Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 12:44 AM EDT

PDB ID	:	1D0I
Title	:	CRYSTAL STRUCTURE OF TYPE II DEHYDROQUINASE FROM STREPTOMYCES COELICOLOR COMPLEXED WITH PHOSPHATE IONS
Authors	:	Roszak, A.W.; Krell, T.; Hunter, I.S.; Coggins, J.R.; Lapthorn, A.J.
Deposited on	:	1999-09-10
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

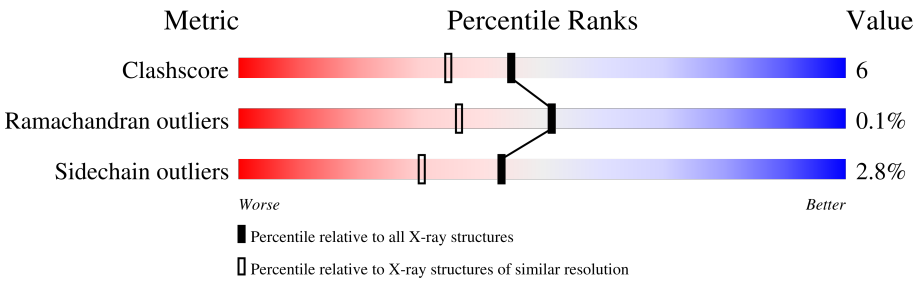
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.80 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	156	80% 13% • •
1	B	156	83% 12% •• •
1	C	156	82% 13% • •
1	D	156	82% 12% • •
1	E	156	85% 9% • • •
1	F	156	80% 14% • • •
1	G	156	84% 10% • • •
1	H	156	83% 12% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	156	83% 10%
1	J	156	79% 13%
1	K	156	85% 10%
1	L	156	84% 11%

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
2	PO4	A	3002	-	X	-	-
2	PO4	E	3006	-	X	-	-
2	PO4	G	3010	-	X	-	-
2	PO4	J	3013	-	X	-	-

2 Entry composition (i)

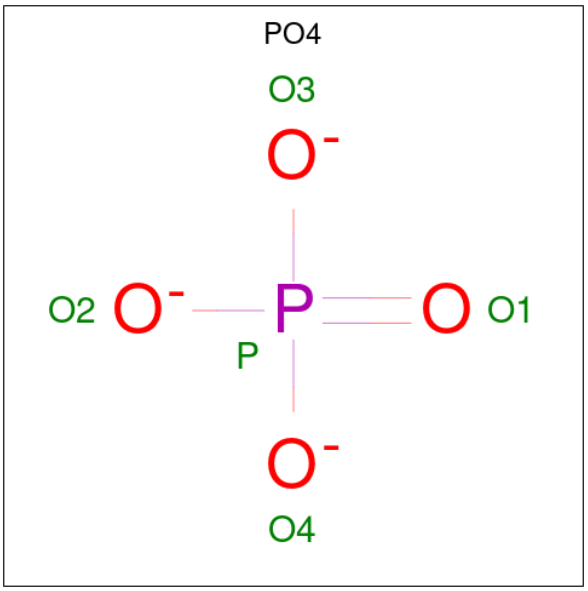
There are 4 unique types of molecules in this entry. The entry contains 15962 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TYPE II 3-DEHYDROQUINATE HYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	150	1153	716	218	213	6	0	5	0
1	B	150	1143	711	215	211	6	0	3	0
1	C	150	1143	711	210	216	6	0	5	0
1	D	151	1154	717	214	217	6	0	6	0
1	E	152	1157	718	220	213	6	0	5	0
1	F	151	1152	716	216	214	6	0	4	0
1	G	151	1152	716	217	213	6	0	4	0
1	H	153	1168	724	221	217	6	0	5	0
1	I	150	1144	711	212	215	6	0	4	0
1	J	150	1160	721	219	214	6	0	7	0
1	K	151	1153	716	216	215	6	0	5	0
1	L	151	1148	714	216	212	6	0	3	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



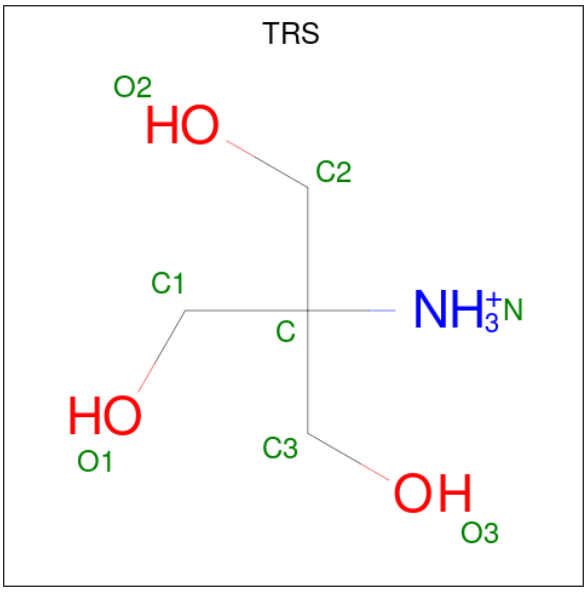
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P			
2	A	1	5	4	1		0	0
			Total	O	P			
2	A	1	5	4	1		0	0
			Total	O	P			
2	B	1	5	4	1		0	0
			Total	O	P			
2	C	1	5	4	1		0	0
			Total	O	P			
2	D	1	5	4	1		0	0
			Total	O	P			
2	E	1	5	4	1		0	0
			Total	O	P			
2	E	1	5	4	1		0	0
			Total	O	P			
2	F	1	5	4	1		0	0
			Total	O	P			
2	G	1	5	4	1		0	0
			Total	O	P			
2	G	1	5	4	1		0	0
			Total	O	P			
2	H	1	5	4	1		0	0
			Total	O	P			
2	I	1	5	4	1		0	0
			Total	O	P			
2	J	1	5	4	1		0	0
			Total	O	P			
2	K	1	5	4	1		0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P			
2	K	1	5	4	1		0	0
			Total	O	P			
2	L	1	5	4	1		0	0

