



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:10 PM UTC

PDB ID : 1M7R / pdb_00001m7r
Title : Crystal Structure of Myotubularin-related Protein-2 (MTMR2) Complexed with Phosphate
Authors : Begley, M.J.; Taylor, G.S.; Kim, S.-A.; Veine, D.M.; Dixon, J.E.; Stuckey, J.A.
Deposited on : 2002-07-22
Resolution : 2.60 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

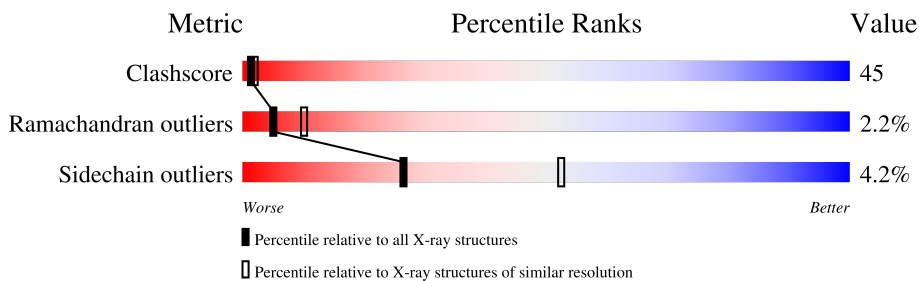
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	657	
1	B	657	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	656	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8632 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 Myotubularin-related Protein-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	75	0	0
			4189	2679	729	764	17			
1	B	513	Total	C	N	O	S	114	0	0
			4189	2679	729	764	17			

There are 30 discrepancies between the modelled and reference sequences:

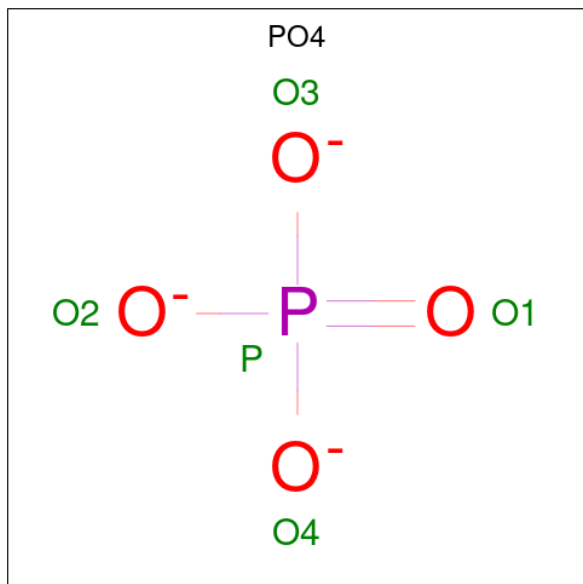
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	cloning artifact	UNP Q13614
A	-1	ALA	-	cloning artifact	UNP Q13614
A	0	SER	-	cloning artifact	UNP Q13614
A	417	SER	CYS	engineered mutation	UNP Q13614
A	644	ALA	-	expression tag	UNP Q13614
A	645	ALA	-	expression tag	UNP Q13614
A	646	ALA	-	expression tag	UNP Q13614
A	647	LEU	-	expression tag	UNP Q13614
A	648	GLU	-	expression tag	UNP Q13614
A	649	HIS	-	expression tag	UNP Q13614
A	650	HIS	-	expression tag	UNP Q13614
A	651	HIS	-	expression tag	UNP Q13614
A	652	HIS	-	expression tag	UNP Q13614
A	653	HIS	-	expression tag	UNP Q13614
A	654	HIS	-	expression tag	UNP Q13614
B	-2	MET	-	cloning artifact	UNP Q13614
B	-1	ALA	-	cloning artifact	UNP Q13614
B	0	SER	-	cloning artifact	UNP Q13614
B	417	SER	CYS	engineered mutation	UNP Q13614
B	644	ALA	-	expression tag	UNP Q13614
B	645	ALA	-	expression tag	UNP Q13614
B	646	ALA	-	expression tag	UNP Q13614
B	647	LEU	-	expression tag	UNP Q13614
B	648	GLU	-	expression tag	UNP Q13614
B	649	HIS	-	expression tag	UNP Q13614

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Chain	Residue	Modelled	Actual	Comment	Reference
B	650	HIS	-	expression tag	UNP Q13614
B	651	HIS	-	expression tag	UNP Q13614
B	652	HIS	-	expression tag	UNP Q13614
B	653	HIS	-	expression tag	UNP Q13614
B	654	HIS	-	expression tag	UNP Q13614

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 3 is water.

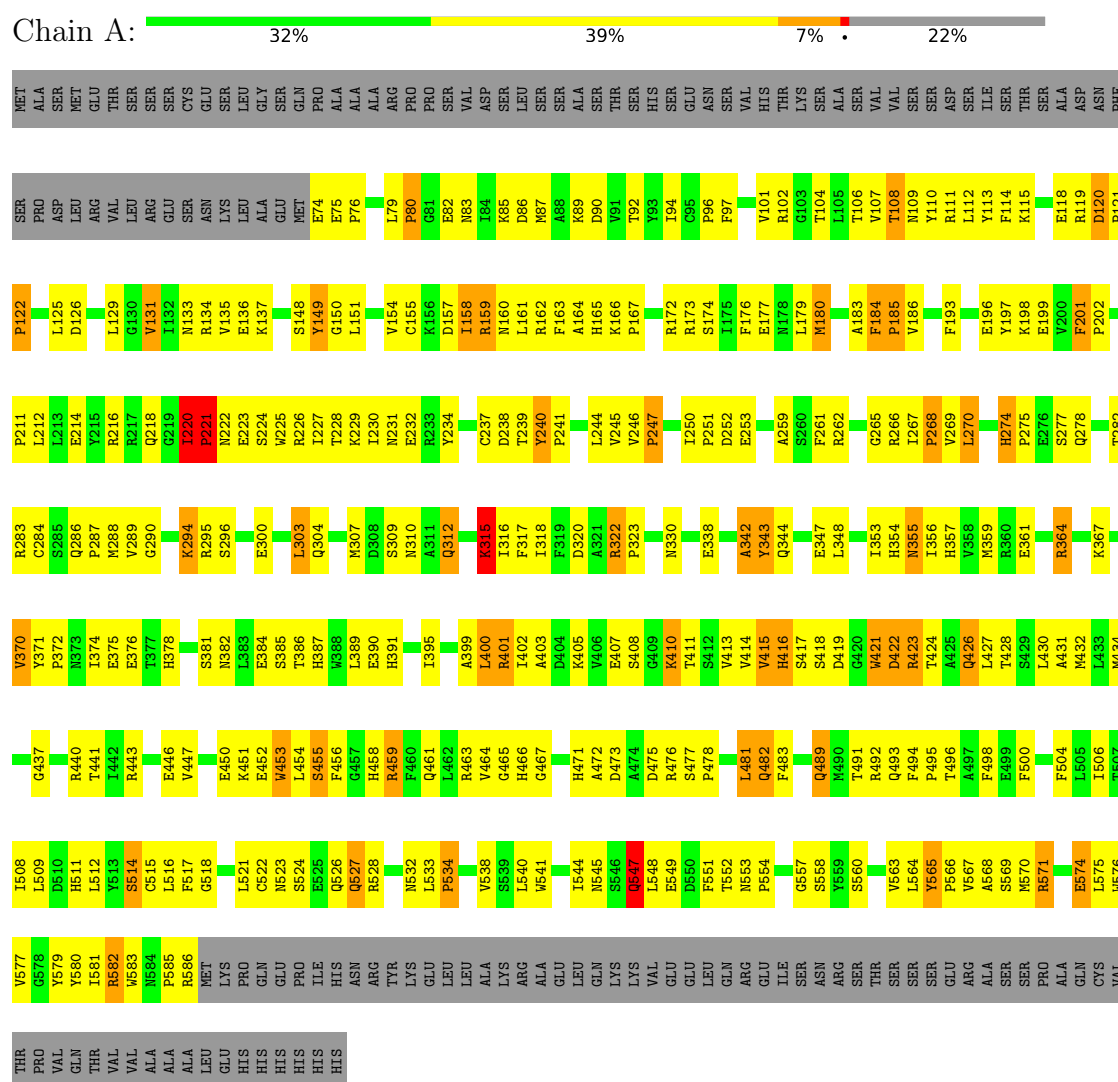
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	88	Total	O	0	0
			88	88		

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: Myotubularin-related Protein-2



• Molecule 1: Myotubularin-related Protein-2





4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.25Å 82.66Å 100.13Å 90.00° 117.93° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.1 (8.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8632	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.98	35/4300 (0.8%)	1.22	52/5829 (0.9%)
1	B	0.97	31/4300 (0.7%)	1.23	51/5829 (0.9%)
All	All	0.98	66/8600 (0.8%)	1.22	103/11658 (0.9%)

