



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:55 AM UTC

PDB ID : 1BPD / pdb_00001bpd
Title : CRYSTAL STRUCTURE OF RAT DNA POLYMERASE BETA: EVIDENCE FOR A COMMON POLYMERASE MECHANISM
Authors : Sawaya, M.R.; Pelletier, H.; Kumar, A.; Wilson, S.H.; Kraut, J.
Deposited on : 1994-04-12
Resolution : 3.60 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

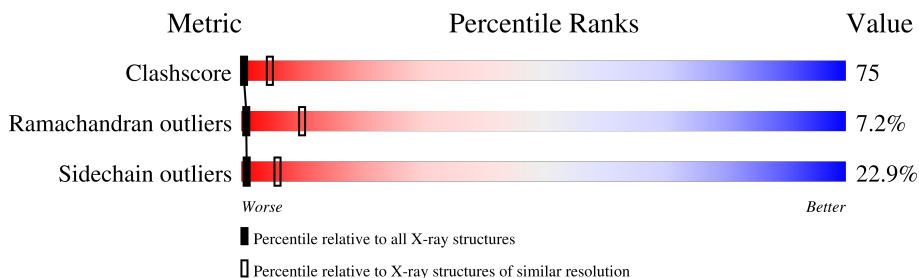
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

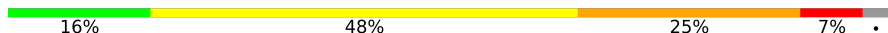
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)

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	335	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2533 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 DNA POLYMERASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2528	1594	446	479	9	0	0	0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



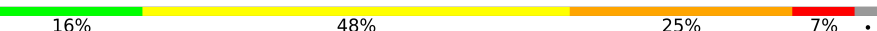
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0

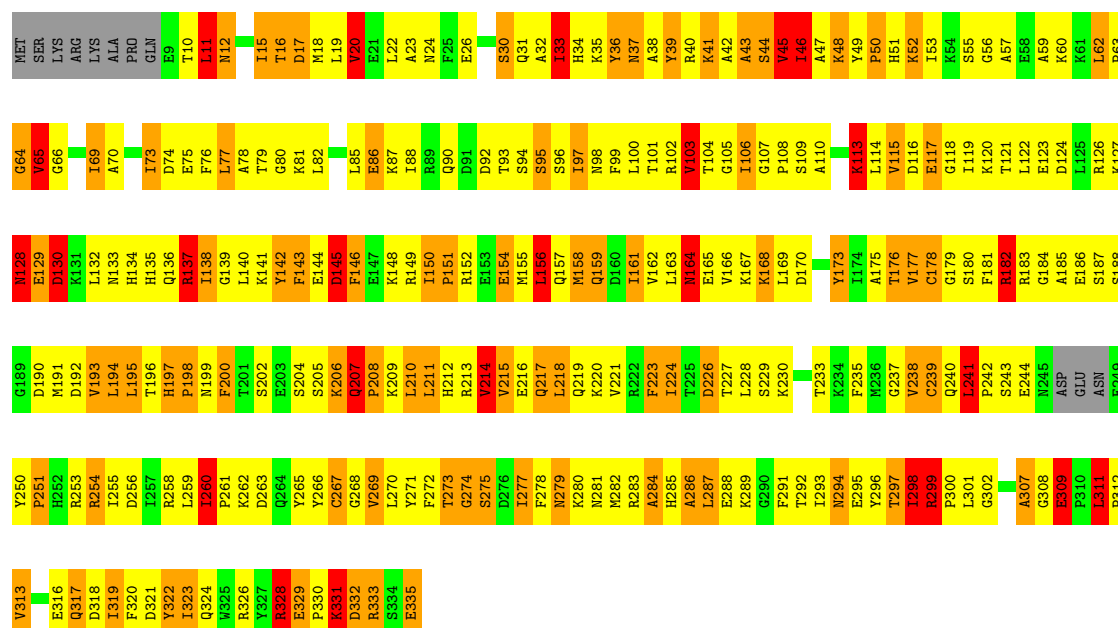
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: DNA POLYMERASE BETA

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.50 Å 68.17 Å 75.28 Å 90.00° 91.68° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2533	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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	1.51	20/2574 (0.8%)	2.14	116/3473 (3.3%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	SER	C-N	8.44	1.48	1.33
1	A	254	ARG	C-N	-8.19	1.24	1.33
1	A	255	ILE	N-CA	-6.57	1.37	1.46
1	A	322	TYR	CA-C	-6.26	1.44	1.52
1	A	256	ASP	CA-C	-6.08	1.45	1.52
1	A	137	ARG	NE-CZ	6.06	1.39	1.33
1	A	298	ILE	CA-CB	-5.95	1.47	1.54
1	A	255	ILE	CA-CB	-5.93	1.48	1.55
1	A	224	ILE	CA-CB	-5.77	1.47	1.54
1	A	214	VAL	N-CA	-5.72	1.39	1.46
1	A	65	VAL	N-CA	-5.49	1.40	1.46
1	A	298	ILE	N-CA	-5.44	1.39	1.46
1	A	45	VAL	N-CA	-5.40	1.40	1.46
1	A	45	VAL	C-N	-5.38	1.27	1.33
1	A	161	ILE	C-N	-5.38	1.27	1.33
1	A	256	ASP	N-CA	-5.37	1.39	1.46
1	A	213	ARG	C-N	-5.15	1.27	1.33
1	A	255	ILE	CA-C	-5.14	1.46	1.52
1	A	267	CYS	CA-C	-5.10	1.45	1.52
1	A	255	ILE	C-N	-5.06	1.27	1.33

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ILE	C-N-CD	-11.27	78.80	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	THR	CA-C-N	-10.51	108.81	122.37
1	A	176	THR	C-N-CA	-10.51	108.81	122.37
1	A	129	GLU	CA-C-N	10.18	133.92	120.28