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	194	194	194	0	0
			Total	O		
4	B	139	139	139	0	0
			Total	O		
4	C	114	114	114	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	171	171	171	0	0
			Total	O		
4	E	205	205	205	0	0
			Total	O		
4	F	174	174	174	0	0
			Total	O		
4	G	205	205	205	0	0
			Total	O		
4	H	190	190	190	0	0
			Total	O		
4	I	197	197	197	0	0
			Total	O		
4	J	116	116	116	0	0
			Total	O		
4	K	183	183	183	0	0
			Total	O		
4	L	135	135	135	0	0

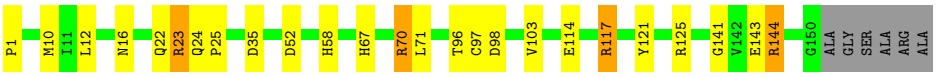
3 Residue-property plots (i)

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.

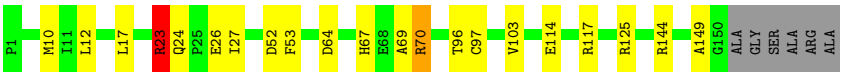
• Molecule 1: TYPE II 3-DEHYDROQUINATE HYDRATASE

Chain A:



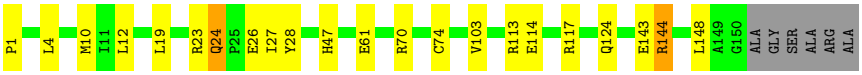
• Molecule 1: TYPE II 3-DEHYDROQUINATE HYDRATASE

Chain B:



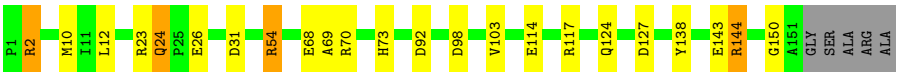
• Molecule 1: TYPE II 3-DEHYDROQUINATE HYDRATASE

Chain C:



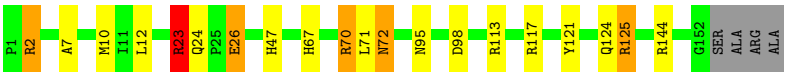
• Molecule 1: TYPE II 3-DEHYDROQUINATE HYDRATASE

Chain D:



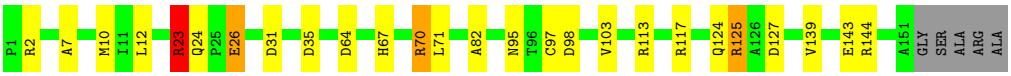
• Molecule 1: TYPE II 3-DEHYDROQUINATE HYDRATASE

Chain E:



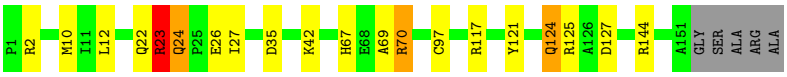
• Molecule 1: TYPE II 3-DEHYDROQUINATE HYDRATASE

Chain F:



• Molecule 1: TYPE II 3-DEHYDROQUINATE HYDRATASE

Chain G:

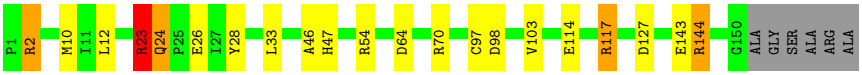


• Molecule 1: TYPE II 3-DEHYDROQUINATE HYDRATASE

Chain H:

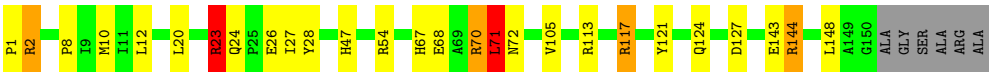
• Molecule 1: TYPE II 3-DEHYDROQUINATE HYDRATASE

Chain I:



• Molecule 1: TYPE II 3-DEHYDROQUINATE HYDRATASE

Chain J:

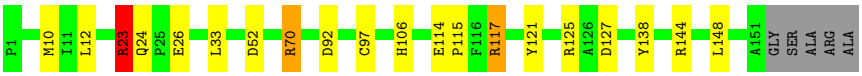


• Molecule 1: TYPE II 3-DEHYDROQUINATE HYDRATASE

Chain K:

• Molecule 1: TYPE II 3-DEHYDROQUINATE HYDRATASE

Chain L:



4 Data and refinement statistics (i)

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	113.20Å 137.50Å 140.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.03 – 1.80	Depositor
% Data completeness (in resolution range)	98.7 (45.03-1.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.171 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15962	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.74	0/1202	1.57	13/1634 (0.8%)
1	B	0.72	0/1182	1.50	11/1608 (0.7%)
1	C	0.68	0/1192	1.52	9/1623 (0.6%)
1	D	0.77	0/1208	1.43	11/1644 (0.7%)
1	E	0.84	0/1207	1.55	10/1641 (0.6%)
1	F	0.76	0/1196	1.56	17/1627 (1.0%)
1	G	0.86	0/1196	1.57	17/1627 (1.0%)
1	H	0.75	0/1217	1.65	19/1654 (1.1%)
1	I	0.84	0/1189	1.67	16/1619 (1.0%)
1	J	1.51	10/1219 (0.8%)	1.98	37/1657 (2.2%)
1	K	0.83	0/1202	1.59	14/1635 (0.9%)
1	L	0.75	0/1187	1.48	14/1615 (0.9%)
All	All	0.86	10/14397 (0.1%)	1.60	188/19584 (1.0%)

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	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	71[A]	LEU	CB-CG	22.81	2.18	1.52
1	J	71[B]	LEU	CB-CG	22.81	2.18	1.52
1	J	71[A]	LEU	CG-CD1	13.03	2.00	1.51
1	J	71[B]	LEU	CG-CD1	13.03	2.00	1.51
1	J	71[A]	LEU	CA-CB	12.95	1.83	1.53
1	J	71[B]	LEU	CA-CB	12.95	1.83	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	71[A]	LEU	CG-CD2	12.81	1.99	1.51
1	J	71[B]	LEU	CG-CD2	12.81	1.99	1.51
1	J	71[A]	LEU	N-CA	5.05	1.56	1.46
1	J	71[B]	LEU	N-CA	5.05	1.56	1.46