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	7
1	B	0	2
All	All	0	9

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	554	PRO	N-CD	-17.99	1.22	1.47
1	A	220	ILE	CA-C	-14.82	1.37	1.52
1	A	575	LEU	C-N	-8.46	1.23	1.33
1	A	354	HIS	C-N	8.00	1.43	1.33
1	B	562	HIS	C-O	7.78	1.32	1.23
1	A	565	TYR	C-N	7.58	1.43	1.33
1	B	413	VAL	C-N	-7.46	1.24	1.33
1	B	576	TRP	C-N	7.41	1.42	1.33
1	A	268	PRO	C-N	-7.35	1.24	1.33
1	B	323	PRO	C-N	-7.32	1.24	1.33
1	A	567	VAL	C-N	-6.84	1.24	1.33
1	A	159	ARG	C-N	-6.82	1.24	1.33
1	B	147	ASN	C-N	-6.74	1.24	1.33
1	A	410	LYS	C-N	-6.72	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	ASP	C-N	6.68	1.43	1.33
1	B	187	SER	C-N	6.55	1.43	1.33
1	B	341	ASP	C-O	6.43	1.31	1.24
1	A	323	PRO	C-N	-6.27	1.26	1.33
1	A	90	ASP	C-O	6.10	1.32	1.23
1	B	415	VAL	C-N	-6.10	1.25	1.33
1	A	198	LYS	C-O	6.07	1.32	1.24
1	B	532	ASN	C-N	5.92	1.42	1.33
1	A	500	PHE	C-N	-5.80	1.25	1.33
1	A	464	VAL	C-O	5.76	1.29	1.23
1	B	441	THR	C-N	-5.75	1.26	1.33
1	A	514	SER	C-N	-5.74	1.25	1.33
1	B	530	LYS	C-N	5.73	1.42	1.33
1	B	158	ILE	C-N	5.72	1.40	1.33
1	B	112	LEU	C-N	-5.70	1.25	1.33
1	A	342	ALA	C-N	-5.65	1.24	1.33
1	B	339	SER	C-N	5.64	1.41	1.33
1	B	110	TYR	C-O	5.61	1.31	1.24
1	A	283	ARG	C-N	-5.56	1.25	1.33
1	A	408	SER	C-N	-5.51	1.24	1.33
1	B	323	PRO	N-CD	5.45	1.55	1.47
1	B	251	PRO	N-CD	5.44	1.55	1.47
1	B	585	PRO	N-CD	5.44	1.55	1.47
1	B	247	PRO	N-CD	5.43	1.55	1.47
1	B	235	GLU	C-N	-5.42	1.26	1.33
1	B	77	PRO	N-CD	5.42	1.55	1.47
1	A	585	PRO	N-CD	5.41	1.55	1.47
1	A	534	PRO	N-CD	5.41	1.55	1.47
1	B	80	PRO	N-CD	5.41	1.55	1.47
1	A	158	ILE	C-O	5.41	1.30	1.24
1	A	122	PRO	N-CD	5.40	1.55	1.47
1	B	122	PRO	N-CD	5.39	1.55	1.47
1	A	323	PRO	N-CD	5.39	1.55	1.47
1	A	247	PRO	N-CD	5.38	1.55	1.47
1	B	202	PRO	N-CD	5.38	1.55	1.47
1	A	268	PRO	N-CD	5.38	1.55	1.47
1	A	185	PRO	N-CD	5.38	1.55	1.47
1	A	80	PRO	N-CD	5.38	1.55	1.47
1	A	211	PRO	N-CD	5.38	1.55	1.47
1	B	268	PRO	N-CD	5.37	1.55	1.47
1	B	460	PHE	C-O	5.37	1.30	1.24
1	A	251	PRO	N-CD	5.37	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	495	PRO	N-CD	5.36	1.55	1.47
1	A	221	PRO	N-CD	5.36	1.55	1.47
1	B	534	PRO	N-CD	5.36	1.55	1.47
1	B	211	PRO	N-CD	5.32	1.55	1.47
1	B	156	LYS	C-N	-5.30	1.27	1.33
1	A	133	ASN	C-N	-5.28	1.26	1.33
1	A	421	TRP	NE1-CE2	-5.22	1.31	1.37
1	A	465	GLY	C-N	5.17	1.40	1.33
1	A	355	ASN	C-N	5.11	1.40	1.33
1	B	567	VAL	C-N	5.03	1.39	1.33

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	GLN	OE1-CD-NE2	-9.87	112.73	122.60
1	A	547	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	B	278	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	A	344	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	A	426	GLN	OE1-CD-NE2	-9.83	112.77	122.60
1	B	489	GLN	OE1-CD-NE2	-9.83	112.77	122.60
1	A	526	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	B	426	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	B	547	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	B	218	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	A	482	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	B	286	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	A	489	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	B	527	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	A	527	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	A	218	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	A	312	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	A	493	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	B	312	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	A	494	PHE	CA-C-N	9.34	131.51	119.84
1	A	494	PHE	C-N-CA	9.34	131.51	119.84
1	A	220	ILE	CB-CA-C	8.82	127.42	111.36
1	B	388	TRP	O-C-N	8.32	131.08	122.09
1	B	323	PRO	CA-C-O	-7.88	111.99	122.08
1	B	494	PHE	CA-C-N	7.65	129.40	119.84
1	B	494	PHE	C-N-CA	7.65	129.40	119.84
1	B	416	HIS	N-CA-C	7.61	119.24	108.74
1	A	532	ASN	CA-C-N	7.50	129.47	120.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ASN	C-N-CA	7.50	129.47	120.09
1	B	532	ASN	O-C-N	-7.50	113.58	122.58
1	A	221	PRO	O-C-N	6.79	131.81	122.64
1	B	286	GLN	CG-CD-NE2	6.72	126.49	116.40
1	A	526	GLN	CG-CD-NE2	6.71	126.47	116.40
1	B	304	GLN	CG-CD-NE2	6.71	126.47	116.40
1	A	344	GLN	CG-CD-NE2	6.70	126.45	116.40
1	A	312	GLN	CG-CD-NE2	6.69	126.44	116.40
1	A	547	GLN	CG-CD-NE2	6.69	126.44	116.40
1	A	527	GLN	CG-CD-NE2	6.69	126.43	116.40
1	B	278	GLN	CG-CD-NE2	6.66	126.39	116.40
1	A	426	GLN	CG-CD-NE2	6.66	126.39	116.40
1	B	426	GLN	CG-CD-NE2	6.66	126.39	116.40
1	B	218	GLN	CG-CD-NE2	6.65	126.38	116.40
1	B	312	GLN	CG-CD-NE2	6.63	126.35	116.40
1	A	489	GLN	CG-CD-NE2	6.63	126.34	116.40
1	B	489	GLN	CG-CD-NE2	6.62	126.33	116.40
1	A	482	GLN	CG-CD-NE2	6.62	126.33	116.40
1	B	547	GLN	CG-CD-NE2	6.62	126.33	116.40
1	A	218	GLN	CG-CD-NE2	6.62	126.32	116.40
1	A	493	GLN	CG-CD-NE2	6.61	126.31	116.40
1	B	527	GLN	CG-CD-NE2	6.60	126.30	116.40
1	A	410	LYS	O-C-N	-6.41	114.60	122.55
1	B	285	SER	CA-C-O	-6.27	114.55	121.89
1	B	410	LYS	CA-C-N	-6.16	114.00	122.93
1	B	410	LYS	C-N-CA	-6.16	114.00	122.93
1	B	340	GLU	CA-C-N	6.15	128.52	120.28
1	B	340	GLU	C-N-CA	6.15	128.52	120.28
1	B	562	HIS	N-CA-C	6.08	119.28	109.79
1	A	323	PRO	CA-C-O	-6.07	114.26	121.67
1	B	192	LEU	CA-C-O	-5.99	114.45	121.16
1	A	309	SER	CA-C-N	-5.95	114.58	122.85
1	A	309	SER	C-N-CA	-5.95	114.58	122.85
1	B	112	LEU	CA-C-O	-5.92	114.18	120.40
1	A	184	PHE	CA-C-N	5.88	125.08	118.97
1	A	184	PHE	C-N-CA	5.88	125.08	118.97
1	A	565	TYR	CA-C-N	-5.87	114.57	120.21
1	A	565	TYR	C-N-CA	-5.87	114.57	120.21
1	B	416	HIS	O-C-N	5.81	129.71	122.92
1	A	201	PHE	CA-C-N	5.76	125.86	119.87
1	A	201	PHE	C-N-CA	5.76	125.86	119.87
1	B	576	TRP	O-C-N	5.67	130.14	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	TYR	CA-C-O	-5.66	115.38	121.38
1	B	516	LEU	N-CA-C	-5.60	105.17	112.23
1	B	154	VAL	CA-C-O	-5.57	114.14	120.65
1	B	165	HIS	CB-CA-C	-5.56	100.58	109.75
1	A	250	ILE	CA-C-N	5.54	125.52	120.21
1	A	250	ILE	C-N-CA	5.54	125.52	120.21
1	B	554	PRO	N-CD-CG	5.52	111.48	103.20
1	A	274	HIS	CB-CA-C	-5.47	100.64	109.67
1	A	560	SER	O-C-N	5.47	129.86	122.59
1	A	565	TYR	O-C-N	5.45	125.63	121.27
1	A	120	ASP	O-C-N	-5.43	115.07	121.32
1	A	441	THR	CA-C-O	-5.29	115.47	121.72
1	B	201	PHE	CA-C-N	5.28	126.44	119.84
1	B	201	PHE	C-N-CA	5.28	126.44	119.84
1	B	315	LYS	CA-C-O	-5.28	115.79	121.38
1	B	416	HIS	CA-C-O	-5.26	115.78	121.36
1	A	287	PRO	CB-CA-C	-5.24	104.24	111.21
1	A	322	ARG	CA-C-O	5.19	126.36	120.70
1	B	325	VAL	CA-C-N	5.18	128.00	120.79
1	B	325	VAL	C-N-CA	5.18	128.00	120.79
1	A	343	TYR	CA-C-N	5.14	127.94	120.79
1	A	343	TYR	C-N-CA	5.14	127.94	120.79
1	A	274	HIS	CA-CB-CG	-5.11	108.69	113.80
1	B	165	HIS	CA-CB-CG	-5.09	108.71	113.80
1	B	547	GLN	O-C-N	-5.09	115.61	122.22
1	A	547	GLN	O-C-N	-5.09	115.38	122.20
1	B	458	HIS	CA-CB-CG	-5.07	108.73	113.80
1	B	441	THR	CA-C-O	-5.05	115.30	121.36
1	A	270	LEU	N-CA-C	5.03	117.50	109.96
1	B	314	HIS	CB-CA-C	-5.02	102.40	110.74
1	B	494	PHE	O-C-N	-5.02	116.87	121.34
1	A	571	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	A	416	HIS	O-C-N	5.00	128.77	122.92

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	TYR	Mainchain
1	A	180	MET	Mainchain
1	A	220	ILE	Mainchain,Peptide
1	A	315	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	453	TRP	Mainchain
1	A	547	GLN	Mainchain
1	B	266	ARG	Mainchain
1	B	562	HIS	Mainchain

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	4189	0	4113	332	0
1	B	4189	0	4113	403	0
2	A	10	0	0	2	0
2	B	10	0	0	1	0
3	A	146	0	0	16	0
3	B	88	0	0	14	0
All	All	8632	0	8226	731	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 45.