1	A	129	GLU	C-N-CA	10.18	133.92	120.28
1	A	170	ASP	CA-CB-CG	10.11	122.71	112.60
1	A	137	ARG	CD-NE-CZ	9.88	138.23	124.40
1	A	33	ILE	CA-C-N	9.71	133.65	120.44
1	A	33	ILE	C-N-CA	9.71	133.65	120.44
1	A	274	GLY	N-CA-C	8.56	123.67	110.91
1	A	62	LEU	CA-C-N	8.12	128.15	119.78
1	A	62	LEU	C-N-CA	8.12	128.15	119.78
1	A	273	THR	CA-C-N	-7.81	109.69	121.09
1	A	273	THR	C-N-CA	-7.81	109.69	121.09
1	A	309	GLU	CA-C-N	7.66	129.41	119.84
1	A	309	GLU	C-N-CA	7.66	129.41	119.84
1	A	11	LEU	N-CA-C	7.64	119.39	111.14
1	A	50	PRO	CB-CA-C	-7.54	99.12	111.56
1	A	319	ILE	CB-CA-C	-7.43	102.28	111.87
1	A	311	LEU	CA-C-N	7.38	127.65	119.90
1	A	311	LEU	C-N-CA	7.38	127.65	119.90
1	A	20	VAL	N-CA-CB	7.34	118.62	110.62
1	A	45	VAL	N-CA-C	7.34	117.47	110.42
1	A	113	LYS	N-CA-C	7.33	119.35	111.36
1	A	48	LYS	N-CA-C	-7.26	103.36	111.28
1	A	20	VAL	N-CA-C	7.22	117.31	110.30
1	A	279	ASN	N-CA-C	-7.20	103.12	110.97
1	A	223	PHE	N-CA-C	-7.04	104.84	113.50
1	A	207	GLN	C-N-CD	-7.00	96.32	125.00
1	A	24	ASN	N-CA-CB	6.98	120.97	110.22
1	A	226	ASP	CA-CB-CG	6.93	119.53	112.60
1	A	299	ARG	O-C-N	6.88	126.11	121.71
1	A	73	ILE	CB-CA-C	-6.67	103.28	112.02
1	A	195	LEU	N-CA-CB	-6.63	99.19	111.53
1	A	117	GLU	N-CA-C	-6.50	104.38	112.90
1	A	137	ARG	NE-CZ-NH1	6.42	127.92	121.50
1	A	182	ARG	N-CA-CB	6.36	119.24	110.01
1	A	269	VAL	CB-CA-C	-6.28	103.93	111.97
1	A	241	LEU	N-CA-C	6.28	118.74	110.08
1	A	52	LYS	N-CA-CB	6.25	121.04	110.49
1	A	50	PRO	CA-C-N	-6.19	113.10	122.81
1	A	50	PRO	C-N-CA	-6.19	113.10	122.81
1	A	207	GLN	N-CA-C	6.17	123.46	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	HIS	CA-CB-CG	-6.15	107.65	113.80
1	A	87	LYS	CA-C-N	6.14	128.38	120.70
1	A	87	LYS	C-N-CA	6.14	128.38	120.70
1	A	12	ASN	CA-CB-CG	-6.07	106.53	112.60
1	A	103	VAL	N-CA-C	6.07	117.41	109.58
1	A	321	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	229	SER	CA-C-N	-6.02	112.98	121.72
1	A	229	SER	C-N-CA	-6.02	112.98	121.72
1	A	329	GLU	CA-C-N	6.02	127.36	119.84
1	A	329	GLU	C-N-CA	6.02	127.36	119.84
1	A	193	VAL	CB-CA-C	-5.96	103.52	110.91
1	A	197	HIS	C-N-CD	-5.92	100.71	125.00
1	A	44	SER	N-CA-C	-5.91	103.82	111.02
1	A	103	VAL	N-CA-CB	5.90	119.34	110.13
1	A	130	ASP	N-CA-CB	-5.85	101.52	110.12
1	A	260	ILE	CB-CA-C	-5.85	100.72	111.36
1	A	297	THR	N-CA-C	5.84	117.13	108.60
1	A	45	VAL	N-CA-CB	5.84	117.38	110.55
1	A	317	GLN	N-CA-CB	5.76	118.52	109.94
1	A	267	CYS	O-C-N	5.75	128.76	122.20