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	71[A]	LEU	CA-CB-CG	-25.16	57.44	115.30
1	J	71[B]	LEU	CA-CB-CG	-25.16	57.44	115.30
1	F	117	ARG	NE-CZ-NH2	-17.65	111.48	120.30
1	K	144[A]	ARG	NE-CZ-NH2	-16.28	112.16	120.30
1	K	144[B]	ARG	NE-CZ-NH2	-16.28	112.16	120.30
1	I	144[A]	ARG	NE-CZ-NH2	-16.23	112.19	120.30
1	I	144[B]	ARG	NE-CZ-NH2	-16.23	112.19	120.30
1	H	144[A]	ARG	NE-CZ-NH2	-14.86	112.87	120.30
1	H	144[B]	ARG	NE-CZ-NH2	-14.86	112.87	120.30
1	C	117	ARG	NE-CZ-NH2	-14.84	112.88	120.30
1	H	144[A]	ARG	NE-CZ-NH1	13.81	127.21	120.30
1	H	144[B]	ARG	NE-CZ-NH1	13.81	127.21	120.30
1	B	117	ARG	NE-CZ-NH2	-13.25	113.67	120.30
1	A	144[A]	ARG	NE-CZ-NH1	-13.25	113.67	120.30
1	A	144[B]	ARG	NE-CZ-NH1	-13.25	113.67	120.30
1	J	71[A]	LEU	CB-CA-C	12.94	134.79	110.20
1	J	71[B]	LEU	CB-CA-C	12.94	134.79	110.20
1	A	144[A]	ARG	NE-CZ-NH2	12.84	126.72	120.30
1	A	144[B]	ARG	NE-CZ-NH2	12.84	126.72	120.30
1	I	144[A]	ARG	NE-CZ-NH1	12.77	126.69	120.30
1	I	144[B]	ARG	NE-CZ-NH1	12.77	126.69	120.30
1	C	70	ARG	CD-NE-CZ	12.58	141.21	123.60
1	I	2	ARG	NE-CZ-NH1	-12.27	114.16	120.30
1	J	71[A]	LEU	CD1-CG-CD2	11.46	144.88	110.50
1	J	71[B]	LEU	CD1-CG-CD2	11.46	144.88	110.50
1	E	144[A]	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	E	144[B]	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	E	144[A]	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	E	144[B]	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	J	117	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	H	70[A]	ARG	CD-NE-CZ	10.56	138.39	123.60
1	H	70[B]	ARG	CD-NE-CZ	10.56	138.39	123.60
1	G	117	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	J	70[A]	ARG	CA-C-N	10.39	140.06	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	70[B]	ARG	CA-C-N	10.39	140.06	117.20
1	I	70	ARG	NE-CZ-NH2	10.32	125.46	120.30
1	J	127	ASP	CB-CG-OD2	9.91	127.22	118.30
1	I	54	ARG	NE-CZ-NH2	9.66	125.13	120.30
1	H	23	ARG	NE-CZ-NH2	9.56	125.08	120.30
1	J	71[A]	LEU	CB-CG-CD1	-9.52	94.82	111.00
1	J	71[B]	LEU	CB-CG-CD1	-9.52	94.82	111.00
1	I	70	ARG	CD-NE-CZ	9.46	136.85	123.60
1	G	144[A]	ARG	NE-CZ-NH2	-9.17	115.71	120.30
1	G	144[B]	ARG	NE-CZ-NH2	-9.17	115.71	120.30
1	K	144[A]	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	K	144[B]	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	B	70[A]	ARG	CD-NE-CZ	9.11	136.35	123.60
1	B	70[B]	ARG	CD-NE-CZ	9.11	136.35	123.60
1	E	70[A]	ARG	CD-NE-CZ	9.01	136.22	123.60
1	E	70[B]	ARG	CD-NE-CZ	9.01	136.22	123.60
1	K	70[A]	ARG	CD-NE-CZ	9.00	136.21	123.60
1	K	70[B]	ARG	CD-NE-CZ	9.00	136.21	123.60
1	H	117	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	D	127	ASP	CB-CG-OD2	8.84	126.25	118.30
1	F	125	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	A	70[A]	ARG	CD-NE-CZ	8.69	135.77	123.60
1	A	70[B]	ARG	CD-NE-CZ	8.69	135.77	123.60
1	G	70[A]	ARG	CD-NE-CZ	8.69	135.76	123.60
1	G	70[B]	ARG	CD-NE-CZ	8.69	135.76	123.60
1	J	113	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	G	23	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	L	23	ARG	NE-CZ-NH1	-8.05	116.28	120.30
1	G	144[A]	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	G	144[B]	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	L	23	ARG	NE-CZ-NH2	7.99	124.30	120.30
1	F	64	ASP	CB-CG-OD1	7.73	125.26	118.30
1	J	71[A]	LEU	CB-CG-CD2	-7.72	97.87	111.00
1	J	71[B]	LEU	CB-CG-CD2	-7.72	97.87	111.00
1	F	117	ARG	NH1-CZ-NH2	7.70	127.87	119.40
1	C	70	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	F	127	ASP	CB-CG-OD2	7.62	125.16	118.30
1	F	31	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	A	117	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	A	121	TYR	CB-CG-CD1	-7.49	116.51	121.00
1	D	70	ARG	CD-NE-CZ	7.49	134.08	123.60
1	H	70[A]	ARG	NE-CZ-NH2	7.42	124.01	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	70[B]	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	I	2	ARG	NH1-CZ-NH2	7.35	127.48	119.40
1	C	117	ARG	NH1-CZ-NH2	7.17	127.29	119.40
1	B	52	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	G	125	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	J	70[A]	ARG	O-C-N	-6.96	111.56	122.70
1	J	70[B]	ARG	O-C-N	-6.96	111.56	122.70
1	D	144[A]	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	D	144[B]	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	L	127	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	F	125	ARG	CD-NE-CZ	6.80	133.12	123.60
1	H	52	ASP	CB-CG-OD1	6.76	124.38	118.30
1	C	113	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	G	127	ASP	CB-CA-C	6.71	123.81	110.40
1	B	23	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	F	23	ARG	NE-CZ-NH2	6.57	123.58	120.30
1	G	121	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	A	70[A]	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	A	70[B]	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	F	113	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	J	127	ASP	CB-CG-OD1	-6.47	112.47	118.30
1	F	23	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	L	92	ASP	CB-CG-OD2	-6.43	112.52	118.30
1	F	70[A]	ARG	NE-CZ-NH2	6.41	123.51	120.30
1	F	70[B]	ARG	NE-CZ-NH2	6.41	123.51	120.30
1	E	113	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	K	117	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	B	53	PHE	CB-CG-CD2	-6.35	116.36	120.80
1	I	117	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	D	31	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	A	35	ASP	CB-CG-OD2	6.33	124.00	118.30
1	L	70[A]	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	L	70[B]	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	I	127	ASP	CB-CG-OD2	6.32	123.99	118.30
1	D	138	TYR	CB-CG-CD2	-6.29	117.22	121.00
1	D	54	ARG	NE-CZ-NH2	6.21	123.41	120.30
1	B	114	GLU	OE1-CD-OE2	-6.13	115.94	123.30
1	J	71[A]	LEU	N-CA-C	-6.13	94.45	111.00
1	J	71[B]	LEU	N-CA-C	-6.13	94.45	111.00
1	L	117	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	I	2	ARG	CG-CD-NE	-6.07	99.05	111.80
1	L	125	ARG	NE-CZ-NH2	6.04	123.32	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	144[A]	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	J	144[B]	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	F	70[A]	ARG	CD-NE-CZ	5.96	131.94	123.60
1	F	70[B]	ARG	CD-NE-CZ	5.96	131.94	123.60
1	H	70[A]	ARG	CG-CD-NE	5.93	124.26	111.80
1	H	70[B]	ARG	CG-CD-NE	5.93	124.26	111.80
1	B	117	ARG	NH1-CZ-NH2	5.93	125.92	119.40
1	G	127	ASP	O-C-N	-5.92	113.14	123.20
1	H	35	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	C	117	ARG	CG-CD-NE	-5.83	99.56	111.80
1	C	61	GLU	OE1-CD-OE2	5.78	130.24	123.30
1	C	144[A]	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	C	144[B]	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	D	138	TYR	CB-CG-CD1	5.75	124.45	121.00
1	E	125	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	J	54	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	125	ARG	CD-NE-CZ	5.72	131.60	123.60
1	E	47	HIS	CA-CB-CG	-5.71	103.89	113.60
1	L	117	ARG	CG-CD-NE	-5.70	99.83	111.80
1	J	70[A]	ARG	CA-C-O	-5.69	108.14	120.10
1	J	70[B]	ARG	CA-C-O	-5.69	108.14	120.10
1	K	54	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	K	23	ARG	CD-NE-CZ	5.66	131.53	123.60
1	K	125	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	52	ASP	CB-CG-OD1	5.66	123.39	118.30
1	D	70	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	I	23	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	H	125	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	K	72	ASN	N-CA-CB	-5.54	100.64	110.60
1	H	54	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	E	23	ARG	CD-NE-CZ	5.53	131.34	123.60
1	F	35	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	149	ALA	CB-CA-C	5.52	118.37	110.10
1	B	64	ASP	CB-CG-OD1	5.51	123.26	118.30
1	D	92	ASP	CB-CG-OD2	5.51	123.26	118.30
1	G	121	TYR	CB-CG-CD2	5.50	124.30	121.00
1	G	35	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	J	54	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	J	70[A]	ARG	CD-NE-CZ	5.46	131.24	123.60
1	J	70[B]	ARG	CD-NE-CZ	5.46	131.24	123.60
1	J	71[A]	LEU	O-C-N	-5.44	113.99	122.70
1	J	71[B]	LEU	O-C-N	-5.44	113.99	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	52	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	J	23[A]	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	J	23[B]	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	G	124[A]	GLN	CA-CB-CG	5.43	125.34	113.40
1	G	124[B]	GLN	CA-CB-CG	5.43	125.34	113.40
1	I	2	ARG	CD-NE-CZ	5.33	131.06	123.60
1	L	138	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	J	68	GLU	O-C-N	-5.30	114.22	122.70
1	K	83	TYR	CB-CG-CD2	5.29	124.17	121.00
1	L	52	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	J	105	VAL	CA-CB-CG1	5.26	118.79	110.90
1	H	24	GLN	CB-CG-CD	5.25	125.25	111.60
1	F	82	ALA	CB-CA-C	-5.25	102.23	110.10
1	L	127	ASP	CB-CG-OD2	5.22	123.00	118.30
1	J	8	PRO	O-C-N	5.17	130.97	122.70
1	B	125	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	L	121	TYR	CB-CG-CD2	5.14	124.08	121.00
1	F	124	GLN	OE1-CD-NE2	5.12	133.68	121.90
1	G	127	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	I	64	ASP	CB-CG-OD1	5.11	122.90	118.30
1	J	54	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	L	106	HIS	CA-CB-CG	-5.10	104.94	113.60
1	D	127	ASP	CB-CA-C	5.08	120.56	110.40
1	I	127	ASP	CB-CA-C	5.08	120.55	110.40
1	J	2	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	H	23	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	K	125	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	K	42	LYS	CG-CD-CE	5.00	126.91	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	72	ASN	Mainchain

