



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:55 am GMT

PDB ID : 1TSI  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

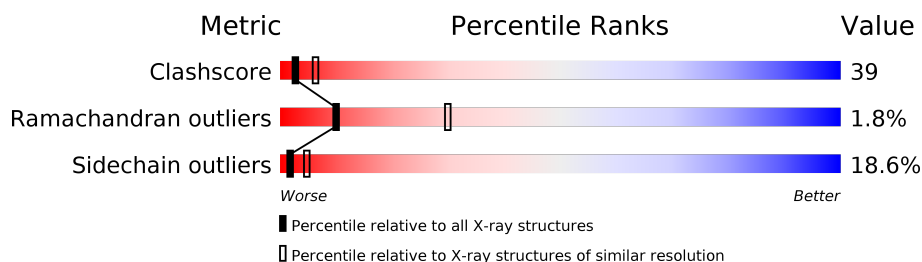
# 1 Overall quality at a glance

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	112137	3975 (2.88-2.80)
Ramachandran outliers	110173	3902 (2.88-2.80)
Sidechain outliers	110143	3905 (2.88-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	
1	B	250	

## 2 Entry composition [i](#)

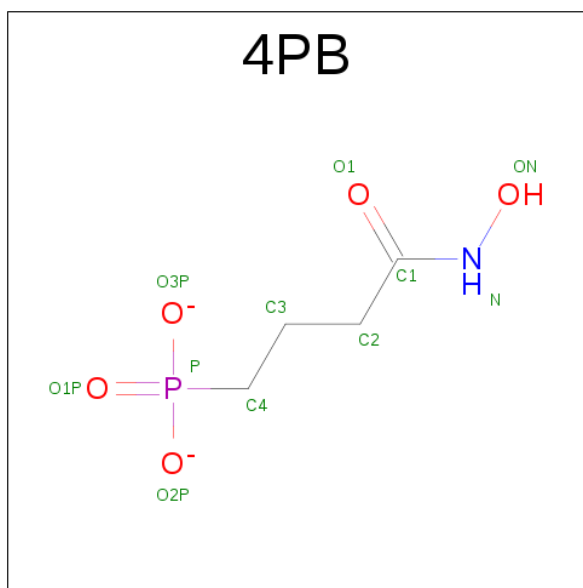
There are 3 unique types of molecules in this entry. The entry contains 3835 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 4PB) (formula: C<sub>4</sub>H<sub>8</sub>NO<sub>5</sub>P).



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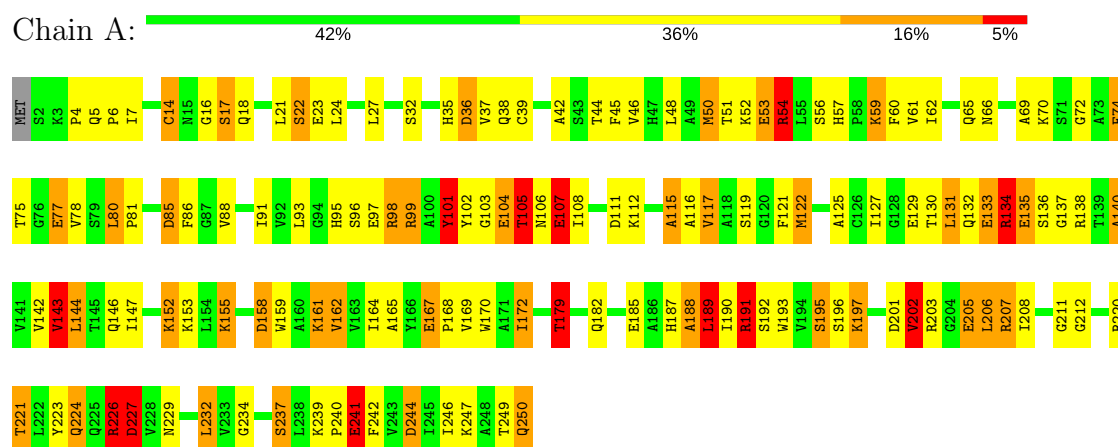
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	25	Total	O	0	0
			25	25		