All (731) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:PHE:CE1	1:A:405:LYS:HD2	1.60	1.36
1:A:454:LEU:HD13	3:A:1207:HOH:O	1.38	1.23
1:B:393:LYS:HG3	1:B:568:ALA:O	1.37	1.20
1:A:261:PHE:O	1:A:288:MET:HG2	1.42	1.16
1:B:370:VAL:CG1	1:B:581:ILE:HG12	1.75	1.14
1:B:137:LYS:HE3	1:B:176:PHE:CD2	1.83	1.13
1:B:230:ILE:HD11	1:B:256:LYS:HE2	1.22	1.12
1:B:511:HIS:HD2	1:B:540:LEU:CD1	1.62	1.11
1:A:112:LEU:HD13	1:A:179:LEU:HD21	1.31	1.11
1:B:511:HIS:HD2	1:B:540:LEU:HD11	0.98	1.11
1:B:511:HIS:CD2	1:B:540:LEU:CD1	2.32	1.11
1:B:337:TYR:CD1	1:B:348:LEU:CD2	2.34	1.11
1:A:74:GLU:HB3	1:A:115:LYS:HD3	1.31	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LYS:HE2	1:B:176:PHE:CG	1.86	1.10
1:B:432:MET:HE1	1:B:452:GLU:HG3	1.29	1.10
1:A:359:MET:HE3	1:A:482:GLN:HE22	1.10	1.10
1:B:410:LYS:HE2	3:B:1093:HOH:O	0.92	1.09
1:B:94:ILE:HD11	1:B:147:ASN:HB3	1.28	1.07
1:A:544:ILE:HG23	1:A:551:PHE:CE1	1.89	1.07
1:B:337:TYR:HD1	1:B:348:LEU:CD2	1.67	1.06
1:B:511:HIS:CD2	1:B:540:LEU:HD11	1.88	1.06
1:A:317:PHE:CE1	1:A:405:LYS:CD	2.41	1.04
1:B:94:ILE:HD11	1:B:147:ASN:CB	1.90	1.02
1:A:274:HIS:CD2	1:A:275:PRO:HD2	1.96	0.99
1:B:337:TYR:CD1	1:B:348:LEU:HD21	1.96	0.98
1:B:314:HIS:CD2	1:B:315:LYS:HB2	1.97	0.98
1:B:370:VAL:HG13	1:B:581:ILE:HG12	1.45	0.98
1:B:261:PHE:O	1:B:288:MET:HG2	1.64	0.97
1:B:137:LYS:HE2	1:B:176:PHE:CB	1.94	0.97
1:B:91:VAL:HG22	1:B:165:HIS:ND1	1.78	0.96
1:B:137:LYS:CE	1:B:176:PHE:CD2	2.47	0.96
1:B:337:TYR:CD1	1:B:348:LEU:HD23	2.01	0.96
1:B:370:VAL:HG11	1:B:581:ILE:HG12	1.45	0.96
1:A:158:ILE:HG23	1:A:367:LYS:HG3	1.46	0.95
1:A:110:TYR:HB2	1:A:193:PHE:CD1	2.02	0.95
1:B:432:MET:HE1	1:B:452:GLU:CG	1.97	0.94
1:B:137:LYS:CE	1:B:176:PHE:CG	2.49	0.94
1:A:101:VAL:CG2	1:A:119:ARG:HH21	1.81	0.93
1:B:229:LYS:O	1:B:232:GLU:HG2	1.70	0.91
1:B:274:HIS:ND1	1:B:275:PRO:HD2	1.86	0.91
1:A:317:PHE:HE1	1:A:405:LYS:HD2	1.35	0.90
1:A:165:HIS:CD2	1:A:172:ARG:HG2	2.06	0.89
1:A:544:ILE:HG23	1:A:551:PHE:CD1	2.08	0.89
1:B:137:LYS:HG2	1:B:176:PHE:CD1	2.08	0.89
1:B:338:GLU:HB3	1:B:343:TYR:CD1	2.08	0.88
1:B:402:ILE:HG23	1:B:413:VAL:HG21	1.56	0.88
1:A:390:GLU:HG2	3:A:1037:HOH:O	1.74	0.87
1:B:74:GLU:HB3	1:B:115:LYS:HD3	1.58	0.86
1:B:389:LEU:HB2	1:B:570:MET:HE1	1.56	0.86
1:B:314:HIS:HD2	1:B:315:LYS:HB2	1.39	0.85
1:B:511:HIS:CD2	1:B:540:LEU:HD13	2.10	0.85
1:A:545:ASN:HA	1:A:548:LEU:HD21	1.59	0.84
1:A:74:GLU:CB	1:A:115:LYS:HD3	2.07	0.83
1:B:320:ASP:OD1	1:B:322:ARG:HG3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:HD21	1:B:161:LEU:HD22	1.60	0.83
1:A:274:HIS:CG	1:A:275:PRO:HD2	2.13	0.82
1:B:138:ILE:HD13	1:B:162:ARG:NH1	1.94	0.82
1:B:400:LEU:HD23	1:B:434:MET:SD	2.19	0.82
1:A:267:ILE:O	1:A:269:VAL:HG13	1.80	0.82
1:B:120:ASP:HB3	1:B:121:PRO:HD3	1.60	0.82
1:A:387:HIS:O	1:A:391:HIS:CD2	2.33	0.81
1:B:231:ASN:HD22	1:B:236:LEU:H	1.27	0.81
1:B:432:MET:CE	1:B:452:GLU:HG3	2.09	0.81
1:A:378:HIS:HB2	1:A:382:ASN:HD21	1.46	0.80
1:A:277:SER:O	1:A:278:GLN:HB2	1.79	0.80
1:A:261:PHE:CE1	1:A:288:MET:O	2.34	0.80
1:B:338:GLU:HA	1:B:343:TYR:CE1	2.15	0.80
1:B:295:ARG:HH11	1:B:342:ALA:HA	1.48	0.79
1:A:353:ILE:HD13	1:A:395:ILE:HD13	1.64	0.79
1:B:110:TYR:HB2	1:B:193:PHE:CD1	2.19	0.78
1:B:330:ASN:HA	1:B:333:LYS:HE3	1.64	0.78
1:B:375:GLU:OE2	1:B:377:THR:HB	1.83	0.78
1:B:567:VAL:HG11	1:B:572:HIS:CD2	2.18	0.78
1:A:518:GLY:HA2	1:A:521:LEU:CD1	2.13	0.78
1:B:138:ILE:CD1	1:B:162:ARG:NH1	2.46	0.78
1:B:466:HIS:CD2	1:B:521:LEU:HD23	2.17	0.78
1:B:393:LYS:CG	1:B:568:ALA:O	2.27	0.78
1:B:545:ASN:HA	1:B:548:LEU:HD21	1.64	0.78
1:B:137:LYS:HG3	1:B:176:PHE:CE1	2.19	0.77
1:A:317:PHE:CD1	1:A:405:LYS:HG2	2.19	0.77
1:A:259:ALA:HA	1:A:267:ILE:CG2	2.14	0.77
1:B:307:MET:CE	1:B:316:ILE:HG22	2.15	0.77
1:A:212:LEU:O	1:A:216:ARG:HG3	1.85	0.76
1:B:110:TYR:HB2	1:B:193:PHE:CG	2.19	0.76
1:A:137:LYS:HD3	1:A:172:ARG:NH1	2.00	0.75
1:A:120:ASP:HB3	1:A:121:PRO:HD3	1.68	0.75
1:A:267:ILE:O	1:A:267:ILE:HG13	1.84	0.75
1:B:159:ARG:HB3	1:B:583:TRP:CD1	2.22	0.75
1:B:314:HIS:CG	1:B:315:LYS:N	2.55	0.75
1:B:504:PHE:CZ	1:B:508:ILE:HD11	2.21	0.75
1:B:135:VAL:HG22	1:B:153:THR:HG22	1.67	0.75
1:A:268:PRO:HA	1:A:284:CYS:HB3	1.69	0.74
1:B:340:GLU:HG2	3:B:1227:HOH:O	1.86	0.74
1:B:461:GLN:HE22	1:B:466:HIS:HB2	1.53	0.74
1:B:216:ARG:HD2	1:B:216:ARG:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:TYR:HE1	1:B:266:ARG:NH1	1.86	0.74
1:A:185:PRO:HD2	1:A:467:GLY:HA3	1.70	0.74
1:B:295:ARG:NH1	1:B:342:ALA:HA	2.02	0.74
1:A:101:VAL:HG23	1:A:119:ARG:HH21	1.51	0.73
1:A:134:ARG:NH1	1:A:136:GLU:HG3	2.03	0.73
1:B:545:ASN:HA	1:B:548:LEU:CD2	2.19	0.73
1:A:509:LEU:HD12	1:A:579:TYR:CE1	2.24	0.73
1:B:340:GLU:HG3	1:B:341:ASP:N	2.04	0.73
1:A:166:LYS:HB3	1:A:167:PRO:HD2	1.71	0.73
1:A:374:ILE:HD11	1:A:581:ILE:HD13	1.69	0.73
1:B:337:TYR:HD1	1:B:348:LEU:HD23	1.40	0.73
1:B:137:LYS:CG	1:B:176:PHE:CD1	2.71	0.72
1:B:286:GLN:OE1	1:B:322:ARG:NH1	2.22	0.72
1:A:101:VAL:CG2	1:A:119:ARG:HE	2.02	0.72
1:A:186:VAL:HG22	1:A:467:GLY:O	1.89	0.72
1:B:343:TYR:O	1:B:345:ASN:N	2.22	0.72
1:B:526:GLN:HG2	1:B:530:LYS:HE3	1.69	0.72
1:A:101:VAL:CG2	1:A:119:ARG:NH2	2.53	0.72
1:A:387:HIS:O	1:A:391:HIS:HD2	1.72	0.72
1:A:359:MET:HE3	1:A:482:GLN:NE2	1.95	0.72
1:A:399:ALA:C	1:A:434:MET:HE1	2.15	0.72
1:B:383:LEU:HD11	1:B:575:LEU:HD13	1.72	0.72
1:A:511:HIS:HA	1:A:514:SER:OG	1.90	0.72
1:B:137:LYS:HE2	1:B:176:PHE:HB3	1.70	0.72
1:B:138:ILE:HD13	1:B:162:ARG:HH12	1.54	0.71
1:A:437:GLY:HA2	1:A:440:ARG:NH1	2.04	0.71
1:B:329:ALA:O	1:B:333:LYS:HG3	1.91	0.71
1:B:268:PRO:HA	1:B:284:CYS:HB3	1.71	0.71
1:A:89:LYS:HG2	1:A:104:THR:OG1	1.90	0.71
1:B:340:GLU:CG	1:B:341:ASP:H	2.04	0.71
1:B:185:PRO:CG	1:B:192:LEU:HD23	2.20	0.70
1:A:158:ILE:HG12	1:A:367:LYS:HB2	1.74	0.70
1:B:295:ARG:HD2	1:B:300:GLU:OE2	1.90	0.70
1:A:289:VAL:O	1:A:294:LYS:HG3	1.91	0.70
1:A:222:ASN:O	1:A:224:SER:N	2.25	0.70
1:A:399:ALA:O	1:A:434:MET:HE1	1.91	0.70
1:B:518:GLY:HA2	1:B:521:LEU:CD1	2.21	0.70
1:B:86:ASP:OD1	1:B:87:MET:N	2.25	0.70
1:B:370:VAL:HG11	1:B:580:TYR:O	1.92	0.69
1:B:370:VAL:HG13	1:B:581:ILE:CG1	2.21	0.69
1:A:338:GLU:HB3	1:A:343:TYR:CD1	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ALA:HB2	1:B:434:MET:HE3	1.73	0.69
1:A:509:LEU:CD1	1:A:579:TYR:CE1	2.76	0.69
1:B:401:ARG:HD2	3:B:1197:HOH:O	1.89	0.69
1:B:400:LEU:HD21	1:B:566:PRO:HD2	1.75	0.69
1:B:518:GLY:HA2	1:B:521:LEU:HD12	1.75	0.69
1:A:125:LEU:HD21	1:A:161:LEU:HD13	1.75	0.69
1:A:491:THR:HG22	1:A:498:PHE:CD1	2.27	0.69
1:B:458:HIS:NE2	1:B:463:ARG:HG3	2.08	0.69
1:A:317:PHE:CZ	1:A:405:LYS:NZ	2.61	0.68
1:A:361:GLU:OE2	1:A:364:ARG:NH1	2.27	0.68
1:B:495:PRO:HD2	3:B:1217:HOH:O	1.93	0.68
1:A:158:ILE:HG22	1:A:158:ILE:O	1.92	0.68
1:A:422:ASP:OD1	1:A:458:HIS:CE1	2.47	0.68
1:B:220:ILE:HG23	1:B:221:PRO:HA	1.76	0.68
1:A:286:GLN:OE1	1:A:322:ARG:NH1	2.23	0.68
1:A:518:GLY:HA2	1:A:521:LEU:HD12	1.76	0.68
1:B:266:ARG:HD2	1:B:419:ASP:O	1.94	0.68
1:B:185:PRO:HG2	1:B:192:LEU:CD2	2.23	0.68
1:B:231:ASN:ND2	1:B:236:LEU:H	1.91	0.68
1:B:291:VAL:HG12	3:B:1211:HOH:O	1.93	0.68
1:B:322:ARG:NH2	1:B:336:GLY:O	2.22	0.68
1:B:399:ALA:C	1:B:434:MET:HE1	2.18	0.68
1:A:220:ILE:HD12	1:A:225:TRP:HB2	1.75	0.67
1:B:338:GLU:HG3	1:B:343:TYR:CZ	2.29	0.67
1:B:314:HIS:CD2	1:B:315:LYS:N	2.62	0.67
1:A:356:ILE:HG13	1:A:357:HIS:N	2.08	0.67
1:B:79:LEU:HG	1:B:111:ARG:NH2	2.09	0.67
1:B:91:VAL:CG2	1:B:165:HIS:ND1	2.56	0.67
1:B:450:GLU:CD	1:B:454:LEU:HD12	2.19	0.67
1:B:254:GLU:HG3	1:B:257:ARG:NH2	2.08	0.67
1:A:296:SER:O	1:A:300:GLU:HG3	1.95	0.67
1:A:466:HIS:ND1	1:A:515:CYS:SG	2.68	0.67
1:B:154:VAL:HA	1:B:160:ASN:OD1	1.93	0.67
1:A:101:VAL:HG22	1:A:119:ARG:HE	1.58	0.67
1:B:340:GLU:HG3	1:B:341:ASP:H	1.59	0.67
1:A:120:ASP:HB3	1:A:121:PRO:CD	2.24	0.66
1:A:317:PHE:HB2	1:A:413:VAL:HG12	1.76	0.66
1:B:231:ASN:HD21	1:B:237:CYS:H	1.43	0.66
1:B:359:MET:CE	1:B:482:GLN:HE22	2.08	0.66
1:B:356:ILE:HG13	1:B:357:HIS:N	2.10	0.66
1:A:378:HIS:CB	1:A:382:ASN:ND2	2.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:NE	3:A:1130:HOH:O	2.29	0.66
1:A:378:HIS:CB	1:A:382:ASN:HD21	2.09	0.66
1:A:74:GLU:HB3	1:A:115:LYS:CD	2.17	0.66
1:A:452:GLU:O	1:A:456:PHE:HB2	1.96	0.66
1:B:230:ILE:CD1	1:B:256:LYS:HE2	2.14	0.66
1:A:266:ARG:HD2	1:A:419:ASP:O	1.95	0.66
