



● Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



● Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.74Å 93.86Å 163.44Å 87.62° 80.39° 68.29°	Depositor
Resolution (Å)	34.37 – 1.70 34.37 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.9 (34.37-1.70) 94.9 (34.37-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 1.70Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.203 , 0.252 0.225 , 0.225	Depositor DCC
R_{free} test set	26636 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 80.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	46082	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.25% 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: PO4, OXY, HMQ, HQ9, FE, M8O, OMD

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	0.88	1/3485 (0.0%)	1.17	11/4746 (0.2%)
1	B	0.86	1/3472 (0.0%)	1.19	11/4729 (0.2%)
1	C	0.89	1/3461 (0.0%)	1.22	18/4716 (0.4%)
1	D	0.90	2/3492 (0.1%)	1.19	14/4756 (0.3%)
1	E	0.93	3/3462 (0.1%)	1.25	16/4716 (0.3%)
1	F	0.88	2/3483 (0.1%)	1.22	18/4743 (0.4%)
1	G	0.86	0/3450	1.19	14/4702 (0.3%)
1	H	0.89	5/3451 (0.1%)	1.22	20/4702 (0.4%)
1	I	0.87	3/3440 (0.1%)	1.20	12/4689 (0.3%)
1	J	0.91	3/3461 (0.1%)	1.23	19/4715 (0.4%)
1	K	0.85	2/3462 (0.1%)	1.23	23/4716 (0.5%)
1	L	0.87	1/3434 (0.0%)	1.22	20/4680 (0.4%)
All	All	0.88	24/41553 (0.1%)	1.21	196/56610 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	81[A]	ARG	CA-C	13.89	1.71	1.52
1	E	81[B]	ARG	CA-C	13.89	1.71	1.52
1	D	391	MET	SD-CE	-11.03	1.51	1.79
1	F	391	MET	SD-CE	-9.41	1.56	1.79
1	C	391	MET	SD-CE	-9.19	1.56	1.79
1	I	391	MET	SD-CE	-9.06	1.56	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	391	MET	SD-CE	-8.03	1.59	1.79
1	J	391	MET	SD-CE	-7.82	1.60	1.79
1	J	82	GLN	C-N	7.08	1.42	1.34
1	A	82	GLN	C-O	-6.64	1.18	1.24
1	H	169	MET	SD-CE	-6.53	1.63	1.79
1	I	82	GLN	C-N	6.46	1.41	1.34
1	H	82	GLN	C-N	6.39	1.42	1.34
1	K	81	ARG	C-O	-6.12	1.16	1.24
1	F	82	GLN	C-N	5.97	1.40	1.34
1	H	306	MET	SD-CE	-5.89	1.64	1.79
1	E	83	PRO	N-CD	5.45	1.55	1.47
1	K	82	GLN	C-N	5.42	1.40	1.34
1	B	336	ASN	CA-C	-5.41	1.46	1.52
1	I	82	GLN	C-O	-5.35	1.18	1.24
1	L	83	PRO	N-CD	5.33	1.55	1.47
1	D	306	MET	SD-CE	-5.23	1.66	1.79
1	H	83	PRO	N-CD	5.14	1.54	1.47
1	J	83	PRO	N-CD	5.04	1.54	1.47

