



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:59 AM UTC

PDB ID : 1TSI / pdb_00001tsi
Title : STRUCTURE OF THE COMPLEX BETWEEN TRYPANOSOMAL
TRIOSEPHOSPHATE ISOMERASE AND N-HYDROXY-4-PHOSPHONO-
BUTANAMIDE: BINDING AT THE ACTIVE SITE DESPITE AN "OPEN"
FLEXIBLE LOOP
Authors : Verlinde, C.L.M.J.
Deposited on : 1992-11-19
Resolution : 2.84 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

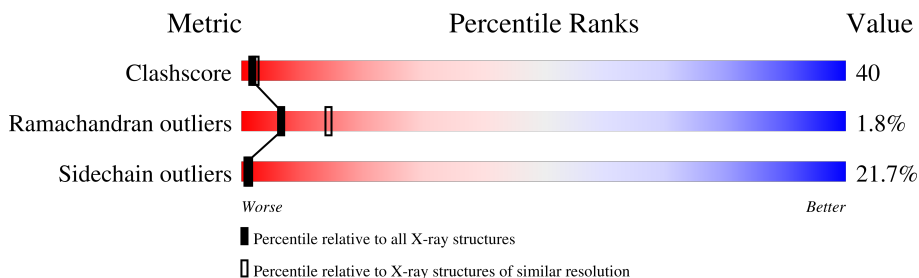
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)

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	250	33% 38% 24% 6%
1	B	250	32% 44% 21% .

2 Entry composition [i](#)

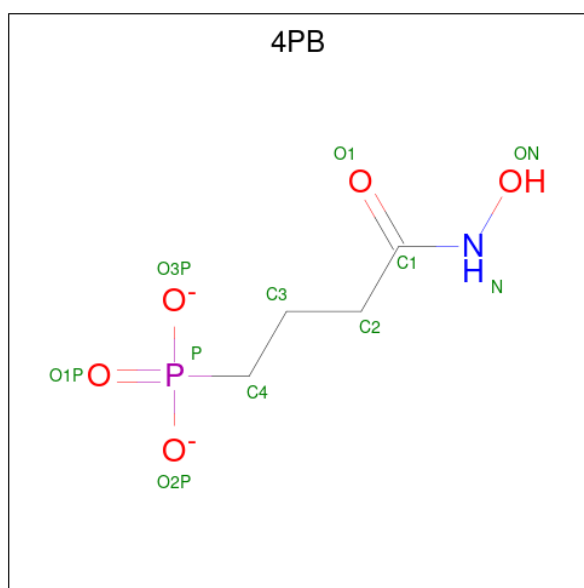
There are 3 unique types of molecules in this entry. The entry contains 3835 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1889	1200	334	350	5			
1	B	249	Total	C	N	O	S	0	0	0
			1882	1197	333	347	5			

- Molecule 2 is N-HYDROXY-4-PHOSPHONO-BUTANAMIDE (CCD ID: 4PB) (formula: $C_4H_8NO_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			11	4	1	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		

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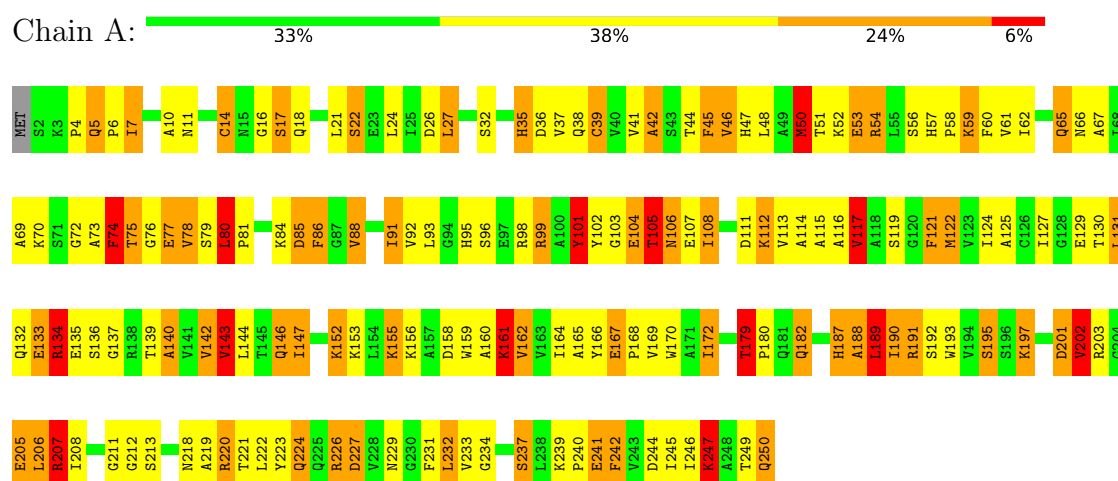
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	25	Total	O	0	0
			25	25		

3 Residue-property plots

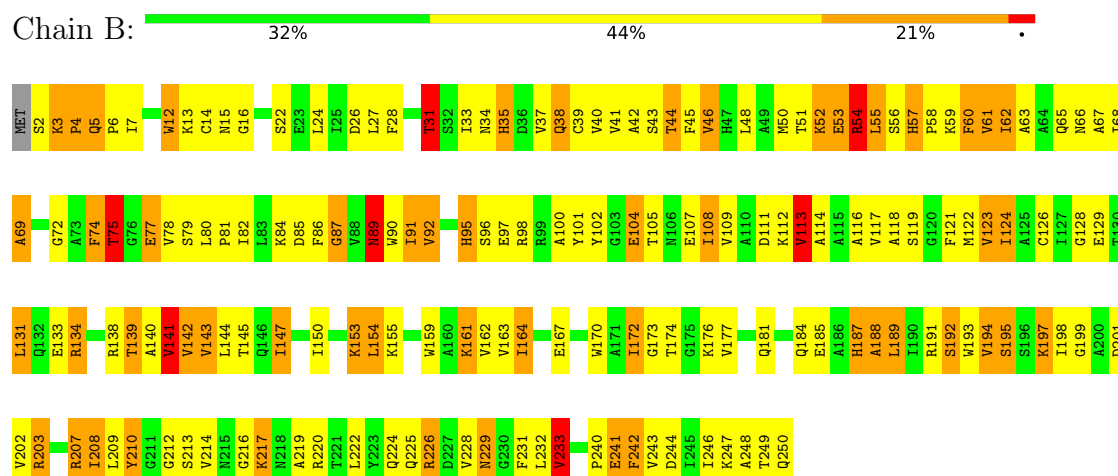
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



• 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.34Å 97.15Å 46.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.84	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.84)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.115 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3835	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: 4PB

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	1.05	0/1923	2.32	113/2606 (4.3%)
1	B	1.02	0/1916	2.24	96/2597 (3.7%)
All	All	1.03	0/3839	2.28	209/5203 (4.0%)

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	B	3	0

There are no bond length outliers.