1	A	298	ILE	N-CA-C	-5.74	100.13	108.17
1	A	146	PHE	CA-CB-CG	-5.71	108.09	113.80
1	A	17	ASP	CA-CB-CG	-5.70	106.90	112.60
1	A	269	VAL	N-CA-CB	5.69	117.21	110.55
1	A	322	TYR	O-C-N	5.67	127.91	122.07
1	A	228	LEU	N-CA-CB	5.66	118.51	110.13
1	A	143	PHE	CA-CB-CG	-5.65	108.15	113.80
1	A	318	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	286	ALA	N-CA-C	-5.63	105.06	111.14
1	A	24	ASN	CA-CB-CG	5.56	118.16	112.60
1	A	30	SER	CA-C-N	-5.54	112.61	122.42
1	A	30	SER	C-N-CA	-5.54	112.61	122.42
1	A	142	TYR	CB-CA-C	-5.54	100.49	110.35
1	A	207	GLN	CA-C-N	5.53	126.75	119.84
1	A	207	GLN	C-N-CA	5.53	126.75	119.84
1	A	43	ALA	O-C-N	5.52	127.83	122.09
1	A	284	ALA	N-CA-C	5.50	116.96	111.07
1	A	178	CYS	CA-CB-SG	-5.49	101.78	114.40
1	A	243	SER	N-CA-C	5.44	118.56	109.96
1	A	95	SER	N-CA-C	-5.43	105.28	111.14
1	A	65	VAL	N-CA-CB	5.41	117.67	111.39
1	A	154	GLU	O-C-N	5.41	127.66	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	VAL	N-CA-C	5.41	116.37	108.58
1	A	30	SER	CB-CA-C	-5.37	107.69	114.40
1	A	65	VAL	O-C-N	5.37	128.53	122.68
1	A	156	LEU	N-CA-C	-5.36	105.43	111.28
1	A	215	VAL	N-CA-CB	5.34	116.23	110.62
1	A	287	LEU	N-CA-C	-5.33	104.89	111.33
1	A	39	TYR	N-CA-C	-5.30	104.92	111.33
1	A	319	ILE	O-C-N	5.29	127.60	121.94
1	A	94	SER	N-CA-CB	5.29	118.36	110.22
1	A	145	ASP	N-CA-C	-5.29	105.63	111.71
1	A	328	ARG	N-CA-CB	5.29	118.23	110.35
1	A	333	ARG	N-CA-C	5.26	119.46	112.30
1	A	46	ILE	N-CA-C	5.25	117.65	111.09
1	A	128	ASN	CA-CB-CG	5.25	117.84	112.60
1	A	34	HIS	CB-CA-C	5.20	119.12	110.90
1	A	138	ILE	O-C-N	5.20	127.14	121.94
1	A	164	ASN	CA-CB-CG	-5.19	107.41	112.60
1	A	313	VAL	N-CA-C	5.19	115.45	107.77
1	A	191	MET	CB-CA-C	-5.15	103.74	111.73
1	A	24	ASN	CB-CA-C	5.15	120.16	110.63
1	A	192	ASP	N-CA-C	5.12	117.63	108.17
1	A	200	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	331	LYS	N-CA-C	-5.09	104.81	111.02
1	A	254	ARG	CA-C-N	-5.07	114.20	121.95
1	A	254	ARG	C-N-CA	-5.07	114.20	121.95
1	A	238	VAL	CB-CA-C	-5.06	102.59	110.69
1	A	121	THR	N-CA-C	5.05	118.25	110.42
1	A	268	GLY	N-CA-C	-5.03	101.26	113.18
1	A	326	ARG	N-CA-CB	5.03	117.34	109.85
1	A	197	HIS	CA-C-N	5.02	126.12	119.84
1	A	197	HIS	C-N-CA	5.02	126.12	119.84

There are no chirality outliers.

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	2528	0	2459	374	0
2	A	5	0	0	0	0
All	All	2533	0	2459	374	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 75.

