



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:35 AM UTC

PDB ID : 1GU0 / pdb_00001gu0
Title : CRYSTAL STRUCTURE OF TYPE II DEHYDROQUINASE FROM STREPTOMYCES COELICOLOR
Authors : Roszak, A.W.; Krell, T.; Robinson, D.; Hunter, I.S.; Coggins, J.R.; Lapthorn, A.J.
Deposited on : 2002-01-22
Resolution : 2.00 Å(reported)

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

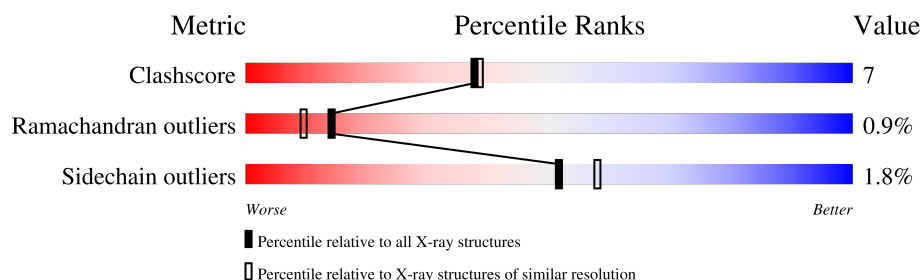
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	156	
1	B	156	
1	C	156	
1	D	156	
1	E	156	
1	F	156	
1	G	156	
1	H	156	

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Mol	Chain	Length	Quality of chain
1	I	156	 78% 17% .
1	J	156	 81% 13% . .
1	K	156	 78% 16% . .
1	L	156	 83% 11% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15099 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 3-DEHYDROQUINATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1110	691	207	207	5			
1	B	149	Total	C	N	O	S	0	0	0
			1110	691	207	207	5			
1	C	149	Total	C	N	O	S	0	0	0
			1110	691	207	207	5			
1	D	149	Total	C	N	O	S	0	0	0
			1110	691	207	207	5			
1	E	149	Total	C	N	O	S	0	0	0
			1110	691	207	207	5			
1	F	149	Total	C	N	O	S	0	0	0
			1110	691	207	207	5			
1	G	149	Total	C	N	O	S	0	0	0
			1117	696	208	208	5			
1	H	149	Total	C	N	O	S	0	0	0
			1110	691	207	207	5			
1	I	149	Total	C	N	O	S	0	0	0
			1110	691	207	207	5			
1	J	149	Total	C	N	O	S	0	0	0
			1110	691	207	207	5			
1	K	149	Total	C	N	O	S	0	0	0
			1110	691	207	207	5			
1	L	149	Total	C	N	O	S	0	0	0
			1110	691	207	207	5			

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		
2	G	1	Total	C	N	O	0	0
			8	4	1	3		
2	J	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	157	Total	O	0	6
			157	157		
3	B	133	Total	O	0	0
			133	133		
3	C	99	Total	O	0	0
			99	99		
3	D	156	Total	O	0	3
			156	156		
3	E	167	Total	O	0	0
			167	167		
3	F	151	Total	O	0	2
			151	151		
3	G	178	Total	O	0	2
			178	178		
3	H	171	Total	O	0	1
			171	171		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	158	Total 158	O 158	0	0
3	J	95	Total 95	O 95	0	0
3	K	156	Total 156	O 156	0	1
3	L	119	Total 119	O 119	0	0

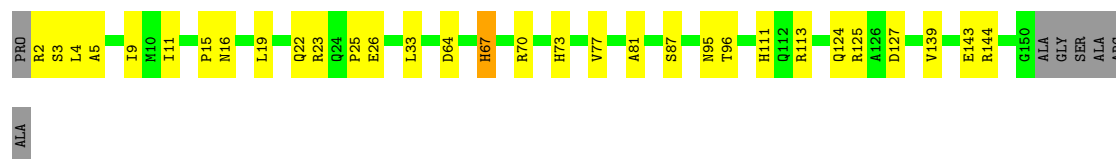
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain A: 



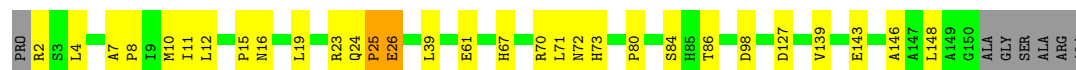
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain B: 



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain C: 



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain D: 



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain E: 