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	GLU	CB-CA-C	-14.75	93.12	110.08
1	B	123	VAL	N-CA-C	12.81	127.03	108.58
1	A	122	MET	N-CA-C	-11.06	92.36	110.17
1	B	69	ALA	N-CA-C	10.71	122.53	111.07
1	B	34	ASN	N-CA-C	9.91	123.11	111.71
1	B	5	GLN	CA-C-O	9.66	125.57	119.29
1	B	210	TYR	CB-CA-C	9.40	125.92	110.22
1	A	10	ALA	CA-C-N	-9.39	109.76	122.72
1	A	10	ALA	C-N-CA	-9.39	109.76	122.72
1	B	162	VAL	N-CA-C	9.03	121.59	108.58
1	A	182	GLN	CA-C-N	8.67	132.09	120.65
1	A	182	GLN	C-N-CA	8.67	132.09	120.65
1	A	202	VAL	CB-CA-C	8.64	122.75	111.70
1	B	74	PHE	CA-CB-CG	-8.51	105.29	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	THR	CA-C-N	-8.37	114.43	123.30
1	B	75	THR	C-N-CA	-8.37	114.43	123.30
1	B	113	VAL	N-CA-CB	8.35	119.78	110.51
1	A	101	TYR	CB-CA-C	-8.34	96.44	110.44
1	B	249	THR	N-CA-CB	8.28	122.57	110.57
1	A	10	ALA	CA-C-O	8.27	129.43	120.58
1	A	86	PHE	CA-CB-CG	-7.95	105.85	113.80
1	A	179	THR	CA-CB-OG1	-7.83	97.86	109.60
1	B	77	GLU	N-CA-C	7.73	122.61	110.32
1	B	141	VAL	N-CA-C	-7.62	103.37	110.53
1	A	233	VAL	N-CA-C	7.55	119.48	109.21
1	A	88	VAL	N-CA-CB	7.49	119.97	111.21
1	A	134	ARG	CD-NE-CZ	-7.43	113.99	124.40
1	B	95	HIS	CA-CB-CG	-7.41	106.39	113.80
1	B	108	ILE	CB-CA-C	-7.39	102.33	112.02
1	A	142	VAL	N-CA-C	7.39	118.19	110.72
1	B	123	VAL	CB-CA-C	-7.29	101.87	110.91
1	A	189	LEU	N-CA-CB	-7.26	99.54	110.07
1	B	197	LYS	N-CA-C	7.24	120.04	111.71
1	A	47	HIS	CA-CB-CG	-7.20	106.61	113.80
1	B	16	GLY	N-CA-C	7.16	123.41	112.81
1	A	232	LEU	CA-C-N	7.12	132.38	121.71
1	A	232	LEU	C-N-CA	7.12	132.38	121.71
1	A	11	ASN	CA-CB-CG	7.04	119.64	112.60
1	A	139	THR	N-CA-C	7.03	118.59	111.07
1	A	77	GLU	N-CA-C	7.00	120.83	110.48
1	A	140	ALA	N-CA-CB	6.92	120.40	110.16
1	A	167	GLU	CA-C-O	-6.92	114.79	119.29
1	A	188	ALA	CA-C-O	6.90	127.90	120.10
1	A	14	CYS	CA-CB-SG	-6.90	98.54	114.40
1	B	16	GLY	CA-C-O	6.89	128.91	122.57
1	A	218	ASN	N-CA-C	6.87	121.33	113.15
1	B	219	ALA	CA-C-N	6.83	130.29	120.79
1	B	219	ALA	C-N-CA	6.83	130.29	120.79
1	A	162	VAL	N-CA-CB	6.78	122.55	111.44
1	A	207	ARG	N-CA-C	-6.76	98.19	109.07
1	B	153	LYS	N-CA-C	6.68	121.17	112.89
1	B	35	HIS	N-CA-C	6.61	120.32	109.94
1	A	79	SER	N-CA-C	6.56	120.23	110.52
1	A	146	GLN	O-C-N	6.56	129.63	122.15
1	B	54	ARG	N-CA-C	6.55	122.35	113.97
1	B	31	THR	CA-C-N	-6.54	113.47	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	THR	C-N-CA	-6.54	113.47	122.30
1	A	189	LEU	N-CA-C	-6.50	104.12	111.14
1	B	61	VAL	N-CA-CB	6.47	122.06	111.45
1	A	167	GLU	O-C-N	6.45	126.45	121.23
1	B	101	TYR	N-CA-C	6.44	121.31	113.38
1	B	233	VAL	N-CA-C	6.39	118.59	108.87
1	B	229	ASN	CA-C-O	6.37	127.01	119.56
1	B	233	VAL	N-CA-CB	6.36	119.34	110.56
1	A	172	ILE	CB-CA-C	-6.34	100.89	111.29
1	A	76	GLY	CA-C-O	-6.33	112.56	119.59
1	A	187	HIS	CA-CB-CG	-6.31	107.49	113.80
1	B	209	LEU	N-CA-C	6.28	119.02	110.55
1	A	5	GLN	N-CA-C	6.27	117.29	109.57
1	B	131	LEU	CB-CA-C	-6.24	100.82	110.81
1	B	89	ASN	N-CA-C	6.22	120.90	112.88
1	B	15	ASN	CA-C-N	6.20	131.05	122.06
1	B	15	ASN	C-N-CA	6.20	131.05	122.06
1	B	50	MET	CA-C-N	6.17	128.87	120.54
1	B	50	MET	C-N-CA	6.17	128.87	120.54
1	A	65	GLN	N-CA-C	6.17	120.67	113.20
1	B	231	PHE	N-CA-C	6.16	119.22	109.50
1	A	17	SER	CB-CA-C	6.12	119.85	109.99
1	A	10	ALA	O-C-N	-6.12	115.59	122.93
1	A	45	PHE	N-CA-CB	6.12	119.11	110.12
1	A	119	SER	CB-CA-C	6.11	119.82	109.55
1	A	188	ALA	N-CA-CB	-6.11	100.80	110.22
1	A	114	ALA	CA-C-N	6.09	128.73	120.38
1	A	114	ALA	C-N-CA	6.09	128.73	120.38
1	A	242	PHE	N-CA-C	-6.09	104.70	111.71
1	B	57	HIS	CA-C-N	6.06	125.68	119.56
1	B	57	HIS	C-N-CA	6.06	125.68	119.56
1	B	5	GLN	CB-CG-CD	-6.01	102.38	112.60
1	B	57	HIS	CA-CB-CG	5.96	119.76	113.80
1	A	50	MET	O-C-N	5.95	128.20	122.07
1	A	41	VAL	N-CA-CB	-5.93	104.31	110.95
1	B	113	VAL	O-C-N	5.90	127.84	121.94
1	A	105	THR	CA-CB-CG2	-5.89	100.48	110.50
1	A	58	PRO	N-CA-CB	5.88	108.93	103.46
1	A	190	ILE	N-CA-CB	5.87	117.02	110.62
1	B	150	ILE	CB-CA-C	-5.87	104.34	112.02
1	A	84	LYS	N-CA-C	-5.84	104.60	110.97
1	B	54	ARG	NE-CZ-NH1	-5.84	115.66	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ARG	CD-NE-CZ	-5.84	116.23	124.40
1	B	111	ASP	CA-CB-CG	-5.82	106.78	112.60
1	A	70	LYS	N-CA-CB	-5.82	100.60	111.13
1	B	224	GLN	N-CA-C	-5.81	106.04	113.01
1	A	84	LYS	CA-C-O	-5.80	114.91	121.00
1	A	104	GLU	N-CA-C	5.80	123.15	110.80
1	A	117	VAL	CA-CB-CG1	-5.79	100.55	110.40