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	81[A]	ARG	CA-C-O	-12.45	107.09	121.66
1	E	81[B]	ARG	CA-C-O	-12.45	107.09	121.66
1	C	409	GLU	CA-C-N	8.94	133.61	120.83
1	C	409	GLU	C-N-CA	8.94	133.61	120.83
1	K	308	ASN	N-CA-C	-8.93	101.52	111.07
1	E	333	ASN	CA-CB-CG	8.17	120.77	112.60
1	L	347	ASP	N-CA-C	7.88	121.83	111.75
1	B	308	ASN	N-CA-C	-7.78	102.73	111.14
1	C	308	ASN	N-CA-C	-7.77	102.89	111.36
1	D	308	ASN	N-CA-C	-7.77	102.75	111.07
1	G	215	GLY	N-CA-C	7.69	120.58	111.35
1	J	347	ASP	N-CA-C	7.67	122.07	112.87
1	H	308	ASN	N-CA-C	-7.65	102.88	111.07
1	J	308	ASN	N-CA-C	-7.62	102.92	111.07
1	H	409	GLU	CA-C-N	7.61	131.71	120.83
1	H	409	GLU	C-N-CA	7.61	131.71	120.83
1	F	343	ASN	CA-CB-CG	7.60	120.20	112.60
1	D	215	GLY	N-CA-C	7.54	120.40	111.35
1	J	82	GLN	CA-C-N	-7.43	112.14	119.87
1	J	82	GLN	C-N-CA	-7.43	112.14	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	409	GLU	CA-C-N	7.26	130.53	120.65
1	B	409	GLU	C-N-CA	7.26	130.53	120.65
1	I	308	ASN	N-CA-C	-7.24	103.47	111.36
1	F	333	ASN	CA-CB-CG	7.18	119.78	112.60
1	C	347	ASP	N-CA-C	7.12	119.95	111.33
1	A	109	ASP	CA-CB-CG	7.02	119.62	112.60
1	L	109	ASP	CA-CB-CG	6.99	119.59	112.60
1	F	308	ASN	N-CA-C	-6.96	103.63	111.07
1	H	30	VAL	N-CA-CB	6.87	118.20	110.72
1	E	395	PHE	CA-CB-CG	6.81	120.61	113.80
1	I	215	GLY	N-CA-C	6.76	119.47	111.35
1	A	145	PHE	CA-CB-CG	6.73	120.53	113.80
1	E	215	GLY	N-CA-C	6.60	119.27	111.35
1	G	308	ASN	N-CA-C	-6.60	104.09	111.28
1	L	145	PHE	CA-CB-CG	6.58	120.38	113.80
1	J	210	ASP	N-CA-C	-6.57	100.56	110.28
1	F	82	GLN	CA-C-N	-6.54	113.41	119.82
1	F	82	GLN	C-N-CA	-6.54	113.41	119.82
1	G	109	ASP	CA-CB-CG	6.52	119.12	112.60
1	K	55	ALA	N-CA-C	-6.50	101.51	110.35
1	C	8	ASP	CA-C-N	6.40	129.80	120.71
1	C	8	ASP	C-N-CA	6.40	129.80	120.71
1	J	294	PHE	CA-CB-CG	6.40	120.20	113.80
1	I	82	GLN	CA-C-N	-6.38	113.24	119.87
1	I	82	GLN	C-N-CA	-6.38	113.24	119.87
1	H	215	GLY	N-CA-C	6.37	118.99	111.35
1	K	82	GLN	CA-C-N	-6.36	113.14	119.56
1	K	82	GLN	C-N-CA	-6.36	113.14	119.56
1	H	94	ASN	N-CA-C	6.34	119.43	110.50
1	J	333	ASN	CA-CB-CG	6.22	118.82	112.60
1	L	124	GLU	CB-CG-CD	6.21	123.15	112.60
1	L	333	ASN	CA-CB-CG	6.17	118.77	112.60
1	D	333	ASN	CA-CB-CG	6.16	118.76	112.60
1	L	346	TYR	CA-C-N	6.15	129.36	120.38
1	L	346	TYR	C-N-CA	6.15	129.36	120.38
1	K	296	VAL	N-CA-C	-6.14	105.84	111.67
1	E	310	ASP	CA-CB-CG	6.13	118.73	112.60
1	L	387	ILE	N-CA-C	-6.13	99.75	108.58
1	J	409	GLU	CA-C-N	6.11	129.57	120.83
1	J	409	GLU	C-N-CA	6.11	129.57	120.83
1	C	215	GLY	N-CA-C	6.11	118.68	111.35
1	K	405	LEU	CA-C-N	6.11	128.46	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	405	LEU	C-N-CA	6.11	128.46	120.28
1	B	211	LEU	N-CA-C	6.10	120.33	113.01
1	H	82	GLN	CA-C-N	-6.09	113.41	119.56
1	H	82	GLN	C-N-CA	-6.09	113.41	119.56
1	E	210	ASP	N-CA-C	-6.07	100.67	109.59
1	G	409	GLU	CA-C-N	6.06	128.89	120.65
1	G	409	GLU	C-N-CA	6.06	128.89	120.65
1	I	66	ARG	N-CA-C	6.05	119.40	109.72
1	J	144	PHE	CA-CB-CG	6.02	119.82	113.80
1	L	308	ASN	N-CA-C	-6.02	104.80	111.36
1	J	215	GLY	N-CA-C	6.01	118.56	111.35
1	I	141	GLU	N-CA-C	-5.98	106.14	113.50
1	G	387	ILE	N-CA-C	-5.95	101.87	109.30
1	G	380	ALA	N-CA-C	5.92	118.64	110.35
1	D	210	ASP	CA-CB-CG	5.89	118.50	112.60
1	H	382	LEU	N-CA-C	5.89	117.64	109.15
1	C	66	ARG	N-CA-C	5.87	119.25	110.14
1	C	284	VAL	N-CA-C	-5.86	107.04	112.43
1	A	94	ASN	N-CA-C	5.86	118.31	110.35
1	L	82	GLN	CA-C-N	-5.83	113.81	119.87
1	L	82	GLN	C-N-CA	-5.83	113.81	119.87
1	A	308	ASN	N-CA-C	-5.78	105.06	111.36
1	K	145	PHE	CA-CB-CG	5.77	119.57	113.80
1	E	409	GLU	CA-C-N	5.75	132.16	121.69
1	E	409	GLU	C-N-CA	5.75	132.16	121.69
1	A	409	GLU	CA-C-N	5.75	128.47	120.65
1	A	409	GLU	C-N-CA	5.75	128.47	120.65
1	F	145	PHE	CA-CB-CG	5.71	119.51	113.80
1	G	333	ASN	CA-CB-CG	5.71	118.31	112.60
1	J	353	PHE	CA-CB-CG	5.71	119.51	113.80
1	B	215	GLY	N-CA-C	5.68	118.17	111.35
1	I	410	CYS	N-CA-C	5.68	117.74	109.84
1	B	66	ARG	N-CA-C	5.68	118.47	109.50
1	C	9	LEU	N-CA-C	5.67	118.46	110.23
1	A	294	PHE	CA-CB-CG	5.67	119.47	113.80
1	D	370	ASP	CA-CB-CG	5.65	118.25	112.60
1	K	372	GLU	CA-C-N	5.64	128.10	120.38
1	K	372	GLU	C-N-CA	5.64	128.10	120.38
1	F	347	ASP	N-CA-C	5.62	118.18	111.71
1	L	395	PHE	CA-CB-CG	5.60	119.40	113.80
1	I	210	ASP	N-CA-C	-5.57	101.60	109.96
1	F	382	LEU	N-CA-C	5.54	117.77	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	330	PHE	CA-CB-CG	-5.54	108.26	113.80
1	C	150	GLU	N-CA-C	-5.54	102.28	110.48
1	H	343	ASN	CA-CB-CG	5.54	118.14	112.60
1	J	388	ASP	CA-CB-CG	5.54	118.14	112.60
1	D	409	GLU	CA-C-N	5.54	128.74	120.83
1	D	409	GLU	C-N-CA	5.54	128.74	120.83
1	D	210	ASP	N-CA-C	-5.53	101.71	109.96
1	E	81[A]	ARG	N-CA-C	5.52	118.39	108.17
1	E	81[B]	ARG	N-CA-C	5.52	118.39	108.17
1	B	387	ILE	N-CA-C	-5.51	102.41	109.30
1	H	374	CYS	CA-C-N	5.51	127.94	120.38
1	H	374	CYS	C-N-CA	5.51	127.94	120.38
1	F	346	TYR	CA-C-N	5.50	128.20	120.28
1	F	346	TYR	C-N-CA	5.50	128.20	120.28
1	D	395	PHE	CA-CB-CG	5.50	119.30	113.80
1	H	10	HIS	N-CA-C	5.48	119.00	110.17
1	D	103	ILE	N-CA-C	-5.48	103.58	108.95
1	F	109	ASP	CA-CB-CG	5.48	118.08	112.60
1	J	95	ARG	N-CA-C	-5.47	101.76	109.96
1	L	284	VAL	N-CA-C	-5.46	106.09	111.88
1	D	145	PHE	CA-CB-CG	5.45	119.25	113.80
1	K	301	THR	N-CA-C	-5.43	102.13	109.95
1	H	284	VAL	N-CA-C	-5.43	107.44	112.43
1	F	94	ASN	N-CA-C	5.43	117.73	110.35
1	H	145	PHE	CA-CB-CG	5.42	119.22	113.80
1	E	308	ASN	N-CA-C	-5.42	105.27	111.07
1	L	94	ASN	N-CA-C	5.41	117.71	110.35
1	B	301	THR	N-CA-C	-5.41	101.90	109.69
1	H	333	ASN	CA-CB-CG	5.38	117.98	112.60
1	L	30	VAL	N-CA-CB	5.38	116.97	110.95
1	E	274	ASP	CA-CB-CG	5.38	117.97	112.60
1	E	346	TYR	CA-C-N	5.38	128.23	120.38
1	E	346	TYR	C-N-CA	5.38	128.23	120.38
1	C	370	ASP	CA-CB-CG	5.35	117.95	112.60
1	E	59	LEU	N-CA-C	5.34	118.06	110.10
1	A	210	ASP	N-CA-C	-5.34	101.95	109.96
1	I	334	LEU	N-CA-C	-5.32	105.65	111.82
1	A	343	ASN	CA-CB-CG	5.32	117.92	112.60
1	J	145	PHE	CA-CB-CG	5.31	119.11	113.80
1	J	422	ALA	N-CA-C	5.30	117.80	111.71
1	K	109	ASP	CA-CB-CG	5.30	117.90	112.60
1	G	149	GLY	CA-C-N	5.29	128.98	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	149	GLY	C-N-CA	5.29	128.98	121.42
1	H	294	PHE	CA-CB-CG	5.29	119.09	113.80
1	K	66	ARG	CA-C-N	5.28	127.22	120.56
1	K	66	ARG	C-N-CA	5.28	127.22	120.56
1	A	333	ASN	CA-CB-CG	5.27	117.87	112.60
1	J	66	ARG	N-CA-C	5.26	118.16	109.85
1	C	337	GLU	N-CA-C	5.26	117.29	107.99
1	L	210	ASP	N-CA-C	-5.26	102.08	109.96
1	I	284	VAL	N-CA-C	-5.25	106.31	111.88
1	H	66	ARG	N-CA-C	5.24	118.13	109.85
1	B	260	ASP	CA-CB-CG	5.23	117.83	112.60
1	J	363	VAL	CB-CA-C	-5.22	102.73	111.29
1	G	422	ALA	N-CA-C	5.21	118.42	111.75
1	K	315	PRO	N-CA-C	5.21	117.06	110.70
1	L	422	ALA	N-CA-C	5.21	117.64	111.33
1	G	349	LYS	CA-C-N	5.18	127.47	120.38
1	G	349	LYS	C-N-CA	5.18	127.47	120.38
1	I	400	VAL	N-CA-CB	5.15	118.79	110.13
1	C	210	ASP	N-CA-C	-5.15	102.43	110.10
1	G	211	LEU	N-CA-C	5.15	118.82	112.54
1	H	405	LEU	CA-C-N	5.14	127.17	120.28
1	H	405	LEU	C-N-CA	5.14	127.17	120.28
1	K	333	ASN	CA-CB-CG	5.13	117.73	112.60
1	F	405	LEU	CA-C-N	5.12	127.46	120.54
1	F	405	LEU	C-N-CA	5.12	127.46	120.54
1	J	274	ASP	CA-CB-CG	5.12	117.72	112.60
1	K	409	GLU	CA-C-N	5.12	134.28	121.80
1	K	409	GLU	C-N-CA	5.12	134.28	121.80
1	F	149	GLY	CA-C-N	5.11	128.73	121.42
1	F	149	GLY	C-N-CA	5.11	128.73	121.42
1	C	109	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	422	ALA	N-CA-C	5.10	118.28	111.75
1	F	144	PHE	CA-CB-CG	5.10	118.90	113.80
1	B	18	GLU	N-CA-C	-5.09	99.03	107.99
1	K	149	GLY	CA-C-N	5.09	128.69	121.42
1	K	149	GLY	C-N-CA	5.09	128.69	121.42
1	K	388	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	8	ASP	CA-CB-CG	5.08	117.68	112.60
1	C	387	ILE	N-CA-C	-5.07	102.20	108.89
1	A	387	ILE	N-CA-C	-5.05	101.30	108.58
1	I	109	ASP	CA-CB-CG	5.05	117.66	112.60
1	D	109	ASP	CA-CB-CG	5.05	117.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	VAL	N-CA-C	-5.04	106.88	111.67
1	D	422	ALA	N-CA-C	5.02	116.75	111.28
1	K	83	PRO	CA-N-CD	-5.02	104.98	112.00
1	L	13	SER	N-CA-C	5.01	117.92	109.95
1	C	168	VAL	N-CA-C	5.01	115.53	108.36
1	L	217	ASN	CA-CB-CG	5.01	117.61	112.60
1	F	286	PHE	CA-CB-CG	5.01	118.81	113.80
1	K	17	ASN	N-CA-C	5.01	117.16	110.35

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	81[A]	ARG	Mainchain
1	E	81[B]	ARG	Mainchain

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	3365	0	3291	26	0
1	B	3358	0	3276	18	0
1	C	3350	0	3261	21	0
1	D	3372	0	3300	30	0
1	E	3351	0	3267	26	0
1	F	3366	0	3297	28	0
1	G	3339	0	3254	23	0
1	H	3343	0	3254	32	0
1	I	3335	0	3241	43	0
1	J	3350	0	3269	21	0
1	K	3351	0	3266	43	0
1	L	3332	0	3236	28	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	14	0	6	2	0
4	B	12	0	5	2	0
4	D	12	0	5	0	0
4	E	12	0	5	0	0
4	G	12	0	5	0	0
4	H	12	0	5	0	0
4	I	12	0	6	2	0
4	J	12	0	5	0	0
4	K	12	0	5	1	0
5	C	2	0	0	2	0
6	C	12	0	6	2	0
7	E	5	0	0	0	0
8	F	14	0	6	1	0
8	L	14	0	7	1	0
9	A	543	0	0	9	0
9	B	523	0	0	3	0
9	C	490	0	0	1	0
9	D	547	0	0	10	0
9	E	500	0	0	4	0
9	F	471	0	0	5	0
9	G	434	0	0	3	0
9	H	475	0	0	6	0
9	I	404	0	0	13	0
9	J	501	0	0	3	0
9	K	403	0	0	4	1
9	L	410	0	0	7	1
All	All	46082	0	39278	329	1

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 4.