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain F:  78% 16%



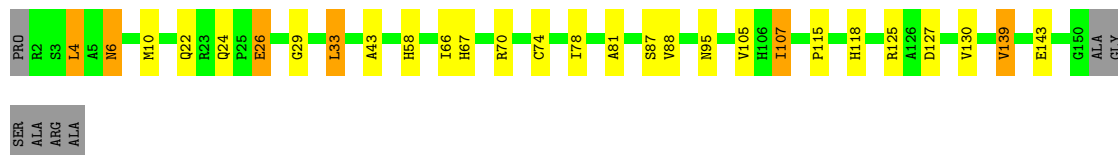
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain G:  79% 14%



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain H:  78% 14%



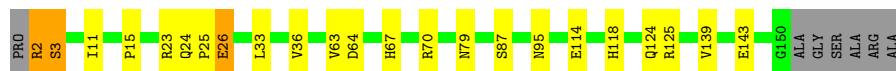
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain I:  78% 17%



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain J:  81% 13%



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain K:  78% 16%



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain L:  83% 11%

PRO	R2	S3	L4	A5	M6	I11	E26	I27	Y28	G29	H67	R70	C74	V77	I78	N95	V103	S123	Q124	R125	A131	G150	ALA	GLY	SER	ALA	ARG	ALA
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.20Å 138.40Å 141.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.00 – 2.00	Depositor
% Data completeness (in resolution range)	66.9 (24.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.200 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15099	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.10	1/1133 (0.1%)	1.36	6/1545 (0.4%)
1	B	1.09	0/1133	1.34	8/1545 (0.5%)
1	C	1.04	2/1133 (0.2%)	1.37	1/1545 (0.1%)
1	D	1.12	1/1133 (0.1%)	1.40	7/1545 (0.5%)
1	E	1.08	1/1133 (0.1%)	1.29	5/1545 (0.3%)
1	F	1.10	1/1133 (0.1%)	1.42	9/1545 (0.6%)
1	G	1.22	3/1140 (0.3%)	1.42	5/1554 (0.3%)
1	H	1.18	5/1133 (0.4%)	1.43	8/1545 (0.5%)
1	I	1.26	3/1133 (0.3%)	1.41	10/1545 (0.6%)
1	J	1.00	0/1133	1.37	4/1545 (0.3%)
1	K	1.16	1/1133 (0.1%)	1.40	5/1545 (0.3%)
1	L	0.99	2/1133 (0.2%)	1.28	6/1545 (0.4%)
All	All	1.11	20/13603 (0.1%)	1.37	74/18549 (0.4%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	105	VAL	CA-CB	-7.19	1.45	1.54
1	H	10	MET	SD-CE	7.09	1.97	1.79
1	I	66	ILE	CA-CB	-6.97	1.46	1.54
1	L	123	SER	C-O	-6.36	1.16	1.24
1	G	89	ALA	CA-CB	5.94	1.62	1.53
1	K	139	VAL	CA-CB	5.86	1.61	1.54
1	C	146	ALA	CA-CB	-5.80	1.44	1.53
1	D	102	VAL	CA-C	-5.71	1.45	1.52
1	A	77	VAL	CA-CB	-5.64	1.47	1.54
1	E	126	ALA	CA-CB	-5.51	1.44	1.53
1	C	86	THR	C-O	-5.50	1.17	1.24
1	H	66	ILE	CA-CB	-5.50	1.47	1.54
1	G	118	HIS	C-O	-5.48	1.16	1.24
1	L	103	VAL	C-O	-5.47	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	88	VAL	CA-CB	-5.44	1.46	1.54
1	F	11	ILE	CA-CB	-5.42	1.47	1.54
1	H	43	ALA	CA-CB	5.38	1.61	1.53
1	G	105	VAL	CA-CB	5.32	1.61	1.54
1	I	105	VAL	CA-C	5.20	1.58	1.52
1	I	67	HIS	C-O	-5.04	1.18	1.24

