



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 04:43 PM UTC

PDB ID : 1TMH / pdb_00001tmh
Title : MODULAR MUTAGENESIS OF A TIM-BARREL ENZYME: THE CRYSTAL STRUCTURE OF A CHIMERIC E. COLI TIM HAVING THE EIGHTH (BETA-ALPHA)-UNIT REPLACED BY THE EQUIVALENT UNIT OF CHICKEN TIM
Authors : Radha Kishan, K.V.; Zeelen, J.Ph.; Wierenga, R.K.
Deposited on : 1994-03-22
Resolution : 2.80 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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

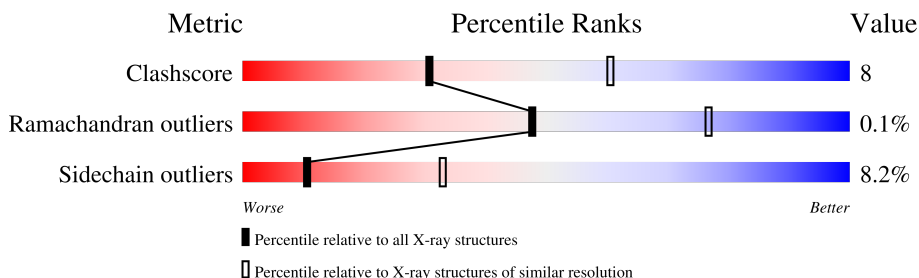
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	254	59% 32% 7% •
1	B	254	62% 32% 5% •
1	C	254	63% 31% 5% •
1	D	254	62% 33% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7628 atoms, of which 4 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 TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	254	Total	C	H	N	O	S	0	0	0
			1902	1193	1	334	364	10			
1	B	254	Total	C	H	N	O	S	0	0	0
			1902	1193	1	334	364	10			
1	C	254	Total	C	H	N	O	S	0	0	0
			1902	1193	1	334	364	10			
1	D	254	Total	C	H	N	O	S	0	0	0
			1902	1193	1	334	364	10			

There are 40 discrepancies between the modelled and reference sequences:

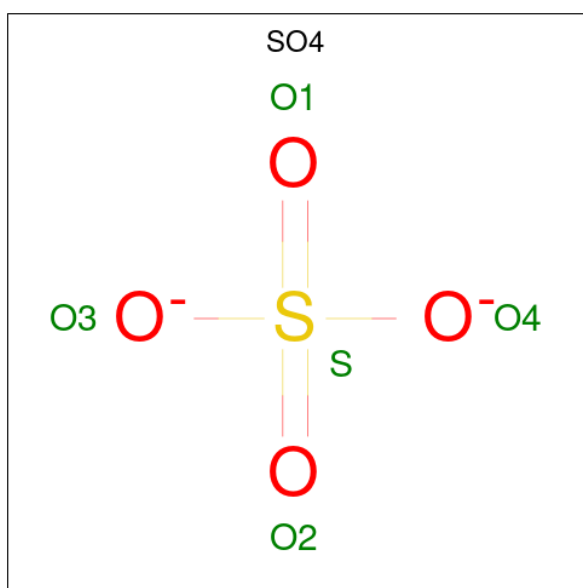
Chain	Residue	Modelled	Actual	Comment	Reference
A	227	HIS	PRO	engineered mutation	UNP P0A858
A	229	VAL	ILE	engineered mutation	UNP P0A858
A	232	PHE	ALA	engineered mutation	UNP P0A858
A	241	PRO	ALA	engineered mutation	UNP P0A858
A	?	-	ASP	deletion	UNP P0A858
A	243	GLU	ALA	engineered mutation	UNP P0A858
A	245	VAL	ALA	engineered mutation	UNP P0A858
A	246	ASP	VAL	engineered mutation	UNP P0A858
A	248	ILE	VAL	engineered mutation	UNP P0A858
A	249	ASN	LYS	engineered mutation	UNP P0A858
B	227	HIS	PRO	engineered mutation	UNP P0A858
B	229	VAL	ILE	engineered mutation	UNP P0A858
B	232	PHE	ALA	engineered mutation	UNP P0A858
B	241	PRO	ALA	engineered mutation	UNP P0A858
B	?	-	ASP	deletion	UNP P0A858
B	243	GLU	ALA	engineered mutation	UNP P0A858
B	245	VAL	ALA	engineered mutation	UNP P0A858
B	246	ASP	VAL	engineered mutation	UNP P0A858
B	248	ILE	VAL	engineered mutation	UNP P0A858
B	249	ASN	LYS	engineered mutation	UNP P0A858
C	227	HIS	PRO	engineered mutation	UNP P0A858

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Chain	Residue	Modelled	Actual	Comment	Reference
C	229	VAL	ILE	engineered mutation	UNP P0A858
C	232	PHE	ALA	engineered mutation	UNP P0A858
C	241	PRO	ALA	engineered mutation	UNP P0A858
C	?	-	ASP	deletion	UNP P0A858
C	243	GLU	ALA	engineered mutation	UNP P0A858
C	245	VAL	ALA	engineered mutation	UNP P0A858
C	246	ASP	VAL	engineered mutation	UNP P0A858
C	248	ILE	VAL	engineered mutation	UNP P0A858
C	249	ASN	LYS	engineered mutation	UNP P0A858
D	227	HIS	PRO	engineered mutation	UNP P0A858
D	229	VAL	ILE	engineered mutation	UNP P0A858
D	232	PHE	ALA	engineered mutation	UNP P0A858
D	241	PRO	ALA	engineered mutation	UNP P0A858
D	?	-	ASP	deletion	UNP P0A858
D	243	GLU	ALA	engineered mutation	UNP P0A858
D	245	VAL	ALA	engineered mutation	UNP P0A858
D	246	ASP	VAL	engineered mutation	UNP P0A858
D	248	ILE	VAL	engineered mutation	UNP P0A858
D	249	ASN	LYS	engineered mutation	UNP P0A858