All (329) 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)
8:F:2001:HMQ:O7	8:F:2001:HMQ:O6	1.53	1.24
8:L:2001:HMQ:O7	8:L:2001:HMQ:O6	1.57	1.21
1:L:287:ASP:H	1:L:324:THR:HG21	1.21	1.05
1:E:287:ASP:H	1:E:324:THR:HG21	1.27	0.97
1:F:287:ASP:H	1:F:324:THR:HG21	1.31	0.95
1:I:287:ASP:H	1:I:324:THR:HG21	1.34	0.90
5:C:1999:OXY:O2	6:C:2001:HQ9:H6'	1.73	0.88
1:B:146:ASN:HD22	1:B:151:LEU:HD11	1.38	0.88
1:H:136:ALA:HB1	9:H:3196:HOH:O	1.73	0.87
1:K:287:ASP:H	1:K:324:THR:HG21	1.38	0.87
1:D:287:ASP:H	1:D:324:THR:HG21	1.42	0.82
1:L:287:ASP:N	1:L:324:THR:HG21	1.93	0.81
1:A:250:TRP:HB3	9:A:3160:HOH:O	1.80	0.81
1:H:287:ASP:H	1:H:324:THR:HG21	1.46	0.79
1:H:313:ILE:HB	1:H:391:MET:CE	2.14	0.78
1:K:287:ASP:N	1:K:324:THR:HG21	2.01	0.76
9:A:3280:HOH:O	1:C:363:VAL:HG22	1.85	0.76
1:D:317:ARG:HG3	9:D:3423:HOH:O	1.84	0.76
1:E:287:ASP:N	1:E:324:THR:HG21	2.00	0.75
1:F:287:ASP:N	1:F:324:THR:HG21	2.00	0.75
1:D:319:MET:SD	9:D:3423:HOH:O	2.44	0.75
1:A:322:GLU:O	1:A:324:THR:HG23	1.89	0.73
1:F:129[A]:VAL:HG11	1:F:397:THR:HG21	1.71	0.73
1:I:202:HIS:HA	9:I:3176:HOH:O	1.89	0.71
9:D:3098:HOH:O	1:G:335:MET:SD	2.49	0.71
1:I:313:ILE:HB	1:I:391:MET:CE	2.21	0.71
1:I:93:PRO:HD2	9:I:3110:HOH:O	1.90	0.70
5:C:1999:OXY:O1	6:C:2001:HQ9:H6'	1.90	0.70
1:A:76:PHE:HB3	9:A:3160:HOH:O	1.91	0.70
1:A:287:ASP:H	1:A:324:THR:HG21	1.57	0.70
1:B:146:ASN:HD22	1:B:151:LEU:CD1	2.04	0.69
1:F:287:ASP:H	1:F:324:THR:CG2	2.04	0.69
1:I:149:GLY:HA2	9:I:3176:HOH:O	1.94	0.68
1:I:179:ILE:HG22	9:I:3207:HOH:O	1.93	0.68
1:J:287:ASP:H	1:J:324:THR:HG21	1.58	0.68
1:J:313:ILE:HB	1:J:391:MET:CE	2.23	0.68
1:I:287:ASP:N	1:I:324:THR:HG21	2.09	0.67
1:I:322:GLU:O	1:I:324:THR:HG23	1.93	0.67
1:D:287:ASP:N	1:D:324:THR:HG21	2.10	0.67
1:I:181:ARG:NH2	9:I:3176:HOH:O	2.29	0.66
1:H:313:ILE:HB	1:H:391:MET:HE2	1.76	0.66
1:H:79:LEU:HD21	1:H:251:ALA:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:262:VAL:HG23	9:K:3283:HOH:O	1.96	0.65
1:H:320:VAL:HG12	1:H:384:PRO:HB3	1.79	0.65
1:H:371:ALA:O	1:H:375:GLU:OE1	2.15	0.65
1:I:313:ILE:HB	1:I:391:MET:HE2	1.77	0.64
1:L:33:ASN:ND2	9:L:3057:HOH:O	2.30	0.64
1:J:363:VAL:CG2	1:J:400:VAL:HG12	2.28	0.64
1:H:287:ASP:N	1:H:324:THR:HG21	2.13	0.63
1:D:58:GLU:HG3	1:D:207:ARG:NH2	2.14	0.63
1:F:126:PRO:HG2	9:F:3241:HOH:O	1.98	0.63
1:B:129:VAL:HG22	9:B:3309:HOH:O	1.98	0.63
1:D:410:CYS:SG	1:D:412:GLN:HB2	2.39	0.62
1:F:274:ASP:OD1	1:F:276:ARG:HD3	2.00	0.62
1:B:328:PRO:HB3	4:B:2001:OMD:C4'	2.30	0.61
1:C:313:ILE:HD12	1:C:391:MET:HE1	1.83	0.61
1:C:88:LEU:HD21	1:C:122:GLY:HA2	1.82	0.61
1:E:322:GLU:O	1:E:324:THR:HG22	2.01	0.61
1:A:287:ASP:H	1:A:324:THR:CG2	2.14	0.60
1:L:224:ASP:HB2	9:L:3275:HOH:O	2.01	0.60
1:L:278:PHE:O	9:L:3308:HOH:O	2.16	0.60
1:J:313:ILE:HB	1:J:391:MET:HE1	1.82	0.60
1:B:126:PRO:HA	9:B:3226:HOH:O	2.01	0.60
1:I:84:LEU:N	1:I:84:LEU:HD12	2.17	0.60
1:K:140[B]:MET:HE3	1:K:187:VAL:H	1.67	0.60
1:A:219:LEU:HD11	9:A:3422:HOH:O	2.02	0.60
1:C:11:TYR:HB3	1:C:226:LEU:HB3	1.82	0.60
1:K:401:LEU:HD11	9:K:3328:HOH:O	2.02	0.60
1:H:294:PHE:HB2	1:H:312:VAL:HG13	1.83	0.60
1:H:369:PRO:HB2	1:H:373:THR:OG1	2.02	0.59
1:H:313:ILE:HB	1:H:391:MET:HE1	1.82	0.59
1:L:161:ARG:HD3	1:L:188:GLU:OE1	2.01	0.59
1:D:129:VAL:HG21	1:D:309:MET:HB3	1.84	0.59
1:B:129:VAL:HG21	1:B:309:MET:HB3	1.84	0.58
1:D:313:ILE:HB	1:D:391:MET:CE	2.33	0.58
1:I:83:PRO:HG2	1:I:84:LEU:HD12	1.84	0.58
1:K:387:ILE:HG21	9:K:3311:HOH:O	2.03	0.58
1:A:354:LEU:HD13	1:F:193:GLN:HE22	1.68	0.58
1:L:129:VAL:HG21	1:L:309:MET:HB3	1.85	0.58
1:F:322:GLU:O	1:F:324:THR:HG23	2.03	0.58
1:K:83:PRO:HG2	1:K:84:LEU:HG	1.86	0.58
1:K:274:ASP:OD1	1:K:276:ARG:HD3	2.04	0.58
1:F:174:LEU:HB3	1:F:276:ARG:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:67:ILE:HG12	1:L:260:ASP:HB2	1.86	0.57
1:C:294:PHE:HB2	1:C:312:VAL:HG13	1.87	0.57
1:I:175:GLU:HB3	9:I:3206:HOH:O	2.03	0.57
1:B:329:TRP:NE1	9:B:3390:HOH:O	2.34	0.57
1:H:109:ASP:HA	9:H:3196:HOH:O	2.03	0.57
1:A:287:ASP:N	1:A:324:THR:HG21	2.19	0.56
1:K:207:ARG:HD3	1:K:300:PRO:HD3	1.86	0.56
1:I:294:PHE:HB2	1:I:312:VAL:HG13	1.87	0.56
1:J:103:ILE:HD13	1:J:135:ARG:HB3	1.88	0.56
1:F:317:ARG:NH1	9:F:3384:HOH:O	2.37	0.56
1:I:94:ASN:ND2	9:I:3110:HOH:O	2.40	0.55
1:J:241:LEU:HD23	9:J:3130:HOH:O	2.07	0.55
1:F:328:PRO:O	1:F:369:PRO:HD3	2.06	0.55
1:I:129:VAL:HG21	1:I:309:MET:HB3	1.88	0.55
1:J:363:VAL:HG22	1:J:400:VAL:HG12	1.87	0.54
1:D:126:PRO:HA	9:D:3239:HOH:O	2.06	0.54
1:F:129[A]:VAL:CG1	1:F:397:THR:HG21	2.37	0.54
1:L:171:VAL:HG21	1:L:177:ALA:HB2	1.89	0.54
1:L:287:ASP:H	1:L:324:THR:CG2	2.08	0.54
1:A:328:PRO:HB3	3:A:2001:M8O:C1	2.37	0.54
1:J:313:ILE:HB	1:J:391:MET:HE2	1.89	0.54
1:L:28:LEU:HD21	1:L:265:HIS:HB3	1.90	0.54
1:A:251:ALA:N	9:A:3160:HOH:O	2.41	0.54
1:B:152:LEU:HB3	1:B:199:ALA:HB3	1.90	0.53
1:G:160:LEU:HG	1:G:187:VAL:HG13	1.90	0.53
1:H:9:LEU:HD22	1:H:170:GLU:OE1	2.09	0.53
1:I:313:ILE:HB	1:I:391:MET:HE1	1.89	0.53
1:H:341:LEU:HD21	1:H:344:GLY:O	2.08	0.53
1:E:195:ARG:NH1	9:E:3170:HOH:O	2.42	0.53
1:F:28:LEU:HD13	1:F:263:ALA:HB1	1.89	0.53
1:H:81:ARG:HB3	9:H:3153:HOH:O	2.08	0.53
1:I:64:LEU:HD22	1:I:261:VAL:HG21	1.92	0.52
1:D:47:LEU:HD21	9:D:3325:HOH:O	2.09	0.52
1:J:129:VAL:HG21	1:J:309:MET:HB3	1.91	0.52
1:I:329:TRP:CZ3	4:I:2001:OMD:H5'	2.44	0.52
1:J:287:ASP:N	1:J:324:THR:HG21	2.23	0.52
1:H:129:VAL:HG21	1:H:309:MET:HB3	1.91	0.52
1:I:173:PRO:O	1:I:174:LEU:HB2	2.10	0.52
1:E:153:LEU:HD22	1:E:198:ILE:HD12	1.92	0.51
1:F:50:THR:HB	1:F:54:MET:HG3	1.92	0.51
1:I:83:PRO:HG2	1:I:84:LEU:CD1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:PRO:HB3	4:B:2001:OMD:C5'	2.41	0.51
1:D:58:GLU:HG3	1:D:207:ARG:HH22	1.73	0.51
1:K:174:LEU:HB3	1:K:276:ARG:HD2	1.92	0.51
1:H:69:PRO:HG2	1:K:424:LEU:HD22	1.93	0.51
1:L:207:ARG:HD3	1:L:300:PRO:HD3	1.93	0.51
1:D:207:ARG:HD3	1:D:300:PRO:HD3	1.91	0.51
1:K:321:ALA:HB1	1:K:324:THR:HG23	1.93	0.51
1:I:424:LEU:HD13	1:K:69:PRO:HG2	1.93	0.51
1:A:69:PRO:HG2	1:C:424:LEU:HD13	1.92	0.50
1:E:129:VAL:HG21	1:E:309:MET:HB3	1.92	0.50
1:C:275:LEU:HB3	1:C:391:MET:HE2	1.93	0.50
1:G:81:ARG:HD3	9:G:3124:HOH:O	2.11	0.50
1:D:38:ALA:HB2	9:D:3062:HOH:O	2.12	0.50
1:D:60:ARG:NH1	9:D:3128:HOH:O	2.44	0.50
1:D:313:ILE:HB	1:D:391:MET:HE1	1.93	0.50
1:I:318:TRP:HE3	9:I:3306:HOH:O	1.93	0.50
1:B:314:PHE:HB2	1:B:392:ALA:HB3	1.93	0.50
1:I:29:PRO:HB3	1:I:35:PRO:HG3	1.94	0.50
1:F:84:LEU:HA	9:F:3136:HOH:O	2.12	0.49
1:I:272:LYS:HB2	9:I:3206:HOH:O	2.11	0.49
1:K:294:PHE:HB2	1:K:312:VAL:HG13	1.92	0.49
1:K:316:PRO:HB3	1:K:388:ASP:HA	1.94	0.49
1:D:214[B]:ILE:HD12	1:D:281:ILE:HG21	1.94	0.49
1:G:254:LEU:HD12	1:G:258:PRO:HG3	1.94	0.49
1:K:118:ALA:HB1	1:K:401:LEU:HB3	1.94	0.49
1:K:341:LEU:HD21	1:K:344:GLY:O	2.11	0.49
1:F:84:LEU:O	1:F:84:LEU:HD22	2.13	0.49
1:J:124:GLU:OE1	1:J:125:LYS:HG3	2.13	0.49
1:F:275:LEU:HB3	1:F:391:MET:HE2	1.93	0.49
1:K:161:ARG:HB2	1:K:190:LEU:HD13	1.94	0.49
1:L:312:VAL:HG22	1:L:394:MET:HB3	1.95	0.49
1:C:159:ARG:HB2	1:C:190:LEU:HB2	1.94	0.49
1:H:84:LEU:HD12	1:H:116:PRO:HG3	1.95	0.49
1:K:110:PHE:HB3	1:K:140[B]:MET:HE2	1.94	0.49
1:A:50:THR:HB	1:A:54:MET:HG3	1.95	0.48
1:C:46:LEU:HD13	1:C:63:TRP:CE2	2.47	0.48
1:A:129:VAL:HG21	1:A:309:MET:HB3	1.94	0.48
1:A:171:VAL:HB	9:A:3306:HOH:O	2.12	0.48
1:F:129[A]:VAL:HG11	1:F:397:THR:CG2	2.42	0.48
1:I:287:ASP:H	1:I:324:THR:CG2	2.16	0.48