1	A	99	ARG	CA-C-N	5.79	130.48	120.58
1	A	99	ARG	C-N-CA	5.79	130.48	120.58
1	A	146	GLN	CB-CG-CD	-5.78	102.78	112.60
1	B	188	ALA	CB-CA-C	5.76	120.03	110.81
1	A	219	ALA	N-CA-C	5.75	117.55	111.28
1	B	242	PHE	N-CA-CB	5.72	118.64	110.06
1	B	155	LYS	N-CA-C	-5.68	101.79	110.14
1	A	231	PHE	N-CA-C	5.67	117.81	109.24
1	A	201	ASP	N-CA-C	-5.66	103.94	111.24
1	B	95	HIS	N-CA-CB	5.65	117.99	109.34
1	A	121	PHE	CA-CB-CG	-5.65	108.15	113.80
1	A	106	ASN	CA-C-O	5.65	126.53	120.55
1	A	219	ALA	CA-C-N	5.63	128.28	120.29
1	A	219	ALA	C-N-CA	5.63	128.28	120.29
1	B	104	GLU	CA-C-N	5.63	133.49	121.45
1	B	104	GLU	C-N-CA	5.63	133.49	121.45
1	A	213	SER	N-CA-C	5.61	117.60	108.63
1	B	134	ARG	O-C-N	5.59	127.90	122.09
1	A	133	GLU	O-C-N	5.57	130.00	122.59
1	B	188	ALA	N-CA-CB	5.57	118.24	109.94
1	B	192	SER	N-CA-C	-5.56	105.13	111.14
1	A	111	ASP	N-CA-C	-5.55	104.86	111.69
1	A	117	VAL	N-CA-CB	5.53	117.02	110.55
1	B	119	SER	N-CA-C	-5.53	106.39	113.02
1	B	249	THR	CA-C-N	5.52	131.64	121.70
1	B	249	THR	C-N-CA	5.52	131.64	121.70
1	B	101	TYR	CA-CB-CG	5.52	123.83	113.90
1	A	133	GLU	CA-CB-CG	-5.51	103.07	114.10
1	A	26	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	160	ALA	N-CA-C	-5.51	106.52	113.18
1	B	87	GLY	O-C-N	5.50	128.93	122.38
1	B	100	ALA	CA-C-N	-5.49	112.76	122.26
1	B	100	ALA	C-N-CA	-5.49	112.76	122.26
1	A	75	THR	CA-C-N	-5.49	113.97	122.86
1	A	75	THR	C-N-CA	-5.49	113.97	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	VAL	CA-C-N	5.46	130.22	123.12
1	B	162	VAL	C-N-CA	5.46	130.22	123.12
1	A	182	GLN	O-C-N	5.42	129.28	122.23
1	A	161	LYS	N-CA-CB	-5.42	102.33	110.73
1	B	232	LEU	N-CA-CB	5.41	120.63	110.56
1	A	166	TYR	CA-C-O	-5.41	115.14	120.98
1	A	45	PHE	CA-CB-CG	5.40	119.20	113.80
1	B	38	GLN	CA-C-N	-5.39	114.59	122.19
1	B	38	GLN	C-N-CA	-5.39	114.59	122.19
1	A	53	GLU	N-CA-C	5.38	118.96	112.93
1	A	188	ALA	O-C-N	-5.38	115.93	122.22
1	A	80	LEU	CA-C-N	5.37	124.88	119.19
1	A	80	LEU	C-N-CA	5.37	124.88	119.19
1	A	70	LYS	N-CA-C	5.37	117.93	108.75
1	B	139	THR	CB-CA-C	-5.36	101.94	110.84
1	B	60	PHE	N-CA-C	5.33	118.75	110.17
1	B	84	LYS	CA-C-N	5.32	127.41	120.28
1	B	84	LYS	C-N-CA	5.32	127.41	120.28
1	B	231	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	143	VAL	CA-CB-CG1	5.31	119.43	110.40
1	B	92	VAL	N-CA-C	-5.30	100.01	107.75
1	A	99	ARG	NE-CZ-NH1	-5.29	116.21	121.50
1	A	179	THR	N-CA-C	-5.29	101.31	109.41
1	B	228	VAL	CA-C-O	-5.26	114.53	120.74
1	A	74	PHE	N-CA-C	-5.24	98.68	107.32
1	A	7	ILE	N-CA-CB	5.23	120.03	111.45
1	B	177	VAL	N-CA-C	5.23	115.31	107.51
1	B	228	VAL	CB-CA-C	-5.22	104.97	111.08
1	A	101	TYR	CA-CB-CG	5.21	123.28	113.90
1	B	187	HIS	N-CA-C	-5.20	105.69	111.36
1	A	39	CYS	CA-C-N	-5.19	115.05	122.84
1	A	39	CYS	C-N-CA	-5.19	115.05	122.84
1	B	145	THR	CA-CB-CG2	-5.19	101.68	110.50
1	A	85	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	12	TRP	O-C-N	5.17	129.60	122.46
1	B	4	PRO	N-CA-CB	5.17	108.68	103.25
1	B	46	VAL	CA-C-N	-5.17	114.41	122.73
1	B	46	VAL	C-N-CA	-5.17	114.41	122.73
1	B	57	HIS	CB-CA-C	5.15	118.00	109.56
1	A	27	LEU	N-CA-C	-5.14	105.59	111.14
1	A	119	SER	CA-C-O	5.13	124.70	119.05
1	A	41	VAL	N-CA-C	5.13	116.13	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	LYS	CB-CA-C	-5.13	101.43	109.22
1	B	233	VAL	CA-CB-CG2	5.12	119.11	110.40
1	B	241	GLU	CB-CA-C	-5.12	99.53	110.32
1	A	108	ILE	N-CA-CB	5.11	117.11	110.57
1	A	50	MET	CA-C-N	5.10	129.31	120.58
1	A	50	MET	C-N-CA	5.10	129.31	120.58
1	A	73	ALA	N-CA-C	5.09	117.59	108.17
1	B	143	VAL	CA-C-N	5.09	127.36	120.44
1	B	143	VAL	C-N-CA	5.09	127.36	120.44
1	A	92	VAL	CA-C-O	-5.09	114.96	120.71
1	B	118	ALA	N-CA-C	5.09	118.95	112.34
1	A	147	ILE	N-CA-C	-5.08	105.59	110.72
1	A	220	ARG	CB-CA-C	-5.07	102.24	110.85
1	A	201	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	143	VAL	N-CA-C	5.05	119.85	109.34
1	A	42	ALA	CA-C-O	5.05	126.29	120.84
1	A	182	GLN	CA-CB-CG	-5.05	104.00	114.10
1	A	46	VAL	N-CA-C	5.04	118.13	111.17
1	B	119	SER	CB-CA-C	-5.04	101.40	110.37
1	A	166	TYR	CB-CA-C	-5.03	102.54	111.05
1	B	210	TYR	N-CA-CB	5.03	118.62	110.17
1	A	146	GLN	CB-CA-C	-5.03	102.30	110.85
1	A	247	LYS	N-CA-CB	5.03	118.07	110.28
1	A	189	LEU	CB-CA-C	-5.02	102.96	110.90
1	B	194	VAL	N-CA-CB	5.02	116.66	110.64
1	A	222	LEU	CB-CA-C	-5.01	101.39	110.56
1	B	225	GLN	N-CA-CB	5.01	117.71	109.95