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

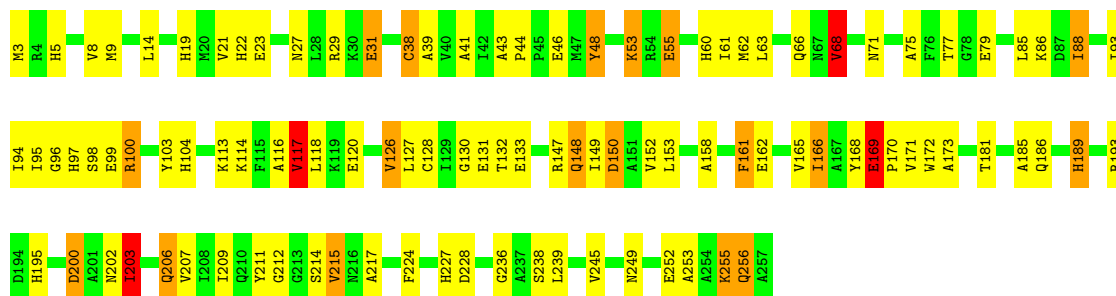
3 Residue-property plots [i](#)

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.

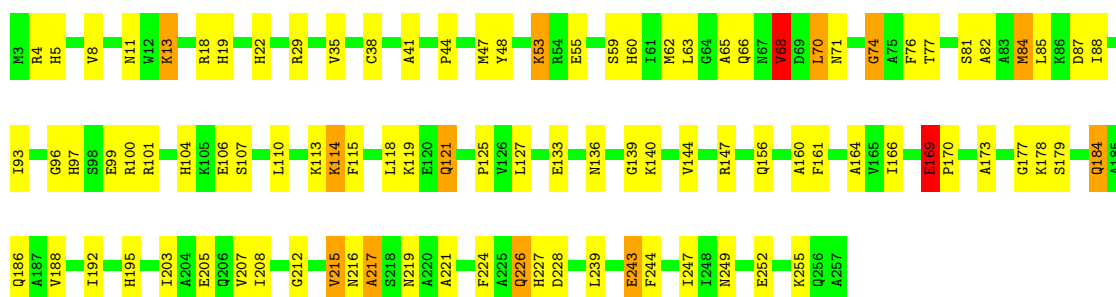
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A: 



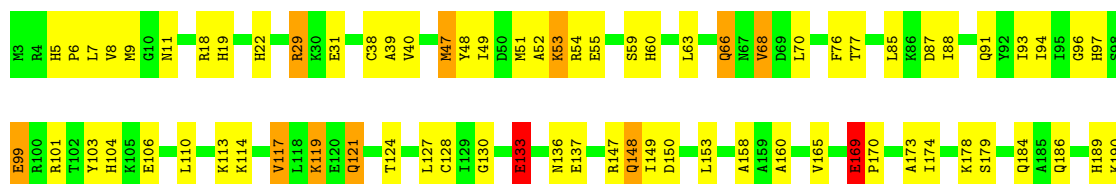
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B: 



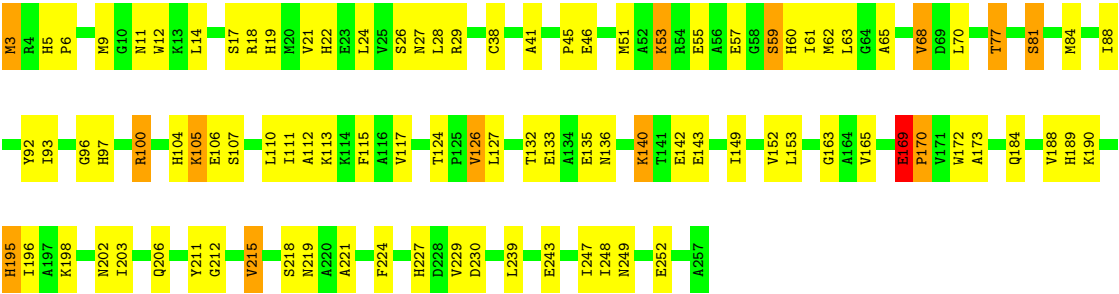
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain C: 





● Molecule 1: TRIOSEPHOSPHATE ISOMERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.64Å 118.31Å 58.98Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	35.10 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (35.10-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7628	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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	1.31	16/1932 (0.8%)	2.05	68/2612 (2.6%)
1	B	1.25	11/1932 (0.6%)	1.99	50/2612 (1.9%)
1	C	1.28	11/1932 (0.6%)	1.98	48/2612 (1.8%)
1	D	1.24	11/1932 (0.6%)	1.94	51/2612 (2.0%)
All	All	1.27	49/7728 (0.6%)	1.99	217/10448 (2.1%)

