Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 12:49 PM EDT

PDB ID	:	1TMH
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 following versions of software and data (see references ⓘ) were used in the production of this report:

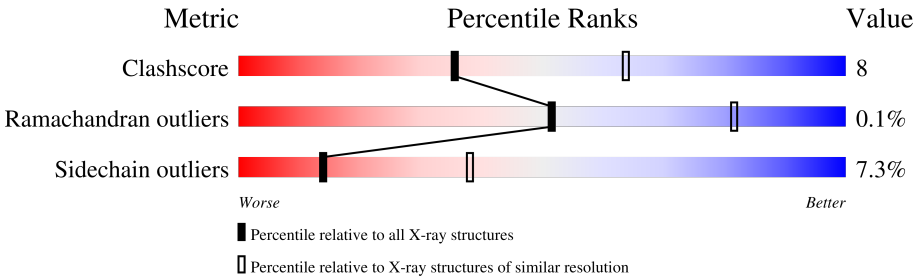
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	254	72% 22% 6%
1	B	254	72% 24% .
1	C	254	73% 21% 6%
1	D	254	71% 23% 6%

2 Entry composition (i)

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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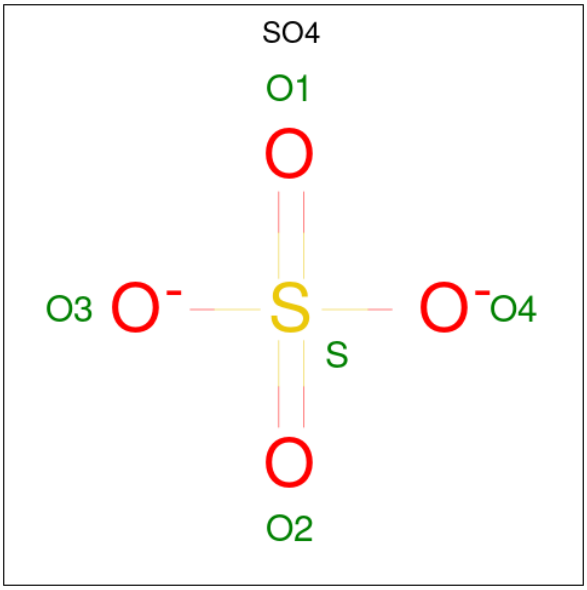
Chain	Residue	Modelled	Actual	Comment	Reference
C	229	VAL	ILE	engineered mutation	UNP P0A858
C	232	PHE	ALA	engineered mutation	UNP P0A858
C	241	PRO	ALA	engineered mutation	UNP P0A858
C	?	-	ASP	deletion	UNP P0A858
C	243	GLU	ALA	engineered mutation	UNP P0A858
C	245	VAL	ALA	engineered mutation	UNP P0A858
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 (three-letter code: SO4) (formula: O_4S).



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 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

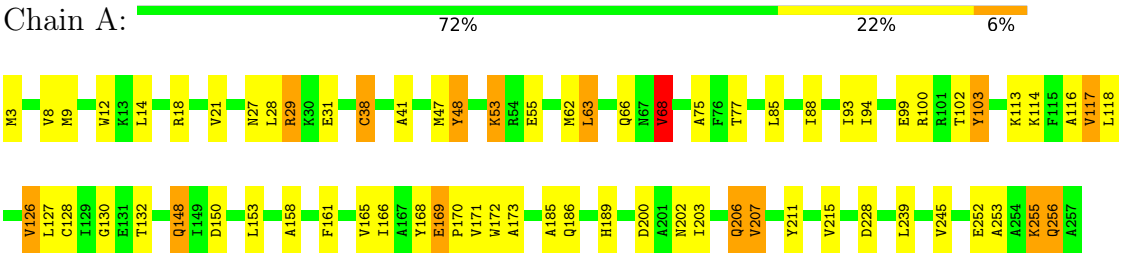
3 Residue-property plots (i)

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.