### 3 Residue-property plots

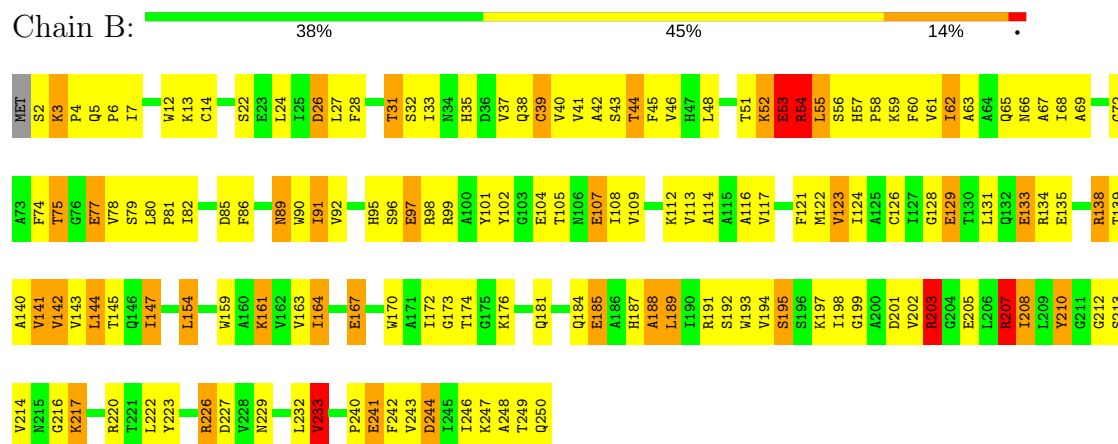
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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	0.89	12/1923 (0.6%)	1.82	44/2606 (1.7%)
1	B	0.86	11/1916 (0.6%)	1.71	30/2597 (1.2%)
All	All	0.88	23/3839 (0.6%)	1.77	74/5203 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	3	0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	GLU	CD-OE2	7.15	1.33	1.25
1	A	241	GLU	CD-OE1	6.71	1.33	1.25
1	B	185	GLU	CD-OE1	6.59	1.32	1.25
1	B	97	GLU	CD-OE2	6.52	1.32	1.25
1	B	241	GLU	CD-OE2	6.24	1.32	1.25
1	A	205	GLU	CD-OE1	6.23	1.32	1.25
1	A	135	GLU	CD-OE2	6.20	1.32	1.25
1	A	23	GLU	CD-OE1	6.19	1.32	1.25
1	B	205	GLU	CD-OE1	6.09	1.32	1.25
1	A	77	GLU	CD-OE2	5.99	1.32	1.25
1	A	107	GLU	CD-OE2	5.99	1.32	1.25
1	A	185	GLU	CD-OE2	5.78	1.32	1.25
1	B	107	GLU	CD-OE1	5.74	1.31	1.25
1	A	133	GLU	CD-OE1	5.68	1.31	1.25
1	B	77	GLU	CD-OE2	5.66	1.31	1.25
1	B	129	GLU	CD-OE2	5.52	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	GLU	CD-OE2	5.48	1.31	1.25
1	A	167	GLU	CD-OE1	5.47	1.31	1.25
1	A	97	GLU	CD-OE2	5.46	1.31	1.25
1	A	104	GLU	CD-OE2	5.42	1.31	1.25
1	B	53	GLU	CD-OE2	5.35	1.31	1.25
1	B	135	GLU	CD-OE2	5.28	1.31	1.25
1	B	167	GLU	CD-OE1	5.23	1.31	1.25