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	3	SER	N-CA-C	8.30	121.23	110.53
1	H	87	SER	N-CA-C	7.97	122.97	107.98
1	D	127	ASP	N-CA-C	-7.49	103.06	111.14
1	F	87	SER	N-CA-C	7.24	121.62	107.57
1	H	81	ALA	CB-CA-C	-7.11	108.36	116.54
1	J	3	SER	N-CA-C	6.95	120.66	110.59
1	H	139	VAL	N-CA-C	-6.88	103.77	110.72
1	H	107	ILE	N-CA-C	6.84	116.99	110.42
1	A	3	SER	N-CA-C	6.83	119.34	110.53
1	I	62	LEU	N-CA-C	-6.59	104.10	111.28
1	G	24	GLN	N-CA-C	6.41	119.60	110.24
1	F	6	ASN	N-CA-C	6.37	119.18	111.40
1	E	58	HIS	N-CA-C	6.36	119.10	108.73
1	I	30	SER	N-CA-C	-6.35	106.12	114.31
1	D	3	SER	N-CA-C	6.26	118.60	110.53
1	I	87	SER	N-CA-C	6.25	119.69	107.57
1	A	67	HIS	N-CA-C	-6.25	104.57	111.82
1	B	3	SER	N-CA-C	6.16	118.48	110.53
1	I	77	VAL	N-CA-C	-6.05	99.03	107.80
1	F	140	PHE	N-CA-C	-6.04	104.61	111.07
1	K	143	GLU	CB-CA-C	-5.96	100.73	110.85
1	E	6	ASN	N-CA-C	5.94	119.00	111.69
1	J	87	SER	N-CA-C	5.86	118.93	107.57
1	F	81	ALA	CB-CA-C	-5.81	109.89	116.63
1	F	77	VAL	N-CA-C	-5.81	99.38	107.80
1	K	145	ILE	N-CA-C	-5.80	104.86	110.72
1	H	130	VAL	CB-CA-C	-5.78	102.07	110.63
1	G	78	ILE	N-CA-C	5.77	116.43	108.12
1	A	87	SER	N-CA-C	5.76	118.74	107.57
1	L	131	ALA	N-CA-C	5.73	118.81	109.06
1	B	58	HIS	N-CA-C	5.68	118.51	109.24
1	L	27	ILE	N-CA-C	-5.66	106.94	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	77	VAL	N-CA-C	-5.66	100.25	108.17
1	D	138	TYR	N-CA-C	-5.64	105.27	111.82
1	L	6	ASN	CB-CA-C	-5.64	100.38	110.70
1	J	36	VAL	CB-CA-C	-5.63	104.53	112.14
1	I	78	ILE	N-CA-C	5.61	116.19	108.12
1	F	61	GLU	N-CA-C	-5.60	104.80	111.69
1	H	78	ILE	N-CA-C	5.60	116.18	108.12
1	K	143	GLU	N-CA-C	5.58	117.45	111.36
1	I	77	VAL	N-CA-CB	5.56	118.47	111.46
1	F	76	ILE	N-CA-C	5.54	116.10	108.12
1	K	87	SER	N-CA-C	5.47	117.92	107.75
1	A	144	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	G	127	ASP	N-CA-C	-5.46	105.41	111.36
1	G	140	PHE	N-CA-C	-5.44	105.35	111.28
1	E	105	VAL	N-CA-C	5.42	115.92	108.12
1	D	129	VAL	CB-CA-C	-5.40	101.74	110.28
1	B	6	ASN	CB-CA-C	-5.40	100.82	110.70
1	B	59	GLU	CA-C-N	5.31	125.87	119.98
1	B	59	GLU	C-N-CA	5.31	125.87	119.98
1	E	15	PRO	CA-C-O	5.29	127.70	121.56
1	A	9	ILE	CB-CA-C	-5.29	104.36	110.91
1	I	129	VAL	CB-CA-C	-5.28	102.94	110.12
1	F	105	VAL	N-CA-C	5.28	115.72	108.12
1	F	58	HIS	N-CA-C	5.25	117.28	108.73
1	I	122	VAL	N-CA-C	5.24	115.97	110.62
1	D	58	HIS	N-CA-C	5.24	117.26	108.73
1	B	120	SER	CA-C-N	5.23	127.29	120.28
1	B	120	SER	C-N-CA	5.23	127.29	120.28
1	K	3	SER	N-CA-C	5.20	118.13	110.59
1	L	78	ILE	N-CA-C	5.20	115.77	108.17
1	G	2	ARG	CA-CB-CG	-5.20	103.71	114.10
1	C	127	ASP	N-CA-C	-5.18	105.55	111.14
1	E	3	SER	N-CA-C	5.17	117.53	110.55
1	H	6	ASN	CB-CA-C	-5.16	102.34	110.86
1	A	81	ALA	CB-CA-C	-5.11	110.66	116.54
1	D	9	ILE	N-CA-CB	-5.11	105.17	111.00
1	B	27	ILE	N-CA-C	-5.10	106.17	111.58
1	H	58	HIS	N-CA-C	5.09	117.53	109.24
1	D	33	LEU	N-CA-C	-5.05	105.91	111.71
1	I	14	GLY	CA-C-N	5.04	124.95	119.76
1	I	14	GLY	C-N-CA	5.04	124.95	119.76
1	J	15	PRO	N-CA-C	5.04	119.10	111.19