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	1153	0	1133	17	0
1	B	1143	0	1122	13	0
1	C	1143	0	1110	14	0
1	D	1154	0	1124	14	0
1	E	1157	0	1133	11	0
1	F	1152	0	1129	14	0
1	G	1152	0	1131	12	0
1	H	1168	0	1146	13	0
1	I	1144	0	1113	16	0
1	J	1160	0	1144	37	0
1	K	1153	0	1130	10	0
1	L	1148	0	1127	7	0
2	A	10	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	10	0	0	0	0
2	F	5	0	0	0	0
2	G	10	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	10	0	0	0	0
2	L	5	0	0	0	0
3	A	8	0	12	0	0
3	D	8	0	12	0	0
3	G	8	0	12	0	0
3	J	8	0	12	0	0
4	A	194	0	0	5	0
4	B	139	0	0	1	0
4	C	114	0	0	2	0
4	D	171	0	0	3	0
4	E	205	0	0	3	0
4	F	174	0	0	2	0
4	G	205	0	0	3	0
4	H	190	0	0	4	0
4	I	197	0	0	5	0
4	J	116	0	0	4	0
4	K	183	0	0	4	0
4	L	135	0	0	1	0
All	All	15962	0	13590	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (177) 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:J:71[A]:LEU:CG	1:J:71[A]:LEU:CD2	1.99	1.41
1:J:71[A]:LEU:CG	1:J:71[A]:LEU:CD1	2.00	1.39
1:J:71[B]:LEU:CG	1:J:71[B]:LEU:CD1	2.07	1.33
1:C:124[B]:GLN:HG2	4:C:1895:HOH:O	1.40	1.18
1:K:143[B]:GLU:OE2	4:K:3179:HOH:O	1.61	1.17
1:C:124[B]:GLN:OE1	4:C:1850:HOH:O	1.70	1.06
1:K:143[B]:GLU:OE1	4:K:3178:HOH:O	1.75	1.02
1:J:71[A]:LEU:HD21	1:J:72:ASN:HD21	1.30	0.94
1:J:67:HIS:HA	1:J:70[B]:ARG:HD3	1.53	0.90
1:J:10[A]:MET:SD	1:J:12:LEU:HD21	2.11	0.89
1:J:71[A]:LEU:HD21	1:J:72:ASN:ND2	1.88	0.88
1:B:70[A]:ARG:HG2	1:B:97:CYS:HB2	1.56	0.87
1:I:10[A]:MET:SD	1:I:12:LEU:HD21	2.15	0.86
1:H:143[B]:GLU:OE1	4:H:3020:HOH:O	1.93	0.84
1:B:67:HIS:HA	1:B:70[B]:ARG:HD3	1.60	0.83
1:D:10[A]:MET:SD	1:D:12:LEU:HD21	2.22	0.79
1:A:143[A]:GLU:OE1	4:A:3360:HOH:O	1.99	0.78
1:A:67:HIS:HA	1:A:70[B]:ARG:HD3	1.65	0.78
1:L:70[B]:ARG:HG2	1:L:97:CYS:HB2	1.64	0.77
1:D:143[B]:GLU:OE1	4:D:3312:HOH:O	2.03	0.76
1:B:17:LEU:HD21	4:B:3056:HOH:O	1.88	0.74
1:E:67:HIS:HA	1:E:70[B]:ARG:HD3	1.69	0.73
1:F:10[A]:MET:SD	1:F:12:LEU:HD21	2.30	0.71
1:E:10[A]:MET:SD	1:E:12:LEU:HD21	2.31	0.71
1:C:103:VAL:HG21	1:C:144[B]:ARG:HG2	1.71	0.71
1:H:10[A]:MET:SD	1:H:12:LEU:HD21	2.31	0.71
1:I:143[B]:GLU:OE1	4:I:3018:HOH:O	2.09	0.71
1:D:98:ASP:HA	4:D:3460:HOH:O	1.91	0.70
1:H:18:ASN:H	1:H:18:ASN:HD22	1.41	0.68
1:F:103:VAL:HG21	1:F:144[B]:ARG:HG2	1.75	0.67
1:G:10[A]:MET:SD	1:G:12:LEU:HD21	2.36	0.66
1:F:98:ASP:HA	4:F:3083:HOH:O	1.94	0.65
1:F:143[B]:GLU:OE1	4:H:3020:HOH:O	2.14	0.65
1:A:98:ASP:HA	4:A:3453:HOH:O	1.97	0.64
1:B:103:VAL:HG21	1:B:144[B]:ARG:HG2	1.78	0.64
1:I:114[A]:GLU:OE2	1:I:117:ARG:NE	2.28	0.64
1:B:24:GLN:HB2	1:B:27:ILE:HD12	1.78	0.63
1:K:71:LEU:HB2	1:K:72:ASN:ND2	2.13	0.63
1:I:2:ARG:HG2	4:I:3050:HOH:O	1.98	0.63
1:J:71[A]:LEU:HG	1:J:72:ASN:N	2.13	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:TYR:O	1:E:124[B]:GLN:HG2	2.00	0.61
1:B:10[A]:MET:SD	1:B:12:LEU:HD21	2.41	0.61
1:I:114[A]:GLU:CD	1:I:117:ARG:HE	2.04	0.61
1:A:98:ASP:HB2	4:A:3444:HOH:O	2.00	0.60
1:A:70[A]:ARG:HG2	1:A:97:CYS:HB2	1.82	0.60
1:A:23:ARG:HG2	1:A:24:GLN:HE21	1.66	0.60
1:B:70[A]:ARG:HG2	1:B:97:CYS:CB	2.31	0.60
1:A:22:GLN:HG3	4:A:3463:HOH:O	2.01	0.59
1:C:103:VAL:CG2	1:C:144[B]:ARG:HG2	2.33	0.59
1:C:10[A]:MET:SD	1:C:12:LEU:HD21	2.44	0.58
1:L:10[A]:MET:SD	1:L:12:LEU:HD21	2.43	0.58
1:J:71[A]:LEU:CD2	1:J:72:ASN:ND2	2.66	0.57
1:A:23:ARG:H	1:A:23:ARG:HD3	1.69	0.57
1:A:23:ARG:CG	1:A:24:GLN:HE21	2.18	0.56
1:J:117:ARG:HD3	4:J:694:HOH:O	2.04	0.56
1:G:10[A]:MET:HE1	1:G:69:ALA:HB2	1.87	0.56
1:D:10[A]:MET:SD	1:D:12:LEU:CD2	2.95	0.55
1:F:67:HIS:HA	1:F:70[B]:ARG:HD3	1.87	0.55
1:C:24:GLN:HB2	1:C:27:ILE:HD12	1.89	0.55
1:K:70[A]:ARG:HG2	1:K:97:CYS:HB2	1.88	0.55
1:A:10[A]:MET:SD	1:A:12:LEU:HD21	2.47	0.55
1:G:10[A]:MET:CE	1:G:69:ALA:HB2	2.37	0.54
1:F:70[A]:ARG:HG2	1:F:97:CYS:HB2	1.90	0.54
1:F:103:VAL:CG2	1:F:144[B]:ARG:HG2	2.38	0.54
1:C:24:GLN:HG3	1:C:28:TYR:HD2	1.74	0.53
1:H:22:GLN:HG3	4:H:3074:HOH:O	2.08	0.53
1:H:98:ASP:HA	4:H:3096:HOH:O	2.10	0.52
1:J:71[A]:LEU:CD2	1:J:71[A]:LEU:HG	2.25	0.51
1:H:10[A]:MET:HG2	1:H:12:LEU:HG	1.93	0.51
1:B:10[A]:MET:SD	1:B:69:ALA:HB2	2.51	0.51
1:H:24:GLN:HG3	1:H:28:TYR:HD2	1.76	0.50
1:A:96:THR:HG21	1:C:19:LEU:HD12	1.91	0.50
1:H:2[B]:ARG:HB3	1:H:6:ASN:OD1	2.11	0.50
1:E:117:ARG:HD3	4:E:3033:HOH:O	2.11	0.50
1:I:23:ARG:HB2	1:I:24:GLN:HE21	1.77	0.49
1:B:103:VAL:CG2	1:B:144[B]:ARG:HG2	2.41	0.49
1:D:54:ARG:HH22	1:D:68[A]:GLU:CD	2.16	0.49
1:E:2[B]:ARG:HD3	1:E:7:ALA:HB2	1.94	0.49
1:D:23:ARG:O	1:D:24:GLN:C	2.49	0.48
1:J:1:PRO:HD3	4:J:595:HOH:O	2.12	0.48
1:J:27:ILE:HA	4:J:1489:HOH:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:10[A]:MET:HG2	1:I:12:LEU:HG	1.96	0.47