1:H:138:ARG:O	9:H:3196:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LEU:HD11	1:C:244:LYS:HE2	1.96	0.48
1:L:131:ILE:HG13	9:L:3173:HOH:O	2.14	0.48
1:C:137:ASN:HA	1:C:193:GLN:HG2	1.96	0.48
1:C:313:ILE:CD1	1:C:391:MET:HE1	2.43	0.48
1:J:79:LEU:HD21	1:J:251:ALA:HB3	1.96	0.48
1:A:84:LEU:HD21	1:A:114:TRP:HB2	1.96	0.47
1:D:313:ILE:HB	1:D:391:MET:HE2	1.95	0.47
1:L:28:LEU:HD13	1:L:263:ALA:HB1	1.95	0.47
1:A:207:ARG:HD3	1:A:300:PRO:HD3	1.96	0.47
1:E:142[A]:ARG:HH11	1:E:242:VAL:HG21	1.79	0.47
1:I:28:LEU:HD13	1:I:263:ALA:HB1	1.96	0.47
1:K:322:GLU:O	1:K:324:THR:HG22	2.14	0.47
1:E:242:VAL:HG22	1:E:251:ALA:HB2	1.96	0.47
9:D:3298:HOH:O	1:I:81:ARG:HD2	2.14	0.47
1:E:287:ASP:H	1:E:324:THR:CG2	2.14	0.47
1:K:78:ARG:HE	1:K:248:GLU:CD	2.23	0.47
1:K:328:PRO:HB3	4:K:2001:OMD:C4'	2.45	0.47
1:K:385:HIS:CE1	1:K:387:ILE:HG22	2.50	0.47
1:B:410:CYS:SG	1:B:412:GLN:HB2	2.54	0.47
1:I:166:LEU:HD22	1:I:264:TRP:CG	2.50	0.47
1:G:312:VAL:HG22	1:G:394:MET:HB3	1.96	0.47
1:H:314:PHE:HB2	1:H:392:ALA:HB3	1.96	0.47
1:K:314:PHE:HB2	1:K:392:ALA:HB3	1.97	0.47
1:B:309:MET:HA	1:B:396:GLU:O	2.14	0.46
1:H:151:LEU:O	1:H:178:VAL:HA	2.14	0.46
1:F:126:PRO:HA	9:F:3195:HOH:O	2.14	0.46
1:A:178:VAL:HG23	9:A:3320:HOH:O	2.15	0.46
1:D:84:LEU:HD21	1:D:114:TRP:HB2	1.97	0.46
1:H:287:ASP:H	1:H:324:THR:CG2	2.23	0.46
1:K:109:ASP:HB2	1:K:140[B]:MET:HG2	1.97	0.46
1:B:341:LEU:HD21	1:B:344:GLY:O	2.16	0.46
1:K:58:GLU:HG2	1:K:207:ARG:NH2	2.31	0.46
1:H:8:ASP:HB3	1:H:9:LEU:H	1.59	0.46
1:L:174:LEU:HD13	1:L:276:ARG:HD2	1.98	0.46
1:B:159:ARG:HB3	1:B:190:LEU:HD12	1.98	0.45
1:F:144:PHE:HA	1:F:242:VAL:O	2.16	0.45
1:L:221:ASN:O	9:L:3275:HOH:O	2.21	0.45
1:A:77:GLU:N	9:A:3160:HOH:O	2.50	0.45
1:A:295:THR:HA	1:A:312:VAL:HG12	1.99	0.45
1:G:84:LEU:HD21	1:G:114:TRP:HB2	1.98	0.45
1:L:81:ARG:NH1	1:L:112:GLU:HB3	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:PRO:HB3	3:A:2001:M8O:C50	2.47	0.45
1:D:424:LEU:HB2	1:E:72:LEU:HG	1.98	0.45
1:E:349:LYS:NZ	1:E:368:GLY:O	2.50	0.45
1:D:180:PRO:HB2	9:D:3325:HOH:O	2.16	0.45
1:K:113:GLY:HA3	1:K:135:ARG:O	2.16	0.45
1:F:78:ARG:NH2	9:F:3121:HOH:O	2.49	0.45
1:L:84:LEU:HD13	1:L:244:LYS:HE2	1.99	0.45
1:B:50:THR:HB	1:B:54:MET:HG3	1.97	0.45
1:D:328:PRO:O	1:D:369:PRO:HD3	2.16	0.45
1:J:341:LEU:HD23	1:J:354:LEU:C	2.41	0.45
1:H:302:SER:HB3	1:I:302:SER:HB2	1.98	0.45
1:H:331:HIS:CE1	1:H:333:ASN:HB2	2.52	0.45
1:H:417:TYR:HA	9:H:3181:HOH:O	2.17	0.45
1:I:328:PRO:HB3	4:I:2001:OMD:C4'	2.47	0.45
9:A:3422:HOH:O	1:G:213:PRO:HB2	2.17	0.45
1:E:424:LEU:HD13	1:G:69:PRO:HG2	1.97	0.45
1:L:95:ARG:HD3	1:L:366:ALA:O	2.16	0.45
1:D:294:PHE:HB2	1:D:312:VAL:HG13	1.99	0.44
1:E:309:MET:HA	1:E:396:GLU:O	2.18	0.44
1:D:159:ARG:HG2	1:D:172:GLU:HB3	1.98	0.44
1:H:179:ILE:HG21	1:H:185:PHE:CD1	2.53	0.44
1:C:328:PRO:O	1:C:369:PRO:HD3	2.17	0.44
1:D:406[A]:GLN:CD	1:D:406[A]:GLN:H	2.25	0.44
9:D:3098:HOH:O	1:G:334:LEU:HD23	2.18	0.44
1:G:95:ARG:HD3	1:G:366:ALA:O	2.17	0.44
1:I:174:LEU:HD13	1:I:276:ARG:HD2	1.99	0.44
1:K:339:MET:HE2	1:K:339:MET:HB3	1.91	0.44
1:A:428:PHE:HA	1:B:40:TYR:O	2.18	0.44
1:E:232:TYR:CD1	1:E:262:VAL:HG22	2.53	0.44
9:E:3155:HOH:O	1:G:76:PHE:HD2	2.00	0.44
1:J:316:PRO:HB3	1:J:388:ASP:HA	2.00	0.44
1:E:93:PRO:HB3	1:G:245:PHE:CG	2.53	0.44
1:F:312:VAL:HG22	1:F:394:MET:HB3	1.99	0.44
1:C:50:THR:HB	1:C:54:MET:HG3	2.00	0.44
1:G:274:ASP:OD1	1:G:276:ARG:HB2	2.17	0.44
1:I:56:ARG:NH2	9:I:3063:HOH:O	2.49	0.44
1:I:89:GLY:HA3	1:I:408:LEU:HD12	2.00	0.44
1:J:322:GLU:O	1:J:324:THR:HG22	2.17	0.44
1:K:341:LEU:HD22	9:K:3335:HOH:O	2.17	0.44
1:L:316:PRO:HB3	1:L:388:ASP:HA	1.99	0.44
1:J:161:ARG:HB2	1:J:190:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:ILE:HG21	1:E:185:PHE:CD1	2.53	0.43
1:L:273:TYR:HE1	9:L:3275:HOH:O	2.01	0.43
9:H:3136:HOH:O	1:K:424:LEU:HD13	2.18	0.43
1:K:142:ARG:HD2	1:K:240:GLN:HE21	1.84	0.43
1:J:252:CYS:SG	9:J:3130:HOH:O	2.61	0.43
1:C:59:LEU:HD13	9:C:3096:HOH:O	2.19	0.43
1:E:249:HIS:HD2	9:E:3125:HOH:O	2.01	0.43
1:E:83:PRO:HG2	1:E:112:GLU:HA	2.01	0.43
1:E:134:TYR:CD2	1:E:198:ILE:HD11	2.53	0.43
1:G:361:HIS:HE1	9:G:3383:HOH:O	2.02	0.43
1:G:129:VAL:HG21	1:G:309:MET:HB3	2.00	0.43
1:H:162:ILE:HG12	1:H:187:VAL:HG22	1.99	0.43
1:I:58:GLU:HG2	9:I:3222:HOH:O	2.18	0.43
1:A:309:MET:HA	1:A:396:GLU:O	2.18	0.43
1:J:84:LEU:HD21	1:J:114:TRP:HB2	2.00	0.42
1:F:24:LEU:HD12	1:F:262:VAL:HG11	2.01	0.42
1:G:103:ILE:HD13	1:G:135:ARG:HB3	1.99	0.42
1:I:93:PRO:HB3	1:K:245:PHE:CG	2.54	0.42
1:K:317:ARG:NH1	1:K:387:ILE:HD11	2.35	0.42
1:C:339:MET:O	1:C:358:ALA:HA	2.19	0.42
1:E:58:GLU:OE2	1:E:207:ARG:NH2	2.52	0.42
1:E:410:CYS:SG	1:E:412:GLN:HB2	2.58	0.42
1:I:197:TYR:HB3	9:I:3161:HOH:O	2.19	0.42
1:J:179:ILE:HG21	1:J:185:PHE:CD1	2.54	0.42
1:K:321:ALA:HB1	1:K:324:THR:CG2	2.49	0.42
1:L:342:ILE:HD12	1:L:391:MET:HG3	2.01	0.42
1:H:374:CYS:O	1:H:378:ILE:HG12	2.19	0.42
1:K:96:LEU:HD22	1:K:413:LEU:HD11	2.02	0.42
1:A:341:LEU:HD21	1:A:344:GLY:O	2.19	0.42
1:F:405:LEU:O	1:F:409:GLU:HB2	2.19	0.42
1:J:415:ALA:HB3	9:J:3477:HOH:O	2.18	0.42
1:G:142:ARG:HD2	1:G:240:GLN:OE1	2.19	0.42
1:H:328:PRO:O	1:H:369:PRO:HD3	2.20	0.42
1:D:111:ILE:HG21	1:D:144:PHE:CG	2.55	0.42
1:K:317:ARG:H	1:K:387:ILE:HG13	1.84	0.42
1:D:391:MET:HE3	1:D:391:MET:HA	2.02	0.42
1:L:145:PHE:O	1:L:243:GLN:HA	2.20	0.42
1:C:275:LEU:HD13	1:C:391:MET:CE	2.51	0.41
1:I:309:MET:HA	1:I:396:GLU:O	2.20	0.41
1:K:150:GLU:HB3	1:K:201:ASN:HB3	2.01	0.41
1:D:232:TYR:CD1	1:D:262:VAL:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:ARG:HB3	1:F:188:GLU:HB3	2.01	0.41
1:G:132:TYR:HB2	1:G:198:ILE:HB	2.02	0.41
1:L:50:THR:HB	1:L:54:MET:HG3	2.02	0.41
1:H:124:GLU:H	1:H:124:GLU:CD	2.29	0.41
1:K:78:ARG:NH2	1:K:82:GLN:HG3	2.35	0.41
1:G:98:TRP:HB3	9:G:3155:HOH:O	2.19	0.41
1:A:144:PHE:HA	1:A:242:VAL:O	2.21	0.41
1:E:240:GLN:NE2	9:E:3324:HOH:O	2.53	0.41
1:B:93:PRO:HB3	1:C:245:PHE:CG	2.55	0.41
1:D:143:VAL:HG11	1:D:258:PRO:HG2	2.03	0.41
1:E:294:PHE:HB2	1:E:312:VAL:HG13	2.03	0.41
1:F:278:PHE:CG	1:F:313:ILE:HD11	2.56	0.41
1:G:274:ASP:OD1	1:G:276:ARG:HD3	2.21	0.41
1:I:58:GLU:HG2	1:I:207:ARG:NH2	2.35	0.41
1:I:317:ARG:NH2	9:I:3304:HOH:O	2.46	0.41
1:F:95:ARG:HD3	1:F:366:ALA:O	2.20	0.41
1:I:320:VAL:HG12	1:I:384:PRO:HB3	2.03	0.41
1:G:207[A]:ARG:HD3	1:G:300:PRO:HD3	2.02	0.41
1:I:162:ILE:HG12	1:I:187:VAL:HG22	2.03	0.41
1:C:129:VAL:HG21	1:C:309:MET:HB3	2.03	0.41
1:D:302:SER:HB3	1:E:302:SER:HB2	2.03	0.41
1:L:97:ARG:NH2	1:L:420:CYS:SG	2.93	0.41
1:L:314:PHE:HA	9:L:3326:HOH:O	2.19	0.41
1:A:245:PHE:CG	1:C:93:PRO:HB3	2.55	0.41
1:H:9:LEU:HD21	1:H:168:VAL:O	2.21	0.41
1:K:341:LEU:HD23	1:K:355:PRO:N	2.36	0.41
1:E:50:THR:HB	1:E:54:MET:HG3	2.04	0.40
1:J:46:LEU:HD13	1:J:63:TRP:CE2	2.56	0.40
1:K:374:CYS:O	1:K:378:ILE:HG13	2.21	0.40
1:A:424:LEU:HD13	1:B:69:PRO:HG2	2.02	0.40
1:I:410:CYS:SG	1:I:412:GLN:HG2	2.61	0.40
1:D:318:TRP:CD1	1:D:386:LYS:HD3	2.57	0.40
1:E:144:PHE:HA	1:E:242:VAL:O	2.21	0.40
1:K:84:LEU:HD13	1:K:244:LYS:HE2	2.03	0.40
1:K:294:PHE:HB3	1:K:313:ILE:O	2.22	0.40
1:K:342:ILE:HD12	1:K:391:MET:HG3	2.02	0.40
1:C:275:LEU:HB3	1:C:391:MET:CE	2.51	0.40
1:F:275:LEU:HB3	1:F:391:MET:CE	2.52	0.40
1:G:294:PHE:HB3	1:G:313:ILE:O	2.22	0.40
1:G:328:PRO:HD2	1:G:348:ALA:HB2	2.03	0.40
1:L:113:GLY:HA3	1:L:135:ARG:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:3260:HOH:O	9:L:3057:HOH:O[1_644]	2.14	0.06