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	1110	0	1070	23	0
1	B	1110	0	1070	17	0
1	C	1110	0	1070	21	0
1	D	1110	0	1070	8	0
1	E	1110	0	1070	12	0
1	F	1110	0	1070	15	0
1	G	1117	0	1085	18	0
1	H	1110	0	1070	13	0
1	I	1110	0	1070	17	0
1	J	1110	0	1070	13	0
1	K	1110	0	1070	23	0
1	L	1110	0	1070	7	0
2	A	8	0	12	0	0
2	D	8	0	12	0	0
2	G	8	0	12	0	0
2	J	8	0	12	0	0
3	A	157	0	0	7	1
3	B	133	0	0	4	0
3	C	99	0	0	2	0
3	D	156	0	0	3	0
3	E	167	0	0	4	1
3	F	151	0	0	8	0
3	G	178	0	0	8	0
3	H	171	0	0	5	0
3	I	158	0	0	4	0
3	J	95	0	0	3	0
3	K	156	0	0	8	0
3	L	119	0	0	1	0
All	All	15099	0	12903	183	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 7.

All (183) 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:H:22:GLN:NE2	3:H:2036:HOH:O	1.61	1.32
1:I:2:ARG:NH2	1:I:70:ARG:O	1.74	1.20
1:C:2:ARG:NH1	1:C:72:ASN:HA	1.69	1.06
1:G:6:ASN:ND2	3:G:2012:HOH:O	1.89	1.05
1:F:22:GLN:NE2	3:F:2028:HOH:O	1.87	1.04
1:K:2:ARG:NH2	1:K:71:LEU:C	2.17	1.02
1:G:31:ASP:OD2	3:G:2052:HOH:O	1.82	0.97
1:E:6:ASN:ND2	3:E:2006:HOH:O	2.01	0.93
1:I:2:ARG:HH22	1:I:70:ARG:C	1.77	0.92
1:F:93:ALA:O	3:F:2106:HOH:O	1.91	0.88
1:I:2:ARG:NH1	1:I:73:HIS:H	1.73	0.86
1:B:74:CYS:O	3:B:2075:HOH:O	1.92	0.86
1:K:111:HIS:NE2	3:K:2118:HOH:O	1.93	0.83
1:I:124:GLN:HB3	3:I:2144:HOH:O	1.79	0.81
1:B:124:GLN:HB3	3:B:2115:HOH:O	1.81	0.80
1:F:53:PHE:O	3:F:2074:HOH:O	2.00	0.79
1:I:2:ARG:NH1	1:I:73:HIS:N	2.29	0.79
1:I:2:ARG:HH12	1:I:73:HIS:H	1.26	0.79
1:K:2:ARG:HH22	1:K:71:LEU:HA	1.47	0.78
1:K:2:ARG:HH22	1:K:71:LEU:CA	2.01	0.74
1:F:97:CYS:N	3:F:2106:HOH:O	2.16	0.74
1:G:42:LYS:HE2	3:G:2070:HOH:O	1.89	0.72
1:K:107:ILE:O	3:K:2114:HOH:O	2.07	0.72
1:C:2:ARG:CZ	1:C:72:ASN:HA	2.20	0.71
1:E:114:GLU:OE2	3:E:2138:HOH:O	2.08	0.71
1:F:21:GLY:O	3:F:2025:HOH:O	2.07	0.71
1:K:124:GLN:HG3	3:K:2138:HOH:O	1.91	0.71
1:L:124:GLN:OE1	3:L:2104:HOH:O	2.09	0.71
1:G:143:GLU:OE2	3:G:2172:HOH:O	2.08	0.70
1:L:2:ARG:N	1:L:2:ARG:HD2	2.08	0.69
1:G:2:ARG:NH2	1:G:72:ASN:HA	2.07	0.69
1:K:2:ARG:HH22	1:K:71:LEU:C	2.04	0.66
1:B:2:ARG:HH21	1:B:7:ALA:HB2	1.61	0.66
1:J:95:ASN:HD22	1:J:125:ARG:HD3	1.59	0.66
1:A:23:ARG:O	1:A:25:PRO:HD3	1.97	0.65
1:A:124:GLN:HB3	3:A:2144:HOH:O	1.96	0.64
1:K:61:GLU:OE2	3:K:2091:HOH:O	2.15	0.64
1:J:2:ARG:N	1:J:2:ARG:HD2	2.11	0.64
1:D:124:GLN:HB3	3:D:2140:HOH:O	1.99	0.63
1:K:31:ASP:HB2	3:K:2044:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:GLN:HA	1:G:25:PRO:O	2.00	0.62
1:A:95:ASN:HD22	1:A:125:ARG:HD3	1.65	0.61
1:F:2:ARG:HG3	1:F:2:ARG:HH21	1.65	0.61
1:F:23:ARG:O	1:F:25:PRO:HD3	2.00	0.61
1:I:2:ARG:HH11	1:I:73:HIS:N	1.98	0.61
1:C:139:VAL:O	1:C:143:GLU:HG2	2.00	0.61
1:K:2:ARG:NH2	1:K:71:LEU:O	2.35	0.60
1:A:5:ALA:N	3:A:2002:HOH:O	2.31	0.60
1:F:22:GLN:CD	3:F:2028:HOH:O	2.34	0.60
1:C:61:GLU:OE2	3:C:2043:HOH:O	2.17	0.60
1:C:23:ARG:O	1:C:25:PRO:HD3	2.02	0.59