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	2
1	D	0	1
All	All	0	3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	HIS	CD2-NE2	-8.98	1.27	1.37
1	C	97	HIS	CD2-NE2	-7.70	1.29	1.37
1	B	215	VAL	CA-CB	7.52	1.64	1.54
1	D	215	VAL	CA-CB	7.43	1.63	1.54
1	C	195	HIS	CD2-NE2	-7.25	1.29	1.37
1	A	104	HIS	CD2-NE2	-6.84	1.30	1.37
1	C	5	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	195	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	5	HIS	CD2-NE2	-6.70	1.30	1.37
1	B	60	HIS	CD2-NE2	-6.68	1.30	1.37
1	B	104	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	22	HIS	CD2-NE2	-6.56	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	HIS	CD2-NE2	-6.51	1.30	1.37
1	B	19	HIS	CD2-NE2	-6.48	1.30	1.37
1	C	215	VAL	CA-CB	6.45	1.62	1.54
1	C	189	HIS	CD2-NE2	-6.43	1.30	1.37
1	D	104	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	60	HIS	CD2-NE2	-6.38	1.30	1.37
1	D	60	HIS	CD2-NE2	-6.26	1.30	1.37
1	D	22	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	19	HIS	CD2-NE2	-6.12	1.31	1.37
1	D	5	HIS	CD2-NE2	-6.05	1.31	1.37
1	B	97	HIS	CD2-NE2	-6.04	1.31	1.37
1	C	19	HIS	CD2-NE2	-6.04	1.31	1.37
1	B	195	HIS	CD2-NE2	-6.03	1.31	1.37
1	A	44	PRO	CA-CB	-6.01	1.48	1.54
1	D	19	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	227	HIS	CD2-NE2	-5.92	1.31	1.37
1	C	60	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	215	VAL	CA-CB	5.83	1.61	1.54
1	B	192	ILE	CA-CB	5.80	1.61	1.54
1	C	104	HIS	CD2-NE2	-5.79	1.31	1.37
1	D	97	HIS	CD2-NE2	-5.77	1.31	1.37
1	C	22	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	245	VAL	CA-CB	5.74	1.61	1.54
1	D	195	HIS	CD2-NE2	-5.74	1.31	1.37
1	B	5	HIS	CD2-NE2	-5.67	1.31	1.37
1	D	169	GLU	CA-CB	5.65	1.60	1.53
1	B	227	HIS	CD2-NE2	-5.61	1.31	1.37
1	B	22	HIS	CD2-NE2	-5.56	1.31	1.37
1	A	209	ILE	CA-CB	5.52	1.60	1.53
1	D	189	HIS	CD2-NE2	-5.42	1.31	1.37
1	B	5	HIS	CG-ND1	-5.37	1.32	1.38
1	D	5	HIS	CG-ND1	-5.35	1.32	1.38
1	A	60	HIS	CG-ND1	-5.21	1.32	1.38
1	A	195	HIS	CG-ND1	-5.18	1.32	1.38
1	A	97	HIS	CG-ND1	-5.17	1.32	1.38
1	C	227	HIS	CD2-NE2	-5.13	1.32	1.37
1	C	60	HIS	CG-ND1	-5.03	1.32	1.38

