Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 10:37 PM EST

PDB ID	:	8TIM
Title	:	TRIOSE PHOSPHATE ISOMERASE
Authors	:	Artymiuk, P.J.; Taylor, W.R.; Phillips, D.C.
Deposited on	:	1998-08-25
Resolution	:	2.50 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:

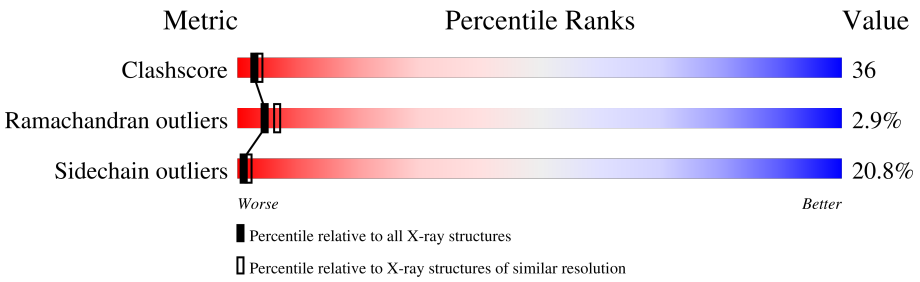
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	247	30% 36% 25% 9%
1	B	247	32% 40% 22% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3778 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.

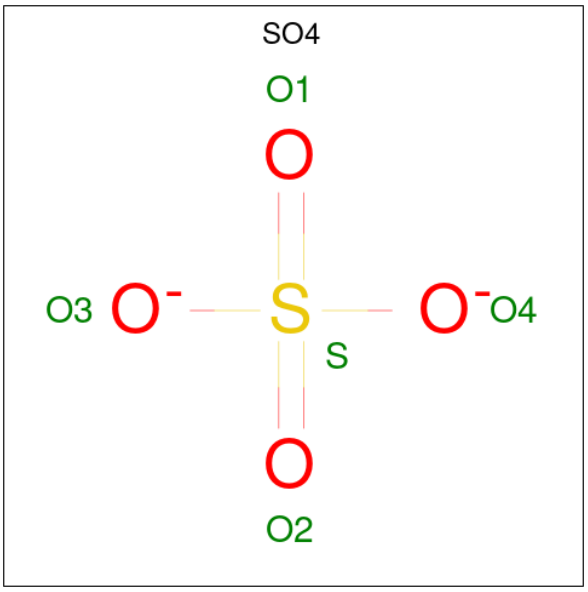
- Molecule 1 is a protein called TRIOSE PHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	247	1867	1184	327	350	6	0	0	0
1	B	247	1867	1184	327	350	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	THR	SER	conflict	UNP P00940
B	194	THR	SER	conflict	UNP P00940

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	B	1	5	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	18	18	18	0	0
			Total	O		
3	B	16	16	16	0	0

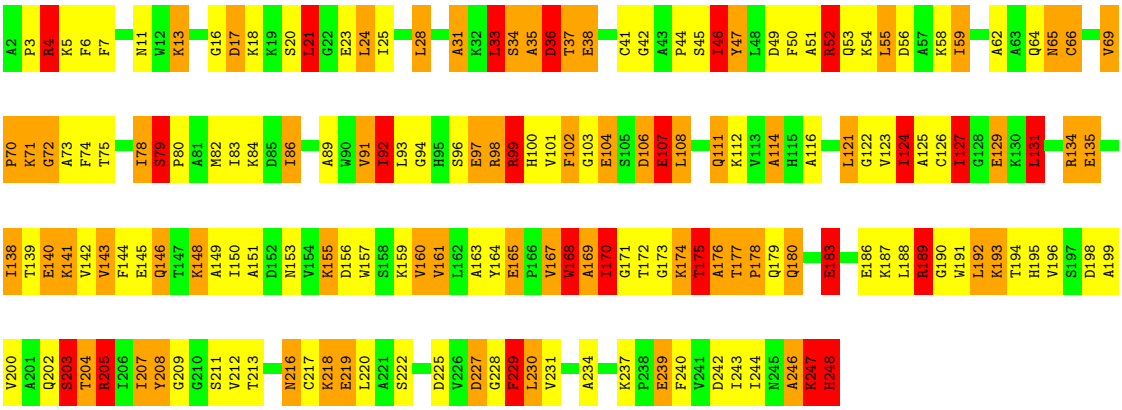
3 Residue-property plots (i)

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.

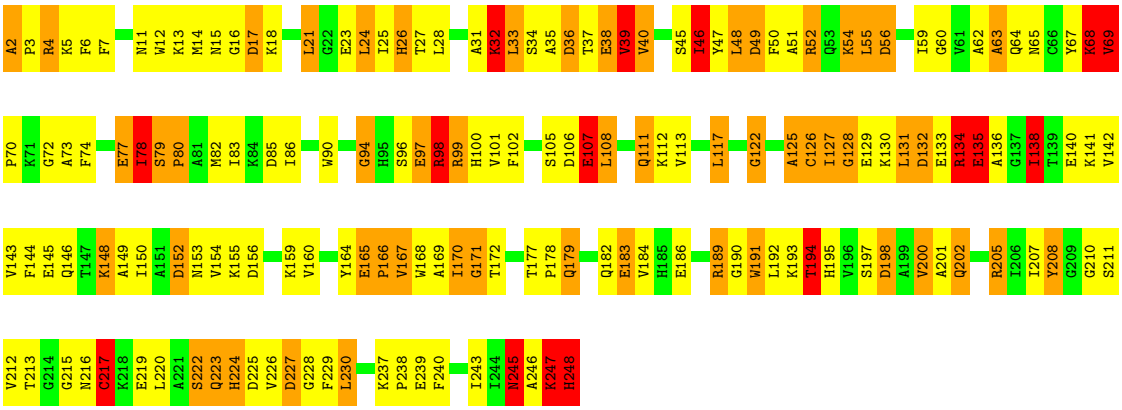
• Molecule 1: TRIOSE PHOSPHATE ISOMERASE

Chain A: 30% 36% 25% 9%



• Molecule 1: TRIOSE PHOSPHATE ISOMERASE

Chain B: 32% 40% 22% 6%



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	106.01Å 74.76Å 61.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	100.0 (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3778	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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: SO4

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	1.35	7/1903 (0.4%)	2.85	193/2571 (7.5%)
1	B	1.30	6/1903 (0.3%)	2.65	137/2571 (5.3%)
All	All	1.33	13/3806 (0.3%)	2.75	330/5142 (6.4%)

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	A	0	4
1	B	0	3
All	All	0	7

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	122	GLY	CA-C	6.44	1.62	1.51
1	A	79	SER	CB-OG	-6.30	1.34	1.42
1	B	190	GLY	N-CA	6.28	1.55	1.46
1	B	79	SER	CB-OG	6.09	1.50	1.42
1	A	170	ILE	C-O	5.99	1.34	1.23
1	B	105	SER	CB-OG	5.99	1.50	1.42
1	B	222	SER	CB-OG	5.71	1.49	1.42
1	A	100	HIS	CA-CB	5.64	1.66	1.53
1	A	174	LYS	CA-CB	5.55	1.66	1.53
1	A	96	SER	CB-OG	-5.50	1.35	1.42
1	A	72	GLY	N-CA	-5.25	1.38	1.46
1	A	66	CYS	CB-SG	5.16	1.91	1.82
1	B	38	GLU	CD-OE2	5.03	1.31	1.25