1:H:70[A]:ARG:HG2	1:H:97:CYS:HB2	1.97	0.47
1:K:122:VAL:HG23	4:K:3086:HOH:O	2.14	0.47
1:L:114:GLU:CD	1:L:117:ARG:HE	2.18	0.47
1:D:2[A]:ARG:HG3	4:D:3442:HOH:O	2.14	0.47
1:B:23:ARG:O	1:B:24:GLN:C	2.53	0.46
1:K:23:ARG:O	1:K:24:GLN:C	2.53	0.46
1:C:4:LEU:HD12	1:C:74:CYS:SG	2.56	0.46
1:J:70[B]:ARG:NH2	1:J:70[B]:ARG:HB2	2.31	0.46
1:E:121:TYR:O	1:E:124[A]:GLN:HG2	2.15	0.46
1:G:23:ARG:HB2	1:G:24:GLN:OE1	2.15	0.46
1:G:67:HIS:HA	1:G:70[B]:ARG:HE	1.80	0.46
1:C:23:ARG:O	1:C:24:GLN:C	2.53	0.46
1:F:2:ARG:HD2	1:F:7:ALA:HB2	1.97	0.45
1:I:47:HIS:NE2	1:I:143[A]:GLU:OE1	2.49	0.45
1:J:23[A]:ARG:HD2	1:K:96:THR:HG22	1.98	0.45
1:J:121:TYR:O	1:J:124[A]:GLN:HG2	2.16	0.45
1:I:46:ALA:HB3	4:I:3108:HOH:O	2.15	0.45
1:J:144[B]:ARG:NH1	1:J:148:LEU:HD21	2.31	0.45
1:G:70[B]:ARG:HG2	1:G:97:CYS:HB2	1.97	0.45
1:L:33:LEU:HD12	1:L:33:LEU:HA	1.86	0.45
1:B:70[A]:ARG:HD2	1:B:96:THR:OG1	2.16	0.44
1:F:95:ASN:OD1	1:F:125:ARG:HD3	2.18	0.44
1:H:121:TYR:O	1:H:124:GLN:HG2	2.18	0.44
1:F:139:VAL:O	1:F:143[B]:GLU:HG3	2.18	0.44
1:F:10[A]:MET:HG2	1:F:12:LEU:HG	1.99	0.44
1:D:114:GLU:OE1	1:D:117:ARG:NE	2.49	0.44
1:J:20:LEU:CD1	1:J:28:TYR:HB3	2.47	0.44
1:C:10[A]:MET:HG2	1:C:12:LEU:HG	2.00	0.44
1:A:16:ASN:O	1:A:23:ARG:NH1	2.51	0.43
1:E:95:ASN:OD1	1:E:125:ARG:HD3	2.18	0.43
1:F:23:ARG:HA	4:F:3154:HOH:O	2.19	0.43
1:I:33:LEU:HD12	1:I:33:LEU:HA	1.92	0.43
1:B:67:HIS:O	1:B:70[A]:ARG:HB2	2.17	0.43
1:I:28:TYR:HE2	4:I:3168:HOH:O	2.01	0.43
1:C:47:HIS:HE2	1:C:143[A]:GLU:CD	2.22	0.43
1:H:70[A]:ARG:HD2	1:H:96:THR:OG1	2.18	0.43
1:L:23:ARG:O	1:L:24:GLN:C	2.57	0.43
1:K:10[A]:MET:HG2	1:K:12:LEU:HG	2.00	0.43
1:G:24:GLN:HB2	1:G:27:ILE:HD12	2.00	0.43
1:I:103:VAL:HG21	1:I:144[A]:ARG:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:GLN:HA	1:E:26:GLU:OE2	2.19	0.42
1:J:47:HIS:HE2	1:J:143[A]:GLU:CD	2.23	0.42
1:I:10[A]:MET:SD	1:I:12:LEU:CD2	2.98	0.42
1:G:2:ARG:HA	4:G:3365:HOH:O	2.20	0.42
1:A:114:GLU:CD	1:A:117:ARG:HE	2.22	0.42
1:E:98:ASP:HB2	4:E:3045:HOH:O	2.20	0.42
1:J:23[A]:ARG:HG3	4:K:3143:HOH:O	2.20	0.42
1:I:97:CYS:SG	4:I:3093:HOH:O	2.59	0.42
1:L:97:CYS:HB3	4:L:3038:HOH:O	2.20	0.42
1:F:24:GLN:HA	1:F:26:GLU:OE2	2.20	0.41
1:A:58:HIS:ND1	2:A:3002:PO4:O1	2.46	0.41
1:G:42:LYS:HE3	4:G:3381:HOH:O	2.20	0.41
1:K:10[A]:MET:SD	1:K:12:LEU:HD21	2.61	0.41
1:L:144[B]:ARG:NH2	1:L:148:LEU:HD21	2.36	0.41
1:B:70[A]:ARG:CG	1:B:97:CYS:HB2	2.40	0.41
1:C:47:HIS:NE2	1:C:143[A]:GLU:OE1	2.53	0.41
1:E:23:ARG:HG3	4:E:3183:HOH:O	2.20	0.41
1:J:27:ILE:HD12	4:J:1970:HOH:O	2.21	0.41
1:H:24:GLN:HG3	1:H:28:TYR:CD2	2.55	0.41
1:D:26:GLU:H	1:D:26:GLU:CD	2.23	0.41
1:D:69:ALA:HA	1:D:73:HIS:ND1	2.36	0.41
1:D:103:VAL:HG21	1:D:144[A]:ARG:HB3	2.02	0.41
1:E:71:LEU:HB2	1:E:72:ASN:ND2	2.35	0.41
1:A:24:GLN:N	1:A:25:PRO:HD3	2.36	0.41
1:I:23:ARG:O	1:I:24:GLN:C	2.60	0.41
1:I:24:GLN:HG3	1:I:28:TYR:HD2	1.86	0.41
1:A:103:VAL:HG11	1:A:141:GLY:HA2	2.04	0.40
1:G:22:GLN:HG3	4:G:3372:HOH:O	2.20	0.40
1:J:20:LEU:HD11	1:J:28:TYR:HB3	2.03	0.40
1:C:144[B]:ARG:NH2	1:C:148:LEU:HD21	2.36	0.40
1:F:139:VAL:O	1:F:143[A]:GLU:HG2	2.20	0.40
1:D:114:GLU:CD	1:D:117:ARG:HE	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	153/156 (98%)	151 (99%)	2 (1%)	0	100	100
1	B	151/156 (97%)	147 (97%)	4 (3%)	0	100	100
1	C	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	D	155/156 (99%)	149 (96%)	5 (3%)	1 (1%)	25	12
1	E	155/156 (99%)	151 (97%)	4 (3%)	0	100	100
1	F	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	G	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
1	H	156/156 (100%)	150 (96%)	6 (4%)	0	100	100
1	I	152/156 (97%)	148 (97%)	4 (3%)	0	100	100
1	J	155/156 (99%)	151 (97%)	4 (3%)	0	100	100
1	K	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
1	L	152/156 (97%)	148 (97%)	4 (3%)	0	100	100
All	All	1842/1872 (98%)	1791 (97%)	50 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	150	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	123/120 (102%)	120 (98%)	3 (2%)	49	36
1	B	121/120 (101%)	119 (98%)	2 (2%)	60	51
1	C	122/120 (102%)	117 (96%)	5 (4%)	30	16
1	D	123/120 (102%)	120 (98%)	3 (2%)	49	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	122/120 (102%)	118 (97%)	4 (3%)	38	23
1	F	122/120 (102%)	119 (98%)	3 (2%)	47	34
1	G	122/120 (102%)	119 (98%)	3 (2%)	47	34
1	H	124/120 (103%)	119 (96%)	5 (4%)	31	16
1	I	122/120 (102%)	118 (97%)	4 (3%)	38	23
1	J	125/120 (104%)	119 (95%)	6 (5%)	25	11
1	K	123/120 (102%)	120 (98%)	3 (2%)	49	36
1	L	121/120 (101%)	118 (98%)	3 (2%)	47	34
All	All	1470/1440 (102%)	1426 (97%)	44 (3%)	43	27