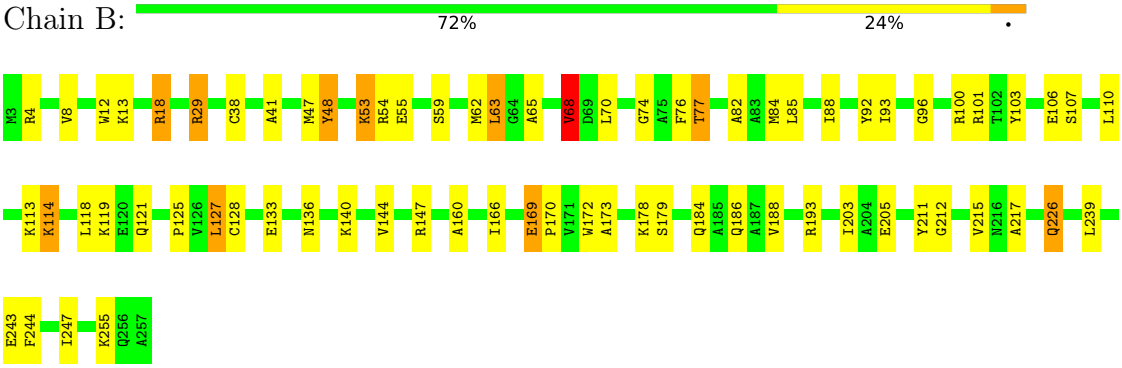
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A:



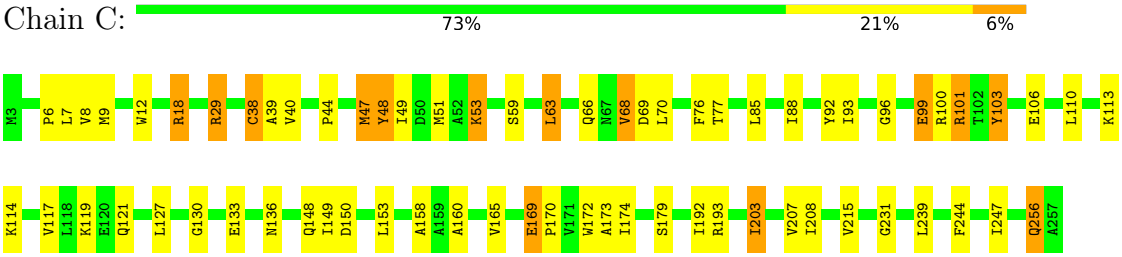
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B:



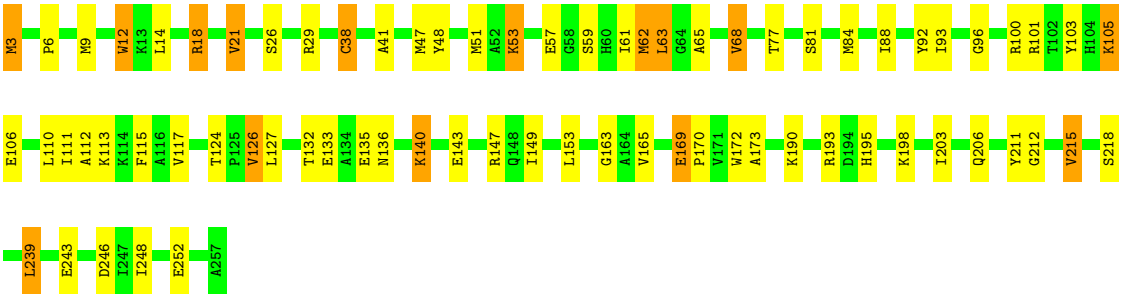
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain C:



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain D:


M3 P6 M9 W12 K13 L14 R18 V21 S26 R29 C38 A41 M47 Y48 M51 A52 K53 E57 G58 S59 H60 I61 M62 L63 G64 A65 V68 T77 S81 M84 I88 Y92 I93 G96 R100 R101 T102 Y103 H104 K105
E106 L110 I111 A112 K113 K114 F115 A116 V117 T124 P125 V126 L127 T132 E133 A134 E135 N136 K140 E143 R147 Q148 I149 L153 G163 A164 V165 E169 P170 V171 W172 A173 K190 R193 D194 H195 K198 I203 Q206 Y211 G212 V215 S218
L239 E243 D246 I247 I248 E252 A257