All (330) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	98	ARG	NE-CZ-NH2	-32.80	103.90	120.30
1	A	98	ARG	NE-CZ-NH1	26.15	133.37	120.30
1	A	107	GLU	CA-CB-CG	22.43	162.75	113.40
1	A	205	ARG	CD-NE-CZ	19.58	151.01	123.60
1	A	35	ALA	N-CA-CB	18.24	135.63	110.10
1	B	52	ARG	NE-CZ-NH2	17.93	129.26	120.30
1	A	98	ARG	NE-CZ-NH2	-13.20	113.70	120.30
1	A	227	ASP	CB-CG-OD2	13.05	130.04	118.30
1	B	98	ARG	NH1-CZ-NH2	12.81	133.49	119.40
1	B	239	GLU	CG-CD-OE2	12.59	143.48	118.30
1	B	189	ARG	NE-CZ-NH1	-12.44	114.08	120.30
1	A	129	GLU	CG-CD-OE2	12.29	142.88	118.30
1	A	227	ASP	CB-CG-OD1	-12.06	107.45	118.30
1	B	152	ASP	CB-CG-OD1	11.96	129.06	118.30
1	B	98	ARG	CD-NE-CZ	11.67	139.94	123.60
1	A	36	ASP	CB-CG-OD1	-11.38	108.06	118.30
1	A	205	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	A	56	ASP	CB-CG-OD1	10.85	128.06	118.30
1	B	4	ARG	NE-CZ-NH1	-10.83	114.88	120.30
1	A	121	LEU	CB-CA-C	10.81	130.74	110.20
1	A	129	GLU	OE1-CD-OE2	-10.29	110.96	123.30
1	A	52	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	B	169	ALA	N-CA-CB	10.10	124.24	110.10
1	B	205	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	A	71	LYS	CA-CB-CG	9.94	135.26	113.40
1	B	134	ARG	NE-CZ-NH1	-9.88	115.36	120.30
1	A	219	GLU	OE1-CD-OE2	9.73	134.97	123.30
1	A	99	ARG	NE-CZ-NH2	9.72	125.16	120.30
1	A	199	ALA	CB-CA-C	9.72	124.67	110.10
1	B	245	ASN	CA-CB-CG	9.71	134.77	113.40
1	B	145	GLU	OE1-CD-OE2	9.67	134.90	123.30
1	B	21	LEU	CB-CA-C	9.52	128.28	110.20
1	B	225	ASP	O-C-N	9.37	137.69	122.70
1	A	160	VAL	CA-CB-CG2	9.27	124.81	110.90
1	B	217	CYS	CA-CB-SG	9.20	130.56	114.00
1	B	239	GLU	OE1-CD-OE2	-9.20	112.26	123.30
1	B	69	VAL	CB-CA-C	9.18	128.84	111.40
1	A	35	ALA	N-CA-C	-9.12	86.38	111.00
1	A	174	LYS	N-CA-C	9.12	135.61	111.00
1	A	38	GLU	CG-CD-OE1	9.02	136.35	118.30
1	A	58	LYS	CA-CB-CG	8.90	132.99	113.40
1	A	100	HIS	CA-CB-CG	-8.88	98.50	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	A	79	SER	CB-CA-C	-8.75	93.47	110.10
1	A	131	LEU	CA-CB-CG	8.56	135.00	115.30
1	B	2	ALA	CB-CA-C	8.53	122.89	110.10
1	A	36	ASP	O-C-N	8.46	136.24	122.70
1	A	138	ILE	CA-CB-CG2	8.46	127.82	110.90
1	B	122	GLY	N-CA-C	-8.46	91.96	113.10
1	A	72	GLY	N-CA-C	8.45	134.23	113.10
1	B	63	ALA	CB-CA-C	8.44	122.76	110.10
1	B	6	PHE	O-C-N	8.43	136.19	122.70
1	A	216	ASN	CA-C-O	8.35	137.63	120.10
1	A	36	ASP	N-CA-C	-8.31	88.56	111.00
1	B	208	TYR	CB-CG-CD1	-8.24	116.05	121.00
1	B	4	ARG	NE-CZ-NH2	8.21	124.40	120.30
1	A	96	SER	CA-CB-OG	8.18	133.29	111.20
1	A	176	ALA	CB-CA-C	8.17	122.36	110.10
1	A	106	ASP	CB-CG-OD2	-8.17	110.95	118.30
1	B	165	GLU	OE1-CD-OE2	8.16	133.09	123.30
1	A	38	GLU	OE1-CD-OE2	-8.12	113.56	123.30
1	B	33	LEU	CA-C-O	-8.09	103.11	120.10
1	B	46	ILE	CA-CB-CG2	7.95	126.80	110.90
1	B	184	VAL	O-C-N	7.94	135.41	122.70
1	A	17	ASP	N-CA-CB	7.93	124.87	110.60
1	A	55	LEU	O-C-N	7.92	135.38	122.70
1	A	183	GLU	CA-CB-CG	7.88	130.74	113.40
1	B	69	VAL	CA-CB-CG1	7.88	122.71	110.90
1	B	100	HIS	CA-CB-CG	-7.83	100.28	113.60
1	A	121	LEU	N-CA-CB	-7.74	94.92	110.40
1	A	174	LYS	N-CA-CB	-7.73	96.69	110.60
1	A	216	ASN	N-CA-C	7.69	131.76	111.00
1	A	114	ALA	CB-CA-C	7.65	121.57	110.10
1	B	106	ASP	CB-CG-OD2	7.64	125.18	118.30
1	B	99	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	170	ILE	CA-C-N	7.62	131.43	116.20
1	A	4	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	35	ALA	CB-CA-C	-7.59	98.71	110.10
1	B	132	ASP	CB-CA-C	7.57	125.53	110.40
1	A	138	ILE	CA-CB-CG1	-7.55	96.64	111.00
1	A	4	ARG	CD-NE-CZ	-7.53	113.06	123.60
1	B	167	VAL	CB-CA-C	7.49	125.63	111.40
1	A	192	LEU	N-CA-CB	-7.48	95.44	110.40
1	A	157	TRP	CA-CB-CG	-7.42	99.60	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	175	THR	CA-CB-CG2	7.41	122.77	112.40
1	A	216	ASN	CB-CA-C	-7.36	95.68	110.40
1	B	62	ALA	N-CA-CB	-7.36	99.80	110.10
1	A	107	GLU	CB-CG-CD	7.35	134.05	114.20
1	B	222	SER	N-CA-CB	-7.35	99.47	110.50
1	A	3	PRO	C-N-CA	7.30	139.95	121.70
1	B	33	LEU	O-C-N	7.27	134.33	122.70
1	A	165	GLU	CA-CB-CG	7.26	129.37	113.40
1	A	216	ASN	N-CA-CB	-7.22	97.59	110.60
1	A	34	SER	CA-C-O	-7.17	105.05	120.10
1	B	208	TYR	CB-CG-CD2	7.17	125.30	121.00
1	B	194	THR	CB-CA-C	-7.14	92.32	111.60
1	A	168	TRP	O-C-N	7.14	134.12	122.70
1	A	114	ALA	N-CA-CB	-7.12	100.14	110.10
1	B	205	ARG	NH1-CZ-NH2	-7.10	111.59	119.40
1	B	68	LYS	CB-CA-C	-7.09	96.21	110.40
1	B	169	ALA	CB-CA-C	-7.08	99.47	110.10
1	A	36	ASP	CB-CA-C	7.07	124.53	110.40
1	A	56	ASP	O-C-N	7.05	133.99	122.70
1	A	234	ALA	N-CA-CB	-7.04	100.25	110.10
1	B	239	GLU	CG-CD-OE1	-7.02	104.26	118.30
1	B	85	ASP	CB-CG-OD2	7.02	124.62	118.30
1	B	85	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	102	PHE	N-CA-CB	-6.98	98.04	110.60
1	B	107	GLU	CA-CB-CG	6.96	128.72	113.40