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ALA	CA-C-N	9.85	126.75	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ALA	C-N-CA	9.85	126.75	119.66
1	D	68	VAL	CB-CA-C	-9.44	96.85	110.82
1	B	161	PHE	CA-CB-CG	-9.25	104.55	113.80
1	A	148	GLN	OE1-CD-NE2	-9.12	113.48	122.60
1	A	97	HIS	CB-CG-CD2	-9.04	119.45	131.20
1	A	249	ASN	OD1-CG-ND2	-9.04	113.56	122.60
1	A	148	GLN	CG-CD-NE2	9.00	129.91	116.40
1	A	206	GLN	OE1-CD-NE2	-8.69	113.91	122.60
1	B	68	VAL	CB-CA-C	-8.69	97.95	110.82
1	B	184	GLN	OE1-CD-NE2	-8.68	113.92	122.60
1	C	55	GLU	N-CA-C	8.66	121.67	111.71
1	D	221	ALA	N-CA-C	8.43	121.30	111.02
1	B	166	ILE	O-C-N	-8.34	114.42	123.18
1	D	169	GLU	CB-CG-CD	8.33	126.76	112.60
1	D	219	ASN	CA-CB-CG	8.25	120.85	112.60
1	B	97	HIS	CA-C-O	-8.20	112.86	121.55
1	A	68	VAL	CB-CA-C	-8.10	96.62	110.30
1	A	224	PHE	CA-CB-CG	-8.07	105.73	113.80
1	A	227	HIS	CA-CB-CG	-8.05	105.75	113.80
1	D	184	GLN	OE1-CD-NE2	-7.92	114.69	122.60
1	A	126	VAL	N-CA-C	-7.85	95.70	106.85
1	B	221	ALA	N-CA-C	7.59	119.24	110.97
1	D	142	GLU	N-CA-C	-7.52	102.77	110.97
1	C	238	SER	O-C-N	7.34	129.90	122.12
1	B	216	ASN	OD1-CG-ND2	-7.28	115.32	122.60
1	C	249	ASN	OD1-CG-ND2	-7.25	115.35	122.60
1	D	11	ASN	OD1-CG-ND2	-7.23	115.37	122.60
1	A	249	ASN	CB-CG-ND2	7.12	127.08	116.40
1	B	219	ASN	CA-CB-CG	7.12	119.72	112.60
1	B	226	GLN	CA-C-O	7.11	129.89	121.36
1	B	100	ARG	CA-CB-CG	-7.07	99.96	114.10
1	D	184	GLN	CG-CD-NE2	6.92	126.78	116.40
1	A	61	ILE	N-CA-C	-6.87	100.71	109.30
1	A	117	VAL	CB-CA-C	-6.81	103.25	111.97
1	C	195	HIS	CB-CG-CD2	-6.80	122.36	131.20
1	C	77	THR	CA-C-O	6.78	128.61	120.81
1	C	68	VAL	N-CA-CB	6.74	122.39	112.35
1	D	247	ILE	N-CA-C	-6.68	104.01	110.42
1	A	104	HIS	CB-CG-CD2	-6.65	122.56	131.20
1	D	188	VAL	N-CA-C	-6.59	104.60	111.58
1	C	148	GLN	CG-CD-NE2	6.57	126.26	116.40
1	C	184	GLN	OE1-CD-NE2	-6.57	116.03	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	LEU	N-CA-C	6.54	121.11	113.20
1	B	164	ALA	CA-C-O	-6.51	113.81	121.16
1	A	212	GLY	O-C-N	-6.50	117.50	123.42
1	C	68	VAL	CB-CA-C	-6.50	100.31	110.52
1	A	217	ALA	N-CA-C	6.46	119.14	111.33
1	C	6	PRO	O-C-N	6.44	130.71	122.91
1	A	161	PHE	CA-CB-CG	-6.43	107.37	113.80
1	A	200	ASP	CA-CB-CG	6.42	119.02	112.60
1	B	184	GLN	CG-CD-NE2	6.41	126.02	116.40
1	D	77	THR	O-C-N	6.41	130.71	122.89
1	A	166	ILE	N-CA-C	-6.37	99.21	108.89
1	B	68	VAL	N-CA-CB	6.36	121.42	112.52
1	D	206	GLN	CA-CB-CG	6.35	126.80	114.10
1	B	35	VAL	N-CA-CB	-6.35	104.67	111.46
1	C	186	GLN	OE1-CD-NE2	-6.34	116.26	122.60
1	A	98	SER	N-CA-C	6.32	119.84	111.75
1	C	190	LYS	N-CA-C	-6.31	104.32	111.14
1	B	169	GLU	CB-CG-CD	6.30	123.31	112.60
1	C	243	GLU	CA-C-N	6.29	128.62	120.44
1	C	243	GLU	C-N-CA	6.29	128.62	120.44
1	B	74	GLY	CA-C-O	6.28	127.45	121.30
1	C	97	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	A	39	ALA	N-CA-C	-6.19	99.63	109.59
1	B	38	CYS	CA-CB-SG	-6.15	100.26	114.40
1	C	256	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	B	249	ASN	OD1-CG-ND2	-6.14	116.45	122.60
1	A	86	LYS	CA-C-N	6.10	128.46	120.28
1	A	86	LYS	C-N-CA	6.10	128.46	120.28
1	B	97	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	B	177	GLY	N-CA-C	-6.09	107.44	114.69
1	D	68	VAL	N-CA-CB	6.07	121.02	112.52
1	A	172	TRP	CG-CD2-CE3	6.07	139.97	133.90
1	B	195	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	C	99	GLU	CA-CB-CG	-6.02	102.06	114.10
1	B	224	PHE	CA-C-O	6.02	126.78	119.38
1	A	131	GLU	CB-CG-CD	5.93	122.69	112.60
1	D	104	HIS	CB-CG-CD2	-5.93	123.49	131.20
1	A	117	VAL	N-CA-C	5.93	116.11	110.42
1	D	46	GLU	N-CA-C	5.92	119.33	111.75
1	D	126	VAL	N-CA-C	-5.92	97.03	109.34
1	B	19	HIS	CB-CG-CD2	-5.92	123.51	131.20
1	D	227	HIS	CA-CB-CG	-5.90	107.90	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	GLU	N-CA-C	-5.89	99.53	108.67
1	A	238	SER	CA-CB-OG	5.88	122.86	111.10
1	A	206	GLN	CG-CD-NE2	5.86	125.18	116.40
1	D	19	HIS	CB-CG-CD2	-5.84	123.60	131.20
1	C	241	PRO	CA-C-N	5.82	128.87	120.38
1	C	241	PRO	C-N-CA	5.82	128.87	120.38
1	C	47	MET	CA-CB-CG	5.80	125.71	114.10
1	A	203	ILE	N-CA-C	-5.80	104.68	111.00
1	C	249	ASN	CB-CG-ND2	5.80	125.09	116.40
1	D	3	MET	N-CA-C	-5.80	94.77	111.00
1	D	229	VAL	N-CA-C	-5.79	99.53	107.99
1	A	48	TYR	CA-C-O	-5.79	112.43	119.32
1	C	137	GLU	CB-CG-CD	5.79	122.44	112.60
1	A	77	THR	CA-C-O	5.78	127.46	120.81
1	B	156	GLN	N-CA-C	5.77	120.48	113.38
1	C	240	LYS	CA-C-N	5.77	125.87	119.87
1	C	240	LYS	C-N-CA	5.77	125.87	119.87
1	D	11	ASN	O-C-N	-5.75	115.94	123.02
1	A	193	ARG	CA-CB-CG	-5.75	102.60	114.10
1	A	23	GLU	N-CA-C	5.74	117.41	111.03
1	B	216	ASN	CA-CB-CG	5.74	118.34	112.60
1	D	224	PHE	CA-CB-CG	-5.73	108.07	113.80
1	B	71	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	A	181	THR	O-C-N	-5.71	115.55	121.60
1	A	133	GLU	CA-CB-CG	-5.69	102.72	114.10
1	D	17	SER	O-C-N	-5.69	117.60	123.29
1	A	71	ASN	OD1-CG-ND2	-5.67	116.94	122.60
1	B	84	MET	CG-SD-CE	-5.66	88.44	100.90
1	C	52	ALA	O-C-N	-5.66	116.12	122.12
1	A	227	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	A	104	HIS	CB-CG-ND1	5.65	131.17	122.70