All (374) 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:115:VAL:HG12	1:A:120:LYS:HG2	1.30	1.14
1:A:62:LEU:HD12	1:A:63:PRO:HD2	1.35	1.09
1:A:182:ARG:HH12	1:A:273:THR:HG23	1.14	1.07
1:A:329:GLU:HG2	1:A:330:PRO:HD2	1.34	1.05
1:A:302:GLY:H	1:A:307:ALA:HB3	1.18	1.03
1:A:66:GLY:H	1:A:69:ILE:HD12	1.26	0.99
1:A:317:GLN:H	1:A:317:GLN:NE2	1.60	0.99
1:A:11:LEU:HG	1:A:52:LYS:HA	1.50	0.94
1:A:299:ARG:HG3	1:A:299:ARG:HH11	1.30	0.94
1:A:182:ARG:NH1	1:A:273:THR:HG23	1.81	0.94
1:A:73:ILE:HG22	1:A:77:LEU:HD22	1.50	0.94
1:A:212:HIS:CE1	1:A:230:LYS:HD3	2.04	0.93
1:A:241:LEU:HD23	1:A:242:PRO:HD2	1.48	0.92
1:A:62:LEU:CD1	1:A:63:PRO:HD2	2.01	0.91
1:A:70:ALA:HA	1:A:73:ILE:HD12	1.52	0.90
1:A:302:GLY:N	1:A:307:ALA:HB3	1.87	0.89
1:A:329:GLU:CG	1:A:330:PRO:HD2	2.03	0.89
1:A:41:LYS:HE2	1:A:64:GLY:HA3	1.55	0.89
1:A:12:ASN:HB3	1:A:46:ILE:CD1	2.03	0.88
1:A:134:HIS:HA	1:A:137:ARG:NH1	1.89	0.87
1:A:152:ARG:NH2	1:A:184:GLY:HA2	1.90	0.86
1:A:227:THR:HG23	1:A:235:PHE:CE1	2.09	0.86
1:A:11:LEU:HB2	1:A:52:LYS:CG	2.06	0.85
1:A:126:ARG:HG3	1:A:140:LEU:HD21	1.58	0.84
1:A:227:THR:HG23	1:A:235:PHE:HE1	1.41	0.82
1:A:19:LEU:HD21	1:A:42:ALA:HB3	1.61	0.82
1:A:197:HIS:ND1	1:A:198:PRO:HD2	1.95	0.81
1:A:218:LEU:HB3	1:A:224:ILE:HG12	1.63	0.81
1:A:197:HIS:CG	1:A:198:PRO:HD2	2.17	0.80
1:A:11:LEU:HD23	1:A:12:ASN:H	1.47	0.80
1:A:241:LEU:CD2	1:A:242:PRO:HD2	2.12	0.79
1:A:62:LEU:HB3	1:A:65:VAL:HG11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:HD23	1:A:175:ALA:HB3	1.64	0.79
1:A:129:GLU:HA	1:A:132:LEU:HD12	1.64	0.79
1:A:98:ASN:O	1:A:101:THR:HG22	1.84	0.78
1:A:115:VAL:CG1	1:A:120:LYS:HG2	2.12	0.78
1:A:110:ALA:HA	1:A:113:LYS:NZ	1.99	0.78
1:A:12:ASN:O	1:A:15:ILE:HG23	1.83	0.78
1:A:219:GLN:HA	1:A:224:ILE:HB	1.67	0.77
1:A:12:ASN:HB3	1:A:46:ILE:HD12	1.67	0.76
1:A:260:ILE:HG22	1:A:261:PRO:HD2	1.65	0.76
1:A:279:ASN:O	1:A:283:ARG:HG2	1.86	0.76
1:A:320:PHE:O	1:A:323:ILE:HG13	1.85	0.76
1:A:70:ALA:O	1:A:73:ILE:HB	1.86	0.75
1:A:183:ARG:O	1:A:331:LYS:HA	1.87	0.75
1:A:12:ASN:ND2	1:A:53:ILE:H	1.85	0.74
1:A:254:ARG:HB3	1:A:254:ARG:NH1	2.01	0.74
1:A:289:LYS:HZ3	1:A:324:GLN:HB2	1.50	0.74
1:A:115:VAL:HG12	1:A:120:LYS:CG	2.16	0.74
1:A:113:LYS:O	1:A:117:GLU:HG2	1.87	0.74
1:A:127:LYS:O	1:A:129:GLU:HG3	1.88	0.73
1:A:285:HIS:O	1:A:288:GLU:HB3	1.88	0.73
1:A:19:LEU:HD21	1:A:42:ALA:CB	2.19	0.73
1:A:36:TYR:CZ	1:A:40:ARG:HD3	2.23	0.73