1	A	239	GLU	CG-CD-OE1	-6.96	104.38	118.30
1	A	174	LYS	CA-CB-CG	-6.95	98.11	113.40
1	B	45	SER	CA-C-O	-6.94	105.53	120.10
1	A	140	GLU	CG-CD-OE1	-6.90	104.50	118.30
1	A	168	TRP	CA-CB-CG	6.87	126.76	113.70
1	A	71	LYS	CB-CA-C	-6.83	96.74	110.40
1	B	33	LEU	CB-CG-CD1	-6.78	99.48	111.00
1	A	100	HIS	O-C-N	6.75	133.50	122.70
1	A	239	GLU	CA-CB-CG	6.73	128.20	113.40
1	A	239	GLU	CG-CD-OE2	6.72	131.74	118.30
1	B	248	HIS	CA-CB-CG	6.71	125.00	113.60
1	B	21	LEU	N-CA-CB	-6.71	96.98	110.40
1	B	97	GLU	OE1-CD-OE2	6.71	131.35	123.30
1	A	143	VAL	O-C-N	6.70	133.42	122.70
1	A	160	VAL	CB-CA-C	-6.65	98.77	111.40
1	B	48	LEU	CB-CA-C	6.64	122.82	110.20
1	B	49	ASP	CB-CG-OD2	6.63	124.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	LYS	O-C-N	6.63	134.47	123.20
1	B	85	ASP	OD1-CG-OD2	-6.61	110.74	123.30
1	B	219	GLU	CA-C-O	6.60	133.96	120.10
1	A	41	CYS	CA-CB-SG	-6.60	102.12	114.00
1	A	143	VAL	CB-CA-C	6.59	123.91	111.40
1	B	107	GLU	OE1-CD-OE2	-6.57	115.42	123.30
1	A	173	GLY	C-N-CA	6.54	138.06	121.70
1	A	205	ARG	N-CA-CB	6.53	122.35	110.60
1	B	239	GLU	CA-CB-CG	6.52	127.73	113.40
1	A	13	LYS	CA-CB-CG	-6.51	99.08	113.40
1	A	155	LYS	N-CA-CB	6.50	122.31	110.60
1	B	197	SER	O-C-N	6.47	133.06	122.70
1	A	177	THR	CA-CB-CG2	6.46	121.45	112.40
1	B	160	VAL	CA-CB-CG1	6.44	120.56	110.90
1	B	152	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	B	138	ILE	CA-CB-CG2	6.43	123.77	110.90
1	B	126	CYS	CA-CB-SG	-6.42	102.44	114.00
1	B	132	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	149	ALA	CB-CA-C	6.37	119.66	110.10
1	A	134	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	200	VAL	O-C-N	6.36	132.88	122.70
1	A	92	ILE	N-CA-CB	6.36	125.42	110.80
1	A	177	THR	N-CA-CB	6.35	122.37	110.30
1	A	34	SER	O-C-N	6.35	132.86	122.70
1	A	52	ARG	NH1-CZ-NH2	6.33	126.37	119.40
1	A	174	LYS	CA-C-O	6.33	133.39	120.10
1	A	69	VAL	CA-CB-CG1	6.32	120.38	110.90
1	A	247	LYS	O-C-N	6.32	132.80	122.70
1	B	125	ALA	C-N-CA	6.29	137.44	121.70
1	A	112	LYS	O-C-N	6.28	132.75	122.70
1	A	217	CYS	CA-CB-SG	6.27	125.29	114.00
1	A	230	LEU	CB-CA-C	6.26	122.09	110.20
1	A	21	LEU	CA-CB-CG	6.23	129.64	115.30
1	A	116	ALA	CB-CA-C	6.23	119.45	110.10
1	A	4	ARG	CA-C-N	-6.22	103.52	117.20
1	A	234	ALA	CB-CA-C	6.20	119.40	110.10
1	A	121	LEU	CA-CB-CG	6.20	129.56	115.30
1	B	182	GLN	CB-CG-CD	6.18	127.68	111.60
1	B	32	LYS	O-C-N	6.18	132.59	122.70
1	B	224	HIS	N-CA-CB	-6.18	99.47	110.60
1	A	151	ALA	O-C-N	6.18	132.59	122.70
1	B	78	ILE	CA-CB-CG1	-6.17	99.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	156	ASP	CB-CG-OD1	-6.14	112.77	118.30
1	B	165	GLU	O-C-N	6.14	132.76	121.10
1	A	99	ARG	N-CA-CB	6.12	121.62	110.60
1	A	123	VAL	CA-CB-CG2	6.12	120.08	110.90
1	A	46	ILE	CA-CB-CG2	6.10	123.11	110.90
1	B	186	GLU	CB-CG-CD	-6.10	97.74	114.20
1	B	138	ILE	CA-CB-CG1	-6.08	99.44	111.00
1	A	193	LYS	CB-CG-CD	6.07	127.39	111.60
1	A	143	VAL	CA-C-O	-6.07	107.35	120.10
1	A	129	GLU	CG-CD-OE1	-6.07	106.16	118.30
1	B	56	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	72	GLY	CA-C-N	-6.05	103.88	117.20
1	B	69	VAL	N-CA-CB	-6.04	98.20	111.50
1	A	31	ALA	N-CA-CB	-6.04	101.64	110.10
1	A	100	HIS	CA-C-O	-6.04	107.43	120.10
1	B	94	GLY	C-N-CA	6.03	136.77	121.70
1	B	170	ILE	CB-CG1-CD1	6.02	130.77	113.90
1	B	97	GLU	CG-CD-OE2	-6.02	106.26	118.30
1	B	207	ILE	O-C-N	6.02	132.33	122.70
1	B	105	SER	O-C-N	6.00	132.31	122.70
1	B	52	ARG	NH1-CZ-NH2	-5.94	112.86	119.40
1	A	173	GLY	CA-C-O	5.94	131.29	120.60
1	B	31	ALA	CB-CA-C	5.94	119.01	110.10
1	B	186	GLU	CA-CB-CG	5.94	126.47	113.40
1	A	189	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	38	GLU	CB-CG-CD	5.92	130.18	114.20
1	B	224	HIS	CA-CB-CG	5.91	123.65	113.60
1	A	4	ARG	NH1-CZ-NH2	5.90	125.89	119.40
1	B	45	SER	O-C-N	5.90	132.14	122.70
1	B	26	HIS	CA-CB-CG	-5.89	103.58	113.60
1	A	167	VAL	CA-C-N	-5.89	104.24	117.20
1	A	98	ARG	NH1-CZ-NH2	-5.88	112.93	119.40
1	A	229	PHE	O-C-N	5.87	132.09	122.70
1	B	102	PHE	N-CA-CB	-5.86	100.05	110.60
1	A	207	ILE	CA-C-N	-5.86	104.32	117.20
1	A	100	HIS	CB-CA-C	-5.85	98.69	110.40
1	A	94	GLY	O-C-N	5.85	132.06	122.70
1	B	217	CYS	N-CA-CB	-5.85	100.07	110.60
1	A	59	ILE	CA-CB-CG1	5.84	122.10	111.00
1	B	135	GLU	OE1-CD-OE2	5.84	130.31	123.30
1	B	80	PRO	CA-C-O	5.82	134.18	120.20
1	A	52	ARG	O-C-N	5.81	132.00	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	170	ILE	C-N-CA	5.81	134.50	122.30
1	A	178	PRO	CA-C-O	5.80	134.13	120.20
1	A	204	THR	CA-C-O	5.80	132.27	120.10
1	A	97	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	B	46	ILE	CA-CB-CG1	-5.79	100.00	111.00
1	B	201	ALA	CA-C-O	5.78	132.24	120.10
1	A	23	GLU	N-CA-CB	5.77	120.98	110.60
1	A	208	TYR	O-C-N	5.77	133.00	123.20
1	B	152	ASP	CA-C-O	-5.75	108.02	120.10