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	429/433 (99%)	417 (97%)	11 (3%)	1 (0%)	43	28
1	B	428/433 (99%)	414 (97%)	14 (3%)	0	100	100
1	C	427/433 (99%)	410 (96%)	16 (4%)	1 (0%)	43	28
1	D	430/433 (99%)	416 (97%)	13 (3%)	1 (0%)	43	28
1	E	427/433 (99%)	412 (96%)	14 (3%)	1 (0%)	43	28
1	F	429/433 (99%)	414 (96%)	14 (3%)	1 (0%)	43	28
1	G	426/433 (98%)	414 (97%)	12 (3%)	0	100	100
1	H	426/433 (98%)	411 (96%)	13 (3%)	2 (0%)	24	12
1	I	425/433 (98%)	416 (98%)	7 (2%)	2 (0%)	24	12
1	J	427/433 (99%)	410 (96%)	15 (4%)	2 (0%)	24	12
1	K	427/433 (99%)	410 (96%)	17 (4%)	0	100	100
1	L	424/433 (98%)	406 (96%)	18 (4%)	0	100	100
All	All	5125/5196 (99%)	4950 (97%)	164 (3%)	11 (0%)	43	28

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	235	ALA
1	E	174	LEU
1	F	363	VAL
1	I	174	LEU

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Mol	Chain	Res	Type
1	H	380	ALA
1	A	363	VAL
1	J	174	LEU
1	J	363	VAL
1	H	363	VAL
1	D	363	VAL
1	I	363	VAL

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	353/355 (99%)	337 (96%)	16 (4%)	24	9
1	B	352/355 (99%)	343 (97%)	9 (3%)	40	23
1	C	351/355 (99%)	340 (97%)	11 (3%)	35	18
1	D	354/355 (100%)	333 (94%)	21 (6%)	18	5
1	E	351/355 (99%)	336 (96%)	15 (4%)	26	10
1	F	353/355 (99%)	340 (96%)	13 (4%)	30	14
1	G	350/355 (99%)	339 (97%)	11 (3%)	35	18
1	H	350/355 (99%)	328 (94%)	22 (6%)	16	5
1	I	349/355 (98%)	333 (95%)	16 (5%)	24	9
1	J	351/355 (99%)	336 (96%)	15 (4%)	26	10
1	K	351/355 (99%)	328 (93%)	23 (7%)	15	4
1	L	348/355 (98%)	327 (94%)	21 (6%)	17	5
All	All	4213/4260 (99%)	4020 (95%)	193 (5%)	24	9