1:A:284:CYS:O	1:A:416:HIS:HB2	1.96	0.66
1:B:137:LYS:CG	1:B:176:PHE:CE1	2.79	0.66
1:A:268:PRO:HG3	1:A:284:CYS:SG	2.36	0.65
1:A:400:LEU:HD11	1:A:566:PRO:O	1.96	0.65
1:B:232:GLU:OE2	1:B:243:LEU:CD2	2.43	0.65
1:B:266:ARG:CD	1:B:419:ASP:O	2.44	0.65
1:B:323:PRO:HD2	1:B:326:ASN:CG	2.21	0.65
1:A:159:ARG:HD3	1:A:583:TRP:CE2	2.31	0.65
1:B:341:ASP:O	1:B:344:GLN:HG2	1.96	0.65
1:A:110:TYR:HB2	1:A:193:PHE:CE1	2.31	0.65
1:A:461:GLN:HB3	1:A:522:CYS:O	1.95	0.65
1:B:340:GLU:CG	1:B:341:ASP:N	2.60	0.65
1:A:107:VAL:HG22	1:A:112:LEU:HD12	1.79	0.65
1:B:307:MET:CE	1:B:316:ILE:CG2	2.75	0.65
1:B:307:MET:HE2	1:B:316:ILE:HB	1.79	0.65
1:A:359:MET:CE	1:A:482:GLN:HE22	1.99	0.65
1:A:150:GLY:HA3	1:A:163:PHE:O	1.97	0.64
1:B:338:GLU:CA	1:B:343:TYR:CE1	2.80	0.64
1:B:91:VAL:O	1:B:102:ARG:HA	1.98	0.64
1:B:287:PRO:HG2	1:B:337:TYR:HA	1.79	0.64
1:A:545:ASN:HA	1:A:548:LEU:CD2	2.27	0.64
1:B:138:ILE:CD1	1:B:162:ARG:HH12	2.08	0.64
1:B:159:ARG:HB3	1:B:583:TRP:NE1	2.13	0.64
1:B:359:MET:HE3	1:B:482:GLN:HE22	1.61	0.64
1:A:378:HIS:HB2	1:A:382:ASN:ND2	2.12	0.63
1:A:426:GLN:O	1:A:430:LEU:HG	1.98	0.63
1:B:137:LYS:HE3	1:B:176:PHE:CE2	2.32	0.63
1:B:450:GLU:HA	1:B:454:LEU:HD12	1.80	0.63
1:B:292:SER:HB2	1:B:294:LYS:NZ	2.14	0.63
1:B:232:GLU:OE2	1:B:243:LEU:HD23	1.97	0.63
1:A:135:VAL:HG12	1:A:176:PHE:CE1	2.33	0.63
1:A:317:PHE:CZ	1:A:405:LYS:HD2	2.30	0.63
1:A:371:TYR:CD1	1:A:372:PRO:HA	2.33	0.63
1:A:403:ALA:HB2	1:A:434:MET:HE3	1.81	0.63
1:B:181:LYS:HA	1:B:188:ASN:ND2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:THR:HG22	3:B:1170:HOH:O	1.97	0.63
1:B:547:GLN:O	1:B:549:GLU:N	2.31	0.63
1:A:489:GLN:NE2	1:A:574:GLU:O	2.31	0.63
1:B:185:PRO:HD2	1:B:467:GLY:HA3	1.80	0.63
1:A:481:LEU:HD12	1:A:481:LEU:O	1.99	0.63
1:B:208:LEU:HD21	1:B:446:GLU:OE1	1.98	0.63
1:A:317:PHE:CD1	1:A:405:LYS:CG	2.81	0.62
1:B:458:HIS:CE1	1:B:463:ARG:HG3	2.34	0.62
1:B:222:ASN:OD1	1:B:224:SER:N	2.31	0.62
1:A:295:ARG:NH2	1:A:342:ALA:HA	2.15	0.62
1:B:330:ASN:HA	1:B:333:LYS:CE	2.28	0.62
1:A:509:LEU:HD12	1:A:579:TYR:CD1	2.33	0.62
1:B:120:ASP:HB3	1:B:121:PRO:CD	2.29	0.62
1:A:403:ALA:CB	1:A:434:MET:HE3	2.29	0.62
1:B:308:ASP:OD1	1:B:312:GLN:HG2	2.00	0.62
1:A:112:LEU:CD1	1:A:179:LEU:HD21	2.19	0.62
1:B:92:THR:HB	1:B:164:ALA:HB3	1.82	0.62
1:B:231:ASN:ND2	1:B:237:CYS:H	1.96	0.62
1:B:365:LYS:HB2	1:B:386:THR:HG22	1.82	0.62
1:B:407:GLU:HB3	3:B:1124:HOH:O	2.00	0.62
1:B:516:LEU:O	1:B:516:LEU:HD23	1.99	0.62
1:B:511:HIS:HA	1:B:514:SER:OG	1.99	0.61
1:B:426:GLN:NE2	1:B:482:GLN:HB3	2.15	0.61
1:B:338:GLU:OE1	1:B:338:GLU:N	2.33	0.61
1:A:261:PHE:O	1:A:288:MET:CG	2.34	0.61
1:A:375:GLU:O	1:A:375:GLU:OE1	2.19	0.61
1:A:268:PRO:CA	1:A:284:CYS:HB3	2.30	0.61
1:B:387:HIS:O	1:B:391:HIS:CD2	2.54	0.61
1:B:185:PRO:HG2	1:B:192:LEU:HD23	1.83	0.61
1:B:290:GLY:HA2	1:B:331:LYS:O	2.00	0.61
1:B:338:GLU:CB	1:B:343:TYR:CE1	2.83	0.61
1:B:363:LEU:HB2	1:B:388:TRP:CZ3	2.34	0.61
1:B:267:ILE:O	1:B:269:VAL:HG13	2.01	0.61
1:B:270:LEU:C	1:B:270:LEU:HD23	2.25	0.61
1:B:375:GLU:C	1:B:375:GLU:OE1	2.43	0.61
1:B:85:LYS:HB3	1:B:182:TYR:CE1	2.36	0.61
1:A:402:ILE:HG23	1:A:413:VAL:HG21	1.82	0.60
1:A:317:PHE:CZ	1:A:405:LYS:CE	2.84	0.60
1:B:85:LYS:HG3	1:B:182:TYR:CE1	2.37	0.60
1:A:227:ILE:HG12	1:A:245:VAL:HG22	1.82	0.60
1:B:321:ALA:HB2	1:B:427:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ILE:HD13	1:B:162:ARG:CZ	2.31	0.60
1:B:157:ASP:OD1	1:B:159:ARG:HG2	2.01	0.60
1:B:246:VAL:HB	1:B:247:PRO:CD	2.32	0.60
1:B:340:GLU:HG3	1:B:341:ASP:OD1	2.02	0.60
1:A:201:PHE:HB3	1:A:202:PRO:HD2	1.83	0.60
1:A:426:GLN:HG2	1:A:453:TRP:HH2	1.67	0.60
1:B:340:GLU:HG3	1:B:341:ASP:CG	2.25	0.60
1:B:400:LEU:CD2	1:B:566:PRO:HD2	2.32	0.60
1:A:135:VAL:HB	1:A:180:MET:SD	2.41	0.59
1:B:389:LEU:CB	1:B:570:MET:HE1	2.29	0.59
1:A:303:LEU:CD2	1:A:318:ILE:HD11	2.32	0.59
1:B:261:PHE:O	1:B:288:MET:CG	2.46	0.59
1:B:323:PRO:HD2	1:B:326:ASN:ND2	2.17	0.59
1:A:74:GLU:HG3	1:A:75:GLU:N	2.17	0.59
1:B:312:GLN:O	1:B:313:SER:C	2.45	0.59
1:B:291:VAL:CG1	3:B:1211:HOH:O	2.50	0.59
1:B:91:VAL:HG22	1:B:165:HIS:CE1	2.37	0.58
1:B:240:TYR:CE1	1:B:266:ARG:NH1	2.69	0.58
1:B:307:MET:HE1	1:B:345:ASN:O	2.03	0.58
1:B:396:LEU:HD21	1:B:486:CYS:HB3	1.85	0.58
1:A:92:THR:OG1	1:A:102:ARG:HG2	2.03	0.58
1:A:149:TYR:CE2	1:A:172:ARG:HG3	2.38	0.58
1:B:423:ARG:O	1:B:427:LEU:HG	2.04	0.58
1:B:377:THR:HG22	1:B:378:HIS:CD2	2.38	0.58
1:B:220:ILE:CD1	1:B:222:ASN:ND2	2.67	0.58
1:B:422:ASP:OD1	1:B:458:HIS:CE1	2.57	0.58
1:A:303:LEU:HD13	1:A:343:TYR:CE2	2.39	0.57
1:B:289:VAL:O	1:B:294:LYS:HG2	2.04	0.57
1:A:266:ARG:O	1:A:284:CYS:HB2	2.04	0.57
1:B:159:ARG:HD3	1:B:583:TRP:CE2	2.38	0.57
1:B:286:GLN:HB3	1:B:417:SER:O	2.04	0.57
1:A:241:PRO:HD2	1:A:244:LEU:HD21	1.85	0.57
1:B:115:LYS:HG3	1:B:124:VAL:HG22	1.85	0.57
1:A:229:LYS:HD3	1:A:232:GLU:OE2	2.04	0.57
1:B:549:GLU:HB2	3:B:1064:HOH:O	2.05	0.57
1:A:461:GLN:CB	1:A:522:CYS:O	2.53	0.57
1:B:186:VAL:HB	1:B:467:GLY:O	2.05	0.57
1:B:403:ALA:CB	1:B:434:MET:HE3	2.35	0.57
1:A:101:VAL:HG22	1:A:119:ARG:HH21	1.69	0.56
1:B:94:ILE:CD1	1:B:147:ASN:HB3	2.19	0.56
1:A:196:GLU:HG3	3:A:1159:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PRO:HG2	1:A:244:LEU:HD23	1.87	0.56
1:A:472:ALA:O	1:A:473:ASP:C	2.47	0.56
1:A:96:PRO:HG2	1:A:97:PHE:CE1	2.41	0.56
1:B:338:GLU:HA	1:B:343:TYR:HE1	1.68	0.56
1:B:567:VAL:HG11	1:B:572:HIS:HD2	1.70	0.56
1:B:126:ASP:OD1	1:B:127:ALA:N	2.38	0.56
1:B:268:PRO:CA	1:B:284:CYS:HB3	2.36	0.56
1:B:129:LEU:HB3	1:B:183:ALA:HA	1.88	0.56
1:B:357:HIS:ND1	1:B:360:ARG:NH2	2.54	0.56
1:A:282:THR:OG1	1:A:414:VAL:HG22	2.05	0.56
1:A:382:ASN:O	1:A:385:SER:OG	2.23	0.56
1:A:86:ASP:OD2	1:A:174:SER:OG	2.18	0.56
1:A:504:PHE:O	1:A:508:ILE:HG13	2.06	0.56
1:B:526:GLN:O	1:B:530:LYS:HG3	2.05	0.56
1:B:584:ASN:C	1:B:586:ARG:H	2.14	0.56
1:A:82:GLU:HG3	1:A:108:THR:OG1	2.06	0.56
1:A:154:VAL:HA	1:A:160:ASN:OD1	2.06	0.56
1:A:443:ARG:HD3	3:A:1075:HOH:O	2.06	0.56
1:B:348:LEU:HD12	1:B:349:VAL:N	2.21	0.55
1:A:107:VAL:HG22	1:A:112:LEU:CD1	2.36	0.55
1:B:547:GLN:C	1:B:549:GLU:H	2.14	0.55
1:A:159:ARG:HD3	1:A:583:TRP:CZ2	2.41	0.55
1:B:185:PRO:CG	1:B:192:LEU:CD2	2.83	0.55
1:B:533:LEU:N	1:B:534:PRO:CD	2.69	0.55
1:A:111:ARG:HD3	1:A:126:ASP:OD1	2.06	0.55
1:B:226:ARG:HD3	1:B:248:ALA:HA	1.88	0.55
1:B:548:LEU:O	1:B:552:THR:OG1	2.16	0.55
1:A:586:ARG:HG3	3:A:1195:HOH:O	2.07	0.55
1:B:338:GLU:CB	1:B:343:TYR:CD1	2.86	0.55
1:A:246:VAL:HB	1:A:247:PRO:CD	2.37	0.55
1:B:78:LEU:HD22	1:B:82:GLU:HG2	1.89	0.55
1:B:307:MET:HE2	1:B:316:ILE:CB	2.37	0.55
1:B:181:LYS:HA	1:B:188:ASN:HD22	1.72	0.54
1:B:220:ILE:HD13	1:B:222:ASN:ND2	2.22	0.54
1:B:338:GLU:HB3	1:B:343:TYR:CE1	2.42	0.54
1:A:294:LYS:HE3	3:A:1106:HOH:O	2.07	0.54
1:A:101:VAL:CG2	1:A:119:ARG:NE	2.69	0.54
1:B:337:TYR:CE1	1:B:348:LEU:HD23	2.41	0.54
1:B:432:MET:HE1	1:B:452:GLU:CD	2.32	0.54
1:B:184:PHE:CG	1:B:469:LYS:HG2	2.43	0.54
1:B:502:GLU:HG3	1:B:576:TRP:HZ2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:VAL:CG1	1:B:572:HIS:CD2	2.90	0.54
1:A:322:ARG:NH1	1:A:330:ASN:HD22	2.06	0.54
1:A:407:GLU:HA	1:A:407:GLU:OE1	2.07	0.54
1:A:415:VAL:HG22	1:A:424:THR:HG23	1.89	0.54
1:B:296:SER:HB3	1:B:299:ASP:HB2	1.89	0.54
1:A:214:GLU:HA	1:A:214:GLU:OE1	2.07	0.54
1:B:209:TYR:CD1	1:B:447:VAL:HG13	2.41	0.54
1:A:110:TYR:CZ	1:A:516:LEU:HD13	2.42	0.54
1:A:547:GLN:O	1:A:547:GLN:HG3	2.08	0.54
1:A:428:THR:O	1:A:432:MET:HE3	2.08	0.54
1:A:521:LEU:O	1:A:522:CYS:HB2	2.08	0.53
1:A:245:VAL:HG11	1:A:270:LEU:HD23	1.89	0.53
1:A:511:HIS:CE1	1:A:517:PHE:HE1	2.27	0.53
1:B:266:ARG:HH21	1:B:421:TRP:HE3	1.56	0.53
1:A:496:THR:HG21	1:A:558:SER:HB2	1.91	0.53
1:A:517:PHE:HB3	1:A:538:VAL:O	2.09	0.53
1:B:79:LEU:HG	1:B:111:ARG:HH22	1.73	0.53
1:B:303:LEU:HD12	1:B:343:TYR:CD2	2.43	0.53
1:B:325:VAL:HG23	3:B:1005:HOH:O	2.08	0.53
1:A:528:ARG:CG	1:A:533:LEU:HD12	2.38	0.53
1:B:112:LEU:HD13	1:B:179:LEU:HD13	1.91	0.53
1:A:126:ASP:OD1	1:A:126:ASP:C	2.51	0.53
1:A:238:ASP:OD1	1:A:239:THR:HG23	2.09	0.53
1:B:119:ARG:O	1:B:120:ASP:C	2.52	0.53
1:B:314:HIS:CG	1:B:315:LYS:H	2.25	0.53
1:B:485:ASP:O	1:B:489:GLN:HG2	2.08	0.53
1:B:266:ARG:CD	1:B:285:SER:HB3	2.39	0.53
1:A:416:HIS:C	1:A:416:HIS:CD2	2.85	0.53
1:A:284:CYS:O	1:A:416:HIS:CB	2.56	0.53