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	B	203	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	A	244	ASP	CB-CG-OD1	-10.23	109.09	118.30
1	B	99	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	B	54	ARG	NE-CZ-NH1	-9.28	115.66	120.30
1	A	101	TYR	CB-CG-CD2	-9.16	115.50	121.00
1	A	167	GLU	CB-CA-C	-8.64	93.12	110.40
1	A	14	CYS	CA-CB-SG	-8.59	98.54	114.00
1	A	105	THR	CA-CB-CG2	-8.51	100.48	112.40
1	B	101	TYR	CB-CG-CD2	-8.46	115.92	121.00
1	A	36	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	A	99	ARG	NE-CZ-NH1	-8.19	116.21	120.30
1	B	210	TYR	CB-CA-C	7.76	125.92	110.40
1	A	111	ASP	CB-CG-OD2	7.71	125.24	118.30
1	B	145	THR	CA-CB-CG2	-7.66	101.68	112.40
1	B	26	ASP	CB-CG-OD2	7.53	125.07	118.30
1	A	140	ALA	N-CA-CB	7.36	120.40	110.10
1	A	227	ASP	CB-CG-OD2	7.32	124.88	118.30
1	A	101	TYR	CB-CG-CD1	7.28	125.37	121.00
1	B	227	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	A	221	THR	CA-CB-CG2	-7.16	102.38	112.40
1	A	101	TYR	CB-CA-C	-6.98	96.44	110.40
1	B	101	TYR	CB-CG-CD1	6.97	125.19	121.00
1	A	111	ASP	CB-CG-OD1	-6.96	112.03	118.30
1	A	122	MET	N-CA-C	-6.90	92.36	111.00
1	A	117	VAL	CA-CB-CG1	-6.90	100.55	110.90
1	A	134	ARG	CD-NE-CZ	-6.86	113.99	123.60
1	B	207	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	A	188	ALA	N-CA-CB	-6.64	100.80	110.10
1	B	188	ALA	CB-CA-C	6.62	120.03	110.10
1	B	203	ARG	NE-CZ-NH2	-6.61	116.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	249	THR	N-CA-CB	6.46	122.57	110.30
1	A	85	ASP	CB-CG-OD2	6.38	124.05	118.30
1	A	138	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	188	ALA	CB-CA-C	6.16	119.34	110.10
1	A	36	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	202	VAL	CB-CA-C	5.98	122.75	111.40
1	B	123	VAL	N-CA-C	5.94	127.03	111.00
1	B	85	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	244	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	B	227	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	226	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	B	188	ALA	N-CA-CB	5.81	118.24	110.10
1	B	244	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	98	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	232	LEU	N-CA-CB	5.73	121.85	110.40
1	A	143	VAL	CA-CB-CG1	5.69	119.43	110.90
1	A	54	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	26	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	A	70	LYS	N-CA-CB	-5.55	100.60	110.60
1	B	101	TYR	CA-CB-CG	5.49	123.83	113.40
1	B	233	VAL	CA-CB-CG2	5.47	119.11	110.90
1	B	241	GLU	CB-CA-C	-5.44	99.53	110.40
1	A	189	LEU	N-CA-CB	-5.43	99.54	110.40
1	A	144	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	B	232	LEU	CB-CG-CD1	5.36	120.11	111.00
1	A	172	ILE	CB-CA-C	-5.36	100.89	111.60
1	A	158	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	115	ALA	N-CA-CB	-5.31	102.67	110.10
1	A	179	THR	CA-CB-OG1	-5.31	97.86	109.00
1	B	138	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	99	ARG	CD-NE-CZ	-5.26	116.23	123.60
1	A	101	TYR	CA-CB-CG	5.20	123.28	113.40
1	A	162	VAL	CA-CB-CG1	5.17	118.65	110.90
1	A	17	SER	CB-CA-C	5.13	119.85	110.10
1	A	119	SER	CB-CA-C	5.12	119.82	110.10
1	A	77	GLU	CG-CD-OE2	-5.11	108.07	118.30
1	B	232	LEU	N-CA-CB	5.11	120.63	110.40
1	B	144	LEU	CA-CB-CG	-5.09	103.58	115.30
1	B	32	SER	N-CA-CB	5.06	118.09	110.50
1	A	162	VAL	N-CA-CB	5.03	122.55	111.50
1	B	123	VAL	CB-CA-C	-5.01	101.87	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	CYS	CA-CB-SG	-5.01	104.99	114.00

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 ⓘ

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	156	2
1	B	1882	0	1917	163	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	300	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 39.