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	115	LEU
1	A	135[A]	ARG

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Mol	Chain	Res	Type
1	A	135[B]	ARG
1	A	171	VAL
1	A	193	GLN
1	A	207	ARG
1	A	236	GLU
1	A	259	LEU
1	A	280	THR
1	A	329	TRP
1	A	375	GLU
1	A	376	LYS
1	A	400	VAL
1	A	416	ASP
1	A	432	ARG
1	B	58	GLU
1	B	81	ARG
1	B	125	LYS
1	B	207	ARG
1	B	243	GLN
1	B	329	TRP
1	B	376	LYS
1	B	416	ASP
1	B	432	ARG
1	C	84	LEU
1	C	115	LEU
1	C	160	LEU
1	C	168	VAL
1	C	207	ARG
1	C	239	VAL
1	C	259	LEU
1	C	329	TRP
1	C	373	THR
1	C	374	CYS
1	C	420	CYS
1	D	8	ASP
1	D	12	LEU
1	D	30	VAL
1	D	72	LEU
1	D	75	ARG
1	D	106	GLU
1	D	142	ARG
1	D	157	GLN
1	D	207	ARG

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Mol	Chain	Res	Type
1	D	243	GLN
1	D	259	LEU
1	D	323	ASN
1	D	324	THR
1	D	329	TRP
1	D	343	ASN
1	D	351	GLU
1	D	373	THR
1	D	388	ASP
1	D	406[A]	GLN
1	D	406[B]	GLN
1	D	432	ARG
1	E	72	LEU
1	E	103	ILE
1	E	124	GLU
1	E	125	LYS
1	E	135	ARG
1	E	141	GLU
1	E	160	LEU
1	E	176	ILE
1	E	207	ARG
1	E	236	GLU
1	E	259	LEU
1	E	312	VAL
1	E	324	THR
1	E	329	TRP
1	E	388	ASP
1	F	84	LEU
1	F	179	ILE
1	F	207	ARG
1	F	272	LYS
1	F	312	VAL
1	F	329	TRP
1	F	363	VAL
1	F	372	GLU
1	F	373	THR
1	F	374	CYS
1	F	400	VAL
1	F	409	GLU
1	F	420	CYS
1	G	72	LEU
1	G	125	LYS

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Mol	Chain	Res	Type
1	G	135	ARG
1	G	160	LEU
1	G	207[A]	ARG
1	G	207[B]	ARG
1	G	210	ASP
1	G	276	ARG
1	G	329	TRP
1	G	349	LYS
1	G	419	SER
1	H	8	ASP
1	H	30	VAL
1	H	84	LEU
1	H	88	LEU
1	H	106	GLU
1	H	111	ILE
1	H	135	ARG
1	H	142	ARG
1	H	157	GLN
1	H	171	VAL
1	H	207	ARG
1	H	210	ASP
1	H	236	GLU
1	H	259	LEU
1	H	276[A]	ARG
1	H	276[B]	ARG
1	H	293	ILE
1	H	322	GLU
1	H	324	THR
1	H	329	TRP
1	H	376	LYS
1	H	387	ILE
1	I	28	LEU
1	I	37	LYS
1	I	58	GLU
1	I	72	LEU
1	I	115	LEU
1	I	124	GLU
1	I	125	LYS
1	I	141	GLU
1	I	176	ILE
1	I	207	ARG
1	I	329	TRP

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Mol	Chain	Res	Type
1	I	378	ILE
1	I	400	VAL
1	I	406	GLN
1	I	412	GLN
1	I	420	CYS
1	J	28	LEU
1	J	30	VAL
1	J	81	ARG
1	J	106	GLU
1	J	124	GLU
1	J	135	ARG
1	J	207	ARG
1	J	234	GLU
1	J	259	LEU
1	J	324	THR
1	J	329	TRP
1	J	347	ASP
1	J	351	GLU
1	J	363	VAL
1	J	419	SER
1	K	30	VAL
1	K	37	LYS
1	K	72	LEU
1	K	141	GLU
1	K	156	GLU
1	K	166	LEU
1	K	190	LEU
1	K	207	ARG
1	K	249	HIS
1	K	259	LEU
1	K	276	ARG
1	K	312	VAL
1	K	324	THR
1	K	329	TRP
1	K	347	ASP
1	K	351	GLU
1	K	354	LEU
1	K	387	ILE
1	K	400	VAL
1	K	413	LEU
1	K	416	ASP
1	K	424	LEU

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Mol	Chain	Res	Type
1	K	432	ARG
1	L	8	ASP
1	L	84	LEU
1	L	115	LEU
1	L	125	LYS
1	L	135	ARG
1	L	138	ARG
1	L	160	LEU
1	L	171	VAL
1	L	179	ILE
1	L	191	ASP
1	L	207	ARG
1	L	243	GLN
1	L	306	MET
1	L	324	THR
1	L	329	TRP
1	L	351	GLU
1	L	354	LEU
1	L	370	ASP
1	L	373	THR
1	L	388	ASP
1	L	389	ASN

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

Mol	Chain	Res	Type
1	A	32	GLN
1	A	101	GLN
1	A	256	HIS
1	A	406	GLN
1	B	32	GLN
1	B	101	GLN
1	B	256	HIS
1	B	323	ASN
1	B	412	GLN
1	C	101	GLN
1	D	101	GLN
1	D	304	HIS
1	D	323	ASN
1	D	343	ASN
1	D	385	HIS
1	D	412	GLN

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Mol	Chain	Res	Type
1	E	32	GLN
1	E	101	GLN
1	E	193	GLN
1	E	249	HIS
1	E	343	ASN
1	E	406	GLN
1	F	17	ASN
1	F	94	ASN
1	F	193	GLN
1	F	217	ASN
1	F	243	GLN
1	F	399	GLN
1	F	406	GLN
1	G	412	GLN
1	G	429	ASN
1	H	101	GLN
1	H	157	GLN
1	H	243	GLN
1	I	193	GLN
1	I	304	HIS
1	I	323	ASN
1	J	217	ASN
1	J	249	HIS
1	J	406	GLN
1	K	240	GLN
1	K	243	GLN
1	K	385	HIS
1	K	406	GLN
1	L	32	GLN
1	L	101	GLN
1	L	385	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 12 are monoatomic - leaving 14 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
4	OMD	H	2001	2	12,12,12	1.22	1 (8%)	16,16,16	2.16	6 (37%)
4	OMD	I	2001	2	12,12,12	1.15	1 (8%)	16,16,16	2.12	5 (31%)
6	HQ9	C	2001	2	10,12,12	2.44	4 (40%)	9,16,16	1.71	3 (33%)
8	HMQ	F	2001	2	11,14,14	2.06	5 (45%)	12,20,20	1.57	4 (33%)
4	OMD	D	2001	2	12,12,12	1.88	4 (33%)	16,16,16	1.62	3 (18%)
4	OMD	E	2001	2	12,12,12	1.29	2 (16%)	16,16,16	2.15	5 (31%)
4	OMD	G	2001	2	12,12,12	1.39	3 (25%)	16,16,16	1.38	2 (12%)
4	OMD	K	2001	2	12,12,12	1.33	1 (8%)	16,16,16	1.54	3 (18%)
7	PO4	E	2002	-	4,4,4	1.25	1 (25%)	6,6,6	0.43	0
8	HMQ	L	2001	2	11,14,14	1.54	3 (27%)	12,20,20	2.68	6 (50%)
3	M8O	A	2001	2	12,13,13	3.22	5 (41%)	12,16,16	2.97	4 (33%)
4	OMD	B	2001	2	12,12,12	1.52	2 (16%)	16,16,16	1.64	4 (25%)
5	OXY	C	1999	2	1,1,1	0.56	0	-		
4	OMD	J	2001	2	12,12,12	1.18	1 (8%)	16,16,16	1.42	3 (18%)