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PRO
1	A	23	ARG
1	A	71	LEU
1	B	23	ARG
1	B	26	GLU
1	C	1	PRO
1	C	24	GLN
1	C	26[A]	GLU
1	C	26[B]	GLU
1	C	114	GLU
1	D	2[A]	ARG
1	D	2[B]	ARG
1	D	24	GLN
1	E	2[A]	ARG
1	E	2[B]	ARG
1	E	23	ARG
1	E	26	GLU
1	F	23	ARG
1	F	26	GLU
1	F	71	LEU
1	G	23	ARG
1	G	24	GLN
1	G	26	GLU
1	H	6	ASN
1	H	18	ASN
1	H	23	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	26	GLU
1	H	153	SER
1	I	23	ARG
1	I	24	GLN
1	I	26	GLU
1	I	98	ASP
1	J	2	ARG
1	J	23[A]	ARG
1	J	23[B]	ARG
1	J	26	GLU
1	J	71[A]	LEU
1	J	71[B]	LEU
1	K	23	ARG
1	K	24	GLN
1	K	26	GLU
1	L	23	ARG
1	L	26	GLU
1	L	115	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	F	24	GLN
1	G	6	ASN
1	H	18	ASN
1	H	24	GLN
1	I	24	GLN
1	J	72	ASN
1	K	6	ASN
1	K	72	ASN
1	L	6	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