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	34	ASN	CA
1	B	210	TYR	CA
1	B	249	THR	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1889	0	1925	161	2
1	B	1882	0	1917	164	0
2	A	11	0	8	3	0
3	A	28	0	0	1	0
3	B	25	0	0	6	0
All	All	3835	0	3850	306	2

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 40.

All (306) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:VAL:HG22	1:B:61:VAL:HG23	1.28	1.10
1:B:5:GLN:NE2	1:B:207:ARG:HH12	1.50	1.07
1:A:91:ILE:HD13	1:A:93:LEU:HD11	1.37	1.04
1:B:5:GLN:HE21	1:B:207:ARG:NH1	1.57	1.01
1:A:195:SER:HB2	1:A:203:ARG:HD3	1.43	1.01
1:B:191:ARG:HG3	1:B:203:ARG:HG3	1.45	0.98
1:B:57:HIS:HD2	1:B:59:LYS:H	1.07	0.94
1:B:5:GLN:HE21	1:B:207:ARG:HH12	0.92	0.89
1:B:133:GLU:HG2	1:B:138:ARG:NH1	1.87	0.89
1:A:69:ALA:HA	1:A:80:LEU:CD2	2.03	0.88
1:A:191:ARG:HD3	1:A:203:ARG:HD2	1.56	0.87
1:B:91:ILE:CG2	1:B:123:VAL:HG22	2.05	0.86
1:B:57:HIS:CD2	1:B:59:LYS:H	1.93	0.85
1:B:69:ALA:HA	1:B:80:LEU:HD12	1.59	0.84
1:B:191:ARG:CG	1:B:203:ARG:HG3	2.07	0.83
1:A:98:ARG:HG2	1:A:98:ARG:HH11	1.44	0.82
1:A:50:MET:O	1:A:54:ARG:HB2	1.80	0.80
1:A:69:ALA:HA	1:A:80:LEU:HD23	1.61	0.80
1:B:52:LYS:HE2	1:B:86:PHE:CE2	2.17	0.79
1:A:195:SER:HB2	1:A:203:ARG:CD	2.12	0.79
1:A:144:LEU:HD21	1:A:189:LEU:CD1	2.13	0.79
1:B:187:HIS:NE2	1:B:210:TYR:HB2	1.98	0.78
1:B:105:THR:OG1	1:B:108:ILE:HG12	1.83	0.78
1:A:98:ARG:HG2	1:A:98:ARG:NH1	1.98	0.77
1:B:55:LEU:HD12	1:B:62:ILE:HD11	1.67	0.77
1:A:195:SER:CB	1:A:203:ARG:HD3	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ILE:HD13	1:A:93:LEU:CD1	2.13	0.75
1:B:91:ILE:HG13	1:B:92:VAL:H	1.49	0.75
1:A:191:ARG:HD3	1:A:203:ARG:CG	2.16	0.75
1:B:248:ALA:O	1:B:250:GLN:HG2	1.88	0.73
1:B:42:ALA:HA	1:B:63:ALA:O	1.88	0.73
1:A:144:LEU:HD21	1:A:189:LEU:HD12	1.71	0.73
1:B:12:TRP:CE3	1:B:43:SER:HB3	2.24	0.73
1:B:68:ILE:HD13	1:B:77:GLU:HB3	1.70	0.72
1:B:113:VAL:O	1:B:117:VAL:HG23	1.90	0.72
1:B:184:GLN:NE2	1:B:188:ALA:HB2	2.04	0.72
1:A:191:ARG:HD3	1:A:203:ARG:CD	2.19	0.71
1:A:77:GLU:HG3	1:B:102:TYR:OH	1.90	0.71
1:A:96:SER:HB3	1:A:167:GLU:OE1	1.89	0.71
1:B:181:GLN:O	1:B:185:GLU:HG3	1.90	0.71
1:B:27:LEU:CD2	1:B:240:PRO:HB3	2.21	0.71
1:B:91:ILE:HG13	1:B:92:VAL:N	2.05	0.71
1:A:191:ARG:NH2	1:A:206:LEU:O	2.24	0.70
1:B:104:GLU:HG3	1:B:108:ILE:HG21	1.73	0.70
1:B:217:LYS:O	1:B:220:ARG:HD2	1.92	0.70
1:A:72:GLY:O	1:B:14:CYS:HB3	1.92	0.69
1:A:172:ILE:HD12	2:A:600:4PB:H22	1.75	0.69
1:B:241:GLU:HA	1:B:244:ASP:OD2	1.93	0.69
1:B:40:VAL:HG22	1:B:61:VAL:CG2	2.15	0.68
1:B:91:ILE:HG23	1:B:123:VAL:HG22	1.74	0.68
1:B:139:THR:O	1:B:143:VAL:HG22	1.93	0.68
1:A:50:MET:HG2	1:A:51:THR:N	2.08	0.68
1:B:89:ASN:HB3	3:B:632:HOH:O	1.92	0.68
1:A:69:ALA:HA	1:A:80:LEU:HD22	1.74	0.68
1:A:74:PHE:HB3	1:B:102:TYR:OH	1.94	0.68
1:B:172:ILE:N	1:B:172:ILE:HD13	2.08	0.68
1:A:191:ARG:CD	1:A:203:ARG:HD2	2.24	0.68
1:B:116:ALA:O	1:B:121:PHE:HB2	1.94	0.68
1:B:55:LEU:CD1	1:B:62:ILE:HD11	2.25	0.67
1:B:124:ILE:HG12	1:B:163:VAL:CG1	2.25	0.66
1:B:226:ARG:NH1	3:B:647:HOH:O	2.28	0.66
1:A:5:GLN:O	1:A:207:ARG:HD2	1.96	0.65
1:B:79:SER:HB2	1:B:81:PRO:HD2	1.79	0.65
1:A:129:GLU:O	1:A:169:VAL:HB	1.97	0.65
1:A:39:CYS:HB3	1:A:60:PHE:CE1	2.32	0.64
1:A:39:CYS:HB2	1:A:59:LYS:O	1.97	0.64
1:B:13:LYS:HA	1:B:65:GLN:OE1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LEU:HD21	1:B:240:PRO:HB3	1.80	0.64
1:A:130:THR:HG22	1:A:133:GLU:CD	2.23	0.64
1:B:5:GLN:NE2	1:B:207:ARG:NH1	2.27	0.64
