Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:15 AM GMT

PDB ID	:	2C57
Title	:	H.PYLORI TYPE II DEHYDROQUINASE IN COMPLEX WITH FA1
Authors	:	Robinson, D.A.; Lapthorn, A.J.
Deposited on	:	2005-10-26
Resolution	:	3.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

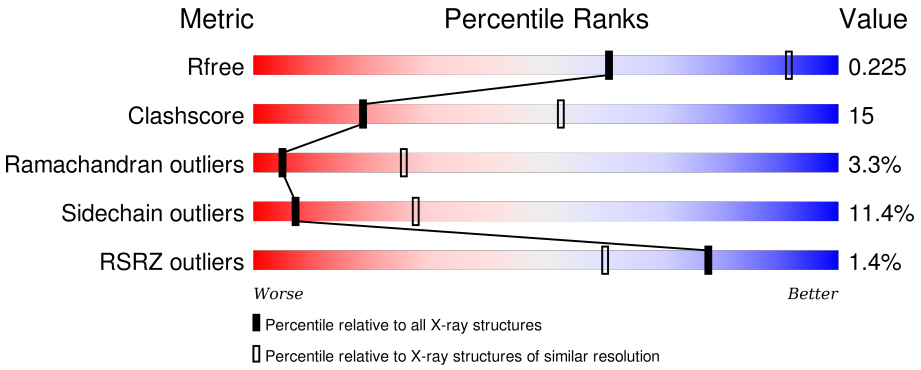
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	180	2% 54% 29% 7% • 9%
1	B	180	2% 52% 26% 7% • 15%
1	C	180	% 56% 24% 5% • 15%
1	D	180	2% 51% 31% 9% • 9%
1	E	180	% 53% 26% 6% • 15%

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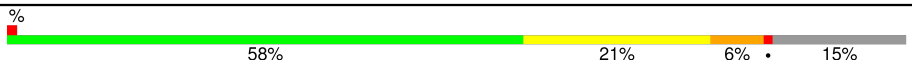
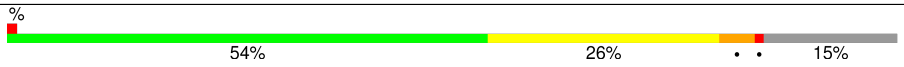
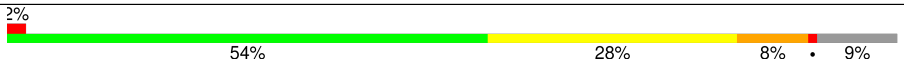
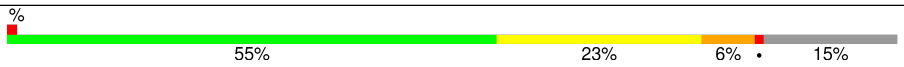
Mol	Chain	Length	Quality of chain
1	F	180	
1	G	180	
1	H	180	
1	I	180	
1	J	180	
1	K	180	
1	L	180	

2 Entry composition (i)

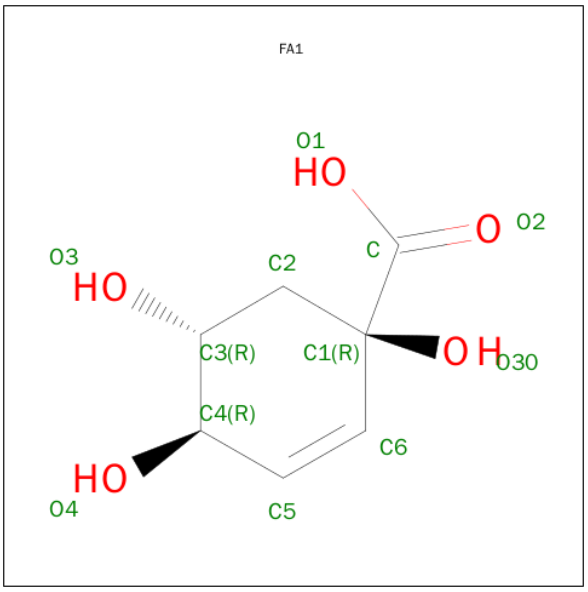
There are 2 unique types of molecules in this entry. The entry contains 14368 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	164	Total	C	N	O	S	0	0	0
			1250	787	215	237	11			
1	B	153	Total	C	N	O	S	0	0	0
			1153	732	190	221	10			
1	C	153	Total	C	N	O	S	0	0	0
			1153	732	190	221	10			
1	D	164	Total	C	N	O	S	0	0	0
			1250	787	215	237	11			
1	E	153	Total	C	N	O	S	0	0	0
			1153	732	190	221	10			
1	F	153	Total	C	N	O	S	0	0	0
			1153	732	190	221	10			
1	G	164	Total	C	N	O	S	0	0	0
			1250	787	215	237	11			
1	H	153	Total	C	N	O	S	0	0	0
			1153	732	190	221	10			
1	I	153	Total	C	N	O	S	0	0	0
			1153	732	190	221	10			
1	J	164	Total	C	N	O	S	0	0	0
			1250	787	215	237	11			
1	K	153	Total	C	N	O	S	0	0	0
			1153	732	190	221	10			
1	L	153	Total	C	N	O	S	0	0	0
			1153	732	190	221	10			

- Molecule 2 is 2,3 -ANHYDRO-QUINIC ACID (three-letter code: FA1) (formula: $C_7H_{10}O_5$).



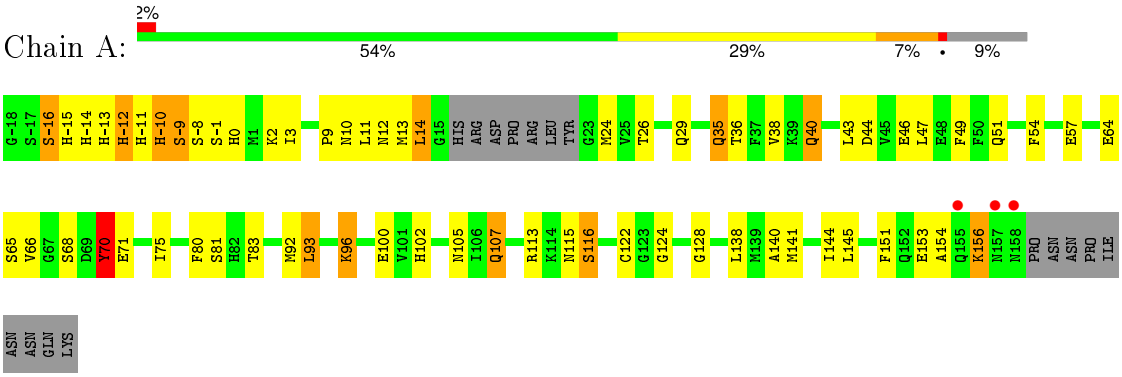
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 7 5	0	0
2	B	1	Total C O 12 7 5	0	0
2	C	1	Total C O 12 7 5	0	0
2	D	1	Total C O 12 7 5	0	0
2	E	1	Total C O 12 7 5	0	0
2	F	1	Total C O 12 7 5	0	0
2	G	1	Total C O 12 7 5	0	0
2	H	1	Total C O 12 7 5	0	0
2	I	1	Total C O 12 7 5	0	0
2	J	1	Total C O 12 7 5	0	0
2	K	1	Total C O 12 7 5	0	0
2	L	1	Total C O 12 7 5	0	0

3 Residue-property plots (i)

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

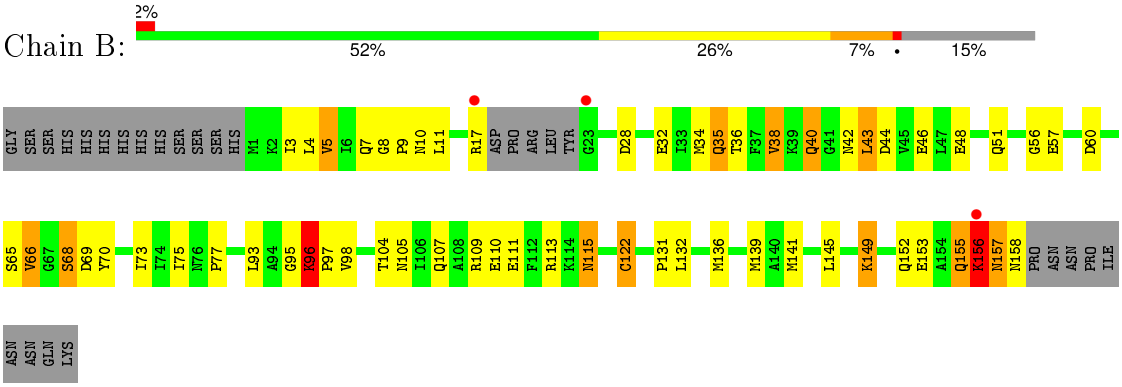
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain A:



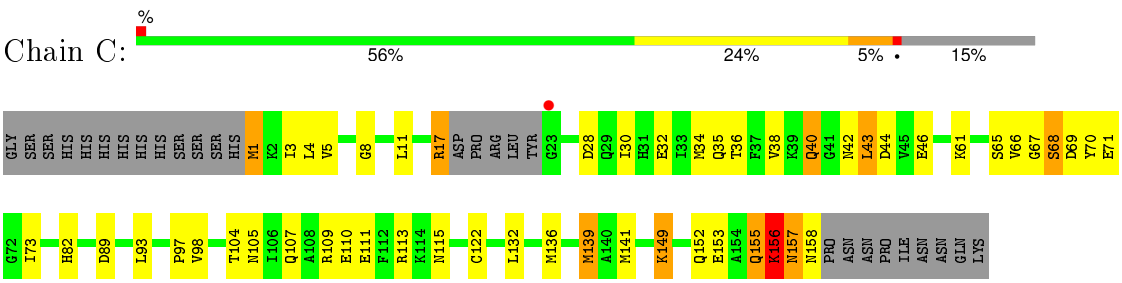
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain B:



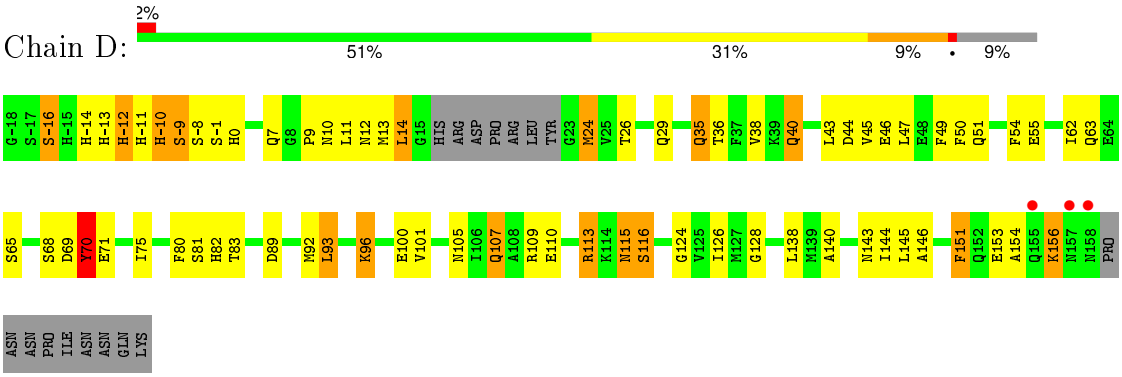
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain C:



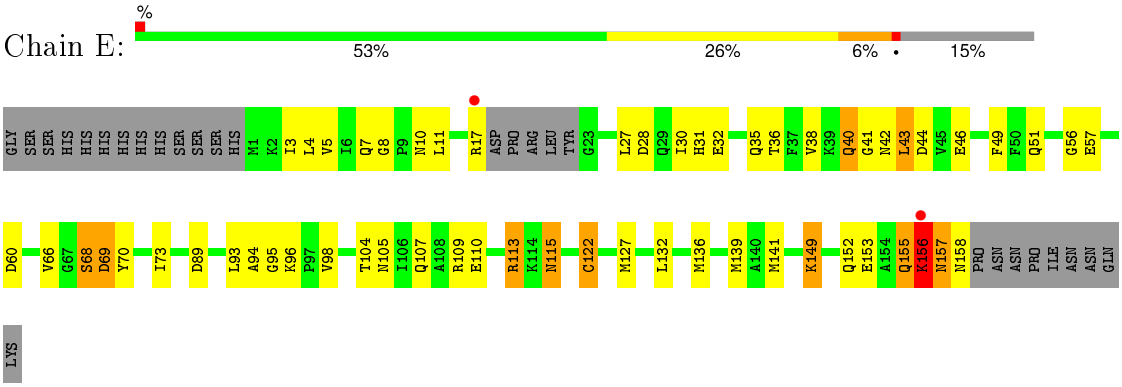
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain D:



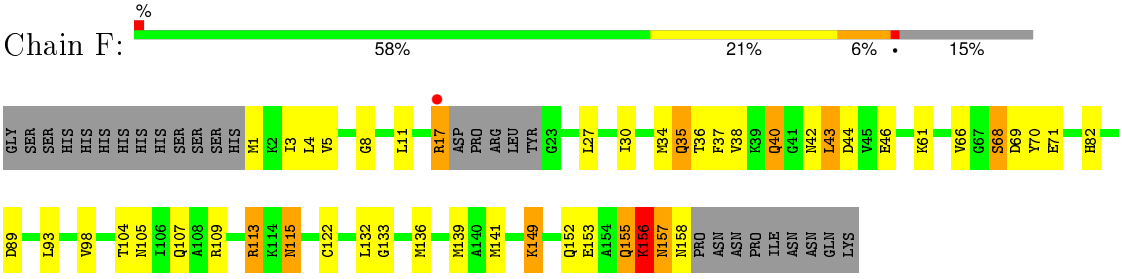
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain E:



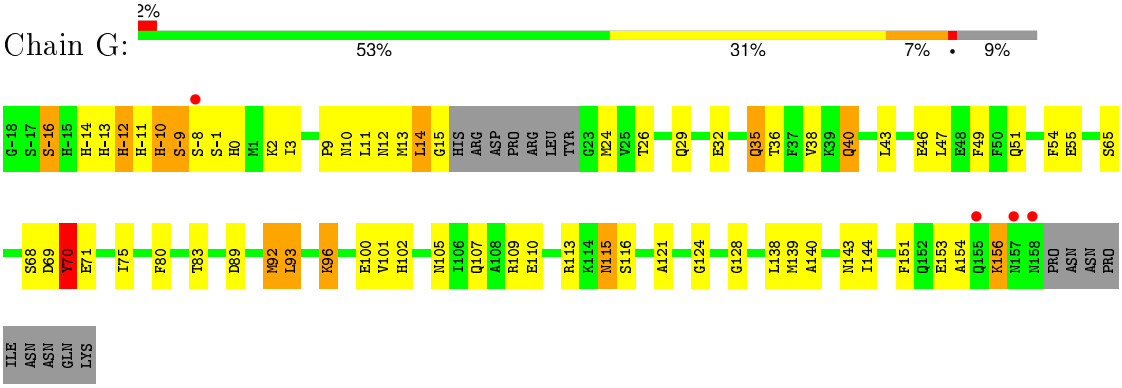
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain F:



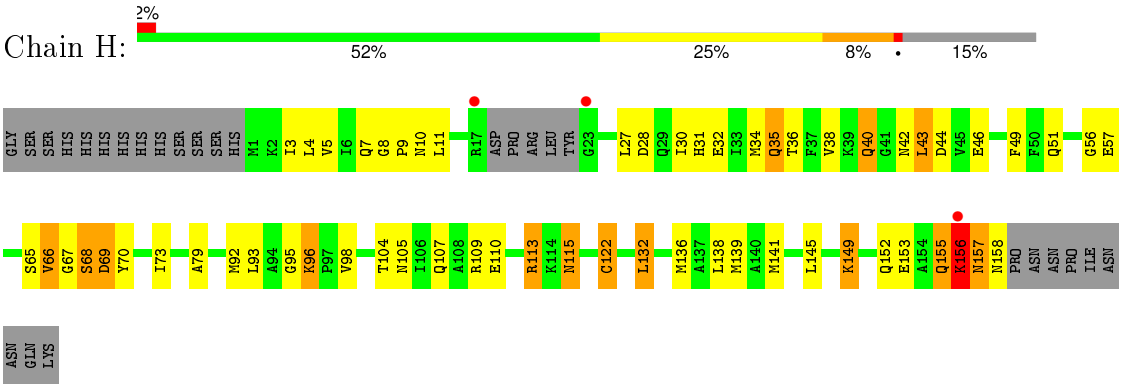
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain G:



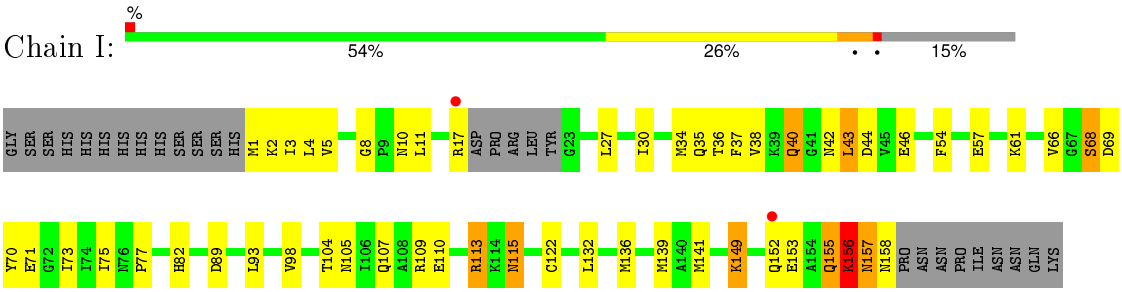
• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain H:



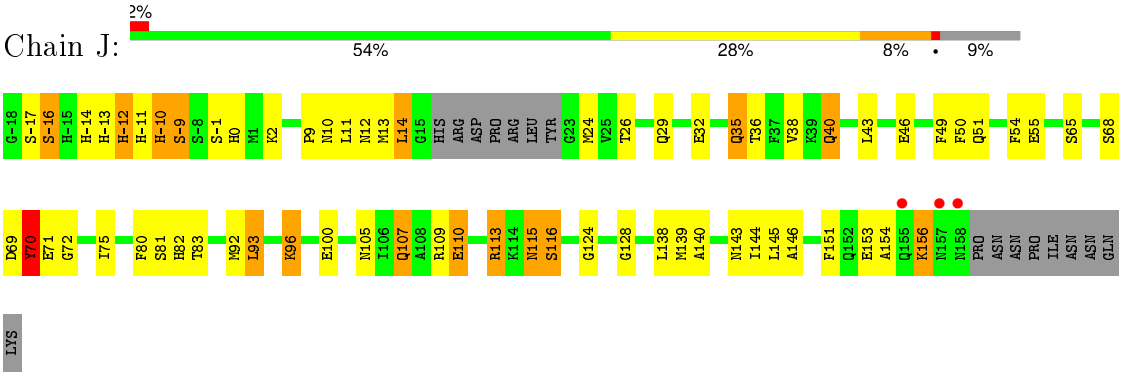
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain I:



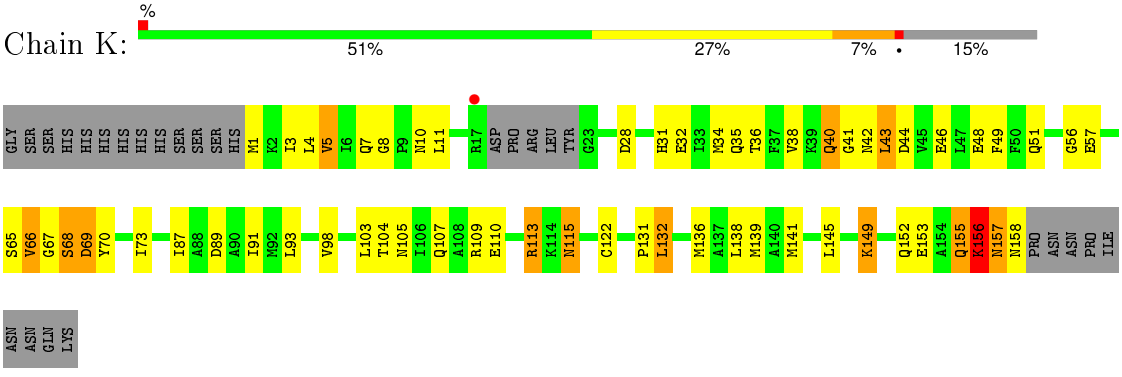
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain J:



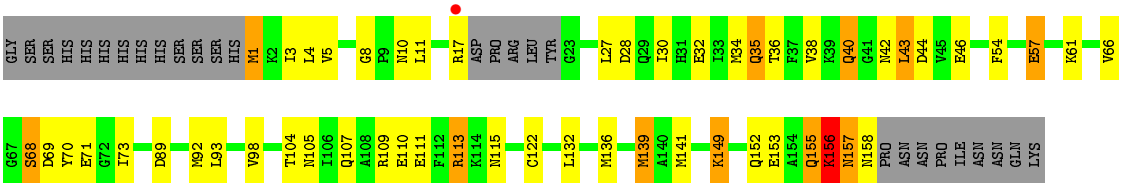
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain K:



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain L:


GLY SER SER HIS HIS HIS HIS HIS SER SER SER HIS M1 K2 I3 L4 V5 G8 P9 N10 L11 R17 ASP PRO ARG LEU TYR G23 L27 D28 Q29 I30 H31 E32 I33 M34 Q35 T36 F37 V38 K39 Q40 G41 N42 L43 D44 V45 E46 F54 E57 K61 V66
G67 S68 D69 Y70 E71 G72 I73 D89 N92 L93 V98 T104 N105 I106 Q107 A108 R109 E110 E111 F112 R113 K114 N115 C122 L132 M136 M139 A140 M141 K149 Q152 E153 A154 Q155 K156 N157 N158 PRO ASN ASN PRO ILE ASN ASN GLN LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	103.86Å 103.86Å 217.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.10 24.95 – 3.10	Depositor EDS
% Data completeness (in resolution range)	83.8 (25.00-3.10) 83.8 (24.95-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.237 0.195 , 0.225	Depositor DCC
R_{free} test set	3968 reflections (11.06%)	DCC
Wilson B-factor (Å^2)	63.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.459 for -h,-k,l 0.468 for h,-h-k,-l 0.460 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 39837 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14368	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FA1

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	1.22	2/1272 (0.2%)	1.09	2/1713 (0.1%)
1	B	1.13	5/1169 (0.4%)	1.05	3/1577 (0.2%)
1	C	1.00	3/1169 (0.3%)	1.00	2/1577 (0.1%)
1	D	1.22	6/1272 (0.5%)	1.14	5/1713 (0.3%)
1	E	1.09	4/1169 (0.3%)	1.05	4/1577 (0.3%)
1	F	1.01	3/1169 (0.3%)	0.99	3/1577 (0.2%)
1	G	1.19	6/1272 (0.5%)	1.08	6/1713 (0.4%)
1	H	1.12	3/1169 (0.3%)	1.07	5/1577 (0.3%)
1	I	1.01	2/1169 (0.2%)	1.00	4/1577 (0.3%)
1	J	1.20	6/1272 (0.5%)	1.08	2/1713 (0.1%)
1	K	1.08	2/1169 (0.2%)	1.05	4/1577 (0.3%)
1	L	1.00	3/1169 (0.3%)	0.99	5/1577 (0.3%)
All	All	1.11	45/14440 (0.3%)	1.05	45/19468 (0.2%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	CYS	CB-SG	-9.38	1.66	1.82
1	D	115	ASN	CB-CG	7.10	1.67	1.51
1	D	55	GLU	CD-OE2	7.05	1.33	1.25
1	B	46	GLU	CG-CD	6.92	1.62	1.51
1	E	46	GLU	CG-CD	6.71	1.62	1.51
1	B	17	ARG	CA-CB	6.68	1.68	1.53
1	B	122	CYS	CB-SG	-6.64	1.71	1.82
1	K	46	GLU	CG-CD	6.53	1.61	1.51
1	E	17	ARG	CA-CB	6.52	1.68	1.53
1	H	46	GLU	CG-CD	6.51	1.61	1.51
1	L	111	GLU	CG-CD	6.48	1.61	1.51
1	E	115	ASN	CB-CG	6.40	1.65	1.51
1	H	115	ASN	CB-CG	6.35	1.65	1.51
1	I	46	GLU	CG-CD	6.34	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	46	GLU	CG-CD	6.34	1.61	1.51
1	J	115	ASN	CB-CG	6.26	1.65	1.51
1	J	70	TYR	CE2-CZ	6.04	1.46	1.38
1	D	70	TYR	CE2-CZ	5.96	1.46	1.38
1	D	55	GLU	CD-OE1	5.76	1.31	1.25
1	C	46	GLU	CG-CD	5.70	1.60	1.51
1	G	32	GLU	CD-OE1	5.57	1.31	1.25
1	G	55	GLU	CD-OE1	5.49	1.31	1.25
1	D	50	PHE	CE2-CZ	5.44	1.47	1.37
1	I	115	ASN	CB-CG	5.43	1.63	1.51
1	B	115	ASN	CB-CG	5.42	1.63	1.51
1	G	15	GLY	N-CA	5.41	1.54	1.46
1	L	57	GLU	CG-CD	-5.38	1.43	1.51
1	F	17	ARG	CA-CB	5.37	1.65	1.53
1	G	115	ASN	CB-CG	5.35	1.63	1.51
1	D	151	PHE	CE1-CZ	5.33	1.47	1.37
1	A	70	TYR	CE2-CZ	5.33	1.45	1.38
1	F	115	ASN	CB-CG	5.31	1.63	1.51
1	B	111	GLU	CG-CD	5.30	1.59	1.51
1	F	46	GLU	CG-CD	5.27	1.59	1.51
1	G	70	TYR	CE2-CZ	5.25	1.45	1.38
1	H	122	CYS	CB-SG	-5.25	1.73	1.81
1	C	111	GLU	CG-CD	5.23	1.59	1.51
1	J	50	PHE	CE2-CZ	5.20	1.47	1.37
1	K	115	ASN	CB-CG	5.18	1.62	1.51
1	J	32	GLU	CD-OE1	5.15	1.31	1.25
1	G	32	GLU	CG-CD	5.15	1.59	1.51
1	J	110	GLU	CG-CD	5.12	1.59	1.51
1	E	122	CYS	CB-SG	-5.07	1.73	1.81
1	C	17	ARG	CA-CB	5.04	1.65	1.53
1	J	55	GLU	CD-OE1	5.03	1.31	1.25

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	92	MET	CG-SD-CE	10.10	116.37	100.20
1	D	92	MET	CG-SD-CE	9.90	116.04	100.20
1	E	44	ASP	CB-CG-OD1	8.97	126.38	118.30
1	H	44	ASP	CB-CG-OD1	8.82	126.24	118.30
1	B	44	ASP	CB-CG-OD1	8.32	125.78	118.30
1	I	44	ASP	CB-CG-OD1	8.13	125.62	118.30
1	D	113	ARG	NE-CZ-NH1	8.09	124.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	92	MET	CG-SD-CE	7.69	112.50	100.20
1	H	113	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	L	44	ASP	CB-CG-OD1	7.51	125.06	118.30
1	C	44	ASP	CB-CG-OD1	7.47	125.03	118.30
1	H	113	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	K	44	ASP	CB-CG-OD1	7.46	125.01	118.30
1	K	89	ASP	CB-CG-OD1	-7.44	111.60	118.30
1	G	113	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	G	89	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	92	MET	CG-SD-CE	6.77	111.03	100.20
1	F	44	ASP	CB-CG-OD1	6.75	124.37	118.30
1	F	113	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	F	89	ASP	CB-CG-OD1	-6.59	112.36	118.30
1	K	113	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	L	89	ASP	CB-CG-OD2	6.40	124.06	118.30
1	E	60	ASP	CB-CG-OD1	6.07	123.76	118.30
1	D	89	ASP	CB-CG-OD1	-6.06	112.84	118.30
1	B	60	ASP	CB-CG-OD1	5.98	123.69	118.30
1	E	89	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	G	89	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	L	113	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	E	113	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	J	113	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	L	89	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	G	113	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	D	70	TYR	CB-CG-CD1	-5.46	117.73	121.00
1	A	113	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	L	92	MET	CB-CG-SD	-5.41	96.17	112.40
1	I	113	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	24	MET	CG-SD-CE	5.31	108.69	100.20
1	I	113	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	K	113	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	G	70	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	H	92	MET	CB-CG-SD	-5.11	97.07	112.40
1	H	44	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	B	38	VAL	CB-CA-C	-5.08	101.76	111.40
1	C	89	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	I	89	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1250	0	1214	49	1
1	B	1153	0	1132	38	0
1	C	1153	0	1132	30	0
1	D	1250	0	1214	49	0
1	E	1153	0	1132	33	0
1	F	1153	0	1132	28	0
1	G	1250	0	1214	45	0
1	H	1153	0	1132	39	0
1	I	1153	0	1132	33	0
1	J	1250	0	1214	47	1
1	K	1153	0	1132	40	0
1	L	1153	0	1132	32	0
2	A	12	0	9	0	0
2	B	12	0	9	1	0
2	C	12	0	9	1	0
2	D	12	0	9	0	0
2	E	12	0	9	1	0
2	F	12	0	9	1	0
2	G	12	0	9	0	0
2	H	12	0	9	1	0
2	I	12	0	9	1	0
2	J	12	0	9	0	0
2	K	12	0	9	1	0
2	L	12	0	9	1	0
All	All	14368	0	14020	438	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 15.