All (300) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:91:ILE:HG23	1:B:123:VAL:HG22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:THR:O	1:B:143:VAL:HG22	1.93	0.68
1:B:40:VAL:HG22	1:B:61:VAL:CG2	2.15	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:27:LEU:HD21	1:B:240:PRO:HB3	1.80	0.64
1:B:13:LYS:HA	1:B:65:GLN:OE1	1.98	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:A:227:ASP:N	1:A:227:ASP:OD1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:130:THR:HG22	1:A:133:GLU:CD	2.23	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
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:B:44:THR:HG23	3:B:603:HOH:O	2.03	0.56
1:B:191:ARG:CD	1:B:203:ARG:HG3	2.36	0.56
1:B:39:CYS:O	1:B:61:VAL:N	2.37	0.56
1:A:62:ILE:HD11	1:A:88:VAL:HG22	1.85	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:A:18:GLN:HA	1:A:50:MET:HE1	1.86	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:172:ILE:CD1	2:A:600:4PB:H22	2.36	0.55
1:A:99:ARG:HG2	1:A:99:ARG:HH11	1.72	0.55
1:B:128:GLY:HA3	1:B:167:GLU:O	2.06	0.55
1:A:191:ARG:O	1:A:195:SER:HB3	2.07	0.54
1:B:139:THR:HG22	1:B:140:ALA:N	2.15	0.54
1:B:124:ILE:HG12	1:B:163:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG23	1:B:78:VAL:HG21	1.89	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:226:ARG:HH11	1:B:226:ARG:HB3	1.72	0.52
1:B:80:LEU:N	1:B:81:PRO:HD2	2.25	0.52
1:A:155:LYS:O	1:A:158:ASP:HB2	2.10	0.52
1:A:188:ALA:O	1:A:192:SER:HB2	2.10	0.52
1:A:80:LEU:HB2	1:A:81:PRO:HD3	1.91	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:CG	1:A:191:ARG:HH11	2.22	0.52
1:B:24:LEU:O	1:B:27:LEU:HB3	2.09	0.52
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:202:VAL:O	1:A:205:GLU:HB2	2.10	0.51
1:A:187:HIS:HB3	1:A:227:ASP:HB2	1.91	0.51
1:A:102:TYR:CZ	1:B:77:GLU:HG3	2.45	0.51
1:A:35:HIS:CD2	1:A:35:HIS:H	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: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:223:TYR:CD2	1:A:249:THR:HA	2.47	0.50
1:A:101:TYR:CE2	1:B:74:PHE:HE1	2.30	0.50
1:B:95:HIS:ND1	1:B:96:SER:N	2.60	0.50
1:A:112:LYS:NZ	3:A:627:HOH:O	2.43	0.49
1:A:133:GLU:O	1:A:136:SER:N	2.46	0.49
1:B:3:LYS:NZ	1:B:223:TYR:O	2.42	0.49
1:B:51:THR:HG21	1:B:62:ILE:HG13	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:194:VAL:HG13	1:B:198:ILE:HD12	1.95	0.48
1:B:80:LEU:N	1:B:81:PRO:CD	2.77	0.48
1:A:18:GLN:HG2	1:A:50:MET:HE1	1.95	0.47
1:A:57:HIS:CD2	1:A:59:LYS:HB2	2.49	0.47
1:B:222:LEU:HA	1:B:222:LEU:HD23	1.75	0.47
1:A:144:LEU:CA	1:A:147:ILE:HG22	2.43	0.47
1:B:194:VAL:HG13	1:B:198:ILE:CD1	2.45	0.47
1:B:147:ILE:HD11	1:B:159:TRP:HH2	1.80	0.47
1:A:134:ARG:HD3	1:A:170:TRP:CD2	2.50	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:250:GLN:HA	3:B:636:HOH:O	2.15	0.47
1:B:40:VAL:CG2	1:B:61:VAL:HG23	2.20	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:130:THR:HG23	1:A:133:GLU:H	1.81	0.46
1:A:45:PHE:HB2	1:B:45:PHE:CB	2.46	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:195:SER:HA	1:B:199:GLY:O	2.15	0.45
1:B:33:ILE:CD1	1:B:246:ILE:HD13	2.46	0.45
1:B:161:LYS:HA	1:B:161:LYS:HD2	1.64	0.45
1:A:135:GLU:C	1:A:137:GLY:H	2.19	0.45
1:A:155:LYS:O	1:A:158:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:HB2	1:A:203:ARG:CG	2.45	0.45
1:B:107:GLU:CD	1:B:107:GLU:H	2.20	0.45
1:A:99:ARG:CG	1:A:99:ARG:HH11	2.25	0.45
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:66:ASN:CG	1:B:67:ALA:H	2.20	0.44
1:B:113:VAL:HG12	1:B:114:ALA:N	2.26	0.44
1:B:68:ILE:HG21	1:B:68:ILE:HD13	1.56	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:B:95:HIS:ND1	1:B:95:HIS:C	2.70	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
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:154:LEU:HD12	1:B:154:LEU:HA	1.62	0.43
1:B:126:CYS:HB3	1:B:167:GLU:OE1	2.18	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:210:TYR:CE1	1:B:222:LEU:CD1	3.02	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:A:48:LEU:O	1:A:52:LYS:HB3	2.19	0.43
1:B:173:GLY:C	1:B:174:THR:HG23	2.39	0.43
1:B:24:LEU:HA	1:B:24:LEU:HD23	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:164:ILE:HA	1:B:164:ILE:HD12	1.64	0.42
1:B:39:CYS:O	1:B:60:PHE:HA	2.19	0.42
1:B:79:SER:HG	1:B:82:ILE:HD12	1.83	0.42
1:A:107:GLU:H	1:A:107:GLU:CD	2.22	0.42
1:B:233:VAL:HA	3:B:650:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ALA:C	1:B:250:GLN:H	2.22	0.42
1:A:102:TYR:CE2	1:B:77:GLU:HG3	2.54	0.42
1:A:134:ARG:HD2	1:A:134:ARG:HH11	1.46	0.42
1:B:124:ILE:HG21	1:B:124:ILE:HD13	1.84	0.42
1:B:193:TRP:O	1:B:197:LYS:HB2	2.20	0.42
1:B:220:ARG:HG3	1:B:220:ARG:H	1.38	0.42
1:B:52:LYS:HE3	1:B:86:PHE:O	2.19	0.42
1:A:95:HIS:CD2	1:B:75:THR:HG21	2.55	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:A:99:ARG:HG2	1:A:99:ARG:NH1	2.32	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:210:TYR:HE1	1:B:222:LEU:CD1	2.33	0.42
1:B:33:ILE:HD11	1:B:246:ILE:HD12	2.02	0.42
1:A:17:SER:O	1:A:21:LEU:HG	2.19	0.41
1:A:191:ARG:CD	1:A:203:ARG:HG2	2.49	0.41
1:A:46:VAL:O	1:A:46:VAL:HG12	2.20	0.41
1:B:191:ARG:CD	1:B:203:ARG:CG	2.98	0.41
1:B:53:GLU:HG2	1:B:54:ARG:HG2	2.02	0.41
1:A:172:ILE:O	1:A:172:ILE:HG22	2.18	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: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:22:SER:O	1:B:26:ASP:N	2.48	0.41
1:B:5:GLN:HA	1:B:6:PRO:HD3	1.63	0.41
1:A:168:PRO:CG	1:A:212:GLY:HA3	2.49	0.41
1:A:57:HIS:CD2	1:A:60:PHE:HD2	2.39	0.41
1:A:42:ALA:O	1:A:65:GLN:NE2	2.41	0.41
1:A:4:PRO:HD2	1:A:229:ASN:ND2	2.35	0.41
1:B:48:LEU:HD12	1:B:48:LEU:HA	1.86	0.41
1:A:65:GLN:O	1:A:66:ASN:HB2	2.20	0.41
1:A:62:ILE:CD1	1:A:88:VAL:HG22	2.51	0.41
1:B:208:ILE:N	1:B:229:ASN:HB2	2.35	0.41
1:B:33:ILE:HD13	1:B:246:ILE:HD13	2.03	0.41
1:B:95:HIS:ND1	1:B:97:GLU:N	2.62	0.40
1:B:57:HIS:HA	1:B:58:PRO:HD3	1.63	0.40
1:A:164:ILE:CG2	1:A:165:ALA:N	2.85	0.40
1:A:232:LEU:HA	1:A:232:LEU:HD12	1.94	0.40
1:A:240:PRO:C	1:A:242:PHE:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:THR:OG1	1:B:13:LYS:HG2	2.21	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 [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	247/250 (99%)	210 (85%)	33 (13%)	4 (2%)	11	33
1	B	247/250 (99%)	210 (85%)	32 (13%)	5 (2%)	9	27
All	All	494/500 (99%)	420 (85%)	65 (13%)	9 (2%)	10	30