1:A:456:PHE:CE1	3:A:1020:HOH:O	2.54	0.53
1:B:584:ASN:OD1	1:B:585:PRO:HD2	2.09	0.53
1:B:220:ILE:CG2	1:B:221:PRO:HA	2.40	0.52
1:B:361:GLU:O	1:B:365:LYS:HG3	2.10	0.52
1:B:461:GLN:O	1:B:465:GLY:HA2	2.08	0.52
1:B:135:VAL:HG12	1:B:176:PHE:CE1	2.45	0.52
1:B:137:LYS:HG3	1:B:176:PHE:CZ	2.45	0.52
1:A:79:LEU:HD11	1:A:111:ARG:NH2	2.25	0.52
1:B:259:ALA:HA	1:B:267:ILE:HG22	1.90	0.52
1:B:459:ARG:HB3	1:B:523:ASN:OD1	2.08	0.52
1:B:468:ASP:HB3	1:B:476:ARG:NH2	2.24	0.52
1:A:122:PRO:HD2	3:A:1152:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LYS:O	1:A:456:PHE:HD1	1.92	0.52
1:B:422:ASP:HB2	2:B:656:PO4:O2	2.09	0.52
1:A:129:LEU:HB3	1:A:183:ALA:HA	1.92	0.52
1:A:267:ILE:O	1:A:268:PRO:C	2.51	0.52
1:B:197:TYR:O	1:B:198:LYS:HD3	2.09	0.52
1:B:466:HIS:CD2	1:B:521:LEU:CD2	2.90	0.52
1:B:468:ASP:HB3	1:B:476:ARG:HH21	1.75	0.52
1:A:430:LEU:HD23	1:A:483:PHE:HE1	1.74	0.52
1:B:375:GLU:OE1	1:B:375:GLU:O	2.28	0.52
1:A:240:TYR:HE1	1:A:266:ARG:NH1	2.08	0.51
1:A:428:THR:C	1:A:432:MET:HE3	2.35	0.51
1:B:240:TYR:CZ	1:B:266:ARG:HB3	2.46	0.51
1:B:246:VAL:HB	1:B:247:PRO:HD2	1.91	0.51
1:B:272:TRP:CZ3	1:B:435:LEU:HD13	2.45	0.51
1:B:521:LEU:O	1:B:522:CYS:HB2	2.10	0.51
1:A:390:GLU:CG	3:A:1037:HOH:O	2.45	0.51
1:B:526:GLN:CG	1:B:530:LYS:HE3	2.38	0.51
1:A:137:LYS:HD3	1:A:172:ARG:HH12	1.73	0.51
1:B:488:TRP:CE2	1:B:576:TRP:CD1	2.99	0.51
1:B:84:ILE:HA	1:B:108:THR:HG22	1.92	0.51
1:B:85:LYS:HG3	1:B:182:TYR:CZ	2.45	0.51
1:A:430:LEU:HD23	1:A:483:PHE:CE1	2.45	0.51
1:A:149:TYR:O	1:A:165:HIS:N	2.42	0.51
1:A:239:THR:HG23	3:A:1032:HOH:O	2.10	0.51
1:A:370:VAL:HG11	1:A:580:TYR:O	2.09	0.51
1:A:131:VAL:HG21	1:A:157:ASP:OD2	2.10	0.51
1:A:173:ARG:O	1:A:177:GLU:HG2	2.10	0.51
1:A:185:PRO:HD2	1:A:467:GLY:CA	2.39	0.51
1:A:461:GLN:HB3	1:A:523:ASN:OD1	2.11	0.51
1:A:183:ALA:O	1:A:184:PHE:CD2	2.63	0.51
1:A:410:LYS:HG3	3:A:1073:HOH:O	2.10	0.51
1:A:315:LYS:NZ	1:A:347:GLU:OE1	2.23	0.51
1:B:307:MET:HE3	1:B:316:ILE:CG2	2.41	0.51
1:A:150:GLY:HA2	1:A:165:HIS:HD2	1.75	0.51
1:A:317:PHE:CE1	1:A:411:THR:HG21	2.45	0.51
1:B:504:PHE:CE2	1:B:508:ILE:CD1	2.94	0.51
1:A:186:VAL:CG2	1:A:467:GLY:O	2.58	0.50
1:B:338:GLU:HB3	1:B:343:TYR:CG	2.46	0.50
1:B:422:ASP:OD1	1:B:458:HIS:HE1	1.94	0.50
1:B:292:SER:HB2	1:B:294:LYS:HZ2	1.76	0.50
1:A:101:VAL:HG21	1:A:119:ARG:NE	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ARG:HH21	1:A:300:GLU:CD	2.19	0.50
1:A:518:GLY:CA	1:A:521:LEU:HD12	2.40	0.50
1:A:547:GLN:O	1:A:549:GLU:N	2.44	0.50
1:A:303:LEU:HD21	1:A:318:ILE:HD11	1.93	0.50
1:A:431:ALA:HA	1:A:434:MET:HE2	1.94	0.50
1:A:443:ARG:O	1:A:447:VAL:HG23	2.11	0.50
1:B:283:ARG:NH1	1:B:452:GLU:OE1	2.43	0.50
1:B:407:GLU:OE1	1:B:407:GLU:HA	2.10	0.50
1:A:86:ASP:OD1	1:A:87:MET:N	2.44	0.50
1:B:206:TRP:CE2	1:B:534:PRO:HA	2.47	0.50
1:A:450:GLU:CD	1:A:454:LEU:HD12	2.37	0.49
1:B:399:ALA:O	1:B:434:MET:HE1	2.11	0.49
1:A:401:ARG:HH11	1:A:401:ARG:HB3	1.76	0.49
1:B:76:PRO:HG3	1:B:106:THR:HG21	1.94	0.49
1:B:320:ASP:CG	1:B:322:ARG:HE	2.20	0.49
1:B:338:GLU:CG	1:B:343:TYR:CZ	2.95	0.49
1:B:500:PHE:CE1	1:B:505:LEU:HD21	2.47	0.49
1:A:421:TRP:CD1	1:A:422:ASP:OD2	2.66	0.49
1:B:446:GLU:HG2	1:B:541:TRP:CE3	2.46	0.49
1:A:114:PHE:HB3	1:A:125:LEU:HB3	1.94	0.49
1:B:186:VAL:HG23	1:B:192:LEU:HD21	1.94	0.49
1:A:131:VAL:HG13	1:A:155:CYS:HB3	1.94	0.49
1:A:240:TYR:HB3	1:A:241:PRO:HD2	1.95	0.49
1:B:310:ASN:O	1:B:311:ALA:HB3	2.13	0.49
1:A:259:ALA:CA	1:A:267:ILE:CG2	2.89	0.49
1:B:323:PRO:HB2	1:B:326:ASN:HD22	1.78	0.49
1:A:582:ARG:O	1:A:582:ARG:HG3	2.12	0.49
1:B:85:LYS:CB	1:B:182:TYR:CE1	2.96	0.49
1:A:259:ALA:HA	1:A:267:ILE:HG22	1.92	0.48
1:A:262:ARG:HG3	1:A:267:ILE:HA	1.95	0.48
1:A:527:GLN:HG3	3:A:1234:HOH:O	2.13	0.48
1:B:241:PRO:HG2	1:B:244:LEU:HD23	1.95	0.48
1:A:557:GLY:O	1:A:558:SER:C	2.55	0.48
1:A:378:HIS:HB3	1:A:382:ASN:ND2	2.27	0.48
1:A:516:LEU:HD23	1:A:517:PHE:CE1	2.49	0.48
1:B:234:TYR:CD2	1:B:526:GLN:HB2	2.47	0.48
1:B:355:ASN:O	1:B:359:MET:HG2	2.13	0.48
1:A:101:VAL:HG21	1:A:119:ARG:HE	1.74	0.48
1:B:78:LEU:HD11	1:B:84:ILE:HG13	1.95	0.48
1:A:430:LEU:O	1:A:434:MET:HG3	2.13	0.48
1:B:75:GLU:HB3	1:B:76:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:THR:OG1	1:B:161:LEU:HB2	2.13	0.48
1:B:348:LEU:HD12	1:B:348:LEU:C	2.38	0.48
1:B:528:ARG:HD3	1:B:533:LEU:HD12	1.94	0.48
1:A:317:PHE:CD1	1:A:411:THR:HG21	2.49	0.48
1:B:283:ARG:NH2	1:B:456:PHE:HB3	2.29	0.48
1:B:340:GLU:CG	3:B:1227:HOH:O	2.54	0.48
1:A:102:ARG:HB2	1:A:118:GLU:OE2	2.14	0.48
1:A:113:TYR:CE1	1:A:126:ASP:HB2	2.49	0.47
1:A:304:GLN:HE22	1:A:307:MET:CE	2.27	0.47
1:B:547:GLN:C	1:B:549:GLU:N	2.72	0.47
1:B:298:GLU:CD	1:B:298:GLU:H	2.22	0.47
1:A:522:CYS:SG	1:A:533:LEU:HD11	2.54	0.47
1:A:318:ILE:O	1:A:348:LEU:HA	2.14	0.47
1:A:563:VAL:HG12	1:A:565:TYR:CE1	2.49	0.47
1:B:135:VAL:HG11	1:B:179:LEU:HD23	1.96	0.47
1:B:316:ILE:HG13	1:B:412:SER:O	2.14	0.47
1:B:450:GLU:OE2	1:B:454:LEU:CD1	2.62	0.47
1:A:85:LYS:O	1:A:86:ASP:HB2	2.15	0.47
1:A:381:SER:HB3	1:B:384:GLU:OE2	2.14	0.47
1:A:509:LEU:HD13	1:A:579:TYR:CE1	2.48	0.47
1:B:149:TYR:O	1:B:164:ALA:HA	2.15	0.47
1:B:282:THR:HG23	3:B:1110:HOH:O	2.14	0.47
1:A:79:LEU:CD1	1:A:111:ARG:NH2	2.78	0.47
1:A:197:TYR:CE2	1:A:199:GLU:HB3	2.50	0.47
1:A:220:ILE:CG2	1:A:221:PRO:N	2.78	0.47
1:A:423:ARG:HH21	2:A:656:PO4:P	2.38	0.47
1:A:446:GLU:HG2	1:A:541:TRP:CE3	2.50	0.47
1:A:541:TRP:CE3	1:A:544:ILE:HD12	2.50	0.47
1:B:85:LYS:HD2	1:B:182:TYR:OH	2.14	0.47
1:B:220:ILE:HD12	1:B:225:TRP:HB2	1.96	0.47
1:B:292:SER:HB2	1:B:294:LYS:HZ1	1.80	0.47
1:A:76:PRO:HB3	1:A:113:TYR:CG	2.50	0.47
1:A:150:GLY:HA2	1:A:165:HIS:CD2	2.49	0.47
1:A:303:LEU:HD13	1:A:343:TYR:HE2	1.80	0.47
1:B:259:ALA:HA	1:B:267:ILE:CG2	2.45	0.47
1:A:76:PRO:HG3	1:A:106:THR:HG21	1.96	0.47
1:B:388:TRP:O	1:B:392:ILE:HG12	2.15	0.47
1:B:502:GLU:HG3	1:B:576:TRP:CZ2	2.49	0.47
1:B:531:GLU:O	1:B:536:ARG:HD3	2.14	0.47
1:B:222:ASN:OD1	1:B:225:TRP:N	2.41	0.47
1:A:237:CYS:HB2	1:A:265:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASP:HB2	1:A:348:LEU:HD11	1.96	0.46
1:A:422:ASP:O	1:A:426:GLN:HG3	2.16	0.46
1:B:383:LEU:HD13	1:B:575:LEU:HD22	1.98	0.46
1:B:296:SER:CB	1:B:299:ASP:HB2	2.45	0.46
1:B:504:PHE:CE2	1:B:508:ILE:HD11	2.49	0.46
1:B:206:TRP:CD1	1:B:534:PRO:HA	2.50	0.46
1:B:415:VAL:HG11	1:B:428:THR:HG22	1.97	0.46
1:A:511:HIS:CD2	1:A:540:LEU:CD1	2.99	0.46
1:A:524:SER:O	1:A:528:ARG:HG3	2.14	0.46
1:B:91:VAL:CG2	1:B:165:HIS:CE1	2.98	0.46
1:B:321:ALA:HB2	1:B:427:LEU:CD1	2.46	0.46
1:B:426:GLN:HE21	1:B:482:GLN:HB3	1.78	0.46
1:A:159:ARG:NE	1:A:583:TRP:CZ2	2.84	0.46
1:A:231:ASN:HD21	1:A:237:CYS:H	1.63	0.46
1:A:511:HIS:CD2	1:A:540:LEU:HD11	2.50	0.46
1:B:158:ILE:HG23	1:B:367:LYS:HG3	1.96	0.46
1:B:212:LEU:HD21	1:B:243:LEU:HD13	1.96	0.46
1:B:245:VAL:HB	1:B:270:LEU:HB3	1.97	0.46
1:B:282:THR:OG1	1:B:414:VAL:HG22	2.15	0.46
1:B:545:ASN:ND2	1:B:548:LEU:HD21	2.31	0.46
1:A:112:LEU:HD13	1:A:179:LEU:CD2	2.22	0.46
1:A:418:SER:HB2	2:A:656:PO4:O3	2.16	0.46
1:A:137:LYS:HE3	1:A:176:PHE:CE2	2.51	0.46
1:A:220:ILE:HG22	1:A:221:PRO:N	2.30	0.46
1:A:222:ASN:O	1:A:222:ASN:OD1	2.33	0.46
1:B:287:PRO:HG2	1:B:337:TYR:CA	2.46	0.46
1:A:423:ARG:O	1:A:427:LEU:HG	2.15	0.46
1:B:138:ILE:HD13	1:B:162:ARG:NH2	2.31	0.46
1:B:270:LEU:HD23	1:B:271:SER:N	2.30	0.46
1:B:396:LEU:HD23	1:B:430:LEU:HD13	1.98	0.46
1:A:113:TYR:CD1	1:A:126:ASP:HB2	2.51	0.46
1:B:310:ASN:O	1:B:310:ASN:OD1	2.34	0.46
1:B:437:GLY:HA2	1:B:440:ARG:NH1	2.30	0.46
1:A:159:ARG:CD	1:A:583:TRP:CZ2	2.99	0.45
1:A:576:TRP:CD1	1:A:576:TRP:C	2.92	0.45
1:B:85:LYS:CG	1:B:182:TYR:CE1	2.99	0.45
1:A:316:ILE:HG23	1:A:316:ILE:O	2.16	0.45
1:A:375:GLU:OE1	1:A:375:GLU:C	2.59	0.45
1:B:95:CYS:O	1:B:98:THR:O	2.34	0.45
1:B:307:MET:CE	1:B:316:ILE:HB	2.46	0.45
1:A:82:GLU:CG	1:A:108:THR:OG1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LYS:HB2	1:A:107:VAL:O	2.17	0.45
1:A:432:MET:HE1	1:A:452:GLU:CD	2.42	0.45
1:B:94:ILE:HD11	1:B:147:ASN:HB2	1.90	0.45
1:B:270:LEU:HA	1:B:282:THR:HG22	1.97	0.45
1:B:459:ARG:NH1	1:B:523:ASN:ND2	2.64	0.45
1:A:274:HIS:CG	1:A:275:PRO:CD	2.93	0.45
1:B:266:ARG:HD2	1:B:285:SER:HB3	1.97	0.45
1:A:318:ILE:O	1:A:348:LEU:HD12	2.16	0.45
1:A:353:ILE:CD1	1:A:395:ILE:HD13	2.41	0.45
1:A:452:GLU:HB2	1:A:453:TRP:CD1	2.52	0.45