20 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	PO4	J	3013	-	4,4,4	2.61	2 (50%)	6,6,6	2.00	3 (50%)
2	PO4	F	3008	-	4,4,4	1.77	1 (25%)	6,6,6	1.04	0
3	TRS	J	3304	-	7,7,7	0.88	0	9,9,9	0.84	0
2	PO4	K	3015	-	4,4,4	1.66	1 (25%)	6,6,6	1.10	1 (16%)
2	PO4	B	3003	-	4,4,4	2.05	1 (25%)	6,6,6	1.60	2 (33%)
2	PO4	D	3005	-	4,4,4	1.76	1 (25%)	6,6,6	1.66	1 (16%)
2	PO4	L	3016	-	4,4,4	1.63	1 (25%)	6,6,6	1.08	0
2	PO4	H	3011	-	4,4,4	1.79	1 (25%)	6,6,6	1.40	1 (16%)
2	PO4	A	3002	-	4,4,4	1.70	1 (25%)	6,6,6	2.31	4 (66%)
2	PO4	C	3004	-	4,4,4	1.98	1 (25%)	6,6,6	1.23	0
2	PO4	E	3006	-	4,4,4	1.81	1 (25%)	6,6,6	2.59	3 (50%)
2	PO4	G	3010	-	4,4,4	2.73	3 (75%)	6,6,6	3.08	5 (83%)
2	PO4	E	3007	-	4,4,4	2.14	2 (50%)	6,6,6	1.53	1 (16%)
2	PO4	A	3001	-	4,4,4	2.34	1 (25%)	6,6,6	1.52	2 (33%)
3	TRS	D	3302	-	7,7,7	1.07	0	9,9,9	1.23	1 (11%)
3	TRS	G	3303	-	7,7,7	1.08	0	9,9,9	0.71	0
2	PO4	I	3012	-	4,4,4	1.77	1 (25%)	6,6,6	1.31	1 (16%)
3	TRS	A	3301	-	7,7,7	0.94	0	9,9,9	1.14	0
2	PO4	G	3009	-	4,4,4	2.08	1 (25%)	6,6,6	1.01	1 (16%)
2	PO4	K	3014	-	4,4,4	2.64	1 (25%)	6,6,6	2.14	1 (16%)