1	B	227	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	96	SER	CA-C-O	-5.73	108.06	120.10
1	A	135	GLU	OE1-CD-OE2	5.73	130.17	123.30
1	B	183	GLU	N-CA-CB	-5.72	100.31	110.60
1	B	145	GLU	CG-CD-OE1	-5.71	106.87	118.30
1	B	52	ARG	O-C-N	5.71	131.83	122.70
1	A	230	LEU	N-CA-C	-5.71	95.59	111.00
1	B	17	ASP	CB-CG-OD1	5.70	123.42	118.30
1	A	150	ILE	O-C-N	5.67	131.77	122.70
1	B	201	ALA	CA-C-N	-5.67	104.73	117.20
1	B	205	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	A	186	GLU	CA-CB-CG	5.63	125.78	113.40
1	A	176	ALA	N-CA-C	-5.62	95.81	111.00
1	A	107	GLU	CG-CD-OE1	5.61	129.53	118.30
1	B	219	GLU	CA-C-N	-5.60	104.88	117.20
1	A	47	TYR	CB-CG-CD2	5.59	124.36	121.00
1	A	157	TRP	O-C-N	5.59	131.64	122.70
1	A	193	LYS	CA-C-N	-5.57	104.95	117.20
1	B	52	ARG	N-CA-CB	5.56	120.61	110.60
1	A	127	ILE	CA-CB-CG1	5.55	121.54	111.00
1	A	168	TRP	CA-C-N	-5.54	105.01	117.20
1	B	48	LEU	N-CA-CB	-5.54	99.32	110.40
1	A	104	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	B	183	GLU	OE1-CD-OE2	5.51	129.91	123.30
1	A	102	PHE	CB-CA-C	5.50	121.41	110.40
1	A	96	SER	O-C-N	5.49	131.48	122.70
1	A	41	CYS	CA-C-N	-5.49	105.23	116.20
1	A	58	LYS	CB-CG-CD	5.49	125.86	111.60
1	A	124	ILE	CA-CB-CG2	5.48	121.86	110.90
1	A	161	VAL	CG1-CB-CG2	-5.48	102.13	110.90
1	A	142	VAL	N-CA-CB	-5.48	99.45	111.50
1	A	230	LEU	CB-CG-CD1	-5.48	101.69	111.00
1	B	78	ILE	CA-CB-CG2	5.47	121.85	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	134	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	B	224	HIS	N-CA-C	5.47	125.78	111.00
1	A	79	SER	O-C-N	5.47	131.50	121.10
1	B	96	SER	O-C-N	5.47	131.45	122.70
1	A	209	GLY	N-CA-C	5.47	126.77	113.10
1	A	36	ASP	CA-C-N	-5.46	105.19	117.20
1	B	169	ALA	CA-C-O	-5.46	108.64	120.10
1	A	157	TRP	CA-C-O	-5.46	108.64	120.10
1	B	230	LEU	N-CA-C	-5.45	96.28	111.00
1	A	33	LEU	O-C-N	5.45	131.42	122.70
1	B	136	ALA	C-N-CA	5.45	133.74	122.30
1	A	36	ASP	OD1-CG-OD2	5.43	133.62	123.30
1	A	193	LYS	CA-C-O	5.43	131.50	120.10
1	A	138	ILE	N-CA-CB	-5.43	98.32	110.80
1	A	170	ILE	CB-CG1-CD1	-5.42	98.72	113.90
1	A	41	CYS	N-CA-CB	5.41	120.34	110.60
1	B	40	VAL	O-C-N	-5.40	114.06	122.70
1	A	175	THR	N-CA-C	5.40	125.58	111.00
1	A	4	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	A	231	VAL	CA-CB-CG2	5.39	118.98	110.90
1	B	215	GLY	CA-C-N	5.38	129.03	117.20
1	B	227	ASP	N-CA-CB	-5.37	100.93	110.60
1	B	155	LYS	CB-CA-C	-5.37	99.66	110.40
1	A	74	PHE	CB-CG-CD1	-5.35	117.05	120.80
1	B	184	VAL	CA-C-O	-5.35	108.86	120.10
1	B	113	VAL	O-C-N	5.35	131.25	122.70
1	A	248	HIS	CA-CB-CG	5.33	122.66	113.60
1	B	39	VAL	CA-C-N	-5.33	105.48	117.20
1	B	46	ILE	CB-CA-C	-5.33	100.95	111.60
1	A	98	ARG	CD-NE-CZ	5.32	131.05	123.60
1	B	49	ASP	CA-CB-CG	5.32	125.10	113.40
1	A	21	LEU	CB-CA-C	5.32	120.30	110.20
1	B	68	LYS	C-N-CA	-5.32	108.41	121.70
1	B	6	PHE	N-CA-CB	5.30	120.15	110.60
1	A	203	SER	O-C-N	5.30	131.18	122.70
1	B	183	GLU	CA-C-O	5.29	131.20	120.10
1	B	40	VAL	C-N-CA	5.28	134.90	121.70
1	A	126	CYS	CA-CB-SG	5.25	123.46	114.00
1	A	193	LYS	CA-CB-CG	5.25	124.95	113.40
1	B	128	GLY	CA-C-O	-5.24	111.16	120.60
1	A	91	VAL	N-CA-CB	5.24	123.02	111.50
1	A	126	CYS	CA-C-O	5.23	131.08	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	112	LYS	C-N-CA	-5.22	108.64	121.70
1	A	164	TYR	O-C-N	5.22	131.06	122.70
1	B	105	SER	CA-C-N	-5.21	105.73	117.20
1	B	156	ASP	N-CA-CB	5.21	119.97	110.60
1	B	170	ILE	CA-C-N	5.21	126.62	116.20
1	A	155	LYS	C-N-CA	5.21	134.72	121.70
1	A	230	LEU	CA-CB-CG	-5.20	103.33	115.30
1	B	74	PHE	O-C-N	5.20	131.02	122.70
1	A	150	ILE	CG1-CB-CG2	5.20	122.84	111.40
1	A	102	PHE	C-N-CA	5.20	133.22	122.30
1	A	74	PHE	CA-CB-CG	-5.19	101.44	113.90
1	A	156	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	170	ILE	CA-C-O	-5.19	109.21	120.10
1	A	183	GLU	CG-CD-OE1	-5.17	107.95	118.30
1	A	70	PRO	O-C-N	-5.17	114.42	122.70
1	A	169	ALA	CA-C-O	-5.13	109.32	120.10
1	B	154	VAL	O-C-N	5.13	130.91	122.70
1	A	216	ASN	O-C-N	-5.11	114.52	122.70
1	B	191	TRP	O-C-N	5.11	130.87	122.70
1	A	103	GLY	O-C-N	5.10	130.85	122.70
1	A	24	LEU	CB-CA-C	-5.08	100.54	110.20
1	A	146	GLN	CA-CB-CG	-5.08	102.22	113.40
1	A	165	GLU	CB-CA-C	-5.08	100.23	110.40
1	B	127	ILE	CB-CG1-CD1	5.08	128.13	113.90
1	B	207	ILE	CA-C-O	-5.07	109.46	120.10
1	A	142	VAL	CA-C-O	5.06	130.73	120.10
1	A	100	HIS	N-CA-C	5.06	124.66	111.00
1	A	160	VAL	O-C-N	5.05	130.79	122.70
1	A	229	PHE	CA-C-N	-5.05	106.08	117.20
1	A	135	GLU	O-C-N	5.05	130.78	122.70
1	A	208	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	A	37	THR	CA-C-N	-5.03	106.14	117.20
1	A	97	GLU	CG-CD-OE2	-5.03	108.25	118.30
1	A	209	GLY	C-N-CA	5.02	132.85	122.30
1	A	127	ILE	CA-CB-CG2	-5.01	100.88	110.90
1	B	69	VAL	CA-CB-CG2	-5.01	103.39	110.90