1:A:290:GLY:HA3	3:A:1106:HOH:O	2.17	0.45
1:A:419:ASP:HB2	1:A:421:TRP:NE1	2.31	0.45
1:B:270:LEU:HD23	1:B:271:SER:C	2.41	0.45
1:B:359:MET:HE1	1:B:391:HIS:CG	2.52	0.45
1:B:383:LEU:CD1	1:B:575:LEU:HD22	2.47	0.45
1:A:431:ALA:HA	1:A:434:MET:CE	2.46	0.45
1:B:220:ILE:HD13	1:B:222:ASN:HD22	1.81	0.45
1:B:460:PHE:O	1:B:464:VAL:HG23	2.16	0.45
1:B:229:LYS:HB3	1:B:232:GLU:CG	2.46	0.45
1:B:461:GLN:HB2	1:B:522:CYS:O	2.17	0.45
1:B:461:GLN:O	1:B:465:GLY:N	2.47	0.45
1:A:135:VAL:HG12	1:A:176:PHE:CD1	2.52	0.45
1:A:353:ILE:HD13	1:A:395:ILE:CD1	2.41	0.45
1:A:506:ILE:CG2	1:A:582:ARG:NH1	2.80	0.45
1:B:113:TYR:CE2	1:B:115:LYS:HB2	2.52	0.45
1:B:222:ASN:OD1	1:B:222:ASN:C	2.60	0.45
1:B:361:GLU:CD	1:B:364:ARG:HE	2.24	0.45
1:B:528:ARG:CG	1:B:533:LEU:HD12	2.46	0.45
1:A:231:ASN:ND2	1:A:234:TYR:HA	2.31	0.44
1:B:125:LEU:HD21	1:B:161:LEU:CD2	2.41	0.44
1:B:291:VAL:C	1:B:293:GLY:H	2.25	0.44
1:A:473:ASP:OD1	1:A:475:ASP:HB2	2.17	0.44
1:B:365:LYS:CB	1:B:386:THR:HG22	2.48	0.44
1:A:74:GLU:CG	1:A:115:LYS:HD3	2.47	0.44
1:A:246:VAL:HB	1:A:247:PRO:HD2	2.00	0.44
1:B:113:TYR:CZ	1:B:124:VAL:HG13	2.52	0.44
1:B:517:PHE:HB3	1:B:538:VAL:O	2.17	0.44
1:B:544:ILE:HG23	1:B:551:PHE:CD1	2.52	0.44
1:A:399:ALA:O	1:A:434:MET:CE	2.63	0.44
1:A:569:SER:C	1:A:571:ARG:N	2.75	0.44
1:B:224:SER:HB3	1:B:309:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:HIS:CG	1:B:515:CYS:SG	3.11	0.44
1:A:134:ARG:NH1	1:A:136:GLU:CG	2.78	0.44
1:A:544:ILE:CG2	1:A:551:PHE:CD1	2.91	0.44
1:A:576:TRP:CD1	1:A:576:TRP:O	2.70	0.44
1:A:74:GLU:CG	1:A:75:GLU:N	2.80	0.44
1:A:266:ARG:NH2	1:A:456:PHE:O	2.43	0.44
1:B:185:PRO:HG3	1:B:192:LEU:HD23	1.98	0.44
1:B:356:ILE:HB	1:B:477:SER:HB2	2.00	0.44
1:B:374:ILE:HD11	1:B:581:ILE:HG21	2.00	0.44
1:A:110:TYR:CE1	1:A:516:LEU:HD13	2.53	0.44
1:A:304:GLN:NE2	1:A:307:MET:HE2	2.33	0.44
1:A:466:HIS:HE1	1:A:512:LEU:O	2.00	0.44
1:A:528:ARG:HG2	1:A:533:LEU:HD12	1.99	0.44
1:A:569:SER:C	1:A:571:ARG:H	2.25	0.44
1:B:85:LYS:HE2	1:B:109:ASN:HB3	1.99	0.44
1:B:267:ILE:HG13	1:B:269:VAL:HG13	1.99	0.43
1:B:460:PHE:CD2	1:B:512:LEU:HD11	2.53	0.43
1:A:423:ARG:HE	1:A:423:ARG:HB2	1.49	0.43
1:B:241:PRO:HD2	1:B:244:LEU:HD21	2.00	0.43
1:A:134:ARG:NH2	3:A:1200:HOH:O	2.51	0.43
1:B:234:TYR:HB2	1:B:526:GLN:NE2	2.33	0.43
1:B:533:LEU:N	1:B:534:PRO:HD3	2.34	0.43
1:A:231:ASN:ND2	1:A:237:CYS:H	2.15	0.43
1:A:440:ARG:HE	1:A:564:LEU:HD12	1.83	0.43
1:B:504:PHE:CE2	1:B:508:ILE:HD12	2.53	0.43
1:A:471:HIS:HA	1:A:476:ARG:NH1	2.33	0.43
1:B:410:LYS:CE	3:B:1093:HOH:O	1.83	0.43
1:A:374:ILE:CD1	1:A:581:ILE:HD13	2.43	0.43
1:A:459:ARG:O	1:A:463:ARG:HG2	2.19	0.43
1:B:509:LEU:HD12	1:B:579:TYR:CD1	2.53	0.43
1:A:222:ASN:OD1	1:A:222:ASN:C	2.61	0.43
1:A:430:LEU:CD2	1:A:483:PHE:CE1	3.01	0.43
1:A:511:HIS:HA	1:A:514:SER:HG	1.82	0.43
1:A:533:LEU:N	1:A:534:PRO:CD	2.82	0.43
1:B:92:THR:OG1	1:B:102:ARG:HG2	2.19	0.43
1:B:451:LYS:O	1:B:456:PHE:HD1	2.02	0.43
1:B:460:PHE:CE2	1:B:512:LEU:HD11	2.53	0.43
1:A:295:ARG:NE	1:A:300:GLU:OE2	2.40	0.43
1:A:322:ARG:HH11	1:A:330:ASN:ND2	2.16	0.43
1:B:75:GLU:HG2	1:B:87:MET:HE1	2.01	0.43
1:B:511:HIS:CG	1:B:540:LEU:HD13	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASP:OD1	1:A:238:ASP:C	2.62	0.42
1:B:298:GLU:O	1:B:302:TYR:N	2.45	0.42
1:B:314:HIS:CD2	1:B:315:LYS:CB	2.85	0.42
1:B:323:PRO:HB2	1:B:326:ASN:ND2	2.34	0.42
1:A:317:PHE:CE1	1:A:405:LYS:CE	2.98	0.42
1:A:437:GLY:CA	1:A:440:ARG:NH1	2.79	0.42
1:B:481:LEU:HD13	1:B:509:LEU:HD13	2.02	0.42
1:A:92:THR:HB	1:A:164:ALA:HB3	2.02	0.42
1:A:234:TYR:HB3	1:A:238:ASP:HA	2.01	0.42
1:B:128:SER:O	1:B:131:VAL:HG12	2.20	0.42
1:B:192:LEU:C	1:B:194:ALA:N	2.77	0.42
1:B:307:MET:HE1	1:B:316:ILE:HG22	2.00	0.42
1:B:97:PHE:CD1	1:B:585:PRO:HD3	2.55	0.42
1:B:114:PHE:HB3	1:B:125:LEU:HB3	2.00	0.42
1:B:401:ARG:HH11	1:B:401:ARG:HB3	1.83	0.42
1:B:461:GLN:O	1:B:465:GLY:CA	2.68	0.42
1:A:82:GLU:HA	1:A:109:ASN:OD1	2.20	0.42
1:A:101:VAL:HG22	1:A:119:ARG:NE	2.30	0.42
1:A:177:GLU:OE1	1:A:177:GLU:HA	2.20	0.42
1:A:576:TRP:O	1:A:577:VAL:C	2.62	0.42
1:B:209:TYR:HB3	3:B:1182:HOH:O	2.19	0.42
1:B:322:ARG:NH1	1:B:327:ALA:HA	2.35	0.42
1:B:354:HIS:CG	1:B:358:VAL:HG11	2.55	0.42
1:B:544:ILE:HG22	1:B:545:ASN:HD22	1.84	0.42
1:B:177:GLU:HA	1:B:177:GLU:OE1	2.20	0.42
1:A:338:GLU:CG	1:A:343:TYR:CE1	3.03	0.42
1:A:563:VAL:CG1	1:A:565:TYR:CE1	3.03	0.42
1:B:545:ASN:HD22	1:B:548:LEU:HD21	1.85	0.42
1:A:378:HIS:HA	1:B:384:GLU:OE1	2.20	0.42
1:A:568:ALA:O	1:A:569:SER:OG	2.33	0.42
1:B:316:ILE:O	1:B:316:ILE:HG23	2.19	0.42
1:A:395:ILE:HG22	1:A:430:LEU:CD1	2.50	0.41
1:A:492:ARG:CD	1:A:574:GLU:OE2	2.67	0.41
1:B:185:PRO:HG2	1:B:192:LEU:HD21	2.01	0.41
1:A:295:ARG:HB2	3:A:1141:HOH:O	2.19	0.41
1:B:584:ASN:O	1:B:586:ARG:N	2.50	0.41
1:A:75:GLU:OE1	1:A:75:GLU:HA	2.20	0.41
1:B:359:MET:HE2	1:B:482:GLN:HE22	1.83	0.41
1:A:492:ARG:HD3	1:A:574:GLU:OE2	2.20	0.41
1:B:226:ARG:HD3	1:B:248:ALA:O	2.21	0.41
1:B:391:HIS:O	1:B:395:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:ASN:O	1:B:504:PHE:HB3	2.20	0.41
1:B:107:VAL:HG22	1:B:112:LEU:HD12	2.01	0.41
1:A:459:ARG:O	1:A:463:ARG:CG	2.68	0.41
1:A:477:SER:OG	1:A:478:PRO:HD2	2.19	0.41
1:B:232:GLU:OE1	1:B:232:GLU:HA	2.20	0.41
1:B:303:LEU:HD12	1:B:343:TYR:HD2	1.85	0.41
1:B:320:ASP:OD2	1:B:322:ARG:NE	2.53	0.41
1:A:79:LEU:H	1:A:82:GLU:HB3	1.86	0.41
1:A:101:VAL:CG2	1:A:119:ARG:CZ	2.98	0.41
1:A:148:SER:HB2	1:A:162:ARG:NH2	2.36	0.41
1:A:416:HIS:CD2	1:A:417:SER:N	2.89	0.41
1:A:422:ASP:OD1	1:A:458:HIS:HE1	1.99	0.41
1:A:458:HIS:NE2	1:A:463:ARG:HG3	2.35	0.41
1:A:553:ASN:OD1	1:A:554:PRO:HD2	2.20	0.41
1:B:223:GLU:HA	1:B:223:GLU:OE1	2.20	0.41
1:B:383:LEU:HD11	1:B:575:LEU:CD1	2.47	0.41
1:B:400:LEU:HA	1:B:434:MET:HE1	2.03	0.41
1:B:401:ARG:HH11	1:B:401:ARG:CG	2.33	0.41
1:B:442:ILE:HG12	1:B:500:PHE:HB3	2.03	0.41
1:B:472:ALA:O	1:B:473:ASP:C	2.64	0.41
1:B:503:TYR:CD2	1:B:551:PHE:CE2	3.09	0.41
1:A:267:ILE:O	1:A:267:ILE:CG1	2.61	0.41
1:A:386:THR:O	1:A:387:HIS:HB2	2.21	0.41
1:B:450:GLU:CD	1:B:454:LEU:CD1	2.92	0.41
1:A:136:GLU:HA	1:A:136:GLU:OE1	2.20	0.41
1:A:222:ASN:O	1:A:225:TRP:N	2.52	0.41
1:A:317:PHE:CE1	1:A:405:LYS:CG	2.98	0.41
1:A:384:GLU:HB2	1:B:380:LEU:HB2	2.02	0.41
1:A:389:LEU:HD12	1:A:570:MET:HE1	2.02	0.41
1:A:400:LEU:CD2	1:A:565:TYR:HD2	2.34	0.41
1:A:576:TRP:O	1:A:576:TRP:CG	2.73	0.41
1:B:74:GLU:HG3	1:B:75:GLU:H	1.86	0.41
1:B:227:ILE:HG12	1:B:245:VAL:HG22	2.03	0.41
1:A:355:ASN:O	1:A:359:MET:HG2	2.21	0.41
1:B:197:TYR:CZ	1:B:199:GLU:HB2	2.56	0.41
1:A:94:ILE:HD12	1:A:162:ARG:HD3	2.02	0.40
1:A:135:VAL:CG1	1:A:176:PHE:CD1	3.04	0.40
1:A:228:THR:OG1	1:A:252:ASP:OD1	2.30	0.40
1:A:304:GLN:HE22	1:A:307:MET:HE2	1.84	0.40
1:B:76:PRO:HA	1:B:77:PRO:HD3	1.95	0.40
1:B:82:GLU:OE1	1:B:111:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:GLN:NE2	1:B:466:HIS:HB2	2.28	0.40
1:A:157:ASP:OD1	1:A:159:ARG:CG	2.70	0.40
1:A:376:GLU:OE2	1:B:569:SER:HB2	2.21	0.40
1:B:278:GLN:HA	1:B:278:GLN:OE1	2.22	0.40
1:B:281:ILE:HG12	1:B:413:VAL:HG22	2.03	0.40
1:B:363:LEU:HD12	1:B:363:LEU:O	2.20	0.40
1:A:186:VAL:HG22	1:A:467:GLY:C	2.47	0.40
1:B:188:ASN:OD1	1:B:469:LYS:HE3	2.22	0.40
1:B:376:GLU:OE1	1:B:376:GLU:HA	2.20	0.40
1:B:443:ARG:O	1:B:447:VAL:HG23	2.21	0.40
1:B:496:THR:O	1:B:556:TYR:HA	2.21	0.40
1:A:149:TYR:CZ	1:A:172:ARG:HG3	2.57	0.40
1:A:230:ILE:HD12	1:A:252:ASP:HB3	2.04	0.40
1:A:428:THR:HB	1:A:432:MET:HE2	2.03	0.40
1:A:450:GLU:O	1:A:455:SER:HB3	2.22	0.40
1:A:524:SER:OG	1:A:527:GLN:HB2	2.21	0.40
1:B:206:TRP:CD2	1:B:534:PRO:HA	2.56	0.40
1:B:236:LEU:CD1	1:B:256:LYS:HD3	2.51	0.40
1:B:370:VAL:CG1	1:B:580:TYR:O	2.66	0.40
1:A:193:PHE:HE2	1:A:197:TYR:CD1	2.39	0.40
1:B:237:CYS:HB3	1:B:240:TYR:HB2	2.04	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	188/657 (29%)	166 (88%)	18 (10%)	4 (2%)	5 11
1	B	176/657 (27%)	165 (94%)	7 (4%)	4 (2%)	5 9
All	All	364/1314 (28%)	331 (91%)	25 (7%)	8 (2%)	5 10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	PRO
1	A	223	GLU
1	B	548	LEU
1	A	220	ILE
1	B	581	ILE
1	A	80	PRO
1	B	585	PRO
1	B	495	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	456/584 (78%)	433 (95%)	23 (5%)	22	46
1	B	456/584 (78%)	441 (97%)	15 (3%)	33	61
All	All	912/1168 (78%)	874 (96%)	38 (4%)	26	52