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

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Mol	Chain	Res	Type
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%)	155 (79%)	42 (21%)	1	3
1	B	195/198 (98%)	164 (84%)	31 (16%)	3	8
All	All	392/396 (99%)	319 (81%)	73 (19%)	2	5

All (73) 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	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	80	LEU
1	A	85	ASP
1	A	101	TYR
1	A	105	THR
1	A	107	GLU
1	A	131	LEU
1	A	143	VAL
1	A	152	LYS
1	A	153	LYS

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Mol	Chain	Res	Type
1	A	155	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	196	SER
1	A	197	LYS
1	A	201	ASP
1	A	202	VAL
1	A	206	LEU
1	A	207	ARG
1	A	221	THR
1	A	224	GLN
1	A	226	ARG
1	A	227	ASP
1	A	237	SER
1	A	239	LYS
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	129	GLU
1	B	131	LEU
1	B	141	VAL
1	B	147	ILE
1	B	154	LEU
1	B	161	LYS
1	B	164	ILE
1	B	176	LYS
1	B	189	LEU

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Mol	Chain	Res	Type
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
1	B	233	VAL

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

Mol	Chain	Res	Type
1	A	35	HIS
1	A	38	GLN
1	A	57	HIS
1	A	250	GLN
1	B	5	GLN
1	B	15	ASN
1	B	35	HIS
1	B	57	HIS
1	B	66	ASN
1	B	89	ASN

### 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 carbohydrates 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	1 (10%)	11,13,13	1.85	3 (27%)

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	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	4PB	P-C4	2.04	1.81	1.78

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	113.32
2	A	600	4PB	ON-N-C1	2.50	123.57	119.81
2	A	600	4PB	O2P-P-C4	2.70	113.29	106.96

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.