All (438) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLN:O	1:B:156:LYS:HG2	1.72	0.90
1:F:152:GLN:O	1:F:156:LYS:HG2	1.73	0.89
1:H:152:GLN:O	1:H:156:LYS:HG2	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:GLN:O	1:E:156:LYS:HG2	1.74	0.87
1:L:152:GLN:O	1:L:156:LYS:HG2	1.73	0.87
1:K:152:GLN:O	1:K:156:LYS:HG2	1.76	0.85
1:I:152:GLN:O	1:I:156:LYS:HG2	1.75	0.85
1:J:-10:HIS:O	1:J:-9:SER:OG	1.94	0.84
1:C:152:GLN:O	1:C:156:LYS:HG2	1.78	0.83
1:A:-10:HIS:O	1:A:-9:SER:OG	1.96	0.82
1:D:-10:HIS:O	1:D:-9:SER:OG	2.00	0.79
1:G:-10:HIS:O	1:G:-9:SER:OG	2.00	0.78
1:A:54:PHE:HZ	1:B:57:GLU:HG3	1.52	0.74
1:E:3:ILE:HD12	1:E:141:MET:HG2	1.71	0.72
1:A:-13:HIS:O	1:A:-12:HIS:CB	2.37	0.72
1:B:3:ILE:HD12	1:B:141:MET:HG2	1.69	0.72
1:K:3:ILE:HD12	1:K:141:MET:HG2	1.70	0.71
1:G:-13:HIS:O	1:G:-12:HIS:CB	2.38	0.71
1:K:8:GLY:H	1:K:11:LEU:HD12	1.53	0.70
1:D:-13:HIS:O	1:D:-12:HIS:CB	2.39	0.70
1:A:-13:HIS:O	1:A:-12:HIS:HB2	1.92	0.69
1:G:-13:HIS:O	1:G:-12:HIS:HB2	1.92	0.69
1:J:153:GLU:OE2	1:J:153:GLU:HA	1.92	0.69
1:F:113:ARG:HD3	2:F:1159:FA1:O3	1.93	0.68
1:E:38:VAL:HA	1:E:43:LEU:HD12	1.75	0.68
1:B:38:VAL:HA	1:B:43:LEU:HD12	1.74	0.67
1:H:8:GLY:H	1:H:11:LEU:HD12	1.59	0.67
1:G:-10:HIS:O	1:G:-9:SER:CB	2.41	0.67
1:A:-10:HIS:O	1:A:-9:SER:CB	2.42	0.67
1:D:-10:HIS:O	1:D:-9:SER:CB	2.42	0.67
1:J:-13:HIS:O	1:J:-12:HIS:CB	2.41	0.67
1:G:9:PRO:O	1:G:10:ASN:HB2	1.93	0.67
1:B:28:ASP:O	1:B:32:GLU:HG2	1.94	0.67
1:H:38:VAL:HA	1:H:43:LEU:HD12	1.74	0.67
1:H:3:ILE:HD12	1:H:141:MET:HG2	1.76	0.67
1:K:38:VAL:HA	1:K:43:LEU:HD12	1.75	0.66
1:C:38:VAL:HA	1:C:43:LEU:HD12	1.76	0.66
1:J:-10:HIS:O	1:J:-9:SER:CB	2.42	0.66
1:I:38:VAL:HA	1:I:43:LEU:HD12	1.77	0.66
1:L:38:VAL:HA	1:L:43:LEU:HD12	1.78	0.65
1:D:54:PHE:HZ	1:E:57:GLU:HG3	1.61	0.65
1:K:28:ASP:O	1:K:32:GLU:HG2	1.96	0.65
1:G:153:GLU:HA	1:G:153:GLU:OE2	1.96	0.65
1:J:-13:HIS:O	1:J:-12:HIS:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:GLU:OE2	1:D:153:GLU:HA	1.97	0.65
1:D:151:PHE:O	1:D:154:ALA:HB3	1.97	0.64
1:K:132:LEU:O	1:K:136:MET:HG3	1.97	0.64
1:J:9:PRO:O	1:J:10:ASN:HB2	1.97	0.64
1:E:110:GLU:OE1	1:E:113:ARG:NE	2.28	0.64
1:B:98:VAL:HG12	1:B:122:CYS:SG	2.37	0.64
1:D:-12:HIS:O	1:D:-11:HIS:HB3	1.97	0.64
1:G:11:LEU:O	1:G:14:LEU:HD12	1.97	0.64
1:D:54:PHE:CZ	1:E:57:GLU:HG3	2.33	0.63
1:E:8:GLY:H	1:E:11:LEU:HD12	1.63	0.63
1:D:11:LEU:O	1:D:14:LEU:HD12	2.00	0.62
1:E:132:LEU:O	1:E:136:MET:HG3	1.99	0.62
1:K:36:THR:O	1:K:40:GLN:HB3	1.99	0.62
1:D:-13:HIS:O	1:D:-12:HIS:HB2	2.00	0.62
1:J:151:PHE:O	1:J:154:ALA:HB3	1.98	0.62
1:C:36:THR:O	1:C:40:GLN:HB3	2.00	0.62
1:B:36:THR:O	1:B:40:GLN:HB3	1.99	0.62
1:F:3:ILE:HD12	1:F:141:MET:HG2	1.82	0.62
1:E:36:THR:O	1:E:40:GLN:HB3	1.99	0.61
1:A:151:PHE:O	1:A:154:ALA:HB3	2.00	0.61
1:A:54:PHE:CZ	1:B:57:GLU:HG3	2.33	0.61
1:C:132:LEU:O	1:C:136:MET:HG3	2.00	0.61
1:E:4:LEU:HB2	1:E:70:TYR:CD2	2.36	0.61
1:A:153:GLU:OE2	1:A:153:GLU:HA	2.00	0.61
1:J:54:PHE:HZ	1:K:57:GLU:HG3	1.66	0.61
1:C:3:ILE:HD12	1:C:141:MET:HG2	1.82	0.61
1:F:155:GLN:O	1:F:158:ASN:N	2.32	0.61
1:A:9:PRO:O	1:A:10:ASN:HB2	1.98	0.61
1:F:38:VAL:HA	1:F:43:LEU:HD12	1.82	0.61
1:H:36:THR:O	1:H:40:GLN:HB3	2.01	0.61
1:K:98:VAL:HG12	1:K:122:CYS:SG	2.41	0.60
1:L:155:GLN:O	1:L:158:ASN:N	2.32	0.60
1:H:132:LEU:O	1:H:136:MET:HG3	2.00	0.60
1:L:36:THR:O	1:L:40:GLN:HB3	2.02	0.60
1:J:12:ASN:HB3	1:J:51:GLN:OE1	2.02	0.60
1:J:54:PHE:CZ	1:K:57:GLU:HG3	2.36	0.60
1:A:38:VAL:HG13	1:A:43:LEU:HB2	1.84	0.60
1:I:36:THR:O	1:I:40:GLN:HB3	2.02	0.60
1:L:132:LEU:O	1:L:136:MET:HG3	2.02	0.60
1:C:4:LEU:HB2	1:C:70:TYR:CD2	2.38	0.59
1:D:93:LEU:HD22	1:F:17:ARG:CB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLU:OE1	1:B:113:ARG:NE	2.33	0.59
1:A:36:THR:O	1:A:40:GLN:CB	2.51	0.59
1:B:113:ARG:HD3	2:B:1159:FA1:O3	2.03	0.59
1:K:110:GLU:OE1	1:K:113:ARG:NE	2.36	0.59
1:C:155:GLN:O	1:C:158:ASN:N	2.35	0.58
1:G:151:PHE:O	1:G:154:ALA:HB3	2.02	0.58
1:G:54:PHE:HZ	1:H:57:GLU:HG3	1.68	0.58
1:G:36:THR:O	1:G:40:GLN:CB	2.51	0.58
1:C:105:ASN:OD1	1:C:107:GLN:HB2	2.04	0.58
1:A:-16:SER:HA	1:A:49:PHE:O	2.03	0.58
1:F:4:LEU:HB2	1:F:70:TYR:CD2	2.39	0.58
1:L:105:ASN:OD1	1:L:107:GLN:HB2	2.04	0.58
1:G:156:LYS:O	1:G:156:LYS:CG	2.52	0.58
1:E:149:LYS:O	1:E:153:GLU:HG3	2.03	0.57
1:I:3:ILE:HD12	1:I:141:MET:HG2	1.85	0.57
1:H:8:GLY:N	1:H:11:LEU:HD12	2.20	0.57
1:G:12:ASN:HB3	1:G:51:GLN:OE1	2.04	0.57
1:I:105:ASN:OD1	1:I:107:GLN:HB2	2.05	0.57
1:J:11:LEU:O	1:J:14:LEU:HD12	2.04	0.57
1:L:3:ILE:HD12	1:L:141:MET:HG2	1.86	0.57
1:D:35:GLN:NE2	1:D:49:PHE:HE2	2.03	0.56
1:J:38:VAL:HG13	1:J:43:LEU:HB2	1.87	0.56
1:J:9:PRO:HG3	1:J:80:PHE:CE2	2.40	0.56
1:H:28:ASP:O	1:H:32:GLU:HG2	2.05	0.56
1:G:140:ALA:O	1:G:144:ILE:HG13	2.05	0.56
1:G:54:PHE:CZ	1:H:57:GLU:HG3	2.40	0.56
1:D:9:PRO:O	1:D:10:ASN:HB2	2.04	0.56
1:D:38:VAL:HG13	1:D:43:LEU:HB2	1.87	0.56
1:F:36:THR:O	1:F:40:GLN:HB3	2.06	0.56
1:E:8:GLY:N	1:E:11:LEU:HD12	2.21	0.56
1:K:4:LEU:HB2	1:K:70:TYR:CD2	2.40	0.55
1:J:-14:HIS:NE2	1:J:46:GLU:OE2	2.39	0.55
1:E:98:VAL:HG12	1:E:122:CYS:SG	2.47	0.55
1:K:8:GLY:N	1:K:11:LEU:HD12	2.20	0.55
1:A:35:GLN:NE2	1:A:49:PHE:HE2	2.04	0.55
1:F:152:GLN:O	1:F:156:LYS:CG	2.53	0.55
1:E:155:GLN:O	1:E:158:ASN:N	2.40	0.55
1:I:155:GLN:O	1:I:158:ASN:N	2.38	0.55
1:A:11:LEU:O	1:A:14:LEU:HD12	2.07	0.55
1:E:113:ARG:HD3	2:E:1159:FA1:O3	2.07	0.55
1:H:149:LYS:O	1:H:153:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:-12:HIS:O	1:G:-11:HIS:HB3	2.06	0.55
1:K:73:ILE:HB	1:K:98:VAL:HG22	1.88	0.55
1:I:132:LEU:O	1:I:136:MET:HG3	2.07	0.55
1:A:35:GLN:HE21	1:A:49:PHE:HE2	1.55	0.54
1:G:75:ILE:O	1:G:100:GLU:HA	2.06	0.54
1:H:73:ILE:HB	1:H:98:VAL:HG22	1.89	0.54
1:C:113:ARG:HD3	2:C:1159:FA1:O3	2.06	0.54
1:B:132:LEU:O	1:B:136:MET:HG3	2.06	0.54
1:K:113:ARG:HD3	2:K:1159:FA1:O3	2.07	0.54
1:G:-16:SER:HA	1:G:49:PHE:O	2.07	0.54
1:E:104:THR:OG1	1:E:109:ARG:NH1	2.41	0.54
1:D:156:LYS:CG	1:D:156:LYS:O	2.56	0.54
1:A:36:THR:O	1:A:40:GLN:HB2	2.07	0.54
1:G:-14:HIS:NE2	1:G:46:GLU:OE2	2.41	0.54
1:B:152:GLN:O	1:B:156:LYS:CG	2.51	0.54
1:J:35:GLN:NE2	1:J:49:PHE:HE2	2.05	0.54
1:K:149:LYS:O	1:K:153:GLU:HG3	2.08	0.53
1:G:35:GLN:NE2	1:G:49:PHE:HE2	2.06	0.53
1:K:104:THR:OG1	1:K:109:ARG:NH1	2.42	0.53
1:A:75:ILE:O	1:A:100:GLU:HA	2.09	0.53
1:I:4:LEU:HB2	1:I:70:TYR:CD2	2.43	0.53
1:A:-12:HIS:O	1:A:-11:HIS:HB3	2.08	0.53
1:F:105:ASN:OD1	1:F:107:GLN:HB2	2.08	0.53
1:J:140:ALA:O	1:J:144:ILE:HG13	2.08	0.53
1:H:27:LEU:HA	1:H:30:ILE:HD12	1.89	0.53
1:G:70:TYR:CD1	1:G:70:TYR:N	2.75	0.53
1:A:156:LYS:O	1:A:156:LYS:CG	2.57	0.53
1:G:36:THR:O	1:G:40:GLN:HB2	2.08	0.53
1:B:65:SER:OG	1:B:66:VAL:N	2.42	0.53
1:J:105:ASN:OD1	1:J:107:GLN:HB2	2.08	0.53
1:L:4:LEU:HB2	1:L:70:TYR:CD2	2.44	0.52
1:K:155:GLN:O	1:K:158:ASN:N	2.39	0.52
1:D:-16:SER:HA	1:D:49:PHE:O	2.08	0.52
1:E:27:LEU:HA	1:E:30:ILE:HD12	1.91	0.52
1:J:26:THR:O	1:J:29:GLN:HB2	2.10	0.52
1:D:0:HIS:HA	1:D:44:ASP:OD2	2.10	0.52
1:D:-14:HIS:NE2	1:D:46:GLU:OE2	2.42	0.52
1:D:75:ILE:O	1:D:100:GLU:HA	2.10	0.52
1:D:124:GLY:HA2	1:J:128:GLY:HA3	1.92	0.52
1:C:68:SER:O	1:C:70:TYR:N	2.43	0.52
1:J:36:THR:O	1:J:40:GLN:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLY:H	1:B:11:LEU:HD12	1.75	0.52
1:A:12:ASN:HB3	1:A:51:GLN:OE1	2.09	0.52
1:A:36:THR:O	1:A:40:GLN:HB3	2.10	0.52
1:G:36:THR:O	1:G:40:GLN:HB3	2.09	0.52
1:F:98:VAL:HG12	1:F:122:CYS:SG	2.49	0.52
1:L:98:VAL:HG12	1:L:122:CYS:SG	2.51	0.51
1:K:34:MET:O	1:K:38:VAL:HG23	2.09	0.51
1:I:8:GLY:H	1:I:11:LEU:HD12	1.75	0.51
1:G:71:GLU:O	1:G:96:LYS:HB2	2.11	0.51
1:J:81:SER:HB3	1:J:116:SER:HB2	1.92	0.51
1:E:28:ASP:O	1:E:32:GLU:HG2	2.10	0.51
1:A:140:ALA:O	1:A:144:ILE:HG13	2.09	0.51
1:D:36:THR:O	1:D:40:GLN:CB	2.59	0.51
1:J:109:ARG:HB3	1:J:110:GLU:OE1	2.11	0.51
1:D:156:LYS:HG3	1:D:156:LYS:O	2.11	0.51
1:E:36:THR:O	1:E:40:GLN:CB	2.58	0.51
1:C:149:LYS:O	1:C:153:GLU:HG3	2.11	0.51
1:G:38:VAL:HG13	1:G:43:LEU:HB2	1.92	0.51
1:E:73:ILE:HB	1:E:98:VAL:HG22	1.93	0.51
1:D:71:GLU:O	1:D:96:LYS:HB2	2.10	0.51
1:B:105:ASN:OD1	1:B:107:GLN:HB2	2.11	0.50
1:D:70:TYR:CD1	1:D:70:TYR:N	2.79	0.50
1:F:104:THR:OG1	1:F:109:ARG:NH1	2.45	0.50
1:L:155:GLN:C	1:L:157:ASN:H	2.14	0.50
1:K:87:ILE:O	1:K:91:ILE:HG13	2.12	0.50
1:G:9:PRO:HG3	1:G:80:PHE:CE2	2.46	0.50
1:G:109:ARG:HB3	1:G:110:GLU:OE1	2.12	0.50
1:B:155:GLN:O	1:B:158:ASN:N	2.45	0.50
1:E:152:GLN:O	1:E:156:LYS:CG	2.54	0.50
1:H:110:GLU:OE1	1:H:113:ARG:NE	2.39	0.50
1:B:68:SER:O	1:B:70:TYR:N	2.45	0.50
1:L:28:ASP:O	1:L:32:GLU:HG2	2.12	0.50
1:J:-12:HIS:O	1:J:-11:HIS:HB3	2.11	0.50
1:J:-16:SER:HA	1:J:49:PHE:O	2.11	0.50
1:B:149:LYS:O	1:B:153:GLU:HG3	2.11	0.50
1:G:26:THR:O	1:G:29:GLN:HB2	2.12	0.50
1:A:81:SER:OG	1:A:102:HIS:HE1	1.95	0.50
1:J:70:TYR:CD1	1:J:70:TYR:N	2.79	0.50
1:H:98:VAL:HG12	1:H:122:CYS:SG	2.52	0.49
1:D:140:ALA:O	1:D:144:ILE:HG13	2.12	0.49
1:I:155:GLN:C	1:I:157:ASN:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ASP:O	1:C:32:GLU:HG2	2.12	0.49
1:J:12:ASN:HB3	1:J:51:GLN:CD	2.32	0.49
1:A:47:LEU:HD13	1:A:49:PHE:CZ	2.46	0.49
1:F:155:GLN:C	1:F:157:ASN:H	2.16	0.49
1:F:149:LYS:O	1:F:153:GLU:HG3	2.13	0.49
1:E:68:SER:O	1:E:70:TYR:N	2.45	0.49
1:G:12:ASN:HB3	1:G:51:GLN:CD	2.32	0.49
1:I:68:SER:O	1:I:70:TYR:N	2.46	0.49
1:L:110:GLU:OE1	1:L:113:ARG:NE	2.45	0.49
1:E:94:ALA:O	1:E:96:LYS:HD2	2.13	0.49