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	108	THR
1	A	131	VAL
1	A	151	LEU
1	A	240	TYR
1	A	253	GLU
1	A	294	LYS
1	A	303	LEU
1	A	310	ASN
1	A	312	GLN
1	A	315	LYS
1	A	364	ARG
1	A	370	VAL
1	A	400	LEU
1	A	401	ARG

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Mol	Chain	Res	Type
1	A	415	VAL
1	A	423	ARG
1	A	455	SER
1	A	459	ARG
1	A	481	LEU
1	A	552	THR
1	A	574	GLU
1	A	582	ARG
1	B	118	GLU
1	B	216	ARG
1	B	239	THR
1	B	240	TYR
1	B	266	ARG
1	B	291	VAL
1	B	299	ASP
1	B	322	ARG
1	B	401	ARG
1	B	408	SER
1	B	415	VAL
1	B	417	SER
1	B	574	GLU
1	B	581	ILE
1	B	582	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	HIS
1	A	178	ASN
1	A	222	ASN
1	A	231	ASN
1	A	278	GLN
1	A	304	GLN
1	A	310	ASN
1	A	330	ASN
1	A	345	ASN
1	A	354	HIS
1	A	373	ASN
1	A	382	ASN
1	A	426	GLN
1	A	482	GLN
1	A	561	ASN