4 Data and refinement statistics (i)

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

5.1 Standard geometry

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	0.96	0/1932	1.63	28/2612 (1.1%)
1	B	0.96	0/1932	1.60	25/2612 (1.0%)
1	C	0.96	0/1932	1.61	24/2612 (0.9%)
1	D	0.94	0/1932	1.58	27/2612 (1.0%)
All	All	0.95	0/7728	1.60	104/10448 (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	A	0	2
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	A	29	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	A	103	TYR	CB-CG-CD2	-9.77	115.14	121.00
1	A	18	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	D	103	TYR	CB-CG-CD2	-9.36	115.38	121.00
1	C	92	TYR	CB-CG-CD2	-9.16	115.50	121.00
1	C	18	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	A	12	TRP	CD1-CG-CD2	8.79	113.33	106.30
1	C	172	TRP	CD1-CG-CD2	8.79	113.33	106.30
1	B	172	TRP	CD1-CG-CD2	8.62	113.20	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	18	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	172	TRP	CD1-CG-CD2	8.46	113.06	106.30
1	B	211	TYR	CB-CG-CD2	-8.31	116.01	121.00
1	C	12	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	C	193	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	172	TRP	CE2-CD2-CG	-7.92	100.96	107.30
1	D	172	TRP	CD1-CG-CD2	7.91	112.62	106.30
1	C	77	THR	CA-C-N	-7.84	100.51	116.20
1	A	68	VAL	CB-CA-C	-7.78	96.62	111.40
1	D	172	TRP	CE2-CD2-CG	-7.76	101.10	107.30
1	C	103	TYR	CB-CG-CD2	-7.71	116.38	121.00
1	D	68	VAL	CB-CA-C	-7.66	96.85	111.40
1	B	38	CYS	CA-CB-SG	-7.63	100.26	114.00
1	D	12	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	B	172	TRP	CE2-CD2-CG	-7.59	101.22	107.30
1	C	172	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	D	92	TYR	CB-CG-CD1	-7.54	116.47	121.00
1	B	12	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	C	29	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	C	12	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	A	245	VAL	CG1-CB-CG2	-7.39	99.07	110.90
1	B	193	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	B	18	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	B	84	MET	CG-SD-CE	-7.35	88.44	100.20
1	C	47	MET	CA-CB-CG	7.30	125.71	113.30
1	A	12	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	B	92	TYR	CB-CG-CD1	-7.10	116.74	121.00
1	B	68	VAL	CB-CA-C	-7.08	97.95	111.40
1	B	193	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	48	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	A	128	CYS	CA-CB-SG	-6.92	101.54	114.00
1	A	172	TRP	CG-CD2-CE3	6.74	139.97	133.90
1	A	63	LEU	CA-CB-CG	-6.68	99.93	115.30
1	A	38	CYS	CA-CB-SG	-6.58	102.17	114.00
1	D	215	VAL	CG1-CB-CG2	-6.52	100.46	110.90
1	C	63	LEU	CA-CB-CG	-6.45	100.46	115.30
1	B	12	TRP	CE2-CD2-CG	-6.39	102.19	107.30
1	C	29	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	18	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	D	101	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	77	THR	CA-C-N	-6.30	103.60	116.20
1	D	12	TRP	CE2-CD2-CG	-6.21	102.33	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	VAL	CA-CB-CG1	-6.18	101.63	110.90
1	D	9	MET	CA-CB-CG	-6.17	102.81	113.30
1	A	18	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	100	ARG	CA-CB-CG	-6.11	99.96	113.40
1	D	206	GLN	CA-CB-CG	6.09	126.80	113.40
1	D	246	ASP	CB-CG-OD1	6.04	123.74	118.30
1	D	3	MET	N-CA-C	-6.01	94.77	111.00
1	C	69	ASP	CB-CG-OD2	5.98	123.68	118.30
1	D	48	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	B	127	LEU	CA-CB-CG	5.95	128.98	115.30
1	B	128	CYS	CA-CB-SG	-5.93	103.32	114.00
1	B	226	GLN	CA-C-N	-5.92	104.18	117.20
1	B	103	TYR	CB-CG-CD2	-5.91	117.46	121.00
1	D	239	LEU	CA-CB-CG	5.90	128.86	115.30
1	D	63	LEU	CA-CB-CG	-5.88	101.77	115.30
1	C	68	VAL	CB-CA-C	-5.84	100.31	111.40
1	C	48	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	C	172	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	A	126	VAL	N-CA-C	-5.67	95.70	111.00
1	C	51	MET	CG-SD-CE	-5.67	91.14	100.20
1	C	38	CYS	CA-CB-SG	-5.66	103.81	114.00
1	A	103	TYR	CB-CG-CD1	5.65	124.39	121.00
1	D	62	MET	CG-SD-CE	5.63	109.21	100.20
1	D	57	GLU	CA-C-N	-5.61	104.98	116.20
1	B	29	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	D	47	MET	CA-CB-CG	5.57	122.78	113.30
1	A	172	TRP	CB-CG-CD1	-5.54	119.80	127.00
1	A	148	GLN	CG-CD-NE2	5.50	129.91	116.70
1	D	243	GLU	N-CA-CB	-5.47	100.75	110.60
1	A	207	VAL	CA-CB-CG2	-5.45	102.73	110.90
1	D	193	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	12	TRP	CG-CD1-NE1	-5.42	104.68	110.10
1	A	48	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	D	38	CYS	CA-CB-SG	-5.37	104.34	114.00
1	D	103	TYR	CB-CG-CD1	5.36	124.22	121.00
1	C	101	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	B	8	VAL	CG1-CB-CG2	-5.30	102.41	110.90
1	D	147	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	206	GLN	CA-CB-CG	5.25	124.94	113.40
1	D	21	VAL	CG1-CB-CG2	-5.22	102.55	110.90
1	B	166	ILE	O-C-N	-5.17	114.42	122.70
1	D	126	VAL	N-CA-C	-5.17	97.03	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	255	LYS	CA-CB-CG	5.16	124.74	113.40
1	C	99	GLU	CA-CB-CG	-5.16	102.06	113.40
1	C	12	TRP	CG-CD1-NE1	-5.15	104.95	110.10
1	A	102	THR	CA-CB-CG2	-5.14	105.20	112.40
1	B	172	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	A	77	THR	CA-C-N	-5.12	105.96	116.20
1	A	28	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	B	54	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	63	LEU	CA-CB-CG	-5.01	103.78	115.30
1	C	6	PRO	O-C-N	5.00	130.71	122.70