1:D:35:GLN:HE21	1:D:49:PHE:HE2	1.59	0.49
1:F:8:GLY:H	1:F:11:LEU:HD12	1.77	0.49
1:K:40:GLN:C	1:K:42:ASN:H	2.15	0.49
1:J:36:THR:O	1:J:40:GLN:HB2	2.13	0.48
1:L:68:SER:O	1:L:70:TYR:N	2.47	0.48
1:A:70:TYR:CD1	1:A:70:TYR:N	2.81	0.48
1:A:105:ASN:OD1	1:A:107:GLN:HB2	2.13	0.48
1:D:82:HIS:CE1	1:D:113:ARG:O	2.66	0.48
1:J:156:LYS:O	1:J:156:LYS:CG	2.61	0.48
1:D:-11:HIS:CE1	1:D:0:HIS:ND1	2.81	0.48
1:K:68:SER:O	1:K:70:TYR:N	2.47	0.48
1:B:73:ILE:HB	1:B:98:VAL:HG22	1.96	0.48
1:L:1:MET:HG3	1:L:71:GLU:OE1	2.14	0.48
1:L:152:GLN:O	1:L:156:LYS:CG	2.55	0.48
1:J:75:ILE:O	1:J:100:GLU:HA	2.13	0.48
1:I:82:HIS:CE1	1:I:113:ARG:O	2.66	0.48
1:L:149:LYS:O	1:L:153:GLU:HG3	2.13	0.48
1:H:68:SER:O	1:H:70:TYR:N	2.47	0.48
1:E:95:GLY:O	1:E:96:LYS:HB3	2.14	0.48
1:L:30:ILE:O	1:L:34:MET:HG3	2.14	0.48
1:K:40:GLN:O	1:K:42:ASN:N	2.47	0.48
1:C:1:MET:HG3	1:C:71:GLU:OE1	2.13	0.47
1:H:152:GLN:O	1:H:156:LYS:CG	2.55	0.47
1:H:155:GLN:O	1:H:158:ASN:N	2.44	0.47
1:I:75:ILE:HG12	1:I:77:PRO:HD3	1.96	0.47
1:H:95:GLY:O	1:H:96:LYS:HB3	2.14	0.47
1:A:54:PHE:HB2	1:A:57:GLU:HB2	1.97	0.47
1:C:155:GLN:C	1:C:157:ASN:H	2.18	0.47
1:J:35:GLN:HE21	1:J:49:PHE:HE2	1.61	0.47
1:D:105:ASN:OD1	1:D:107:GLN:HB2	2.14	0.47
1:L:104:THR:OG1	1:L:109:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:ASN:OD1	1:H:107:GLN:HB2	2.15	0.47
1:L:113:ARG:HD3	2:L:1159:FA1:O3	2.14	0.47
1:H:4:LEU:HB2	1:H:70:TYR:CD2	2.49	0.47
1:J:82:HIS:CE1	1:J:113:ARG:O	2.67	0.47
1:A:54:PHE:CD1	1:B:56:GLY:HA3	2.50	0.47
1:F:82:HIS:CE1	1:F:113:ARG:O	2.68	0.47
1:F:68:SER:O	1:F:70:TYR:N	2.48	0.47
1:D:36:THR:O	1:D:40:GLN:HB3	2.15	0.47
1:B:4:LEU:HB2	1:B:70:TYR:CD2	2.50	0.47
1:I:149:LYS:O	1:I:153:GLU:HG3	2.14	0.47
1:A:71:GLU:O	1:A:96:LYS:HB2	2.14	0.47
1:D:9:PRO:HG3	1:D:80:PHE:CE2	2.50	0.47
1:D:38:VAL:C	1:D:40:GLN:N	2.68	0.47
1:J:71:GLU:O	1:J:96:LYS:HB2	2.15	0.47
1:A:-8:SER:O	1:A:-8:SER:OG	2.32	0.47
1:B:40:GLN:C	1:B:42:ASN:H	2.18	0.47
1:D:81:SER:HB3	1:D:116:SER:HB2	1.97	0.47
1:I:30:ILE:O	1:I:34:MET:HG3	2.15	0.47
1:A:0:HIS:HA	1:A:44:ASP:OD2	2.15	0.47
1:G:156:LYS:O	1:G:156:LYS:HG3	2.14	0.47
1:K:105:ASN:OD1	1:K:107:GLN:HB2	2.14	0.47
1:H:11:LEU:HA	1:H:11:LEU:HD23	1.73	0.46
1:K:65:SER:OG	1:K:66:VAL:N	2.47	0.46
1:D:12:ASN:HB3	1:D:51:GLN:OE1	2.15	0.46
1:I:113:ARG:HD3	2:I:1159:FA1:O3	2.15	0.46
1:K:155:GLN:C	1:K:157:ASN:H	2.18	0.46
1:J:2:LYS:O	1:J:70:TYR:HB3	2.15	0.46
1:H:7:GLN:O	1:H:51:GLN:HA	2.14	0.46
1:B:95:GLY:O	1:B:96:LYS:HB3	2.15	0.46
1:K:36:THR:O	1:K:40:GLN:CB	2.64	0.46
1:L:155:GLN:O	1:L:157:ASN:N	2.49	0.46
1:H:155:GLN:C	1:H:157:ASN:H	2.17	0.46
1:F:1:MET:HG3	1:F:71:GLU:OE1	2.14	0.46
1:K:152:GLN:O	1:K:156:LYS:CG	2.57	0.46
1:C:40:GLN:C	1:C:42:ASN:H	2.18	0.46
1:I:104:THR:OG1	1:I:109:ARG:NH1	2.49	0.46
1:E:155:GLN:C	1:E:157:ASN:H	2.19	0.46
1:G:35:GLN:HE21	1:G:49:PHE:HE2	1.63	0.46
1:A:156:LYS:O	1:A:156:LYS:HG3	2.16	0.46
1:E:40:GLN:C	1:E:42:ASN:H	2.19	0.46
1:I:27:LEU:HA	1:I:30:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:GLN:O	1:E:51:GLN:HA	2.16	0.46
1:I:152:GLN:O	1:I:156:LYS:CG	2.57	0.46
1:B:155:GLN:C	1:B:157:ASN:H	2.19	0.46
1:A:2:LYS:O	1:A:70:TYR:HB3	2.16	0.46
1:A:3:ILE:HD12	1:A:141:MET:HG2	1.98	0.46
1:L:155:GLN:C	1:L:157:ASN:N	2.70	0.45
1:A:3:ILE:HD12	1:A:141:MET:CG	2.46	0.45
1:F:27:LEU:HA	1:F:30:ILE:HD12	1.97	0.45
1:L:8:GLY:N	1:L:11:LEU:HD12	2.31	0.45
1:J:139:MET:O	1:J:143:ASN:ND2	2.49	0.45
1:F:133:GLY:O	1:F:136:MET:HB2	2.17	0.45
1:I:155:GLN:C	1:I:157:ASN:N	2.70	0.45
1:F:30:ILE:O	1:F:34:MET:HG3	2.16	0.45
1:D:145:LEU:O	1:D:146:ALA:C	2.54	0.45
1:H:36:THR:O	1:H:40:GLN:CB	2.65	0.45
1:L:27:LEU:HA	1:L:30:ILE:HD12	1.99	0.45
1:F:132:LEU:O	1:F:136:MET:HG3	2.16	0.45
1:D:26:THR:O	1:D:29:GLN:HB2	2.17	0.45
1:C:104:THR:OG1	1:C:109:ARG:NH1	2.50	0.45
1:I:1:MET:HG3	1:I:71:GLU:OE1	2.17	0.45
1:E:11:LEU:HA	1:E:11:LEU:HD23	1.80	0.45
1:H:31:HIS:CE1	1:H:49:PHE:HB3	2.52	0.45
1:J:36:THR:O	1:J:40:GLN:HB3	2.16	0.45
1:I:98:VAL:HG12	1:I:122:CYS:SG	2.56	0.45
1:H:104:THR:OG1	1:H:109:ARG:NH1	2.50	0.45
1:G:54:PHE:CD1	1:G:54:PHE:N	2.85	0.44
1:J:145:LEU:O	1:J:146:ALA:C	2.56	0.44
1:B:5:VAL:HG23	1:B:48:GLU:O	2.17	0.44
1:C:98:VAL:HG12	1:C:122:CYS:SG	2.56	0.44
1:H:40:GLN:C	1:H:42:ASN:H	2.19	0.44
1:J:156:LYS:O	1:J:156:LYS:HG3	2.16	0.44
1:J:38:VAL:C	1:J:40:GLN:N	2.69	0.44
1:A:124:GLY:HA2	1:G:128:GLY:HA3	2.00	0.44
1:D:109:ARG:HB3	1:D:110:GLU:OE1	2.17	0.44
1:F:8:GLY:N	1:F:11:LEU:HD12	2.32	0.44
1:I:110:GLU:OE1	1:I:113:ARG:NE	2.50	0.44
1:E:127:MET:O	1:E:127:MET:HG3	2.17	0.44
1:C:65:SER:O	1:C:67:GLY:N	2.51	0.44
1:A:54:PHE:CE1	1:B:56:GLY:HA3	2.52	0.44
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.77	0.44
1:I:40:GLN:C	1:I:42:ASN:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:LEU:HD23	1:D:145:LEU:HA	1.79	0.44
1:B:11:LEU:HD23	1:B:11:LEU:HA	1.78	0.44
1:H:145:LEU:HD23	1:H:145:LEU:HA	1.74	0.44
1:F:155:GLN:O	1:F:157:ASN:N	2.51	0.44
1:I:2:LYS:O	1:I:70:TYR:HA	2.18	0.44
1:H:34:MET:O	1:H:35:GLN:C	2.56	0.43
1:K:7:GLN:O	1:K:51:GLN:HA	2.16	0.43
1:A:9:PRO:HG3	1:A:80:PHE:CE2	2.53	0.43
1:J:-11:HIS:CE1	1:J:0:HIS:ND1	2.86	0.43
1:J:54:PHE:CD1	1:K:56:GLY:HA3	2.52	0.43
1:A:38:VAL:C	1:A:40:GLN:N	2.71	0.43
1:K:5:VAL:HG23	1:K:48:GLU:O	2.18	0.43
1:I:11:LEU:HD23	1:I:11:LEU:HA	1.77	0.43
1:F:35:GLN:HB2	1:F:35:GLN:HE21	1.57	0.43
1:A:-11:HIS:CE1	1:A:0:HIS:ND1	2.86	0.43
1:L:8:GLY:H	1:L:11:LEU:HD12	1.83	0.43
1:H:65:SER:OG	1:H:66:VAL:N	2.50	0.43
1:K:31:HIS:CE1	1:K:49:PHE:HB3	2.54	0.43
1:D:36:THR:O	1:D:40:GLN:HB2	2.18	0.43
1:L:40:GLN:C	1:L:42:ASN:H	2.22	0.43
1:G:-11:HIS:CE1	1:G:0:HIS:ND1	2.87	0.43
1:J:54:PHE:CE1	1:K:56:GLY:HA3	2.54	0.43
1:F:155:GLN:C	1:F:157:ASN:N	2.71	0.43
1:E:155:GLN:C	1:E:157:ASN:N	2.72	0.43
1:L:11:LEU:HA	1:L:11:LEU:HD23	1.75	0.43
1:F:40:GLN:C	1:F:42:ASN:H	2.22	0.43
1:B:8:GLY:N	1:B:11:LEU:HD12	2.34	0.43
1:E:105:ASN:OD1	1:E:107:GLN:HB2	2.18	0.43
1:G:93:LEU:HD22	1:I:17:ARG:CB	2.48	0.43
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.72	0.43
1:K:65:SER:O	1:K:67:GLY:N	2.51	0.42
1:D:-8:SER:O	1:D:-8:SER:OG	2.36	0.42
1:G:139:MET:O	1:G:143:ASN:ND2	2.52	0.42
1:K:155:GLN:C	1:K:157:ASN:N	2.72	0.42
1:L:73:ILE:HB	1:L:98:VAL:HG22	2.01	0.42
1:H:155:GLN:C	1:H:157:ASN:N	2.72	0.42
1:J:145:LEU:HD23	1:J:145:LEU:HA	1.71	0.42
1:A:128:GLY:HA3	1:G:124:GLY:HA2	2.00	0.42
1:I:8:GLY:N	1:I:11:LEU:HD12	2.34	0.42
1:L:54:PHE:HB2	1:L:57:GLU:HB2	2.00	0.42
1:J:93:LEU:HD22	1:L:17:ARG:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:GLU:OE1	1:C:113:ARG:NE	2.51	0.42
1:I:54:PHE:HB2	1:I:57:GLU:HB2	2.00	0.42
1:B:104:THR:OG1	1:B:109:ARG:NH1	2.50	0.42
1:A:81:SER:HB3	1:A:116:SER:HB2	2.02	0.42
1:D:101:VAL:HG22	1:D:126:ILE:HB	2.02	0.42
1:B:36:THR:O	1:B:40:GLN:CB	2.67	0.42
1:G:100:GLU:OE2	1:G:102:HIS:NE2	2.43	0.42
1:G:92:MET:HG3	1:G:121:ALA:HB1	2.01	0.42
1:D:54:PHE:CD1	1:E:56:GLY:HA3	2.55	0.42
1:C:155:GLN:C	1:C:157:ASN:N	2.72	0.42
1:C:155:GLN:O	1:C:157:ASN:N	2.53	0.42
1:G:38:VAL:C	1:G:40:GLN:N	2.72	0.42
1:A:12:ASN:HB3	1:A:51:GLN:CD	2.40	0.42
1:K:103:LEU:HD23	1:K:103:LEU:HA	1.91	0.42
1:D:62:ILE:O	1:D:63:GLN:C	2.56	0.42
1:A:3:ILE:HB	1:A:47:LEU:HD23	2.01	0.42
1:D:128:GLY:HA3	1:J:124:GLY:HA2	2.02	0.42
1:L:35:GLN:HE21	1:L:35:GLN:HB2	1.54	0.42
1:C:73:ILE:HB	1:C:98:VAL:HG22	2.00	0.41
1:A:93:LEU:HD22	1:C:17:ARG:CB	2.49	0.41
1:B:131:PRO:O	1:B:132:LEU:C	2.59	0.41
1:D:7:GLN:O	1:D:51:GLN:HG2	2.20	0.41
1:A:-14:HIS:NE2	1:A:46:GLU:OE2	2.53	0.41
1:D:143:ASN:N	1:D:143:ASN:HD22	2.18	0.41
1:B:97:PRO:HB2	1:B:141:MET:SD	2.60	0.41
1:K:34:MET:HB3	1:K:138:LEU:HD11	2.03	0.41
1:C:110:GLU:CD	1:C:110:GLU:H	2.22	0.41
1:B:9:PRO:C	1:B:11:LEU:H	2.24	0.41
1:D:47:LEU:HD13	1:D:49:PHE:CZ	2.55	0.41
1:C:82:HIS:CE1	1:C:113:ARG:O	2.73	0.41
1:B:155:GLN:C	1:B:157:ASN:N	2.73	0.41
1:C:139:MET:CE	1:F:37:PHE:CE1	3.03	0.41
1:C:30:ILE:O	1:C:34:MET:HG3	2.20	0.41
1:C:8:GLY:N	1:C:11:LEU:HD12	2.35	0.41
1:G:54:PHE:CE1	1:H:56:GLY:HA3	2.56	0.41
1:I:155:GLN:O	1:I:157:ASN:N	2.54	0.41
1:J:153:GLU:OE2	1:J:153:GLU:CA	2.65	0.41
1:G:54:PHE:CD1	1:H:56:GLY:HA3	2.55	0.41
1:A:26:THR:O	1:A:29:GLN:HB2	2.20	0.41
1:I:36:THR:O	1:I:40:GLN:CB	2.66	0.41
1:H:65:SER:O	1:H:67:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:ASN:OD1	1:G:107:GLN:HB2	2.20	0.41
1:K:131:PRO:O	1:K:132:LEU:C	2.60	0.41
1:C:40:GLN:O	1:C:42:ASN:N	2.54	0.41
1:C:97:PRO:HB2	1:C:141:MET:SD	2.61	0.41
1:H:40:GLN:O	1:H:42:ASN:N	2.54	0.41
1:G:2:LYS:O	1:G:70:TYR:HB3	2.21	0.41
1:L:73:ILE:O	1:L:98:VAL:HA	2.20	0.41
1:D:12:ASN:HB3	1:D:51:GLN:CD	2.41	0.41
1:H:34:MET:HB3	1:H:138:LEU:HD11	2.03	0.41
1:I:37:PHE:CE1	1:L:139:MET:CE	3.04	0.41
1:G:-8:SER:OG	1:G:-8:SER:O	2.35	0.41
1:G:3:ILE:HB	1:G:47:LEU:HD23	2.03	0.41
1:B:34:MET:O	1:B:35:GLN:C	2.59	0.41
1:A:64:GLU:O	1:A:66:VAL:N	2.54	0.41
1:K:1:MET:HG2	1:K:1:MET:O	2.20	0.41
1:H:113:ARG:HD3	2:H:1159:FA1:O3	2.21	0.40
1:B:7:GLN:O	1:B:51:GLN:HA	2.20	0.40
1:H:9:PRO:C	1:H:11:LEU:H	2.25	0.40
1:J:2:LYS:C	1:J:70:TYR:HB3	2.42	0.40
1:J:72:GLY:HA2	1:J:96:LYS:HG3	2.03	0.40
1:E:31:HIS:CE1	1:E:49:PHE:HB3	2.56	0.40
1:I:73:ILE:HB	1:I:98:VAL:HG22	2.02	0.40
1:B:75:ILE:O	1:B:77:PRO:HD3	2.21	0.40
1:D:38:VAL:HG11	1:D:45:VAL:HB	2.04	0.40
1:K:145:LEU:HD23	1:K:145:LEU:HA	1.79	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)
1:A:-15:HIS:ND1	1:J:-17:SER:OG[3_554]	2.16	0.04