1:A:80:LEU:CB	1:A:81:PRO:HD3	2.28	0.64
1:A:143:VAL:O	1:A:147:ILE:HG22	1.99	0.64
1:B:108:ILE:O	1:B:112:LYS:HG3	1.98	0.63
1:B:133:GLU:HG2	1:B:138:ARG:HH12	1.64	0.63
1:A:22:SER:HB3	1:A:54:ARG:NH2	2.13	0.63
1:A:144:LEU:HA	1:A:147:ILE:HG22	1.80	0.63
1:A:91:ILE:CD1	1:A:93:LEU:HD11	2.23	0.62
1:A:179:THR:OG1	1:A:182:GLN:HB2	1.99	0.62
1:A:202:VAL:O	1:A:205:GLU:N	2.31	0.62
1:B:68:ILE:HD13	1:B:77:GLU:CB	2.28	0.62
1:B:41:VAL:O	1:B:63:ALA:N	2.31	0.61
1:B:37:VAL:HG22	1:B:38:GLN:N	2.16	0.61
1:A:48:LEU:HD13	1:A:88:VAL:HG21	1.83	0.60
1:A:189:LEU:O	1:A:192:SER:HB3	2.00	0.60
1:B:104:GLU:HG2	1:B:109:VAL:HG22	1.82	0.60
1:A:93:LEU:O	1:A:125:ALA:HA	2.01	0.60
1:A:130:THR:HG22	1:A:133:GLU:OE1	2.02	0.60
1:B:28:PHE:O	1:B:31:THR:HB	2.02	0.60
1:A:105:THR:HG23	1:A:108:ILE:HD12	1.83	0.60
1:A:106:ASN:HB2	1:A:107:GLU:OE2	2.02	0.59
1:B:51:THR:CG2	1:B:62:ILE:HG13	2.33	0.59
1:B:41:VAL:N	1:B:61:VAL:O	2.29	0.59
1:B:95:HIS:CE1	1:B:97:GLU:H	2.21	0.59
1:A:18:GLN:HA	1:A:50:MET:HE1	1.84	0.58
1:A:158:ASP:O	1:A:161:LYS:HB2	2.03	0.58
1:B:104:GLU:HG3	1:B:108:ILE:CG2	2.33	0.58
1:A:105:THR:H	1:A:108:ILE:HD12	1.69	0.58
1:A:131:LEU:HB3	1:A:132:GLN:NE2	2.18	0.58
1:B:51:THR:HG22	1:B:62:ILE:CG1	2.33	0.58
1:A:241:GLU:O	1:A:244:ASP:HB2	2.03	0.58
1:A:75:THR:HG23	1:B:65:GLN:HB3	1.86	0.58
1:A:38:GLN:NE2	1:A:61:VAL:HG13	2.18	0.58
1:A:16:GLY:HA2	1:A:21:LEU:HD21	1.86	0.57
1:A:168:PRO:HG2	1:A:212:GLY:HA3	1.86	0.57
1:A:195:SER:HA	1:A:203:ARG:HB2	1.86	0.57
1:B:79:SER:OG	1:B:82:ILE:HD12	2.04	0.57
1:A:127:ILE:HB	1:A:146:GLN:OE1	2.04	0.57
1:A:250:GLN:NE2	1:A:250:GLN:HA	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLY:O	2:A:600:4PB:H21	2.04	0.57
1:A:220:ARG:O	1:A:224:GLN:HB3	2.05	0.57
1:A:227:ASP:OD1	1:A:227:ASP:N	2.34	0.56
1:B:44:THR:HG23	3:B:603:HOH:O	2.03	0.56
1:A:62:ILE:HD11	1:A:88:VAL:HG22	1.85	0.56
1:B:39:CYS:O	1:B:61:VAL:N	2.37	0.56
1:B:191:ARG:CD	1:B:203:ARG:HG3	2.36	0.56
1:A:38:GLN:HE22	1:A:61:VAL:HG13	1.71	0.56
1:A:101:TYR:HE2	1:B:74:PHE:CE1	2.23	0.56
1:A:191:ARG:O	1:A:203:ARG:HG3	2.06	0.56
1:A:6:PRO:HD2	1:A:36:ASP:O	2.05	0.56
1:B:134:ARG:HD2	1:B:170:TRP:CD2	2.41	0.56
1:A:37:VAL:HG22	1:A:38:GLN:N	2.21	0.56
1:A:226:ARG:HB3	1:A:227:ASP:OD1	2.06	0.55
1:B:124:ILE:HA	1:B:163:VAL:HB	1.87	0.55
1:A:131:LEU:HD23	1:A:170:TRP:HB2	1.89	0.55
1:A:249:THR:O	1:A:250:GLN:HB2	2.06	0.55
1:A:99:ARG:HG2	1:A:99:ARG:HH11	1.72	0.55
1:A:172:ILE:CD1	2:A:600:4PB:H22	2.36	0.55
1:B:128:GLY:HA3	1:B:167:GLU:O	2.06	0.55
1:A:46:VAL:HG23	1:B:78:VAL:HG21	1.89	0.54
1:A:191:ARG:O	1:A:195:SER:HB3	2.07	0.54
1:B:124:ILE:HG12	1:B:163:VAL:HG11	1.89	0.54
1:B:139:THR:HG22	1:B:140:ALA:N	2.15	0.54
1:A:234:GLY:O	1:A:237:SER:HB3	2.08	0.54
1:B:26:ASP:OD1	1:B:54:ARG:NH2	2.40	0.54
1:B:12:TRP:CZ3	1:B:43:SER:HB3	2.43	0.54
1:A:144:LEU:HA	1:A:147:ILE:CG2	2.37	0.53
1:B:65:GLN:O	1:B:66:ASN:HB2	2.08	0.53
1:B:134:ARG:HD2	1:B:170:TRP:CG	2.43	0.53
1:B:210:TYR:CE1	1:B:222:LEU:HD13	2.43	0.53
1:A:190:ILE:HB	1:A:208:ILE:HD13	1.91	0.52
1:B:80:LEU:N	1:B:81:PRO:HD2	2.25	0.52
1:B:226:ARG:HH11	1:B:226:ARG:HB3	1.72	0.52
1:A:155:LYS:O	1:A:158:ASP:HB2	2.10	0.52
1:A:80:LEU:HB2	1:A:81:PRO:HD3	1.91	0.52
1:A:188:ALA:O	1:A:192:SER:HB2	2.10	0.52
1:A:45:PHE:CD2	1:A:78:VAL:HG21	2.43	0.52
1:A:101:TYR:CE2	1:B:74:PHE:CE1	2.97	0.52
1:A:191:ARG:HH11	1:A:191:ARG:CG	2.22	0.52
1:B:24:LEU:O	1:B:27:LEU:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HB3	1:A:132:GLN:HE22	1.75	0.52