1	B	99	GLU	CB-CG-CD	5.65	122.20	112.60
1	D	9	MET	CA-CB-CG	-5.64	102.81	114.10
1	D	59	SER	N-CA-C	-5.62	101.08	109.96
1	D	195	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	B	11	ASN	CA-CB-CG	5.61	118.21	112.60
1	C	87	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	104	HIS	CA-CB-CG	-5.61	108.19	113.80
1	D	70	LEU	N-CA-C	5.60	119.84	112.89
1	A	150	ASP	CA-C-O	-5.60	113.77	120.10
1	A	128	CYS	CA-CB-SG	-5.59	101.54	114.40
1	B	228	ASP	CA-CB-CG	-5.59	107.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	230	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	216	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	A	214	SER	N-CA-C	5.55	119.23	111.90
1	B	44	PRO	N-CA-C	-5.55	103.93	110.70
1	D	219	ASN	N-CA-C	5.54	120.20	113.38
1	D	170	PRO	N-CA-C	-5.54	102.43	110.80
1	A	195	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	B	252	GLU	CB-CG-CD	5.53	122.01	112.60
1	C	31	GLU	CB-CG-CD	5.52	121.98	112.60
1	D	81	SER	O-C-N	5.51	129.52	123.01
1	C	124	THR	CA-CB-OG1	-5.49	101.36	109.60
1	D	219	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	B	74	GLY	N-CA-C	5.47	118.58	110.60
1	C	169	GLU	CB-CG-CD	5.46	121.88	112.60
1	D	249	ASN	CB-CG-ND2	5.46	124.58	116.40
1	B	100	ARG	N-CA-C	-5.45	106.31	113.12
1	C	104	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	D	152	VAL	N-CA-C	-5.42	105.83	111.58
1	A	206	GLN	CA-CB-CG	5.42	124.94	114.10
1	D	77	THR	CA-C-N	5.42	129.69	120.91
1	D	77	THR	C-N-CA	5.42	129.69	120.91
1	D	24	LEU	CA-C-O	-5.41	115.14	120.82
1	D	57	GLU	O-C-N	5.40	129.52	122.87
1	A	55	GLU	CA-CB-CG	-5.38	103.35	114.10
1	B	139	GLY	CA-C-O	5.37	124.98	118.86
1	D	227	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	D	227	HIS	N-CA-CB	-5.34	102.31	110.26
1	B	115	PHE	N-CA-C	-5.34	105.13	111.69
1	A	245	VAL	CG1-CB-CG2	-5.33	99.07	110.80
1	A	38	CYS	N-CA-CB	-5.32	102.58	111.20
1	A	255	LYS	CA-CB-CG	5.32	124.74	114.10
1	A	38	CYS	CA-CB-SG	-5.32	102.17	114.40
1	C	148	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	D	97	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	A	169	GLU	CB-CG-CD	5.28	121.57	112.60
1	C	94	ILE	N-CA-C	-5.28	102.70	109.30
1	D	243	GLU	N-CA-CB	-5.26	100.75	110.32
1	B	8	VAL	N-CA-C	-5.26	98.92	107.28
1	A	79	GLU	N-CA-C	5.25	117.50	109.95
1	A	68	VAL	N-CA-CB	5.24	122.06	112.36
1	A	95	ILE	O-C-N	-5.24	117.49	123.10
1	C	121	GLN	CG-CD-NE2	-5.24	108.54	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	GLN	N-CA-C	5.24	119.82	113.38
1	A	96	GLY	CA-C-O	5.23	125.58	119.19
1	D	27	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	C	243	GLU	O-C-N	5.21	128.14	122.20
1	B	243	GLU	O-C-N	-5.21	115.50	122.43
1	B	87	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	115	PHE	CA-CB-CG	5.20	119.00	113.80
1	C	147	ARG	CA-C-O	5.20	126.46	120.90
1	A	172	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	C	117	VAL	N-CA-C	5.19	115.81	110.36
1	A	169	GLU	CA-C-O	5.19	127.28	120.74
1	D	202	ASN	N-CA-CB	-5.18	102.50	110.12
1	D	195	HIS	CB-CG-ND1	5.17	130.45	122.70
1	D	107	SER	N-CA-C	5.16	117.19	110.53
1	C	91	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	A	117	VAL	CA-CB-CG1	-5.16	101.63	110.40
1	B	217	ALA	N-CA-C	5.15	117.29	111.11
1	B	13	LYS	CA-CB-CG	-5.15	103.81	114.10
1	C	11	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	A	147	ARG	CA-C-O	5.13	126.21	120.82
1	D	92	TYR	O-C-N	-5.12	117.24	123.13
1	C	29	ARG	N-CA-C	-5.12	105.70	111.28
1	D	45	PRO	CB-CA-C	5.12	118.06	111.56
1	B	5	HIS	CA-C-N	5.11	125.04	119.78
1	B	5	HIS	C-N-CA	5.11	125.04	119.78
1	A	152	VAL	N-CA-C	-5.10	106.17	111.58
1	A	22	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	C	238	SER	CB-CA-C	-5.09	102.34	110.79
1	D	172	TRP	CE2-CD2-CG	-5.09	101.10	107.20
1	C	230	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	100	ARG	N-CA-C	-5.05	105.47	111.69
1	C	230	ASP	N-CA-C	5.05	119.43	113.16
1	C	224	PHE	CA-CB-CG	-5.05	108.75	113.80
1	B	104	HIS	CB-CG-CD2	-5.05	124.64	131.20
1	B	207	VAL	CB-CA-C	5.04	117.16	110.91
1	C	178	LYS	N-CA-CB	-5.04	102.20	110.21
1	A	236	GLY	N-CA-C	5.03	118.73	112.64
1	A	149	ILE	N-CA-C	-5.03	105.52	111.00
1	B	121	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	C	133	GLU	CA-CB-CG	-5.03	104.04	114.10
1	D	100	ARG	N-CA-C	-5.03	107.28	113.41
1	A	195	HIS	CA-CB-CG	-5.03	108.78	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ILE	O-C-N	5.02	128.15	122.67
1	A	44	PRO	N-CA-CB	5.02	105.83	103.22
1	B	66	GLN	N-CA-C	5.01	119.38	113.16
1	D	196	ILE	N-CA-C	-5.01	105.96	110.82
1	B	249	ASN	CB-CG-ND2	5.01	123.91	116.40
1	C	128	CYS	CA-C-O	-5.00	115.25	120.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	TYR	Sidechain
1	A	211	TYR	Sidechain
1	D	211	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1901	1	1892	36	0
1	B	1901	1	1892	38	0
1	C	1901	1	1892	32	0
1	D	1901	1	1892	33	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
All	All	7624	4	7568	126	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 8.