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	205	ARG	Sidechain
1	A	52	ARG	Sidechain
1	A	99	ARG	Sidechain
1	B	134	ARG	Sidechain
1	B	52	ARG	Sidechain
1	B	99	ARG	Sidechain

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	1867	0	1874	143	0
1	B	1867	0	1874	134	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	18	0	0	0	0
3	B	16	0	0	4	0
All	All	3778	0	3748	266	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 36.

All (266) 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:A:82:MET:HB3	1:B:46:ILE:HD13	1.33	1.08
1:A:129:GLU:OE2	1:A:168:TRP:CD1	2.17	0.97
1:A:84:LYS:HG3	1:A:121:LEU:HD13	1.47	0.97
1:B:178:PRO:HD2	1:B:179:GLN:NE2	1.80	0.97
1:A:49:ASP:O	1:A:53:GLN:HG3	1.68	0.94
1:A:141:LYS:O	1:A:145:GLU:HG3	1.68	0.94
1:A:175:THR:HG22	1:A:177:THR:HG23	1.47	0.92
1:A:124:ILE:CD1	1:A:163:ALA:HB2	2.00	0.92
1:B:69:VAL:HG22	1:B:70:PRO:CD	2.02	0.90
1:A:35:ALA:O	1:A:36:ASP:HB2	1.69	0.89
1:B:25:ILE:HG21	1:B:54:LYS:HB3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ILE:HD12	1:A:171:GLY:N	1.85	0.89
1:B:178:PRO:HD2	1:B:179:GLN:HE22	1.32	0.88
1:A:212:VAL:HA	1:A:216:ASN:HD22	1.39	0.87
1:B:23:GLU:O	1:B:26:HIS:HB3	1.75	0.87
1:A:177:THR:OG1	1:A:180:GLN:HG2	1.74	0.86
1:A:46:ILE:HD12	1:A:47:TYR:H	1.39	0.85
1:B:67:TYR:HB2	1:B:77:GLU:HG3	1.58	0.85
1:B:2:ALA:HB3	1:B:3:PRO:HD3	1.60	0.83
1:B:129:GLU:OE2	1:B:134:ARG:NH1	2.11	0.83
1:A:17:ASP:O	1:A:21:LEU:HB2	1.78	0.81
1:B:177:THR:HB	1:B:179:GLN:NE2	1.96	0.81
1:B:213:THR:O	1:B:217:CYS:HB3	1.79	0.81
1:A:82:MET:SD	1:B:46:ILE:HD11	2.21	0.80
1:B:5:LYS:HE2	1:B:38:GLU:HB2	1.63	0.80
1:A:175:THR:HB	1:A:180:GLN:OE1	1.81	0.79
1:A:178:PRO:HG3	1:A:219:GLU:HG3	1.64	0.79
1:A:247:LYS:O	1:A:248:HIS:CD2	2.36	0.79
1:A:42:GLY:HA2	1:A:62:ALA:O	1.82	0.78
1:A:82:MET:HB3	1:B:46:ILE:CD1	2.13	0.78
1:A:64:GLN:HA	1:A:92:ILE:HG13	1.66	0.77
1:B:17:ASP:O	1:B:21:LEU:HB2	1.83	0.77
1:A:219:GLU:O	1:A:222:SER:OG	2.03	0.76
1:B:69:VAL:HG22	1:B:70:PRO:HD2	1.66	0.76
1:B:107:GLU:HG3	1:B:111:GLN:HE22	1.51	0.76
1:A:246:ALA:O	1:A:248:HIS:N	2.19	0.75
1:B:69:VAL:HG22	1:B:70:PRO:HD3	1.68	0.75
1:B:25:ILE:HG23	1:B:55:LEU:HD13	1.68	0.74
1:A:247:LYS:O	1:A:248:HIS:HD2	1.71	0.74
1:B:189:ARG:NH2	1:B:227:ASP:OD2	2.20	0.74
1:A:46:ILE:HD12	1:A:47:TYR:N	2.03	0.73
1:A:176:ALA:HB1	1:A:208:TYR:OH	1.88	0.73
1:A:75:THR:O	1:B:98:ARG:HD2	1.90	0.72
1:A:35:ALA:O	1:A:36:ASP:CB	2.38	0.72
1:A:104:GLU:HG2	1:A:108:LEU:CD1	2.20	0.72
1:B:192:LEU:HD22	1:B:200:VAL:CG1	2.19	0.72
1:B:7:PHE:O	1:B:228:GLY:HA3	1.90	0.71
1:A:141:LYS:HD2	1:A:145:GLU:OE2	1.91	0.71
1:B:177:THR:HB	1:B:179:GLN:HE22	1.54	0.70
1:B:192:LEU:HD22	1:B:200:VAL:HG12	1.72	0.70
1:A:175:THR:HG22	1:A:177:THR:CG2	2.21	0.70
1:A:218:LYS:HD2	1:A:219:GLU:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:HD12	1:A:46:ILE:N	2.06	0.69
1:A:52:ARG:NH1	1:A:59:ILE:O	2.24	0.69
1:B:194:THR:HB	1:B:195:HIS:CE1	2.28	0.69
1:A:190:GLY:O	1:A:194:THR:HG23	1.92	0.69
1:B:2:ALA:HB3	1:B:3:PRO:CD	2.24	0.68
1:B:5:LYS:HE3	1:B:36:ASP:O	1.94	0.68
2:B:560:SO4:O2	3:B:621:HOH:O	2.12	0.68
1:B:223:GLN:HB3	1:B:226:VAL:CG2	2.23	0.68
1:B:125:ALA:HB1	1:B:150:ILE:HD13	1.76	0.68
1:B:220:LEU:O	1:B:223:GLN:HB2	1.92	0.68
1:B:69:VAL:CG2	1:B:70:PRO:HD3	2.24	0.67
1:A:49:ASP:HB2	1:A:86:ILE:HG12	1.76	0.67
1:A:168:TRP:CE3	1:A:169:ALA:HB2	2.30	0.67
1:B:213:THR:O	1:B:217:CYS:CB	2.43	0.67
1:A:70:PRO:HA	1:A:79:SER:OG	1.94	0.67
1:A:175:THR:CG2	1:A:177:THR:HG23	2.25	0.66
1:B:194:THR:HB	1:B:195:HIS:ND1	2.09	0.66
1:A:44:PRO:HA	3:B:623:HOH:O	1.96	0.66
1:A:129:GLU:OE2	1:A:168:TRP:HD1	1.79	0.66
1:A:34:SER:O	1:A:37:THR:HG22	1.95	0.65
1:A:64:GLN:O	1:A:65:ASN:HB2	1.96	0.65
1:A:122:GLY:HA2	1:A:159:LYS:HB3	1.78	0.65
1:A:124:ILE:HD13	1:A:163:ALA:HB2	1.79	0.65
1:A:131:LEU:HA	1:A:168:TRP:HB2	1.79	0.65
1:B:237:LYS:HB3	1:B:238:PRO:HD2	1.78	0.65
1:B:55:LEU:HG	1:B:59:ILE:HG21	1.79	0.64
1:B:223:GLN:HB3	1:B:226:VAL:HG23	1.79	0.64
1:A:124:ILE:HD11	1:A:163:ALA:HB2	1.77	0.64
1:A:84:LYS:CG	1:A:121:LEU:HD13	2.28	0.62
1:B:178:PRO:CD	1:B:179:GLN:NE2	2.61	0.62