1:B:144:LEU:HD21	1:B:189:LEU:HD22	1.93	0.51
1:A:112:LYS:NZ	3:A:627:HOH:O	2.43	0.51
1:A:187:HIS:HB3	1:A:227:ASP:HB2	1.91	0.51
1:A:202:VAL:O	1:A:205:GLU:HB2	2.10	0.51
1:A:102:TYR:CZ	1:B:77:GLU:HG3	2.45	0.51
1:A:35:HIS:H	1:A:35:HIS:CD2	2.29	0.50
1:A:191:ARG:HD3	1:A:203:ARG:HG2	1.90	0.50
1:B:51:THR:HG22	1:B:62:ILE:HG13	1.93	0.50
1:A:93:LEU:HD22	1:A:112:LYS:HB3	1.94	0.50
1:A:98:ARG:NH1	1:A:102:TYR:CD2	2.79	0.50
1:A:134:ARG:HD3	1:A:170:TRP:CG	2.47	0.50
1:A:135:GLU:C	1:A:137:GLY:H	2.19	0.50
1:A:144:LEU:CD2	1:A:189:LEU:HD12	2.40	0.50
1:B:6:PRO:HA	1:B:229:ASN:O	2.12	0.50
1:B:247:LYS:O	1:B:250:GLN:OE1	2.29	0.50
1:A:101:TYR:CE2	1:B:74:PHE:HE1	2.30	0.50
1:A:223:TYR:CD2	1:A:249:THR:HA	2.47	0.50
1:B:95:HIS:ND1	1:B:96:SER:N	2.60	0.50
1:B:107:GLU:CD	1:B:107:GLU:H	2.20	0.50
1:B:66:ASN:CG	1:B:67:ALA:H	2.20	0.49
1:A:133:GLU:O	1:A:136:SER:N	2.46	0.49
1:B:51:THR:HG21	1:B:62:ILE:HG13	1.95	0.49
1:B:95:HIS:ND1	1:B:95:HIS:C	2.70	0.49
1:A:45:PHE:HB2	1:B:45:PHE:HB2	1.95	0.49
1:B:91:ILE:CG1	1:B:92:VAL:N	2.76	0.49
1:A:142:VAL:O	1:A:146:GLN:HG3	2.13	0.48
1:A:101:TYR:HE2	1:B:74:PHE:CD1	2.30	0.48
1:A:98:ARG:HH11	1:A:98:ARG:CG	2.22	0.48
1:B:66:ASN:ND2	1:B:67:ALA:H	2.11	0.48
1:B:33:ILE:HD11	1:B:246:ILE:CD1	2.43	0.48
1:B:187:HIS:CE1	1:B:210:TYR:HB2	2.48	0.48
1:B:208:ILE:H	1:B:229:ASN:HB2	1.79	0.48
1:A:5:GLN:HG3	1:A:6:PRO:HD2	1.96	0.48
1:B:80:LEU:N	1:B:81:PRO:CD	2.77	0.48
1:B:194:VAL:HG13	1:B:198:ILE:HD12	1.95	0.48
1:A:18:GLN:HG2	1:A:50:MET:HE1	1.95	0.48
1:B:173:GLY:C	1:B:174:THR:HG23	2.39	0.47
1:A:57:HIS:CD2	1:A:59:LYS:HB2	2.49	0.47
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.75	0.47
1:A:144:LEU:CA	1:A:147:ILE:HG22	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLU:CD	1:A:107:GLU:H	2.22	0.47
1:B:147:ILE:HD11	1:B:159:TRP:HH2	1.80	0.47
1:B:194:VAL:HG13	1:B:198:ILE:CD1	2.45	0.47
1:A:134:ARG:HD3	1:A:170:TRP:CD2	2.50	0.47
1:B:248:ALA:C	1:B:250:GLN:H	2.22	0.47
1:A:191:ARG:CG	1:A:191:ARG:NH1	2.77	0.47
1:A:39:CYS:HB3	1:A:60:PHE:CD1	2.49	0.47
1:B:40:VAL:CG2	1:B:61:VAL:HG23	2.20	0.47
1:B:250:GLN:HA	3:B:636:HOH:O	2.15	0.47
1:A:37:VAL:CG2	1:A:38:GLN:N	2.78	0.46
1:B:242:PHE:O	1:B:246:ILE:HG13	2.15	0.46
1:B:2:SER:HB2	3:B:630:HOH:O	2.15	0.46
1:A:18:GLN:O	1:A:22:SER:OG	2.34	0.46
1:B:141:VAL:CG2	1:B:142:VAL:N	2.79	0.46
1:A:45:PHE:HB2	1:B:45:PHE:CB	2.46	0.46
1:A:130:THR:HG23	1:A:133:GLU:H	1.81	0.46
1:A:250:GLN:NE2	1:A:250:GLN:CA	2.79	0.46
1:A:246:ILE:O	1:A:249:THR:OG1	2.34	0.46
1:B:124:ILE:CG1	1:B:163:VAL:HG11	2.46	0.46
1:B:90:TRP:CZ2	1:B:122:MET:HG2	2.51	0.46
1:A:102:TYR:OH	1:B:77:GLU:HG3	2.15	0.45
1:A:164:ILE:HD12	1:A:206:LEU:HD11	1.98	0.45
1:B:37:VAL:CG2	1:B:38:GLN:N	2.79	0.45
1:A:187:HIS:CE1	1:A:208:ILE:HG22	2.51	0.45
1:B:33:ILE:CD1	1:B:246:ILE:HD13	2.46	0.45
1:B:195:SER:HA	1:B:199:GLY:O	2.15	0.45
1:B:161:LYS:HA	1:B:161:LYS:HD2	1.64	0.45
1:A:155:LYS:O	1:A:158:ASP:N	2.50	0.45
1:A:195:SER:HB2	1:A:203:ARG:CG	2.45	0.45
1:A:240:PRO:C	1:A:242:PHE:H	2.25	0.45
1:A:99:ARG:HH11	1:A:99:ARG:CG	2.25	0.45
1:A:66:ASN:CG	1:A:67:ALA:N	2.75	0.44
1:A:105:THR:HG23	1:A:108:ILE:CD1	2.47	0.44
1:A:144:LEU:HD21	1:A:189:LEU:HD11	1.97	0.44
1:B:68:ILE:HD13	1:B:68:ILE:HG21	1.56	0.44
1:B:113:VAL:HG12	1:B:114:ALA:N	2.26	0.44
1:A:103:GLY:O	1:A:108:ILE:HD12	2.17	0.44
1:A:191:ARG:HH11	1:A:191:ARG:HG3	1.82	0.44
1:B:57:HIS:HD2	1:B:59:LYS:N	1.92	0.44