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	OMD	H	2001	2	-	0/4/4/4	0/1/1/1
4	OMD	I	2001	2	-	2/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HQ9	C	2001	2	-	1/4/17/17	0/1/1/1
8	HMQ	F	2001	2	-	2/5/23/23	0/1/1/1
4	OMD	D	2001	2	-	0/4/4/4	0/1/1/1
4	OMD	E	2001	2	-	0/4/4/4	0/1/1/1
4	OMD	G	2001	2	-	0/4/4/4	0/1/1/1
4	OMD	K	2001	2	-	1/4/4/4	0/1/1/1
8	HMQ	L	2001	2	-	0/5/23/23	0/1/1/1
3	M8O	A	2001	2	-	12/13/13/13	-
4	OMD	B	2001	2	-	0/4/4/4	0/1/1/1
4	OMD	J	2001	2	-	0/4/4/4	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	M8O	O6-C50	8.75	1.37	1.23
6	C	2001	HQ9	O3'-C3'	5.80	1.42	1.24
8	F	2001	HMQ	C7-C8	4.30	1.57	1.51
3	A	2001	M8O	C1-C3	3.87	1.58	1.48
8	L	2001	HMQ	O7-O6	3.37	1.57	1.46
4	D	2001	OMD	C5'-C4'	-3.32	1.33	1.38
3	A	2001	M8O	O1-C2	-3.31	1.19	1.30
4	G	2001	OMD	O2-C1	-2.94	1.21	1.30
8	F	2001	HMQ	OD2-C8	-2.89	1.21	1.30
4	D	2001	OMD	C6'-C1'	-2.84	1.36	1.40
4	B	2001	OMD	C6'-C1'	-2.83	1.36	1.40
3	A	2001	M8O	C4-C2	2.69	1.55	1.51
3	A	2001	M8O	C7-C50	2.65	1.56	1.48
4	B	2001	OMD	O3'-C3'	-2.65	1.31	1.37
4	E	2001	OMD	O2-C1	-2.62	1.22	1.30
4	J	2001	OMD	O2-C1	-2.62	1.22	1.30
4	D	2001	OMD	C4'-C3'	-2.59	1.34	1.39
4	D	2001	OMD	O2-C1	-2.53	1.22	1.30
8	L	2001	HMQ	C6-C5	2.51	1.51	1.45
4	H	2001	OMD	O2-C1	-2.46	1.22	1.30
6	C	2001	HQ9	O1-C1	-2.43	1.22	1.30
8	F	2001	HMQ	C6-C5	2.42	1.51	1.45
7	E	2002	PO4	P-O1	2.37	1.56	1.50
4	E	2001	OMD	C2-C1	2.34	1.56	1.51
4	I	2001	OMD	O2-C1	-2.34	1.23	1.30
6	C	2001	HQ9	O6'-C6'	-2.29	1.40	1.43
4	G	2001	OMD	C2-C1	2.15	1.55	1.51
8	F	2001	HMQ	C4-C5	2.13	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	2001	HMQ	OD2-C8	-2.12	1.23	1.30
4	K	2001	OMD	O6'-C6'	-2.12	1.32	1.36
8	F	2001	HMQ	O7-O6	2.10	1.53	1.46
4	G	2001	OMD	O3'-C3'	-2.01	1.32	1.37
6	C	2001	HQ9	C4'-C5'	-2.01	1.29	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	M8O	O5-C5-C4	-7.90	108.99	121.20
8	L	2001	HMQ	C2-C1-C6	4.98	124.67	119.31
4	I	2001	OMD	C4'-C3'-C2'	-4.78	114.94	120.19
4	E	2001	OMD	C4'-C3'-C2'	-4.74	114.98	120.19
4	H	2001	OMD	C2-C1'-C6'	4.44	125.80	120.75
4	E	2001	OMD	C5'-C6'-C1'	-4.23	115.61	120.43
8	L	2001	HMQ	C1-C6-C5	-4.21	118.89	122.72
3	A	2001	M8O	C5-C4-C2	4.13	120.56	112.32
8	L	2001	HMQ	OD1-C8-C7	-3.86	111.10	122.11
4	I	2001	OMD	C5'-C6'-C1'	-3.59	116.34	120.43
4	H	2001	OMD	C2-C1'-C2'	-3.35	114.13	120.06
8	F	2001	HMQ	C2-C1-C6	3.22	122.78	119.31
3	A	2001	M8O	O5-C5-C6	-3.22	116.22	121.20
4	G	2001	OMD	C5'-C6'-C1'	-3.20	116.78	120.43
8	L	2001	HMQ	OD2-C8-C7	3.05	123.95	114.51
4	H	2001	OMD	C5'-C6'-C1'	-3.02	116.99	120.43
4	H	2001	OMD	O6'-C6'-C1'	2.95	126.22	118.79
4	D	2001	OMD	C3'-C2'-C1'	-2.95	117.46	120.77
3	A	2001	M8O	C6-C5-C4	2.86	125.31	118.58
6	C	2001	HQ9	O1-C1-O2	-2.86	115.97	123.33
4	B	2001	OMD	C5'-C6'-C1'	-2.83	117.19	120.43
4	K	2001	OMD	C2-C1'-C6'	-2.82	117.53	120.75
4	D	2001	OMD	C2'-C1'-C6'	2.78	121.37	118.18
4	J	2001	OMD	C5'-C6'-C1'	-2.78	117.26	120.43
4	B	2001	OMD	O1-C1-C2	-2.77	114.57	122.94
4	I	2001	OMD	C3'-C2'-C1'	2.66	123.75	120.77
4	E	2001	OMD	C2'-C1'-C6'	2.64	121.21	118.18
4	B	2001	OMD	C2'-C1'-C6'	2.58	121.14	118.18
4	E	2001	OMD	C3'-C2'-C1'	2.46	123.53	120.77
4	H	2001	OMD	O1-C1-C2	-2.43	115.62	122.94
6	C	2001	HQ9	O2-C1-C2	-2.42	115.21	122.11
8	L	2001	HMQ	O5-C5-C4	-2.42	117.66	121.56
8	F	2001	HMQ	OD2-C8-C7	2.39	121.91	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2001	OMD	C2'-C1'-C6'	2.38	120.92	118.18
4	H	2001	OMD	O2-C1-C2	2.36	122.99	113.98
4	I	2001	OMD	C1'-C2-C1	2.26	117.97	113.10
8	L	2001	HMQ	O5-C5-C6	2.25	124.64	121.43
8	F	2001	HMQ	C4-C5-C6	-2.22	114.87	117.12
4	J	2001	OMD	O6'-C6'-C5'	2.20	125.27	119.36
4	G	2001	OMD	C2'-C1'-C6'	2.19	120.70	118.18
6	C	2001	HQ9	O3'-C3'-C2'	2.18	124.53	121.43
4	K	2001	OMD	C1'-C2-C1	2.17	117.78	113.10
4	D	2001	OMD	C2-C1'-C6'	-2.17	118.28	120.75
4	J	2001	OMD	C4'-C5'-C6'	2.14	122.64	120.50
8	F	2001	HMQ	OD1-C8-C7	-2.14	116.02	122.11
4	B	2001	OMD	C2-C1'-C2'	-2.11	116.32	120.06
4	K	2001	OMD	C4'-C5'-C6'	-2.09	118.41	120.50
4	E	2001	OMD	C4'-C5'-C6'	2.04	122.53	120.50

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	M8O	C3-C1-C7-C50
3	A	2001	M8O	O1-C2-C4-C5
3	A	2001	M8O	C2-C4-C5-O5
3	A	2001	M8O	C7-C1-C3-O4
3	A	2001	M8O	O6-C50-C7-C1
3	A	2001	M8O	C6-C50-C7-C1
3	A	2001	M8O	O6-C50-C6-C5
3	A	2001	M8O	O3-C2-C4-C5
6	C	2001	HQ9	O2-C1-C2-C1'
3	A	2001	M8O	C7-C50-C6-C5
3	A	2001	M8O	O5-C5-C6-C50
8	F	2001	HMQ	C1-C7-C8-OD1
8	F	2001	HMQ	C1-C7-C8-OD2
4	I	2001	OMD	O2-C1-C2-C1'
4	I	2001	OMD	O1-C1-C2-C1'
3	A	2001	M8O	C7-C1-C3-O2
3	A	2001	M8O	C2-C4-C5-C6
4	K	2001	OMD	O1-C1-C2-C1'

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2001	OMD	2	0
6	C	2001	HQ9	2	0
8	F	2001	HMQ	1	0
4	K	2001	OMD	1	0
8	L	2001	HMQ	1	0
3	A	2001	M8O	2	0
4	B	2001	OMD	2	0
5	C	1999	OXY	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	424/433 (97%)	0.30	21 (4%) 34 38	5, 14, 30, 50	10 (2%)
1	B	426/433 (98%)	0.37	15 (3%) 47 52	7, 15, 30, 54	9 (2%)
1	C	426/433 (98%)	0.33	19 (4%) 38 42	6, 15, 29, 44	10 (2%)
1	D	426/433 (98%)	0.31	11 (2%) 57 61	3, 14, 27, 46	11 (2%)
1	E	426/433 (98%)	0.42	19 (4%) 38 42	7, 15, 30, 53	7 (1%)
1	F	426/433 (98%)	0.52	24 (5%) 30 33	7, 17, 32, 50	10 (2%)
1	G	425/433 (98%)	0.36	21 (4%) 35 38	7, 14, 30, 55	7 (1%)
1	H	426/433 (98%)	0.64	38 (8%) 15 16	7, 18, 34, 56	6 (1%)
1	I	426/433 (98%)	0.60	26 (6%) 27 29	5, 18, 33, 52	7 (1%)
1	J	426/433 (98%)	0.41	18 (4%) 40 45	7, 16, 30, 49	8 (1%)
1	K	426/433 (98%)	0.87	49 (11%) 9 9	5, 20, 37, 58	10 (2%)
1	L	426/433 (98%)	0.70	24 (5%) 30 33	7, 19, 33, 49	6 (1%)
All	All	5109/5196 (98%)	0.49	285 (5%) 30 33	3, 16, 32, 58	101 (1%)