1:A:82:MET:CB	1:B:46:ILE:HD13	2.21	0.62
1:B:216:ASN:O	1:B:220:LEU:HD12	2.00	0.61
1:B:211:SER:O	1:B:216:ASN:ND2	2.32	0.61
1:B:55:LEU:HD12	1:B:59:ILE:HD13	1.82	0.61
1:B:168:TRP:O	1:B:172:THR:HG21	1.99	0.61
1:A:175:THR:CB	1:A:180:GLN:OE1	2.49	0.61
1:B:212:VAL:HG12	1:B:243:ILE:HD13	1.82	0.61
1:B:142:VAL:O	1:B:146:GLN:HG3	2.00	0.61
1:B:212:VAL:HA	1:B:216:ASN:HD21	1.66	0.61
1:A:13:LYS:O	1:A:44:PRO:HG3	2.01	0.60
1:B:179:GLN:CD	1:B:179:GLN:H	2.03	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ALA:CB	1:B:3:PRO:HD3	2.30	0.60
1:A:170:ILE:HD12	1:A:170:ILE:C	2.21	0.60
1:A:127:ILE:CG2	1:A:146:GLN:HB3	2.31	0.60
1:A:208:TYR:O	1:A:229:PHE:HA	2.03	0.59
1:B:131:LEU:O	1:B:132:ASP:C	2.41	0.59
1:B:131:LEU:O	1:B:135:GLU:HB2	2.03	0.58
1:B:108:LEU:O	1:B:112:LYS:HG3	2.04	0.58
1:B:178:PRO:CD	1:B:179:GLN:HE22	2.10	0.58
1:B:83:ILE:O	1:B:86:ILE:HG13	2.03	0.57
1:A:73:ALA:HA	1:B:13:LYS:HD2	1.85	0.57
1:B:193:LYS:HB2	1:B:198:ASP:HA	1.85	0.57
1:A:91:VAL:HG22	1:A:93:LEU:HG	1.87	0.57
1:A:167:VAL:C	1:A:169:ALA:N	2.58	0.57
1:A:124:ILE:CD1	1:A:163:ALA:CB	2.78	0.56
1:B:48:LEU:HD21	1:B:63:ALA:HB2	1.87	0.56
1:A:78:ILE:HG21	1:B:46:ILE:HG12	1.87	0.56
1:A:124:ILE:HD11	1:A:163:ALA:CB	2.35	0.56
1:B:144:PHE:O	1:B:148:LYS:HB2	2.06	0.56
1:B:177:THR:CB	1:B:179:GLN:NE2	2.66	0.56
1:B:208:TYR:CZ	1:B:210:GLY:HA3	2.41	0.56
1:A:191:TRP:O	1:A:195:HIS:N	2.38	0.55
1:B:18:LYS:HE2	1:B:50:PHE:CD1	2.41	0.55
1:A:82:MET:SD	1:B:46:ILE:CD1	2.94	0.55
1:A:239:GLU:O	1:A:242:ASP:HB2	2.05	0.55
1:B:159:LYS:HE2	3:B:633:HOH:O	2.07	0.55
1:A:213:THR:OG1	1:A:216:ASN:HB2	2.06	0.55
1:B:216:ASN:C	1:B:220:LEU:HD12	2.27	0.55
1:A:49:ASP:HB2	1:A:86:ILE:CG1	2.37	0.54
1:A:219:GLU:HG2	1:A:220:LEU:N	2.22	0.54
1:B:191:TRP:CD1	1:B:195:HIS:CE1	2.95	0.54
1:A:46:ILE:CD1	1:A:47:TYR:N	2.70	0.54
1:A:98:ARG:HA	1:A:102:PHE:HB2	1.89	0.54
1:A:240:PHE:CE2	1:A:244:ILE:HD11	2.42	0.54
1:B:142:VAL:HG12	1:B:143:VAL:N	2.22	0.54
1:A:131:LEU:O	1:A:135:GLU:HB2	2.08	0.54
1:A:139:THR:O	1:A:143:VAL:HB	2.08	0.53
1:B:16:GLY:HA3	1:B:21:LEU:HD13	1.90	0.53
1:B:4:ARG:HD3	1:B:202:GLN:O	2.08	0.53
1:B:69:VAL:CG2	1:B:70:PRO:CD	2.80	0.53
1:A:89:ALA:HA	1:A:121:LEU:HD12	1.91	0.53
1:A:129:GLU:OE2	1:A:168:TRP:NE1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:MET:O	1:B:14:MET:HG2	2.09	0.53
1:B:149:ALA:O	1:B:153:ASN:ND2	2.41	0.53
1:A:31:ALA:HB3	1:A:33:LEU:HD21	1.91	0.53
1:A:187:LYS:O	1:A:191:TRP:N	2.42	0.52
1:B:171:GLY:N	3:B:624:HOH:O	2.42	0.52
1:A:140:GLU:HG2	1:A:144:PHE:CE2	2.44	0.52
1:A:240:PHE:HA	1:A:243:ILE:HD12	1.90	0.52
1:A:4:ARG:HD3	1:A:202:GLN:O	2.10	0.52
1:B:128:GLY:HA3	1:B:165:GLU:O	2.09	0.52
1:B:50:PHE:HE1	1:B:54:LYS:HZ2	1.58	0.51
1:B:33:LEU:HA	1:B:245:ASN:HD22	1.75	0.51
1:A:129:GLU:CD	1:A:139:THR:HG23	2.31	0.51
1:B:2:ALA:CB	1:B:3:PRO:CD	2.86	0.51
1:A:108:LEU:HD22	1:A:108:LEU:O	2.12	0.50
1:A:175:THR:O	1:A:176:ALA:C	2.47	0.50
1:A:170:ILE:CD1	1:A:171:GLY:N	2.69	0.50
1:B:129:GLU:OE1	1:B:129:GLU:N	2.44	0.50
1:B:165:GLU:O	1:B:167:VAL:HG23	2.11	0.50
1:B:12:TRP:O	1:B:15:ASN:HB2	2.12	0.50
1:A:70:PRO:HA	1:A:79:SER:HG	1.76	0.49
1:A:18:LYS:NZ	1:B:49:ASP:OD1	2.45	0.49
1:A:127:ILE:HG22	1:A:146:GLN:HB3	1.93	0.49
1:A:50:PHE:O	1:A:54:LYS:HG2	2.13	0.49
1:B:5:LYS:HE3	1:B:36:ASP:C	2.33	0.49
1:A:79:SER:HB3	1:A:82:MET:HG3	1.94	0.49
1:A:124:ILE:O	1:A:124:ILE:HG13	2.12	0.49
1:B:46:ILE:HD12	1:B:47:TYR:CE2	2.47	0.49
1:A:246:ALA:O	1:A:247:LYS:C	2.51	0.48
1:A:189:ARG:NE	1:A:225:ASP:OD1	2.45	0.48
1:B:79:SER:HB2	1:B:80:PRO:HD2	1.96	0.48
1:A:97:GLU:O	1:A:101:VAL:HB	2.13	0.48
1:A:104:GLU:HG2	1:A:108:LEU:HD12	1.95	0.48
1:A:212:VAL:HG21	1:A:229:PHE:CD2	2.49	0.48
1:B:80:PRO:HA	1:B:83:ILE:HD12	1.96	0.48
1:B:237:LYS:HB3	1:B:238:PRO:CD	2.43	0.48
1:B:246:ALA:O	1:B:248:HIS:N	2.46	0.48
1:A:168:TRP:CZ3	1:A:169:ALA:HB2	2.49	0.48
1:B:192:LEU:HD22	1:B:200:VAL:HG11	1.94	0.48
1:B:37:THR:HG22	1:B:38:GLU:N	2.29	0.48
1:A:218:LYS:HD2	1:A:218:LYS:C	2.33	0.48
1:B:69:VAL:O	1:B:79:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:HB2	1:A:191:TRP:CZ2	2.49	0.47