All (126) 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:D:65:ALA:HB3	1:D:93:ILE:HD12	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:HE3	1:B:18:ARG:HH22	1.55	0.72
1:A:9:MET:HE2	1:A:94:ILE:HD11	1.71	0.71
1:C:169:GLU:HB2	1:C:174:ILE:HD11	1.76	0.67
1:A:8:VAL:HG23	1:A:38:CYS:SG	2.35	0.67
1:C:8:VAL:HG23	1:C:38:CYS:SG	2.35	0.66
1:B:65:ALA:HB3	1:B:93:ILE:HD12	1.78	0.65
1:C:53:LYS:HE3	1:D:18:ARG:HH22	1.61	0.65
1:A:170:PRO:HG2	1:A:173:ALA:HB3	1.78	0.64
1:C:18:ARG:HH22	1:D:53:LYS:HE3	1.62	0.64
1:D:170:PRO:HD2	1:D:212:GLY:O	1.98	0.63
1:C:119:LYS:HE3	1:C:160:ALA:O	2.01	0.61
1:B:81:SER:HB3	1:B:84:MET:HE3	1.86	0.58
1:A:85:LEU:HD13	1:A:93:ILE:HD12	1.84	0.58
1:C:113:LYS:O	1:C:117:VAL:HG23	2.04	0.57
1:A:88:ILE:HD13	1:B:48:TYR:CE1	2.38	0.57
1:B:106:GLU:HG3	1:B:110:LEU:HD23	1.85	0.57
1:D:169:GLU:HA	1:D:212:GLY:O	2.05	0.57
1:B:70:LEU:HD11	1:B:113:LYS:HE2	1.88	0.56
1:B:244:PHE:HA	1:B:247:ILE:HD12	1.87	0.56
1:A:68:VAL:HG13	1:A:85:LEU:HD12	1.88	0.56
1:A:113:LYS:O	1:A:116:ALA:HB3	2.06	0.56
1:A:99:GLU:O	1:A:103:TYR:HB2	2.06	0.56
1:B:68:VAL:HG23	1:B:114:LYS:HG2	1.86	0.55
1:C:165:VAL:HG13	1:C:208:ILE:HB	1.88	0.55
1:C:106:GLU:HG3	1:C:110:LEU:HD23	1.88	0.54
1:B:144:VAL:O	1:B:147:ARG:HB3	2.08	0.54
1:B:170:PRO:HG2	1:B:173:ALA:HB3	1.90	0.54
1:C:150:ASP:HA	1:C:153:LEU:HB3	1.91	0.53
1:B:169:GLU:HA	1:B:212:GLY:O	2.09	0.53
1:B:53:LYS:NZ	1:B:53:LYS:HB3	2.25	0.52
1:A:53:LYS:NZ	1:A:53:LYS:HB3	2.25	0.52
1:A:252:GLU:O	1:A:255:LYS:HB3	2.10	0.51
1:C:7:LEU:O	1:C:231:GLY:HA3	2.10	0.51
1:C:117:VAL:O	1:C:121:GLN:HG2	2.11	0.51
1:A:93:ILE:HG13	1:A:118:LEU:HD22	1.93	0.50
1:A:150:ASP:HA	1:A:153:LEU:HB3	1.93	0.50
1:C:18:ARG:O	1:C:51:MET:HE1	2.11	0.49
1:A:170:PRO:HG2	1:A:173:ALA:CB	2.43	0.49
1:D:149:ILE:HG22	1:D:153:LEU:HD22	1.95	0.49
1:D:53:LYS:HB3	1:D:53:LYS:NZ	2.28	0.49
1:B:70:LEU:CD1	1:B:113:LYS:HE2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:THR:OG1	1:D:135:GLU:HG3	2.13	0.48
1:A:14:LEU:HD22	1:B:76:PHE:HB2	1.95	0.48
1:D:96:GLY:HA2	1:D:111:ILE:HD13	1.94	0.48
1:D:81:SER:HB3	1:D:84:MET:HB2	1.96	0.48
1:A:53:LYS:HE3	1:B:18:ARG:NH2	2.27	0.48
1:B:4:ARG:HD3	1:B:205:GLU:O	2.13	0.48
1:B:82:ALA:HB3	1:B:121:GLN:HG3	1.96	0.48
1:D:126:VAL:HA	1:D:165:VAL:HB	1.96	0.48
1:A:130:GLY:H	1:A:148:GLN:HE22	1.62	0.47
1:B:118:LEU:HD12	1:B:125:PRO:HB3	1.95	0.47
1:A:21:VAL:HG21	1:A:48:TYR:HB3	1.96	0.47
1:B:119:LYS:HE2	1:B:160:ALA:O	2.15	0.47
1:C:88:ILE:HA	1:C:88:ILE:HD12	1.59	0.46
1:C:149:ILE:HD11	1:C:192:ILE:HG12	1.97	0.46
1:C:48:TYR:CE1	1:D:88:ILE:HD13	2.51	0.46
1:D:26:SER:HA	1:D:29:ARG:NH1	2.30	0.46
1:D:41:ALA:HA	1:D:62:MET:O	2.15	0.46
1:A:186:GLN:OE1	1:A:228:ASP:N	2.48	0.46
1:A:41:ALA:HA	1:A:62:MET:O	2.16	0.46
1:B:41:ALA:HA	1:B:62:MET:O	2.16	0.46
1:B:133:GLU:O	1:B:136:ASN:HB3	2.16	0.46
1:B:173:ALA:HA	1:B:178:LYS:O	2.16	0.45
1:C:99:GLU:O	1:C:103:TYR:HB2	2.16	0.45
1:B:186:GLN:HB2	1:B:226:GLN:HB3	1.97	0.45