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	350	ALA	9.2
1	K	349	LYS	7.9
1	K	346	TYR	7.2
1	L	350	ALA	7.1
1	J	235	ALA	6.7
1	C	350	ALA	6.4
1	J	238	PRO	6.2
1	L	351	GLU	6.1
1	K	348	ALA	5.9
1	H	88	LEU	5.7
1	C	347	ASP	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	350	ALA	5.6
1	L	348	ALA	5.4
1	I	347	ASP	5.2
1	G	86	GLY	5.1
1	A	433	ARG	5.1
1	A	88	LEU	5.1
1	G	87	PRO	5.0
1	K	347	ASP	4.8
1	G	347	ASP	4.6
1	E	347	ASP	4.5
1	J	87	PRO	4.5
1	K	87	PRO	4.4
1	K	88	LEU	4.4
1	D	350	ALA	4.4
1	J	237	GLY	4.3
1	H	382	LEU	4.2
1	K	351	GLU	4.2
1	B	103	ILE	4.2
1	K	103	ILE	4.2
1	E	351	GLU	4.1
1	L	346	TYR	4.1
1	H	378	ILE	4.0
1	H	238	PRO	4.0
1	E	344	GLY	4.0
1	F	424	LEU	3.9
1	F	346	TYR	3.8
1	I	378	ILE	3.8
1	E	85	GLY	3.7
1	H	349	LYS	3.6
1	H	350	ALA	3.5
1	D	237	GLY	3.5
1	E	86	GLY	3.5
1	A	431	ASN	3.5
1	D	235	ALA	3.4
1	A	87	PRO	3.4
1	C	235	ALA	3.4
1	C	87	PRO	3.4
1	G	350	ALA	3.4
1	K	235	ALA	3.4
1	K	189	LEU	3.4
1	D	347	ASP	3.3
1	I	86	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	236	GLU	3.3
1	C	346	TYR	3.3
1	D	346	TYR	3.3
1	K	107	PRO	3.3
1	B	347	ASP	3.3
1	L	105	ALA	3.3
1	I	346	TYR	3.2
1	L	235	ALA	3.2
1	I	236	GLU	3.2
1	G	376	LYS	3.2
1	H	239	VAL	3.2
1	A	371	ALA	3.2
1	K	105	ALA	3.2
1	L	232	TYR	3.1
1	K	190	LEU	3.1
1	F	237	GLY	3.1
1	L	347	ASP	3.1
1	G	373	THR	3.1
1	K	431	ASN	3.1
1	A	86	GLY	3.1
1	K	372	GLU	3.1
1	F	432	ARG	3.1
1	E	107	PRO	3.1
1	H	347	ASP	3.1
1	C	237	GLY	3.1
1	J	236	GLU	3.1
1	K	110	PHE	3.1
1	K	86	GLY	3.0
1	F	351	GLU	3.0
1	F	380	ALA	3.0
1	E	236	GLU	3.0
1	E	346	TYR	3.0
1	F	379	ALA	3.0
1	H	348	ALA	3.0
1	A	84	LEU	3.0
1	H	420	CYS	3.0
1	I	351	GLU	3.0
1	K	104	PRO	3.0
1	I	350	ALA	2.9
1	F	84	LEU	2.9
1	H	235	ALA	2.9
1	H	346	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	237	GLY	2.8
1	H	236	GLU	2.8
1	E	8	ASP	2.8
1	E	235	ALA	2.8
1	H	85	GLY	2.8
1	L	237	GLY	2.8
1	I	430	PRO	2.8
1	L	103	ILE	2.8
1	F	407	ALA	2.8
1	B	425	PRO	2.8
1	E	369	PRO	2.8
1	H	87	PRO	2.8
1	I	87	PRO	2.8
1	K	411	PRO	2.8
1	B	238	PRO	2.7
1	K	387	ILE	2.7
1	J	373	THR	2.7
1	L	373	THR	2.7
1	C	107	PRO	2.7
1	J	410	CYS	2.7
1	K	352	GLY	2.7
1	J	433	ARG	2.7
1	H	84	LEU	2.7
1	F	235	ALA	2.7
1	F	236	GLU	2.6
1	G	238	PRO	2.6
1	F	350	ALA	2.6
1	G	348	ALA	2.6
1	H	351	GLU	2.6
1	H	421	TRP	2.6
1	B	235	ALA	2.6
1	I	107	PRO	2.6
1	B	433	ARG	2.6
1	K	373	THR	2.6
1	K	416	ASP	2.6
1	H	9	LEU	2.6
1	D	303	VAL	2.6
1	A	429	ASN	2.6
1	B	237	GLY	2.5
1	I	85	GLY	2.5
1	E	410	CYS	2.5
1	C	88	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	378	ILE	2.5
1	I	235	ALA	2.5
1	K	238	PRO	2.5
1	K	345	ALA	2.5
1	K	371	ALA	2.5
1	L	371	ALA	2.5
1	I	427	THR	2.5
1	F	376[A]	LYS	2.5
1	H	141	GLU	2.5
1	J	323	ASN	2.5
1	G	8	ASP	2.5
1	A	380	ALA	2.5
1	H	430	PRO	2.5
1	I	380	ALA	2.5
1	J	432	ARG	2.5
1	B	419	SER	2.5
1	L	343	ASN	2.5
1	G	410	CYS	2.5
1	C	8	ASP	2.5
1	J	88	LEU	2.5
1	J	428	PHE	2.5
1	L	254	LEU	2.5
1	J	86	GLY	2.5
1	G	88	LEU	2.4
1	K	383	ALA	2.4
1	B	171	VAL	2.4
1	A	347	ASP	2.4
1	F	410	CYS	2.4
1	C	84	LEU	2.4
1	E	189	LEU	2.4
1	I	424	LEU	2.4
1	K	407	ALA	2.4
1	L	389	ASN	2.4
1	K	229	VAL	2.4
1	K	432	ARG	2.4
1	K	410	CYS	2.4
1	K	401	LEU	2.4
1	C	371	ALA	2.4
1	G	377	ALA	2.4
1	H	380	ALA	2.4
1	I	415	ALA	2.4
1	H	324	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	106	GLU	2.4
1	I	433	ARG	2.4
1	G	378	ILE	2.4
1	H	426[A]	SER	2.3
1	E	238	PRO	2.3
1	A	379	ALA	2.3
1	G	345	ALA	2.3
1	L	380	ALA	2.3
1	K	429	ASN	2.3
1	A	432	ARG	2.3
1	A	415	ALA	2.3
1	H	79	LEU	2.3
1	K	424	LEU	2.3
1	K	39	PRO	2.3
1	K	227	THR	2.3
1	B	55	ALA	2.3
1	E	345	ALA	2.3
1	I	259	LEU	2.3
1	G	351	GLU	2.3
1	J	376	LYS	2.3
1	B	30	VAL	2.3
1	H	171	VAL	2.3
1	H	329	TRP	2.2
1	G	58	GLU	2.2
1	G	235	ALA	2.2
1	J	380	ALA	2.2
1	L	374	CYS	2.2
1	L	383	ALA	2.2
1	G	429	ASN	2.2
1	A	382	LEU	2.2
1	H	37	LYS	2.2
1	A	85	GLY	2.2
1	C	344	GLY	2.2
1	H	86	GLY	2.2
1	A	378	ILE	2.2
1	H	411	PRO	2.2
1	B	421	TRP	2.2
1	K	421	TRP	2.2
1	E	84	LEU	2.2
1	H	28	LEU	2.2
1	G	85	GLY	2.2
1	C	234	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	351	GLU	2.2
1	A	83	PRO	2.2
1	H	427	THR	2.2
1	D	380	ALA	2.2
1	J	379	ALA	2.2
1	K	420	CYS	2.2
1	E	343	ASN	2.2
1	C	238	PRO	2.2
1	L	8	ASP	2.1
1	L	416	ASP	2.1
1	D	236	GLU	2.1
1	B	383	ALA	2.1
1	A	420	CYS	2.1
1	D	85	GLY	2.1
1	H	237	GLY	2.1
1	F	382	LEU	2.1
1	I	382	LEU	2.1
1	F	431	ASN	2.1
1	A	324	THR	2.1
1	F	373	THR	2.1
1	L	234	GLU	2.1
1	F	378	ILE	2.1
1	F	138[A]	ARG	2.1
1	I	30	VAL	2.1
1	K	24	LEU	2.1
1	K	84	LEU	2.1
1	E	141	GLU	2.1
1	J	426	SER	2.1
1	F	427	THR	2.1
1	H	373	THR	2.1
1	F	87	PRO	2.1
1	H	425	PRO	2.1
1	L	87	PRO	2.1
1	A	346	TYR	2.1
1	C	105	ALA	2.1
1	G	237	GLY	2.1
1	J	371	ALA	2.1
1	K	239	VAL	2.1
1	D	410	CYS	2.1
1	F	381	ASP	2.1
1	K	173	PRO	2.1
1	F	428	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	417	TYR	2.1
1	L	192	GLY	2.0
1	C	345	ALA	2.0
1	G	380	ALA	2.0
1	H	371	ALA	2.0
1	I	377	ALA	2.0
1	I	379	ALA	2.0
1	K	236	GLU	2.0
1	I	381	ASP	2.0
1	K	370	ASP	2.0
1	D	420	CYS	2.0
1	K	374	CYS	2.0
1	I	384	PRO	2.0
1	K	83	PRO	2.0
1	F	372	GLU	2.0
1	H	170	GLU	2.0
1	K	106	GLU	2.0
1	B	85	GLY	2.0
1	C	85	GLY	2.0
1	I	431	ASN	2.0
1	H	432	ARG	2.0
1	A	127	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	OMD	K	2001	12/12	0.76	0.16	9,13,18,19	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PO4	E	2002	5/5	0.80	0.16	41,44,44,45	5
4	OMD	J	2001	12/12	0.84	0.11	14,15,18,21	12
8	HMQ	L	2001	14/14	0.84	0.15	10,18,20,20	14
4	OMD	D	2001	12/12	0.85	0.12	13,19,24,25	0
3	M8O	A	2001	14/14	0.87	0.13	7,20,25,30	14
6	HQ9	C	2001	12/12	0.89	0.11	10,17,18,19	12
4	OMD	G	2001	12/12	0.90	0.09	15,18,20,23	0
8	HMQ	F	2001	14/14	0.90	0.11	11,16,20,23	14
4	OMD	E	2001	12/12	0.90	0.10	12,17,20,22	12
4	OMD	I	2001	12/12	0.91	0.10	12,22,25,26	12
4	OMD	H	2001	12/12	0.92	0.10	18,22,23,26	12
4	OMD	B	2001	12/12	0.94	0.07	12,15,20,22	0
5	OXY	C	1999	2/2	0.95	0.11	7,7,7,14	2
2	FE	C	2000	1/1	0.99	0.02	10,10,10,10	0
2	FE	H	2000	1/1	0.99	0.03	14,14,14,14	0
2	FE	G	2000	1/1	1.00	0.01	10,10,10,10	0
2	FE	B	2000	1/1	1.00	0.01	8,8,8,8	1
2	FE	I	2000	1/1	1.00	0.01	15,15,15,15	0
2	FE	J	2000	1/1	1.00	0.01	13,13,13,13	0
2	FE	K	2000	1/1	1.00	0.01	14,14,14,14	0
2	FE	L	2000	1/1	1.00	0.01	13,13,13,13	0
2	FE	A	2000	1/1	1.00	0.01	11,11,11,11	0
2	FE	D	2000	1/1	1.00	0.01	11,11,11,11	0
2	FE	E	2000	1/1	1.00	0.02	12,12,12,12	0
2	FE	F	2000	1/1	1.00	0.01	12,12,12,12	0

6.5 Other polymers

There are no such residues in this entry.