1:A:42:ALA:O	1:A:46:ILE:HG23	1.88	0.73
1:A:56:GLY:HA2	1:A:59:ALA:HB3	1.71	0.73
1:A:62:LEU:O	1:A:65:VAL:HG13	1.89	0.73
1:A:114:LEU:O	1:A:117:GLU:HB2	1.89	0.73
1:A:110:ALA:HA	1:A:113:LYS:HZ1	1.54	0.72
1:A:260:ILE:CG2	1:A:261:PRO:HD2	2.18	0.72
1:A:115:VAL:HG13	1:A:120:LYS:HA	1.71	0.72
1:A:265:TYR:O	1:A:269:VAL:HG23	1.89	0.72
1:A:241:LEU:HD23	1:A:242:PRO:CD	2.20	0.71
1:A:183:ARG:HD3	1:A:274:GLY:HA3	1.71	0.71
1:A:11:LEU:HD12	1:A:52:LYS:HB2	1.72	0.71
1:A:109:SER:O	1:A:113:LYS:HG2	1.90	0.71
1:A:317:GLN:NE2	1:A:317:GLN:N	2.38	0.71
1:A:73:ILE:O	1:A:77:LEU:HD13	1.90	0.71
1:A:104:THR:HG23	1:A:139:GLY:HA2	1.73	0.71
1:A:211:LEU:O	1:A:214:VAL:HG13	1.91	0.71
1:A:16:THR:HG23	1:A:46:ILE:HG13	1.74	0.70
1:A:56:GLY:HA2	1:A:59:ALA:CB	2.21	0.70
1:A:211:LEU:HB2	1:A:259:LEU:HD22	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HG	1:A:52:LYS:CA	2.20	0.70
1:A:311:LEU:HB3	1:A:312:PRO:HD2	1.73	0.69
1:A:56:GLY:O	1:A:59:ALA:HB3	1.90	0.69
1:A:132:LEU:HA	1:A:136:GLN:HE21	1.58	0.69
1:A:41:LYS:O	1:A:44:SER:HB3	1.91	0.69
1:A:209:LYS:HA	1:A:212:HIS:HB2	1.73	0.69
1:A:62:LEU:CG	1:A:63:PRO:HD2	2.22	0.69
1:A:270:LEU:HD12	1:A:270:LEU:O	1.93	0.69
1:A:134:HIS:HA	1:A:137:ARG:HH11	1.56	0.69
1:A:11:LEU:H	1:A:11:LEU:HD22	1.57	0.68
1:A:259:LEU:HD12	1:A:260:ILE:N	2.08	0.68
1:A:22:LEU:HD21	1:A:39:TYR:CE1	2.30	0.67
1:A:206:LYS:C	1:A:208:PRO:HD3	2.19	0.67
1:A:36:TYR:OH	1:A:40:ARG:HD3	1.95	0.67
1:A:241:LEU:CG	1:A:242:PRO:HD2	2.25	0.67
1:A:62:LEU:C	1:A:65:VAL:HG13	2.20	0.67
1:A:205:SER:O	1:A:207:GLN:HG2	1.94	0.67
1:A:46:ILE:O	1:A:49:TYR:HB3	1.94	0.67
1:A:106:ILE:HD13	1:A:106:ILE:N	2.10	0.66
1:A:284:ALA:O	1:A:288:GLU:N	2.29	0.66
1:A:46:ILE:HD13	1:A:53:ILE:HD12	1.77	0.66
1:A:240:GLN:HG2	1:A:241:LEU:N	2.10	0.66
1:A:12:ASN:HD21	1:A:53:ILE:H	1.41	0.66
1:A:162:VAL:O	1:A:166:VAL:HG13	1.96	0.66
1:A:179:GLY:O	1:A:181:PHE:N	2.29	0.66
1:A:270:LEU:HD21	1:A:282:MET:SD	2.37	0.65
1:A:11:LEU:HB2	1:A:52:LYS:CB	2.27	0.65
1:A:152:ARG:HA	1:A:155:MET:HB2	1.79	0.65
1:A:11:LEU:HB2	1:A:52:LYS:HG3	1.77	0.65
1:A:328:ARG:NH1	1:A:328:ARG:HG2	2.11	0.65
1:A:150:ILE:HG22	1:A:151:PRO:N	2.11	0.65
1:A:75:GLU:O	1:A:78:ALA:HB3	1.97	0.64
1:A:286:ALA:HB2	1:A:323:ILE:HG21	1.79	0.64
1:A:299:ARG:HG3	1:A:299:ARG:NH1	2.04	0.64
1:A:41:LYS:O	1:A:41:LYS:HD2	1.97	0.64
1:A:65:VAL:HA	1:A:69:ILE:HD12	1.79	0.64
1:A:166:VAL:O	1:A:169:LEU:HB2	1.97	0.64