1:B:184:GLN:O	1:B:188:VAL:HG23	2.16	0.45
1:D:112:ALA:O	1:D:115:PHE:HB3	2.16	0.45
1:A:14:LEU:HB3	1:B:74:GLY:N	2.32	0.45
1:D:170:PRO:HG2	1:D:173:ALA:HB3	1.98	0.45
1:B:217:ALA:HB2	1:B:243:GLU:HG3	1.97	0.45
1:A:66:GLN:HB3	1:B:77:THR:HG23	1.98	0.45
1:A:161:PHE:CD1	1:A:161:PHE:N	2.84	0.45
1:C:106:GLU:HG3	1:C:110:LEU:CD2	2.47	0.45
1:A:46:GLU:OE2	1:B:47:MET:HE3	2.17	0.44
1:A:27:ASN:O	1:A:31:GLU:HB2	2.17	0.44
1:C:7:LEU:HA	1:C:39:ALA:O	2.17	0.44
1:D:53:LYS:HB3	1:D:53:LYS:HZ2	1.81	0.44
1:C:130:GLY:H	1:C:148:GLN:HE22	1.65	0.44
1:D:12:TRP:HZ3	1:D:21:VAL:HG22	1.82	0.44
1:D:106:GLU:HG3	1:D:110:LEU:HD23	2.00	0.44
1:C:244:PHE:HA	1:C:247:ILE:HD12	1.98	0.44
1:C:158:ALA:HB1	1:C:203:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ILE:HD12	1:B:88:ILE:HA	1.85	0.43
1:A:114:LYS:HA	1:A:117:VAL:HG23	2.01	0.43
1:A:253:ALA:HA	1:A:256:GLN:NE2	2.33	0.43
1:D:133:GLU:O	1:D:136:ASN:HB3	2.18	0.43
1:A:88:ILE:HA	1:A:88:ILE:HD12	1.69	0.43
1:B:169:GLU:HA	1:B:170:PRO:HD2	1.82	0.43
1:C:8:VAL:O	1:C:40:VAL:HA	2.19	0.43
1:D:6:PRO:HG2	1:D:38:CYS:HA	2.01	0.43
1:B:170:PRO:HG2	1:B:173:ALA:CB	2.49	0.43
1:C:85:LEU:HD13	1:C:93:ILE:HD12	2.01	0.43
1:D:248:ILE:HG21	1:D:248:ILE:HD13	1.83	0.43
1:B:29:ARG:HG3	1:B:59:SER:HB3	2.01	0.42
1:D:113:LYS:O	1:D:117:VAL:HG23	2.19	0.42
1:D:140:LYS:O	1:D:143:GLU:HB3	2.18	0.42
1:D:59:SER:OG	1:D:61:ILE:HG13	2.18	0.42
1:B:96:GLY:O	1:B:101:ARG:NH1	2.53	0.42
1:C:76:PHE:HB2	1:D:14:LEU:HD22	2.01	0.42
1:C:49:ILE:O	1:C:53:LYS:HB2	2.20	0.42
1:C:133:GLU:O	1:C:136:ASN:HB3	2.19	0.42
1:A:169:GLU:HA	1:A:170:PRO:HD2	1.83	0.42
1:C:96:GLY:O	1:C:101:ARG:HD2	2.19	0.42
1:D:105:LYS:HD3	1:D:105:LYS:HA	1.80	0.42
1:A:132:THR:HA	1:A:171:VAL:HB	2.01	0.41
1:B:68:VAL:HG13	1:B:85:LEU:HD12	2.02	0.41
1:C:70:LEU:HD21	1:C:114:LYS:HG3	2.02	0.41
1:A:158:ALA:O	1:A:203:ILE:HG21	2.20	0.41
1:D:29:ARG:HG3	1:D:59:SER:HB3	2.03	0.41
1:A:200:ASP:OD1	1:A:202:ASN:HB3	2.19	0.41
1:D:195:HIS:HA	1:D:198:LYS:HE3	2.01	0.41
1:A:75:ALA:HA	1:B:13:LYS:HD3	2.03	0.41
1:B:101:ARG:HH11	1:B:101:ARG:HD2	1.71	0.41
1:D:190:LYS:HA	1:D:190:LYS:HD2	1.91	0.41
1:A:185:ALA:O	1:A:189:HIS:HD2	2.04	0.41
1:C:66:GLN:HB3	1:D:77:THR:CG2	2.51	0.41
1:A:29:ARG:HD3	1:A:55:GLU:O	2.21	0.41
1:B:140:LYS:HA	1:B:140:LYS:HD3	1.87	0.41
1:D:170:PRO:HG2	1:D:173:ALA:CB	2.51	0.41
1:C:170:PRO:HG2	1:C:173:ALA:HB3	2.03	0.40
1:C:29:ARG:HG3	1:C:59:SER:HB3	2.02	0.40
1:D:124:THR:HG23	1:D:163:GLY:O	2.22	0.40
1:B:107:SER:O	1:B:110:LEU:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:HA	1:A:165:VAL:HB	2.03	0.40
1:C:256:GLN:HE21	1:C:256:GLN:HB2	1.76	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	252/254 (99%)	238 (94%)	14 (6%)	0	100	100
1	B	252/254 (99%)	234 (93%)	18 (7%)	0	100	100
1	C	252/254 (99%)	240 (95%)	12 (5%)	0	100	100
1	D	252/254 (99%)	236 (94%)	15 (6%)	1 (0%)	30	60
All	All	1008/1016 (99%)	948 (94%)	59 (6%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	105	LYS