1:A:5:GLN:HG2	1:A:6:PRO:O	2.16	0.44
1:A:240:PRO:O	1:A:242:PHE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:CA	1:A:203:ARG:HB2	2.48	0.44
1:A:91:ILE:O	1:A:91:ILE:HG23	2.18	0.44
1:A:112:LYS:O	1:A:115:ALA:HB3	2.18	0.44
1:A:14:CYS:HB3	1:B:72:GLY:O	2.18	0.43
1:B:113:VAL:HG22	1:B:123:VAL:HG11	2.00	0.43
1:B:198:ILE:CG2	1:B:202:VAL:HG21	2.48	0.43
1:B:243:VAL:O	1:B:243:VAL:HG12	2.17	0.43
1:B:126:CYS:HB3	1:B:167:GLU:OE1	2.18	0.43
1:B:154:LEU:HD12	1:B:154:LEU:HA	1.62	0.43
1:B:210:TYR:CD1	1:B:222:LEU:HD13	2.53	0.43
1:A:117:VAL:HG13	1:A:161:LYS:HB3	2.00	0.43
1:B:7:ILE:HD11	1:B:207:ARG:CZ	2.48	0.43
1:B:107:GLU:CD	1:B:107:GLU:N	2.77	0.43
1:B:210:TYR:CE1	1:B:222:LEU:CD1	3.02	0.43
1:A:48:LEU:O	1:A:52:LYS:HB3	2.19	0.43
1:A:122:MET:SD	1:A:161:LYS:HD2	2.59	0.43
1:A:140:ALA:O	1:A:144:LEU:HG	2.19	0.43
1:B:24:LEU:HD23	1:B:24:LEU:HA	1.83	0.43
1:A:14:CYS:O	1:B:72:GLY:N	2.50	0.42
1:B:33:ILE:HD13	1:B:246:ILE:HG21	2.01	0.42
1:A:86:PHE:CD1	1:B:46:VAL:CG1	3.01	0.42
1:B:68:ILE:CD1	1:B:77:GLU:CB	2.97	0.42
1:B:39:CYS:O	1:B:60:PHE:HA	2.19	0.42
1:B:164:ILE:HD12	1:B:164:ILE:HA	1.64	0.42
1:A:240:PRO:C	1:A:242:PHE:N	2.78	0.42
1:B:233:VAL:HA	3:B:650:HOH:O	2.18	0.42
1:A:102:TYR:CE2	1:B:77:GLU:HG3	2.54	0.42
1:A:95:HIS:CD2	1:B:75:THR:HG21	2.55	0.42
1:A:132:GLN:N	1:A:132:GLN:CD	2.78	0.42
1:A:134:ARG:HH11	1:A:134:ARG:HD2	1.46	0.42
1:B:52:LYS:HE3	1:B:86:PHE:O	2.19	0.42
1:B:124:ILE:HD13	1:B:124:ILE:HG21	1.84	0.42
1:B:193:TRP:O	1:B:197:LYS:HB2	2.20	0.42
1:B:220:ARG:H	1:B:220:ARG:HG3	1.38	0.42
1:A:99:ARG:HG2	1:A:99:ARG:NH1	2.32	0.42
1:A:152:LYS:HA	1:A:152:LYS:HD3	1.45	0.42
1:A:193:TRP:CE2	1:A:197:LYS:HG2	2.54	0.42
1:B:39:CYS:N	1:B:59:LYS:O	2.45	0.42
1:A:116:ALA:HB1	1:A:121:PHE:HB2	2.01	0.42
1:B:33:ILE:HD11	1:B:246:ILE:HD12	2.02	0.42
1:B:66:ASN:CG	1:B:67:ALA:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:TYR:HE1	1:B:222:LEU:CD1	2.33	0.42
1:A:17:SER:O	1:A:21:LEU:HG	2.19	0.41
1:A:46:VAL:O	1:A:46:VAL:HG12	2.20	0.41
1:A:191:ARG:CD	1:A:203:ARG:HG2	2.49	0.41
1:B:53:GLU:HG2	1:B:54:ARG:HG2	2.02	0.41
1:B:191:ARG:CD	1:B:203:ARG:CG	2.98	0.41
1:B:35:HIS:CD2	1:B:35:HIS:H	2.38	0.41
1:B:35:HIS:O	1:B:59:LYS:HE2	2.19	0.41
1:B:85:ASP:C	1:B:87:GLY:N	2.77	0.41
1:B:233:VAL:HG23	1:B:242:PHE:HE1	1.86	0.41
1:B:214:VAL:HB	1:B:233:VAL:HG13	2.03	0.41
1:B:5:GLN:HA	1:B:6:PRO:HD3	1.63	0.41
1:B:22:SER:O	1:B:26:ASP:N	2.48	0.41
1:A:57:HIS:CD2	1:A:60:PHE:HD2	2.39	0.41
1:A:168:PRO:CG	1:A:212:GLY:HA3	2.49	0.41
1:A:180:PRO:C	1:A:182:GLN:N	2.78	0.41
1:A:4:PRO:HD2	1:A:229:ASN:ND2	2.35	0.41
1:A:42:ALA:O	1:A:65:GLN:NE2	2.41	0.41
1:B:48:LEU:HA	1:B:48:LEU:HD12	1.86	0.41
1:A:18:GLN:HG2	1:A:50:MET:CE	2.51	0.41
1:A:62:ILE:CD1	1:A:88:VAL:HG22	2.51	0.41
1:B:33:ILE:HD13	1:B:246:ILE:HD13	2.03	0.41
1:B:208:ILE:N	1:B:229:ASN:HB2	2.35	0.41
1:A:65:GLN:O	1:A:66:ASN:HB2	2.20	0.41
1:B:95:HIS:ND1	1:B:97:GLU:N	2.62	0.40
1:A:247:LYS:C	1:A:249:THR:H	2.27	0.40
1:B:57:HIS:HA	1:B:58:PRO:HD3	1.63	0.40
1:A:75:THR:OG1	1:B:13:LYS:HG2	2.21	0.40
1:A:164:ILE:CG2	1:A:165:ALA:N	2.85	0.40
1:A:232:LEU:HD12	1:A:232:LEU:HA	1.94	0.40
1:B:184:GLN:HE22	1:B:188:ALA:HB2	1.81	0.40
1:B:241:GLU:O	1:B:244:ASP:HB2	2.22	0.40
1:A:105:THR:HG23	1:A:105:THR:H	1.35	0.40
1:B:105:THR:O	1:B:109:VAL:HG23	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LYS:CD	1:A:250:GLN:OE1[2_564]	1.49	0.71
1:A:161:LYS:CE	1:A:250:GLN:OE1[2_564]	1.57	0.63