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Mol	Chain	Res	Type
1	B	83	ASN
1	B	231	ASN
1	B	314	HIS
1	B	326	ASN
1	B	378	HIS
1	B	416	HIS
1	B	426	GLN
1	B	461	GLN
1	B	482	GLN
1	B	511	HIS
1	B	526	GLN
1	B	532	ASN
1	B	545	ASN
1	B	572	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	B	656	-	4,4,4	1.85	3 (75%)	6,6,6	0.45	0
2	PO4	A	656	-	4,4,4	1.85	2 (50%)	6,6,6	0.49	0
2	PO4	B	655	-	4,4,4	1.85	3 (75%)	6,6,6	0.45	0
2	PO4	A	655	-	4,4,4	1.84	3 (75%)	6,6,6	0.48	0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	656	PO4	P-O4	-2.13	1.48	1.54
2	B	655	PO4	P-O2	-2.11	1.48	1.54
2	B	656	PO4	P-O2	-2.09	1.48	1.54
2	B	656	PO4	P-O4	-2.08	1.48	1.54
2	B	655	PO4	P-O3	-2.08	1.48	1.54
2	A	655	PO4	P-O4	-2.06	1.48	1.54
2	A	655	PO4	P-O3	-2.06	1.48	1.54
2	B	656	PO4	P-O3	-2.06	1.48	1.54
2	A	656	PO4	P-O3	-2.05	1.48	1.54
2	A	655	PO4	P-O2	-2.05	1.48	1.54
2	B	655	PO4	P-O4	-2.03	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	656	PO4	1	0
2	A	656	PO4	2	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.