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	191/191 (100%)	173 (91%)	18 (9%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	191/191 (100%)	178 (93%)	13 (7%)	14	42
1	C	191/191 (100%)	175 (92%)	16 (8%)	10	32
1	D	191/191 (100%)	175 (92%)	16 (8%)	10	32
All	All	764/764 (100%)	701 (92%)	63 (8%)	10	33

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	31	GLU
1	A	53	LYS
1	A	63	LEU
1	A	68	VAL
1	A	88	ILE
1	A	100	ARG
1	A	117	VAL
1	A	120	GLU
1	A	127	LEU
1	A	166	ILE
1	A	169	GLU
1	A	203	ILE
1	A	206	GLN
1	A	207	VAL
1	A	215	VAL
1	A	239	LEU
1	A	256	GLN
1	B	53	LYS
1	B	55	GLU
1	B	63	LEU
1	B	68	VAL
1	B	114	LYS
1	B	127	LEU
1	B	169	GLU
1	B	179	SER
1	B	203	ILE
1	B	208	ILE
1	B	215	VAL
1	B	239	LEU
1	B	255	LYS
1	C	9	MET
1	C	47	MET

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Mol	Chain	Res	Type
1	C	53	LYS
1	C	54	ARG
1	C	63	LEU
1	C	68	VAL
1	C	119	LYS
1	C	127	LEU
1	C	133	GLU
1	C	169	GLU
1	C	179	SER
1	C	203	ILE
1	C	207	VAL
1	C	215	VAL
1	C	239	LEU
1	C	256	GLN
1	D	3	MET
1	D	28	LEU
1	D	51	MET
1	D	53	LYS
1	D	55	GLU
1	D	63	LEU
1	D	68	VAL
1	D	100	ARG
1	D	127	LEU
1	D	140	LYS
1	D	169	GLU
1	D	203	ILE
1	D	215	VAL
1	D	218	SER
1	D	239	LEU
1	D	252	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	91	GLN
1	A	136	ASN
1	A	148	GLN
1	A	202	ASN
1	A	210	GLN
1	A	256	GLN
1	B	27	ASN

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Mol	Chain	Res	Type
1	B	148	GLN
1	B	195	HIS
1	B	210	GLN
1	B	249	ASN
1	C	11	ASN
1	C	27	ASN
1	C	67	ASN
1	C	91	GLN
1	C	148	GLN
1	C	210	GLN
1	C	249	ASN
1	C	256	GLN
1	D	27	ASN
1	D	91	GLN
1	D	210	GLN
1	D	226	GLN
1	D	249	ASN
1	D	256	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	556	-	4,4,4	0.35	0	6,6,6	0.41	0
2	SO4	A	555	-	4,4,4	0.48	0	6,6,6	0.22	0
2	SO4	C	557	-	4,4,4	0.28	0	6,6,6	0.22	0
2	SO4	D	558	-	4,4,4	0.51	0	6,6,6	0.41	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.