1:C:10:MET:HE2	1:C:73:HIS:CE1	2.38	0.59
1:A:2:ARG:NH2	1:A:73:HIS:H	2.01	0.58
1:H:127:ASP:O	3:H:2161:HOH:O	2.17	0.58
1:K:2:ARG:NH2	1:K:71:LEU:CA	2.64	0.57
1:E:23:ARG:O	1:E:25:PRO:HD3	2.04	0.57
1:A:2:ARG:HH21	1:A:73:HIS:H	1.53	0.56
1:G:64:ASP:OD2	3:G:2108:HOH:O	2.18	0.56
1:F:2:ARG:NH1	1:F:70:ARG:O	2.38	0.56
1:A:2:ARG:HH21	1:A:73:HIS:N	2.04	0.56
1:C:98:ASP:HA	3:C:2062:HOH:O	2.05	0.56
1:A:22:GLN:NE2	3:A:2034:HOH:O	2.25	0.55
1:A:23:ARG:HD2	1:B:96:THR:HG22	1.88	0.55
1:K:111:HIS:CE1	3:K:2118:HOH:O	2.49	0.55
1:A:113:ARG:C	3:A:2123:HOH:O	2.49	0.55
1:A:139:VAL:O	1:A:143:GLU:HG2	2.06	0.55
1:B:15:PRO:O	1:B:16:ASN:HB2	2.07	0.55
1:G:2:ARG:HH22	1:G:72:ASN:HA	1.70	0.55
1:B:125:ARG:O	1:B:125:ARG:HD2	2.07	0.54
1:K:2:ARG:HH21	1:K:71:LEU:C	2.11	0.54
1:H:139:VAL:O	1:H:143:GLU:HG2	2.08	0.53
1:K:67:HIS:O	1:K:70:ARG:HB3	2.07	0.53
1:G:33:LEU:HD23	3:G:2017:HOH:O	2.08	0.53
1:K:80:PRO:HB2	1:K:84:SER:OG	2.08	0.53
1:E:78:ILE:HG12	1:E:80:PRO:HG3	1.91	0.52
1:I:111:HIS:NE2	3:I:2122:HOH:O	2.25	0.52
1:J:67:HIS:O	1:J:70:ARG:HB3	2.10	0.51
1:C:2:ARG:NH1	1:C:71:LEU:O	2.36	0.51
1:C:10:MET:HE2	1:C:73:HIS:NE2	2.25	0.51
1:F:94:LEU:C	3:F:2106:HOH:O	2.54	0.50
1:B:139:VAL:O	1:B:143:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:GLY:HA3	3:H:2044:HOH:O	2.10	0.50
1:B:23:ARG:O	1:B:25:PRO:HD3	2.11	0.50
1:E:80:PRO:HB2	1:E:84:SER:OG	2.11	0.49
1:G:2:ARG:HA	3:G:2011:HOH:O	2.12	0.49
1:H:95:ASN:HD22	1:H:125:ARG:HD3	1.77	0.49
1:I:79:ASN:OD1	1:I:79:ASN:C	2.53	0.49
1:L:2:ARG:N	1:L:2:ARG:CD	2.74	0.49
1:I:2:ARG:NH1	1:I:73:HIS:O	2.46	0.49
1:A:111:HIS:NE2	3:A:2117:HOH:O	2.29	0.49
1:B:113:ARG:O	1:B:118:HIS:NE2	2.38	0.49
1:L:4:LEU:HD12	1:L:74:CYS:SG	2.53	0.49
1:H:4:LEU:HD12	1:H:74:CYS:SG	2.54	0.48
1:J:95:ASN:ND2	1:J:125:ARG:HD3	2.27	0.48
1:E:24:GLN:O	1:E:26:GLU:N	2.47	0.48
1:H:33:LEU:HD12	1:H:33:LEU:HA	1.60	0.48
1:A:19:LEU:HD11	1:B:67:HIS:CD2	2.48	0.47
1:B:124:GLN:NE2	3:B:2116:HOH:O	2.46	0.47
1:C:80:PRO:HG2	1:C:84:SER:OG	2.15	0.47
1:C:24:GLN:O	1:C:26:GLU:N	2.48	0.47
1:E:95:ASN:HD22	1:E:125:ARG:HD3	1.79	0.47
1:A:64:ASP:OD2	3:A:2094:HOH:O	2.21	0.47
1:J:33:LEU:HD12	1:J:33:LEU:HA	1.76	0.47
1:J:118:HIS:O	3:J:2076:HOH:O	2.20	0.46
1:J:139:VAL:O	1:J:143:GLU:HG2	2.14	0.46
1:D:68:GLU:OE1	3:D:2096:HOH:O	2.21	0.46
1:H:24:GLN:O	1:H:26:GLU:N	2.48	0.46
1:A:2:ARG:NH1	1:A:70:ARG:O	2.49	0.46
1:A:15:PRO:O	1:A:16:ASN:HB2	2.16	0.46
1:E:124:GLN:HB3	3:E:2154:HOH:O	2.16	0.46
1:D:95:ASN:HD22	1:D:125:ARG:HD3	1.80	0.46
1:A:95:ASN:ND2	1:A:125:ARG:HD3	2.30	0.45
1:A:127:ASP:HB3	3:A:2148:HOH:O	2.16	0.45
1:B:23:ARG:C	1:B:25:PRO:HD3	2.42	0.45
1:C:67:HIS:O	1:C:70:ARG:HB3	2.16	0.45
1:D:139:VAL:O	1:D:143:GLU:HG2	2.16	0.45
1:A:96:THR:HG22	1:C:23:ARG:HD2	1.99	0.45
1:F:42:LYS:HG3	3:F:2017:HOH:O	2.17	0.45
1:K:2:ARG:HH21	1:K:72:ASN:N	2.15	0.44