1:A:69:ILE:HG22	1:A:73:ILE:HD11	1.80	0.64
1:A:266:TYR:O	1:A:269:VAL:N	2.30	0.64
1:A:122:LEU:HD12	1:A:123:GLU:N	2.12	0.64
1:A:50:PRO:HG2	1:A:51:HIS:CD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:O	1:A:219:GLN:HG3	1.98	0.64
1:A:37:ASN:O	1:A:40:ARG:HB3	1.98	0.63
1:A:104:THR:CG2	1:A:139:GLY:HA2	2.29	0.63
1:A:259:LEU:HD12	1:A:260:ILE:H	1.64	0.63
1:A:289:LYS:NZ	1:A:324:GLN:HB2	2.14	0.63
1:A:133:ASN:HD21	1:A:135:HIS:HB3	1.65	0.62
1:A:56:GLY:CA	1:A:59:ALA:HB3	2.30	0.62
1:A:35:LYS:O	1:A:38:ALA:HB3	2.00	0.62
1:A:132:LEU:HA	1:A:136:GLN:NE2	2.14	0.62
1:A:144:GLU:OE1	1:A:144:GLU:N	2.29	0.62
1:A:302:GLY:HA3	1:A:307:ALA:CB	2.29	0.62
1:A:63:PRO:C	1:A:65:VAL:H	2.07	0.62
1:A:42:ALA:O	1:A:45:VAL:HG12	1.99	0.62
1:A:270:LEU:CD2	1:A:282:MET:HE1	2.30	0.62
1:A:44:SER:O	1:A:48:LYS:HG3	1.99	0.61
1:A:159:GLN:HG3	1:A:177:VAL:HG11	1.82	0.61
1:A:56:GLY:C	1:A:59:ALA:HB3	2.25	0.61
1:A:46:ILE:HD13	1:A:53:ILE:CD1	2.31	0.61
1:A:137:ARG:HG2	1:A:138:ILE:HD13	1.82	0.61
1:A:73:ILE:HG22	1:A:77:LEU:CD2	2.27	0.60
1:A:36:TYR:CE1	1:A:40:ARG:HD3	2.36	0.60
1:A:218:LEU:O	1:A:221:VAL:HG22	2.00	0.60
1:A:311:LEU:HD22	1:A:311:LEU:H	1.64	0.60
1:A:11:LEU:HB2	1:A:52:LYS:HB2	1.83	0.60
1:A:66:GLY:N	1:A:69:ILE:HD12	2.08	0.60
1:A:206:LYS:O	1:A:208:PRO:HD3	2.02	0.60
1:A:211:LEU:O	1:A:211:LEU:HD12	2.01	0.60
1:A:206:LYS:HA	1:A:206:LYS:NZ	2.17	0.60
1:A:62:LEU:HB3	1:A:65:VAL:CG1	2.32	0.59
1:A:143:PHE:HB3	1:A:144:GLU:OE1	2.02	0.59
1:A:145:ASP:HA	1:A:148:LYS:HD2	1.83	0.59
1:A:270:LEU:HD21	1:A:282:MET:HE1	1.82	0.59
1:A:302:GLY:CA	1:A:307:ALA:HB3	2.33	0.59
1:A:104:THR:HG23	1:A:139:GLY:CA	2.31	0.59
1:A:145:ASP:OD1	1:A:145:ASP:N	2.36	0.59
1:A:211:LEU:HB2	1:A:259:LEU:CD2	2.33	0.59
1:A:311:LEU:HD22	1:A:311:LEU:N	2.17	0.59
1:A:74:ASP:HA	1:A:77:LEU:HB2	1.85	0.59
1:A:162:VAL:HG12	1:A:163:LEU:N	2.16	0.58
1:A:62:LEU:HD12	1:A:63:PRO:CD	2.22	0.58
1:A:41:LYS:HZ3	1:A:42:ALA:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:O	1:A:165:GLU:HG2	2.04	0.58
1:A:254:ARG:HB3	1:A:254:ARG:HH11	1.69	0.58
1:A:11:LEU:HB2	1:A:52:LYS:HD2	1.86	0.58
1:A:260:ILE:HG22	1:A:261:PRO:CD	2.33	0.58
1:A:284:ALA:O	1:A:287:LEU:HB3	2.04	0.57
1:A:11:LEU:HB2	1:A:52:LYS:CD	2.34	0.57
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.69	0.57
1:A:155:MET:O	1:A:158:MET:HG2	2.04	0.57
1:A:263:ASP:N	1:A:263:ASP:OD1	2.31	0.57