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	158/180 (88%)	131 (83%)	23 (15%)	4 (2%)	7	32
1	B	149/180 (83%)	132 (89%)	11 (7%)	6 (4%)	4	21
1	C	149/180 (83%)	133 (89%)	12 (8%)	4 (3%)	6	31
1	D	158/180 (88%)	132 (84%)	22 (14%)	4 (2%)	7	32
1	E	149/180 (83%)	132 (89%)	11 (7%)	6 (4%)	4	21
1	F	149/180 (83%)	135 (91%)	10 (7%)	4 (3%)	6	31
1	G	158/180 (88%)	133 (84%)	21 (13%)	4 (2%)	7	32
1	H	149/180 (83%)	134 (90%)	8 (5%)	7 (5%)	3	17
1	I	149/180 (83%)	134 (90%)	10 (7%)	5 (3%)	5	25
1	J	158/180 (88%)	137 (87%)	17 (11%)	4 (2%)	7	32
1	K	149/180 (83%)	132 (89%)	10 (7%)	7 (5%)	3	17
1	L	149/180 (83%)	134 (90%)	10 (7%)	5 (3%)	5	25
All	All	1824/2160 (84%)	1599 (88%)	165 (9%)	60 (3%)	5	26

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-12	HIS
1	A	68	SER
1	B	66	VAL
1	B	68	SER
1	B	69	ASP
1	C	68	SER
1	C	69	ASP
1	D	-12	HIS
1	D	68	SER
1	E	68	SER
1	E	69	ASP
1	F	68	SER
1	F	69	ASP
1	G	-12	HIS
1	G	68	SER
1	H	68	SER
1	H	69	ASP
1	I	68	SER
1	I	69	ASP