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.54	0.47
1:B:7:PHE:O	1:B:228:GLY:CA	2.62	0.47
1:A:45:SER:OG	1:B:78:ILE:CD1	2.62	0.47
1:A:66:CYS:HB3	1:A:83:ILE:HD11	1.95	0.47
1:B:179:GLN:O	1:B:183:GLU:HB2	2.13	0.47
1:A:169:ALA:O	1:A:170:ILE:C	2.53	0.47
1:A:7:PHE:O	1:A:228:GLY:HA3	2.15	0.47
1:A:46:ILE:CD1	1:A:47:TYR:H	2.19	0.47
1:B:50:PHE:HE1	1:B:54:LYS:NZ	2.13	0.47
1:B:64:GLN:O	1:B:65:ASN:HB2	2.15	0.47
1:A:6:PHE:CE1	1:A:228:GLY:HA2	2.50	0.47
1:A:174:LYS:N	1:A:174:LYS:CD	2.78	0.47
1:B:130:LYS:HE3	1:B:133:GLU:OE2	2.15	0.47
1:A:93:LEU:O	1:A:125:ALA:HA	2.14	0.46
1:B:50:PHE:CE1	1:B:54:LYS:HD3	2.50	0.46
1:B:56:ASP:HB3	1:B:59:ILE:HD12	1.96	0.46
1:B:198:ASP:O	1:B:202:GLN:HB2	2.15	0.46
1:B:55:LEU:HG	1:B:59:ILE:CG2	2.44	0.46
1:A:16:GLY:HA3	1:A:21:LEU:HD13	1.97	0.46
1:A:127:ILE:HD13	1:A:127:ILE:H	1.81	0.46
1:B:11:ASN:OD1	1:B:11:ASN:C	2.54	0.46
1:B:177:THR:CB	1:B:179:GLN:HE21	2.27	0.46
1:A:167:VAL:C	1:A:169:ALA:H	2.19	0.46
1:A:28:LEU:HA	1:A:28:LEU:HD13	1.53	0.46
1:A:79:SER:CB	1:A:82:MET:HG3	2.46	0.46
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.76	0.46
1:B:94:GLY:C	1:B:126:CYS:HB2	2.37	0.46
1:A:4:ARG:NH2	1:A:227:ASP:OD1	2.43	0.45
1:A:4:ARG:HD3	1:A:4:ARG:HH11	1.40	0.45
1:B:167:VAL:HA	1:B:170:ILE:HG12	1.98	0.45
1:A:31:ALA:CB	1:A:33:LEU:HD21	2.47	0.45
1:A:174:LYS:HB3	1:A:175:THR:H	1.06	0.45
1:B:178:PRO:HD2	1:B:179:GLN:CD	2.35	0.45
1:A:25:ILE:HG23	1:A:55:LEU:HD23	1.98	0.45
1:A:45:SER:OG	1:B:78:ILE:HD13	2.17	0.45
1:B:24:LEU:O	1:B:25:ILE:C	2.54	0.45
1:A:114:ALA:HB2	1:A:153:ASN:HB3	1.99	0.44
1:A:38:GLU:OE1	1:A:205:ARG:NH1	2.41	0.44
1:B:50:PHE:CE1	1:B:54:LYS:NZ	2.85	0.44
1:B:69:VAL:O	1:B:79:SER:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASN:O	1:A:219:GLU:HG2	2.18	0.44
1:B:97:GLU:O	1:B:101:VAL:N	2.44	0.44
1:B:48:LEU:HG	1:B:86:ILE:HD11	1.98	0.44
1:B:90:TRP:HA	1:B:122:GLY:O	2.18	0.44
1:B:237:LYS:CB	1:B:238:PRO:HD2	2.47	0.44
1:A:4:ARG:HG2	1:A:203:SER:O	2.18	0.44
1:A:51:ALA:O	1:A:55:LEU:HB2	2.18	0.44
1:A:5:LYS:HG3	1:A:36:ASP:O	2.17	0.44
1:A:79:SER:O	1:A:82:MET:N	2.50	0.43
1:A:192:LEU:O	1:A:196:VAL:N	2.51	0.43
1:B:32:LYS:O	1:B:32:LYS:CG	2.63	0.43
1:A:91:VAL:HG22	1:A:92:ILE:O	2.19	0.43
1:A:212:VAL:HG21	1:A:229:PHE:HD2	1.82	0.43
1:B:117:LEU:HD12	1:B:117:LEU:HA	1.80	0.43
1:A:99:ARG:NH1	1:A:106:ASP:OD1	2.48	0.43
1:A:131:LEU:HD21	1:A:174:LYS:NZ	2.34	0.43
1:A:196:VAL:HG11	1:A:200:VAL:HG21	2.01	0.43
1:A:124:ILE:HA	1:A:161:VAL:O	2.19	0.43
1:B:128:GLY:HA2	1:B:164:TYR:CE1	2.54	0.43
1:B:247:LYS:HA	1:B:247:LYS:HD2	1.39	0.43
1:A:211:SER:O	1:A:216:ASN:ND2	2.52	0.43
1:B:69:VAL:HA	1:B:70:PRO:HD3	1.66	0.43
1:B:177:THR:HB	1:B:178:PRO:CD	2.48	0.42
1:A:192:LEU:O	1:A:196:VAL:HB	2.19	0.42
1:B:146:GLN:O	1:B:150:ILE:HG13	2.19	0.42
1:B:55:LEU:HD13	1:B:55:LEU:HA	1.59	0.42
1:B:213:THR:HA	1:B:243:ILE:HD11	2.01	0.42
1:A:46:ILE:HD13	1:A:47:TYR:CG	2.55	0.42
1:B:179:GLN:NE2	1:B:179:GLN:H	2.18	0.42
1:A:160:VAL:HG12	1:A:161:VAL:N	2.34	0.41
1:B:79:SER:O	1:B:82:MET:N	2.52	0.41
1:B:107:GLU:HG3	1:B:111:GLN:NE2	2.28	0.41
1:A:183:GLU:O	1:A:187:LYS:HG3	2.20	0.41
1:A:107:GLU:O	1:A:111:GLN:NE2	2.52	0.41
1:A:218:LYS:HD2	1:A:219:GLU:CA	2.50	0.41
1:B:166:PRO:O	1:B:170:ILE:HD13	2.21	0.41
1:A:239:GLU:O	1:A:243:ILE:HD12	2.20	0.41
1:B:39:VAL:C	1:B:40:VAL:HG23	2.40	0.41
1:B:40:VAL:HA	1:B:60:GLY:O	2.21	0.41
1:B:238:PRO:C	1:B:240:PHE:N	2.74	0.41
1:B:14:MET:O	1:B:14:MET:CG	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:CD1	1:A:46:ILE:H	2.34	0.40
1:B:230:LEU:HD12	1:B:230:LEU:HA	1.93	0.40
1:A:11:ASN:OD1	1:A:11:ASN:C	2.59	0.40
1:A:64:GLN:O	1:A:65:ASN:CB	2.66	0.40
1:A:72:GLY:N	1:B:14:MET:O	2.51	0.40
1:B:48:LEU:O	1:B:51:ALA:HB3	2.21	0.40
1:A:66:CYS:HB3	1:A:83:ILE:CD1	2.51	0.40
1:B:5:LYS:NZ	1:B:35:ALA:O	2.43	0.40
1:B:195:HIS:ND1	1:B:195:HIS:N	2.69	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	245/247 (99%)	219 (89%)	18 (7%)	8 (3%)	4 5
1	B	245/247 (99%)	221 (90%)	18 (7%)	6 (2%)	6 9
All	All	490/494 (99%)	440 (90%)	36 (7%)	14 (3%)	4 6