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 (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	1901	1	1892	35	0
1	B	1901	1	1892	36	0
1	C	1901	1	1892	31	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	123	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 (123) 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
1:A:53:LYS:HE3	1:B:18:ARG:HH22	1.55	0.72
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: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:9:MET:HE2	1:A:94:ILE:HD11	1.91	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:B:88:ILE:HD12	1:B:88:ILE:HA	1.85	0.43
1:D:53:LYS:HB3	1:D:53:LYS:HZ2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	34	66
All	All	1008/1016 (99%)	948 (94%)	59 (6%)	1 (0%)	51	81

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%)	177 (93%)	14 (7%)	14	38
1	B	191/191 (100%)	178 (93%)	13 (7%)	16	42
1	C	191/191 (100%)	176 (92%)	15 (8%)	12	34
1	D	191/191 (100%)	177 (93%)	14 (7%)	14	38
All	All	764/764 (100%)	708 (93%)	56 (7%)	14	38

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	47	MET
1	A	53	LYS
1	A	63	LEU
1	A	68	VAL
1	A	100	ARG
1	A	127	LEU
1	A	166	ILE
1	A	169	GLU
1	A	206	GLN
1	A	207	VAL
1	A	215	VAL
1	A	239	LEU
1	A	256	GLN
1	B	47	MET
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	215	VAL
1	B	239	LEU
1	B	255	LYS
1	C	9	MET
1	C	44	PRO
1	C	47	MET
1	C	53	LYS
1	C	63	LEU
1	C	68	VAL
1	C	100	ARG
1	C	127	LEU
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

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Mol	Chain	Res	Type
1	D	51	MET
1	D	53	LYS
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	91	GLN
1	A	148	GLN
1	A	256	GLN
1	B	91	GLN
1	B	148	GLN
1	B	210	GLN
1	C	136	ASN
1	C	148	GLN
1	C	210	GLN
1	C	256	GLN
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 monosaccharides 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	0.39	0	6,6,6	0.40	0
2	SO4	D	558	-	4,4,4	0.59	0	6,6,6	0.42	0
2	SO4	C	557	-	4,4,4	0.31	0	6,6,6	0.27	0
2	SO4	A	555	-	4,4,4	0.53	0	6,6,6	0.22	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.