1:G:107:ILE:O	1:G:132:GLY:HA2	2.16	0.44
1:H:107:ILE:HB	3:H:2129:HOH:O	2.16	0.44
1:D:54:ARG:NH2	1:D:68:GLU:OE2	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HA	1:A:33:LEU:HD12	1.59	0.44
1:B:7:ALA:HB1	1:B:8:PRO:HD2	1.99	0.44
1:G:67:HIS:O	1:G:70:ARG:HB3	2.17	0.44
1:E:121:TYR:O	1:E:124:GLN:HG2	2.17	0.44
1:J:23:ARG:O	1:J:25:PRO:HD3	2.17	0.44
1:I:80:PRO:HB2	1:I:84:SER:OG	2.17	0.43
1:E:100:LEU:HD12	1:E:101:PRO:HD2	2.00	0.43
1:F:4:LEU:HD12	1:F:74:CYS:SG	2.57	0.43
1:G:6:ASN:OD1	3:G:2011:HOH:O	2.21	0.43
1:D:4:LEU:HD12	1:D:74:CYS:SG	2.58	0.43
1:I:101:PRO:HB2	1:I:145:ILE:HD13	1.99	0.43
1:K:124:GLN:HB3	3:K:2137:HOH:O	2.17	0.43
1:H:29:GLY:CA	3:H:2044:HOH:O	2.65	0.43
1:I:95:ASN:ND2	3:I:2111:HOH:O	2.50	0.43
1:E:119:HIS:NE2	3:E:2147:HOH:O	2.33	0.43
1:J:114:GLU:OE2	3:J:2071:HOH:O	2.21	0.43
1:B:24:GLN:O	1:B:26:GLU:N	2.52	0.43
1:D:112:GLN:HA	3:D:2117:HOH:O	2.18	0.43
1:C:23:ARG:C	1:C:25:PRO:HD3	2.43	0.43
1:L:67:HIS:O	1:L:70:ARG:HB3	2.19	0.43
1:B:33:LEU:HD12	1:B:33:LEU:HA	1.75	0.42
1:F:10:MET:HE2	1:F:73:HIS:CE1	2.54	0.42
1:C:10:MET:CG	1:C:12:LEU:HD21	2.49	0.42
1:E:95:ASN:HD22	1:E:95:ASN:HA	1.60	0.42
1:C:10:MET:HE2	1:C:73:HIS:CD2	2.54	0.42
1:I:94:LEU:O	1:I:97:CYS:HB2	2.20	0.42
1:A:23:ARG:C	1:A:25:PRO:HD3	2.45	0.42
1:G:7:ALA:HB1	1:G:8:PRO:HD2	2.02	0.42
1:G:24:GLN:HB3	1:G:25:PRO:HA	2.01	0.42
1:L:95:ASN:HD22	1:L:125:ARG:HD3	1.84	0.42
1:J:63:VAL:O	1:J:64:ASP:C	2.61	0.42
1:A:67:HIS:CD2	1:C:19:LEU:HD11	2.55	0.42
1:J:124:GLN:NE2	3:J:2083:HOH:O	2.19	0.42
1:K:23:ARG:O	1:K:25:PRO:HD3	2.19	0.42
1:C:15:PRO:O	1:C:16:ASN:HB2	2.19	0.42
1:I:95:ASN:HD22	1:I:125:ARG:HD3	1.84	0.42
1:K:95:ASN:HD22	1:K:125:ARG:HD3	1.84	0.42
1:K:139:VAL:O	1:K:143:GLU:HG2	2.19	0.42
1:F:24:GLN:O	1:F:26:GLU:N	2.52	0.41
1:F:95:ASN:HD22	1:F:95:ASN:HA	1.60	0.41
1:I:33:LEU:HD12	1:I:33:LEU:HA	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:ASN:HD22	1:G:95:ASN:HA	1.68	0.41
1:K:31:ASP:OD2	3:K:2044:HOH:O	2.22	0.41
1:G:2:ARG:NH2	1:G:72:ASN:C	2.78	0.41
1:H:67:HIS:O	1:H:70:ARG:HB3	2.19	0.41
1:A:67:HIS:O	1:A:70:ARG:HB3	2.20	0.41
1:C:39:LEU:HD23	1:C:39:LEU:HA	1.92	0.41
1:C:7:ALA:HB1	1:C:8:PRO:HD2	2.01	0.41
1:I:124:GLN:CG	3:I:2144:HOH:O	2.69	0.41
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.87	0.41
1:L:95:ASN:HD22	1:L:95:ASN:HA	1.70	0.41
1:H:6:ASN:HD22	1:H:6:ASN:HA	1.63	0.40
1:J:24:GLN:O	1:J:26:GLU:N	2.54	0.40
1:J:79:ASN:OD1	1:J:79:ASN:C	2.60	0.40
1:B:120:SER:HB3	1:B:123:SER:OG	2.21	0.40
1:B:150:GLY:HA3	3:B:2133:HOH:O	2.22	0.40
1:D:6:ASN:HD22	1:D:6:ASN:HA	1.66	0.40
1:H:115:PRO:HA	1:H:118:HIS:CE1	2.57	0.40
1:K:114:GLU:HA	1:K:115:PRO:HD3	1.84	0.40
1:G:139:VAL:O	1:G:143:GLU:HG2	2.22	0.40
1:K:33:LEU:HD12	1:K:33:LEU:HA	1.67	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)
3:A:2026:HOH:O	3:E:2024:HOH:O[2_564]	2.09	0.11