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	ILE
1	B	247	LYS
1	A	36	ASP
1	A	247	LYS
1	B	152	ASP
1	A	168	TRP
1	A	172	THR
1	A	246	ALA
1	B	171	GLY

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Mol	Chain	Res	Type
1	A	4	ARG
1	A	65	ASN
1	B	68	LYS
1	B	73	ALA
1	B	138	ILE

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	192/192 (100%)	153 (80%)	39 (20%)	1 2
1	B	192/192 (100%)	151 (79%)	41 (21%)	1 2
All	All	384/384 (100%)	304 (79%)	80 (21%)	1 2

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	21	LEU
1	A	24	LEU
1	A	28	LEU
1	A	33	LEU
1	A	46	ILE
1	A	69	VAL
1	A	71	LYS
1	A	78	ILE
1	A	79	SER
1	A	80	PRO
1	A	86	ILE
1	A	92	ILE
1	A	107	GLU
1	A	108	LEU
1	A	111	GLN
1	A	124	ILE
1	A	127	ILE

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Mol	Chain	Res	Type
1	A	131	LEU
1	A	138	ILE
1	A	141	LYS
1	A	148	LYS
1	A	155	LYS
1	A	165	GLU
1	A	175	THR
1	A	179	GLN
1	A	180	GLN
1	A	183	GLU
1	A	189	ARG
1	A	193	LYS
1	A	198	ASP
1	A	203	SER
1	A	204	THR
1	A	205	ARG
1	A	207	ILE
1	A	218	LYS
1	A	229	PHE
1	A	237	LYS
1	A	248	HIS
1	B	24	LEU
1	B	27	THR
1	B	28	LEU
1	B	32	LYS
1	B	34	SER
1	B	36	ASP
1	B	39	VAL
1	B	46	ILE
1	B	54	LYS
1	B	55	LEU
1	B	68	LYS
1	B	69	VAL
1	B	77	GLU
1	B	78	ILE
1	B	98	ARG
1	B	107	GLU
1	B	108	LEU
1	B	111	GLN
1	B	117	LEU
1	B	127	ILE
1	B	131	LEU

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Mol	Chain	Res	Type
1	B	134	ARG
1	B	135	GLU
1	B	138	ILE
1	B	140	GLU
1	B	141	LYS
1	B	148	LYS
1	B	166	PRO
1	B	179	GLN
1	B	194	THR
1	B	198	ASP
1	B	202	GLN
1	B	205	ARG
1	B	217	CYS
1	B	222	SER
1	B	223	GLN
1	B	224	HIS
1	B	229	PHE
1	B	245	ASN
1	B	247	LYS
1	B	248	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	179	GLN
1	A	202	GLN
1	A	216	ASN
1	A	248	HIS
1	B	111	GLN
1	B	153	ASN
1	B	179	GLN
1	B	245	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)

2 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	SO4	B	560	-	4,4,4	0.86	0	6,6,6	0.43	0
2	SO4	A	561	-	4,4,4	0.93	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

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	B	560	SO4	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.