1:A:195:LEU:HB3	1:A:258:ARG:O	2.05	0.57
1:A:79:THR:O	1:A:81:LYS:N	2.29	0.57
1:A:143:PHE:O	1:A:146:PHE:HB2	2.05	0.57
1:A:69:ILE:O	1:A:73:ILE:HG13	2.05	0.56
1:A:11:LEU:CB	1:A:52:LYS:HB2	2.35	0.56
1:A:98:ASN:O	1:A:102:ARG:HG3	2.03	0.56
1:A:240:GLN:HG3	1:A:251:PRO:O	2.05	0.56
1:A:63:PRO:O	1:A:65:VAL:HG12	2.04	0.56
1:A:217:GLN:HE21	1:A:217:GLN:HA	1.71	0.56
1:A:126:ARG:NE	1:A:140:LEU:HD11	2.21	0.56
1:A:179:GLY:O	1:A:182:ARG:N	2.30	0.56
1:A:11:LEU:H	1:A:11:LEU:CD2	2.18	0.56
1:A:195:LEU:O	1:A:259:LEU:HD12	2.06	0.56
1:A:164:ASN:OD1	1:A:165:GLU:N	2.39	0.56
1:A:86:GLU:O	1:A:86:GLU:HG2	2.04	0.55
1:A:152:ARG:NH2	1:A:181:PHE:O	2.39	0.55
1:A:168:LYS:HB3	1:A:168:LYS:NZ	2.22	0.55
1:A:41:LYS:NZ	1:A:42:ALA:N	2.55	0.55
1:A:59:ALA:O	1:A:62:LEU:HB3	2.07	0.55
1:A:97:ILE:HG22	1:A:98:ASN:OD1	2.07	0.55
1:A:37:ASN:C	1:A:40:ARG:HB3	2.32	0.55
1:A:128:ASN:N	1:A:128:ASN:HD22	2.03	0.55
1:A:69:ILE:O	1:A:73:ILE:N	2.37	0.54
1:A:126:ARG:CG	1:A:140:LEU:HD21	2.33	0.54
1:A:196:THR:HG21	1:A:265:TYR:CG	2.42	0.54
1:A:214:VAL:O	1:A:217:GLN:HB3	2.06	0.54
1:A:132:LEU:HB3	1:A:136:GLN:HB2	1.88	0.54
1:A:152:ARG:NE	1:A:185:ALA:O	2.41	0.54
1:A:159:GLN:O	1:A:163:LEU:HD12	2.08	0.54
1:A:211:LEU:CB	1:A:259:LEU:HD22	2.38	0.54
1:A:103:VAL:HG12	1:A:104:THR:N	2.22	0.54
1:A:275:SER:OG	1:A:277:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:O	1:A:85:LEU:HB3	2.09	0.53
1:A:70:ALA:CA	1:A:73:ILE:HD12	2.33	0.53
1:A:278:PHE:CE2	1:A:333:ARG:HD3	2.43	0.53
1:A:49:TYR:CG	1:A:50:PRO:HD2	2.43	0.53
1:A:63:PRO:O	1:A:65:VAL:N	2.37	0.53
1:A:79:THR:C	1:A:81:LYS:H	2.15	0.53
1:A:269:VAL:O	1:A:273:THR:OG1	2.27	0.53
1:A:144:GLU:O	1:A:148:LYS:HG3	2.09	0.53
1:A:156:LEU:O	1:A:159:GLN:HB3	2.09	0.53
1:A:11:LEU:CD1	1:A:52:LYS:HB2	2.39	0.53
1:A:106:ILE:HD13	1:A:106:ILE:H	1.73	0.53
1:A:134:HIS:HA	1:A:137:ARG:HH12	1.74	0.53
1:A:163:LEU:HD23	1:A:175:ALA:CB	2.36	0.52
1:A:196:THR:HB	1:A:265:TYR:CD1	2.44	0.52
1:A:49:TYR:CD1	1:A:50:PRO:HD2	2.44	0.52
1:A:134:HIS:O	1:A:138:ILE:HG12	2.10	0.52
1:A:155:MET:HE2	1:A:188:SER:HB2	1.91	0.52
1:A:129:GLU:O	1:A:132:LEU:HB2	2.10	0.52
1:A:283:ARG:HH21	1:A:294:ASN:HA	1.74	0.52
1:A:33:ILE:O	1:A:37:ASN:HB2	2.09	0.52
1:A:134:HIS:CE1	1:A:137:ARG:HH22	2.27	0.52
1:A:149:ARG:NH2	1:A:187:SER:O	2.42	0.52
1:A:281:ASN:OD1	1:A:335:GLU:O	2.28	0.52
1:A:17:ASP:O	1:A:20:VAL:HG13	2.10	0.52
1:A:216:GLU:O	1:A:219:GLN:HB2	2.09	0.52