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	147/156 (94%)	140 (95%)	6 (4%)	1 (1%)	18 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	147/156 (94%)	139 (95%)	6 (4%)	2 (1%)	9	4
1	C	147/156 (94%)	139 (95%)	6 (4%)	2 (1%)	9	4
1	D	147/156 (94%)	140 (95%)	6 (4%)	1 (1%)	18	14
1	E	147/156 (94%)	140 (95%)	6 (4%)	1 (1%)	18	14
1	F	147/156 (94%)	140 (95%)	5 (3%)	2 (1%)	9	4
1	G	147/156 (94%)	142 (97%)	4 (3%)	1 (1%)	18	14
1	H	147/156 (94%)	139 (95%)	7 (5%)	1 (1%)	18	14
1	I	147/156 (94%)	140 (95%)	6 (4%)	1 (1%)	18	14
1	J	147/156 (94%)	140 (95%)	6 (4%)	1 (1%)	18	14
1	K	147/156 (94%)	138 (94%)	8 (5%)	1 (1%)	18	14
1	L	147/156 (94%)	140 (95%)	5 (3%)	2 (1%)	9	4
All	All	1764/1872 (94%)	1677 (95%)	71 (4%)	16 (1%)	14	9

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	25	PRO
1	A	26	GLU
1	B	26	GLU
1	C	26	GLU
1	D	26	GLU
1	E	26	GLU
1	F	26	GLU
1	H	26	GLU
1	I	26	GLU
1	J	26	GLU
1	K	26	GLU
1	L	26	GLU
1	B	29	GLY
1	L	29	GLY
1	C	25	PRO
1	F	25	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	114/120 (95%)	112 (98%)	2 (2%)	51	58
1	B	114/120 (95%)	111 (97%)	3 (3%)	40	44
1	C	114/120 (95%)	112 (98%)	2 (2%)	51	58
1	D	114/120 (95%)	112 (98%)	2 (2%)	51	58
1	E	114/120 (95%)	112 (98%)	2 (2%)	51	58
1	F	114/120 (95%)	113 (99%)	1 (1%)	70	78
1	G	116/120 (97%)	114 (98%)	2 (2%)	53	60
1	H	114/120 (95%)	112 (98%)	2 (2%)	51	58
1	I	114/120 (95%)	114 (100%)	0	100	100
1	J	114/120 (95%)	111 (97%)	3 (3%)	40	44
1	K	114/120 (95%)	111 (97%)	3 (3%)	40	44
1	L	114/120 (95%)	111 (97%)	3 (3%)	40	44
All	All	1370/1440 (95%)	1345 (98%)	25 (2%)	51	58