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
3	TRS	J	3304	-	-	0/9/9/9	-
3	TRS	A	3301	-	-	0/9/9/9	-
3	TRS	D	3302	-	-	0/9/9/9	-
3	TRS	G	3303	-	-	0/9/9/9	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	3014	PO4	P-O1	4.86	1.61	1.50
2	J	3013	PO4	P-O1	4.76	1.61	1.50
2	A	3001	PO4	P-O1	4.54	1.61	1.50
2	G	3009	PO4	P-O1	4.08	1.60	1.50
2	B	3003	PO4	P-O1	3.95	1.59	1.50
2	C	3004	PO4	P-O1	3.73	1.59	1.50
2	H	3011	PO4	P-O1	3.41	1.58	1.50
2	K	3015	PO4	P-O1	3.29	1.58	1.50
2	G	3010	PO4	P-O2	-3.26	1.45	1.54
2	I	3012	PO4	P-O1	3.25	1.58	1.50
2	L	3016	PO4	P-O1	3.22	1.58	1.50
2	D	3005	PO4	P-O1	3.20	1.58	1.50
2	E	3007	PO4	P-O1	3.18	1.58	1.50
2	F	3008	PO4	P-O1	3.17	1.58	1.50
2	G	3010	PO4	P-O4	3.14	1.63	1.54
2	G	3010	PO4	P-O1	2.68	1.56	1.50
2	A	3002	PO4	P-O1	2.61	1.56	1.50
2	E	3006	PO4	P-O1	2.35	1.56	1.50
2	E	3007	PO4	P-O2	-2.15	1.48	1.54
2	J	3013	PO4	P-O2	-2.13	1.48	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	3014	PO4	O4-P-O3	4.38	121.53	107.91
2	G	3010	PO4	O3-P-O2	3.83	119.81	107.91
2	E	3006	PO4	O4-P-O1	-3.72	97.81	110.95
2	G	3010	PO4	O4-P-O3	-3.61	96.69	107.91
2	G	3010	PO4	O4-P-O1	-3.58	98.30	110.95
2	E	3006	PO4	O3-P-O2	3.54	118.94	107.91
2	A	3002	PO4	O3-P-O2	3.26	118.06	107.91
2	J	3013	PO4	O3-P-O2	3.14	117.69	107.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	3010	PO4	O4-P-O2	-3.12	98.21	107.91
3	D	3302	TRS	C3-C-N	3.04	115.93	108.17
2	A	3002	PO4	O4-P-O1	-2.89	100.72	110.95
2	E	3006	PO4	O4-P-O2	-2.73	99.41	107.91
2	E	3007	PO4	O3-P-O2	2.68	116.26	107.91
2	A	3001	PO4	O3-P-O1	-2.64	101.63	110.95
2	B	3003	PO4	O3-P-O2	2.53	115.80	107.91
2	A	3002	PO4	O4-P-O3	-2.37	100.54	107.91
2	J	3013	PO4	O3-P-O1	-2.35	102.65	110.95
2	A	3002	PO4	O3-P-O1	2.34	119.22	110.95
2	J	3013	PO4	O4-P-O2	2.34	115.18	107.91
2	H	3011	PO4	O3-P-O1	-2.27	102.94	110.95
2	D	3005	PO4	O3-P-O1	-2.26	102.95	110.95
2	A	3001	PO4	O3-P-O2	2.24	114.88	107.91
2	G	3009	PO4	O3-P-O2	2.14	114.58	107.91
2	I	3012	PO4	O3-P-O2	2.14	114.56	107.91
2	K	3015	PO4	O4-P-O1	2.07	118.29	110.95
2	G	3010	PO4	O3-P-O1	2.07	118.26	110.95
2	B	3003	PO4	O3-P-O1	-2.04	103.72	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3002	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.