5.3 Torsion angles

5.3.1 Protein backbone

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	247/250 (99%)	210 (85%)	33 (13%)	4 (2%)	7	16
1	B	247/250 (99%)	210 (85%)	32 (13%)	5 (2%)	6	12
All	All	494/500 (99%)	420 (85%)	65 (13%)	9 (2%)	6	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	GLU
1	B	75	THR
1	A	241	GLU
1	A	159	TRP
1	B	212	GLY
1	B	216	GLY
1	A	134	ARG
1	B	142	VAL
1	B	4	PRO

5.3.2 Protein sidechains

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	197/198 (100%)	147 (75%)	50 (25%)	0	0
1	B	195/198 (98%)	160 (82%)	35 (18%)	2	3
All	All	392/396 (99%)	307 (78%)	85 (22%)	1	1

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	22	SER
1	A	24	LEU
1	A	27	LEU
1	A	32	SER
1	A	35	HIS
1	A	44	THR
1	A	50	MET
1	A	53	GLU
1	A	54	ARG
1	A	56	SER
1	A	59	LYS
1	A	74	PHE
1	A	78	VAL
1	A	80	LEU
1	A	85	ASP
1	A	91	ILE
1	A	101	TYR
1	A	105	THR
1	A	112	LYS
1	A	113	VAL
1	A	117	VAL
1	A	124	ILE
1	A	131	LEU
1	A	143	VAL
1	A	152	LYS
1	A	153	LYS
1	A	155	LYS
1	A	156	LYS
1	A	161	LYS
1	A	162	VAL
1	A	179	THR
1	A	189	LEU
1	A	191	ARG
1	A	195	SER
1	A	197	LYS
1	A	201	ASP
1	A	202	VAL
1	A	205	GLU
1	A	206	LEU
1	A	207	ARG
1	A	221	THR

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Mol	Chain	Res	Type
1	A	224	GLN
1	A	226	ARG
1	A	227	ASP
1	A	237	SER
1	A	239	LYS
1	A	245	ILE
1	A	247	LYS
1	A	250	GLN
1	B	3	LYS
1	B	31	THR
1	B	44	THR
1	B	52	LYS
1	B	53	GLU
1	B	54	ARG
1	B	55	LEU
1	B	56	SER
1	B	62	ILE
1	B	89	ASN
1	B	91	ILE
1	B	98	ARG
1	B	113	VAL
1	B	124	ILE
1	B	129	GLU
1	B	131	LEU
1	B	141	VAL
1	B	147	ILE
1	B	153	LYS
1	B	154	LEU
1	B	161	LYS
1	B	164	ILE
1	B	172	ILE
1	B	176	LYS
1	B	189	LEU
1	B	192	SER
1	B	195	SER
1	B	201	ASP
1	B	203	ARG
1	B	207	ARG
1	B	208	ILE
1	B	213	SER
1	B	217	LYS
1	B	226	ARG

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Mol	Chain	Res	Type
1	B	233	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	38	GLN
1	A	57	HIS
1	A	224	GLN
1	A	225	GLN
1	A	250	GLN
1	B	5	GLN
1	B	15	ASN
1	B	34	ASN
1	B	35	HIS
1	B	57	HIS
1	B	66	ASN
1	B	187	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	4PB	A	600	-	10,10,10	0.96	0	12,13,13	1.82	3 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4PB	A	600	-	-	0/9/9/9	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	4PB	C3-C2-C1	-3.65	103.06	113.19
2	A	600	4PB	O2P-P-C4	2.67	113.29	106.91
2	A	600	4PB	ON-N-C1	2.55	123.57	119.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	4PB	3	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 ⓘ

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.