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	11	ILE
1	B	4	LEU
1	B	51	VAL
1	B	143	GLU
1	C	4	LEU
1	C	11	ILE
1	D	2	ARG
1	D	4	LEU
1	E	4	LEU
1	E	84	SER
1	F	4	LEU
1	G	2	ARG
1	G	22	GLN
1	H	4	LEU
1	H	33	LEU
1	J	2	ARG
1	J	3	SER
1	J	11	ILE

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Mol	Chain	Res	Type
1	K	4	LEU
1	K	11	ILE
1	K	143	GLU
1	L	2	ARG
1	L	4	LEU
1	L	11	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	95	ASN
1	B	6	ASN
1	C	6	ASN
1	C	95	ASN
1	D	6	ASN
1	D	95	ASN
1	D	106	HIS
1	E	6	ASN
1	E	95	ASN
1	E	119	HIS
1	F	6	ASN
1	F	95	ASN
1	G	6	ASN
1	G	95	ASN
1	H	6	ASN
1	H	13	ASN
1	H	95	ASN
1	I	95	ASN
1	J	6	ASN
1	J	95	ASN
1	K	6	ASN
1	K	95	ASN
1	L	6	ASN
1	L	95	ASN

5.3.3 RNA ⓘ

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TRS	A	200	-	7,7,7	0.30	0	9,9,9	1.98	5 (55%)
2	TRS	G	200	-	7,7,7	0.61	0	9,9,9	1.62	2 (22%)
2	TRS	D	200	-	7,7,7	0.42	0	9,9,9	1.04	0
2	TRS	J	200	-	7,7,7	0.55	0	9,9,9	1.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	A	200	-	-	4/9/9/9	-
2	TRS	G	200	-	-	0/9/9/9	-
2	TRS	D	200	-	-	0/9/9/9	-
2	TRS	J	200	-	-	0/9/9/9	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	200	TRS	C2-C-N	3.06	115.97	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	200	TRS	C3-C-N	2.94	115.66	108.17
2	A	200	TRS	C1-C-N	-2.50	101.80	108.17
2	A	200	TRS	C3-C-N	2.45	114.43	108.17
2	G	200	TRS	C3-C-C2	-2.36	104.37	110.66
2	A	200	TRS	C3-C-C2	-2.28	104.58	110.66
2	A	200	TRS	C2-C-C1	-2.03	105.25	110.66

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	200	TRS	N-C-C1-O1
2	A	200	TRS	C3-C-C1-O1
2	A	200	TRS	C2-C-C3-O3
2	A	200	TRS	C2-C-C1-O1

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.