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Mol	Chain	Res	Type
1	J	-12	HIS
1	J	68	SER
1	K	66	VAL
1	K	68	SER
1	K	69	ASP
1	L	68	SER
1	L	69	ASP
1	A	65	SER
1	B	10	ASN
1	B	156	LYS
1	C	66	VAL
1	C	156	LYS
1	D	65	SER
1	E	66	VAL
1	E	156	LYS
1	F	156	LYS
1	G	65	SER
1	H	66	VAL
1	H	156	LYS
1	I	156	LYS
1	K	156	LYS
1	L	156	LYS
1	A	-9	SER
1	D	-9	SER
1	G	-9	SER
1	H	79	ALA
1	J	-9	SER
1	J	65	SER
1	L	66	VAL
1	E	10	ASN
1	H	132	LEU
1	I	10	ASN
1	K	132	LEU
1	L	10	ASN
1	F	66	VAL
1	I	66	VAL
1	H	10	ASN
1	K	10	ASN
1	K	41	GLY
1	B	96	LYS
1	E	41	GLY

5.3.2 Protein sidechains (i)

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	133/151 (88%)	116 (87%)	17 (13%)	5	21
1	B	120/151 (80%)	108 (90%)	12 (10%)	9	34
1	C	120/151 (80%)	107 (89%)	13 (11%)	8	30
1	D	133/151 (88%)	115 (86%)	18 (14%)	5	20
1	E	120/151 (80%)	108 (90%)	12 (10%)	9	34
1	F	120/151 (80%)	108 (90%)	12 (10%)	9	34
1	G	133/151 (88%)	115 (86%)	18 (14%)	5	20
1	H	120/151 (80%)	107 (89%)	13 (11%)	8	30
1	I	120/151 (80%)	108 (90%)	12 (10%)	9	34
1	J	133/151 (88%)	115 (86%)	18 (14%)	5	20
1	K	120/151 (80%)	108 (90%)	12 (10%)	9	34
1	L	120/151 (80%)	107 (89%)	13 (11%)	8	30
All	All	1492/1812 (82%)	1322 (89%)	170 (11%)	7	28

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-16	SER
1	A	-10	HIS
1	A	-1	SER
1	A	13	MET
1	A	14	LEU
1	A	24	MET
1	A	35	GLN
1	A	40	GLN
1	A	70	TYR
1	A	83	THR
1	A	93	LEU
1	A	96	LYS
1	A	107	GLN
1	A	115	ASN

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Mol	Chain	Res	Type
1	A	116	SER
1	A	138	LEU
1	A	156	LYS
1	B	5	VAL
1	B	35	GLN
1	B	40	GLN
1	B	43	LEU
1	B	93	LEU
1	B	96	LYS
1	B	115	ASN
1	B	139	MET
1	B	149	LYS
1	B	155	GLN
1	B	156	LYS
1	B	157	ASN
1	C	1	MET
1	C	5	VAL
1	C	35	GLN
1	C	40	GLN
1	C	43	LEU
1	C	61	LYS
1	C	93	LEU
1	C	115	ASN
1	C	139	MET
1	C	149	LYS
1	C	155	GLN
1	C	156	LYS
1	C	157	ASN
1	D	-16	SER
1	D	-10	HIS
1	D	-1	SER
1	D	13	MET
1	D	14	LEU
1	D	24	MET
1	D	35	GLN
1	D	40	GLN
1	D	69	ASP
1	D	70	TYR
1	D	83	THR
1	D	93	LEU
1	D	96	LYS
1	D	107	GLN

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Mol	Chain	Res	Type
1	D	115	ASN
1	D	116	SER
1	D	138	LEU
1	D	156	LYS
1	E	5	VAL
1	E	35	GLN
1	E	40	GLN
1	E	43	LEU
1	E	69	ASP
1	E	93	LEU
1	E	115	ASN
1	E	139	MET
1	E	149	LYS
1	E	155	GLN
1	E	156	LYS
1	E	157	ASN
1	F	5	VAL
1	F	35	GLN
1	F	40	GLN
1	F	43	LEU
1	F	61	LYS
1	F	93	LEU
1	F	115	ASN
1	F	139	MET
1	F	149	LYS
1	F	155	GLN
1	F	156	LYS
1	F	157	ASN
1	G	-16	SER
1	G	-10	HIS
1	G	-1	SER
1	G	13	MET
1	G	14	LEU
1	G	24	MET
1	G	35	GLN
1	G	40	GLN
1	G	69	ASP
1	G	70	TYR
1	G	83	THR
1	G	93	LEU
1	G	96	LYS
1	G	101	VAL

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Mol	Chain	Res	Type
1	G	115	ASN
1	G	116	SER
1	G	138	LEU
1	G	156	LYS
1	H	5	VAL
1	H	35	GLN
1	H	40	GLN
1	H	43	LEU
1	H	69	ASP
1	H	93	LEU
1	H	96	LYS
1	H	115	ASN
1	H	139	MET
1	H	149	LYS
1	H	155	GLN
1	H	156	LYS
1	H	157	ASN
1	I	5	VAL
1	I	35	GLN
1	I	40	GLN
1	I	43	LEU
1	I	61	LYS
1	I	93	LEU
1	I	115	ASN
1	I	139	MET
1	I	149	LYS
1	I	155	GLN
1	I	156	LYS
1	I	157	ASN
1	J	-16	SER
1	J	-10	HIS
1	J	-1	SER
1	J	13	MET
1	J	14	LEU
1	J	24	MET
1	J	35	GLN
1	J	40	GLN
1	J	69	ASP
1	J	70	TYR
1	J	83	THR
1	J	93	LEU
1	J	96	LYS

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Mol	Chain	Res	Type
1	J	107	GLN
1	J	115	ASN
1	J	116	SER
1	J	138	LEU
1	J	156	LYS
1	K	5	VAL
1	K	35	GLN
1	K	40	GLN
1	K	43	LEU
1	K	69	ASP
1	K	93	LEU
1	K	115	ASN
1	K	139	MET
1	K	149	LYS
1	K	155	GLN
1	K	156	LYS
1	K	157	ASN
1	L	1	MET
1	L	5	VAL
1	L	35	GLN
1	L	40	GLN
1	L	43	LEU
1	L	61	LYS
1	L	93	LEU
1	L	115	ASN
1	L	139	MET
1	L	149	LYS
1	L	155	GLN
1	L	156	LYS
1	L	157	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-11	HIS
1	A	115	ASN
1	A	143	ASN
1	B	35	GLN
1	C	35	GLN
1	D	-11	HIS
1	D	143	ASN
1	E	35	GLN

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Mol	Chain	Res	Type
1	F	35	GLN
1	G	-11	HIS
1	G	115	ASN
1	G	143	ASN
1	H	35	GLN
1	I	35	GLN
1	J	-11	HIS
1	J	143	ASN
1	K	35	GLN
1	L	35	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 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	FA1	A	1159	-	7,12,12	0.92	0	7,18,18	2.40	3 (42%)
2	FA1	B	1159	-	7,12,12	2.14	3 (42%)	7,18,18	2.29	4 (57%)
2	FA1	C	1159	-	7,12,12	0.99	0	7,18,18	1.59	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FA1	D	1159	-	7,12,12	2.27	2 (28%)	7,18,18	2.36	3 (42%)
2	FA1	E	1159	-	7,12,12	1.77	3 (42%)	7,18,18	2.34	4 (57%)
2	FA1	F	1159	-	7,12,12	1.45	2 (28%)	7,18,18	1.38	1 (14%)
2	FA1	G	1159	-	7,12,12	1.21	1 (14%)	7,18,18	2.63	3 (42%)
2	FA1	H	1159	-	7,12,12	1.59	1 (14%)	7,18,18	1.88	3 (42%)
2	FA1	I	1159	-	7,12,12	1.20	1 (14%)	7,18,18	1.54	1 (14%)
2	FA1	J	1159	-	7,12,12	0.79	0	7,18,18	1.85	2 (28%)
2	FA1	K	1159	-	7,12,12	1.56	2 (28%)	7,18,18	2.29	4 (57%)
2	FA1	L	1159	-	7,12,12	0.98	0	7,18,18	1.24	1 (14%)

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	FA1	A	1159	-	-	0/0/21/21	0/1/1/1
2	FA1	B	1159	-	-	0/0/21/21	0/1/1/1
2	FA1	C	1159	-	-	0/0/21/21	0/1/1/1
2	FA1	D	1159	-	-	0/0/21/21	0/1/1/1
2	FA1	E	1159	-	-	0/0/21/21	0/1/1/1
2	FA1	F	1159	-	-	0/0/21/21	0/1/1/1
2	FA1	G	1159	-	-	0/0/21/21	0/1/1/1
2	FA1	H	1159	-	-	0/0/21/21	0/1/1/1
2	FA1	I	1159	-	-	0/0/21/21	0/1/1/1
2	FA1	J	1159	-	-	0/0/21/21	0/1/1/1
2	FA1	K	1159	-	-	0/0/21/21	0/1/1/1
2	FA1	L	1159	-	-	0/0/21/21	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1159	FA1	C4-C5	2.03	1.54	1.50
2	K	1159	FA1	C4-C5	2.13	1.54	1.50
2	F	1159	FA1	C2-C3	2.20	1.56	1.53
2	E	1159	FA1	O3-C3	2.27	1.48	1.43
2	B	1159	FA1	C2-C3	2.32	1.56	1.53
2	K	1159	FA1	C1-C6	2.33	1.52	1.50
2	F	1159	FA1	C1-C6	2.35	1.52	1.50
2	G	1159	FA1	O30-C1	2.51	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1159	FA1	C4-C5	2.58	1.55	1.50
2	E	1159	FA1	C1-C6	2.61	1.52	1.50
2	E	1159	FA1	C2-C3	2.67	1.57	1.53
2	H	1159	FA1	C1-C6	3.18	1.53	1.50
2	D	1159	FA1	O30-C1	3.59	1.49	1.43
2	B	1159	FA1	C1-C6	4.06	1.54	1.50
2	D	1159	FA1	C1-C6	4.52	1.54	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1159	FA1	O4-C4-C3	-5.59	100.34	109.73
2	A	1159	FA1	O4-C4-C3	-5.02	101.31	109.73
2	K	1159	FA1	O4-C4-C3	-4.57	102.06	109.73
2	D	1159	FA1	O4-C4-C3	-4.22	102.64	109.73
2	E	1159	FA1	C4-C5-C6	-4.00	119.06	123.36
2	B	1159	FA1	O4-C4-C3	-3.49	103.86	109.73
2	B	1159	FA1	C4-C5-C6	-3.29	119.82	123.36
2	J	1159	FA1	O4-C4-C3	-3.13	104.48	109.73
2	D	1159	FA1	C4-C5-C6	-3.02	120.11	123.36
2	H	1159	FA1	O4-C4-C3	-2.76	105.09	109.73
2	H	1159	FA1	C4-C5-C6	-2.46	120.71	123.36
2	K	1159	FA1	C4-C5-C6	-2.46	120.71	123.36
2	A	1159	FA1	C4-C5-C6	-2.19	121.00	123.36
2	E	1159	FA1	O4-C4-C3	-2.14	106.14	109.73
2	K	1159	FA1	C1-C6-C5	2.00	121.73	115.15
2	H	1159	FA1	C1-C6-C5	2.10	122.07	115.15
2	A	1159	FA1	C1-C6-C5	2.11	122.08	115.15
2	K	1159	FA1	O3-C3-C2	2.12	115.03	109.92
2	J	1159	FA1	C1-C6-C5	2.18	122.33	115.15
2	B	1159	FA1	C1-C6-C5	2.34	122.85	115.15
2	G	1159	FA1	O30-C1-C6	2.38	117.87	108.29
2	L	1159	FA1	C1-C6-C5	2.43	123.15	115.15
2	I	1159	FA1	C1-C6-C5	2.45	123.20	115.15
2	G	1159	FA1	C1-C6-C5	2.48	123.32	115.15
2	F	1159	FA1	C1-C6-C5	2.51	123.39	115.15
2	D	1159	FA1	C1-C6-C5	2.63	123.80	115.15
2	C	1159	FA1	C1-C6-C5	2.68	123.96	115.15
2	B	1159	FA1	O3-C3-C2	2.71	116.42	109.92
2	E	1159	FA1	C1-C6-C5	2.74	124.16	115.15
2	E	1159	FA1	O3-C3-C2	2.92	116.94	109.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1159	FA1	1	0
2	C	1159	FA1	1	0
2	E	1159	FA1	1	0
2	F	1159	FA1	1	0
2	H	1159	FA1	1	0
2	I	1159	FA1	1	0
2	K	1159	FA1	1	0
2	L	1159	FA1	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	164/180 (91%)	-0.35	3 (1%)	71	50	60, 61, 62, 63	0
1	B	153/180 (85%)	-0.46	3 (1%)	68	46	60, 61, 62, 62	0
1	C	153/180 (85%)	-0.41	1 (0%)	89	78	60, 61, 62, 62	0
1	D	164/180 (91%)	-0.34	3 (1%)	71	50	60, 61, 62, 63	0
1	E	153/180 (85%)	-0.45	2 (1%)	79	62	61, 61, 62, 62	0
1	F	153/180 (85%)	-0.40	1 (0%)	89	78	60, 61, 62, 62	0
1	G	164/180 (91%)	-0.35	4 (2%)	62	39	60, 61, 62, 63	0
1	H	153/180 (85%)	-0.46	3 (1%)	68	46	60, 61, 62, 62	0
1	I	153/180 (85%)	-0.40	2 (1%)	79	62	60, 61, 62, 62	0
1	J	164/180 (91%)	-0.36	3 (1%)	71	50	59, 61, 62, 63	0
1	K	153/180 (85%)	-0.45	1 (0%)	89	78	60, 61, 62, 62	0
1	L	153/180 (85%)	-0.39	1 (0%)	89	78	60, 61, 62, 62	0
All	All	1880/2160 (87%)	-0.40	27 (1%)	78	60	59, 61, 62, 63	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	158	ASN	5.2
1	D	158	ASN	5.1
1	A	158	ASN	4.7
1	G	155	GLN	4.4
1	K	17	ARG	4.1
1	D	155	GLN	4.0
1	J	155	GLN	3.9
1	J	158	ASN	3.9
1	A	155	GLN	3.9
1	E	17	ARG	3.6
1	H	17	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	17	ARG	3.5
1	F	17	ARG	2.9
1	J	157	ASN	2.8
1	D	157	ASN	2.8
1	I	17	ARG	2.7
1	G	157	ASN	2.4
1	A	157	ASN	2.3
1	L	17	ARG	2.3
1	B	23	GLY	2.2
1	C	23	GLY	2.2
1	E	156	LYS	2.1
1	H	156	LYS	2.1
1	H	23	GLY	2.1
1	I	152	GLN	2.0
1	B	156	LYS	2.0
1	G	-8	SER	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	FA1	K	1159	12/12	0.97	0.23	1.89	60,61,62,64	0
2	FA1	E	1159	12/12	0.96	0.24	1.50	60,61,62,64	0
2	FA1	B	1159	12/12	0.96	0.22	0.94	60,61,62,64	0
2	FA1	H	1159	12/12	0.97	0.22	0.90	61,61,62,63	0
2	FA1	C	1159	12/12	0.97	0.20	0.90	60,61,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FA1	A	1159	12/12	0.98	0.20	0.65	60,61,62,62	0
2	FA1	G	1159	12/12	0.98	0.20	0.46	60,61,62,62	0
2	FA1	L	1159	12/12	0.96	0.19	0.38	61,61,62,63	0
2	FA1	I	1159	12/12	0.97	0.17	0.15	60,61,62,63	0
2	FA1	F	1159	12/12	0.97	0.17	0.11	61,61,62,63	0
2	FA1	J	1159	12/12	0.97	0.18	-0.12	60,61,62,63	0
2	FA1	D	1159	12/12	0.97	0.17	-0.40	60,61,62,62	0

6.5 Other polymers

There are no such residues in this entry.