1:A:223:PHE:C	1:A:224:ILE:HD13	2.35	0.51
1:A:96:SER:OG	1:A:120:LYS:HB3	2.09	0.51
1:A:173:TYR:OH	1:A:210:LEU:O	2.28	0.51
1:A:41:LYS:HZ2	1:A:42:ALA:N	2.08	0.51
1:A:99:PHE:HA	1:A:102:ARG:HD2	1.93	0.51
1:A:134:HIS:CE1	1:A:137:ARG:NH2	2.78	0.51
1:A:155:MET:HE3	1:A:181:PHE:CD2	2.46	0.51
1:A:103:VAL:O	1:A:106:ILE:HG12	2.11	0.51
1:A:270:LEU:HD21	1:A:282:MET:CE	2.40	0.51
1:A:11:LEU:CG	1:A:52:LYS:HB2	2.41	0.51
1:A:137:ARG:O	1:A:140:LEU:HB3	2.11	0.51
1:A:286:ALA:HB1	1:A:291:PHE:HB2	1.92	0.51
1:A:197:HIS:O	1:A:199:ASN:N	2.44	0.50
1:A:218:LEU:HB3	1:A:224:ILE:CG1	2.39	0.50
1:A:36:TYR:CD2	1:A:37:ASN:N	2.79	0.50
1:A:69:ILE:HG22	1:A:73:ILE:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ALA:HB2	1:A:39:TYR:HB3	1.94	0.49
1:A:298:ILE:HG23	1:A:298:ILE:O	2.12	0.49
1:A:109:SER:C	1:A:113:LYS:HE3	2.37	0.49
1:A:156:LEU:HD12	1:A:159:GLN:NE2	2.28	0.49
1:A:270:LEU:HA	1:A:273:THR:OG1	2.13	0.49
1:A:298:ILE:HD13	1:A:322:TYR:HD2	1.78	0.48
1:A:119:ILE:HA	1:A:124:ASP:CG	2.39	0.48
1:A:129:GLU:CA	1:A:132:LEU:HD12	2.40	0.48
1:A:217:GLN:O	1:A:220:LYS:N	2.46	0.48
1:A:45:VAL:HA	1:A:48:LYS:HD2	1.95	0.48
1:A:166:VAL:HG23	1:A:167:LYS:N	2.29	0.48
1:A:11:LEU:CD2	1:A:11:LEU:N	2.76	0.48
1:A:65:VAL:HA	1:A:69:ILE:CD1	2.43	0.48
1:A:163:LEU:O	1:A:166:VAL:HG22	2.13	0.48
1:A:12:ASN:HD21	1:A:52:LYS:HA	1.79	0.48
1:A:211:LEU:HD12	1:A:211:LEU:C	2.38	0.48
1:A:223:PHE:O	1:A:239:CYS:HA	2.14	0.48
1:A:42:ALA:HA	1:A:45:VAL:HG12	1.97	0.47
1:A:129:GLU:HA	1:A:132:LEU:CD1	2.39	0.47
1:A:176:THR:HG22	1:A:178:CYS:SG	2.54	0.47
1:A:235:PHE:CZ	1:A:237:GLY:HA3	2.49	0.47
1:A:285:HIS:HA	1:A:288:GLU:HB3	1.97	0.47
1:A:60:LYS:HA	1:A:65:VAL:HG22	1.95	0.47
1:A:159:GLN:HG2	1:A:163:LEU:CD1	2.44	0.47
1:A:285:HIS:HA	1:A:288:GLU:CB	2.44	0.47
1:A:286:ALA:CB	1:A:323:ILE:HG21	2.42	0.47
1:A:12:ASN:HD21	1:A:53:ILE:N	2.09	0.47
1:A:36:TYR:CG	1:A:37:ASN:N	2.83	0.47
1:A:238:VAL:HG12	1:A:239:CYS:N	2.30	0.47
1:A:70:ALA:C	1:A:73:ILE:HB	2.40	0.47
1:A:115:VAL:O	1:A:118:GLY:N	2.46	0.47
1:A:150:ILE:CG2	1:A:151:PRO:N	2.78	0.47
1:A:151:PRO:HB2	1:A:154:GLU:HG3	1.97	0.47
1:A:273:THR:HG21	1:A:333:ARG:NH1	2.30	0.47
1:A:17:ASP:N	1:A:17:ASP:OD1	2.48	0.47
1:A:157:GLN:O	1:A:161:ILE:HG13	2.14	0.47
1:A:277:ILE:O	1:A:280:LYS:N	2.48	0.47
1:A:286:ALA:HB1	1:A:291:PHE:CB	2.45	0.47
1:A:133:ASN:HD22	1:A:135:HIS:H	1.62	0.46
1:A:308:GLY:O	1:A:309:GLU:HB2	2.15	0.46
1:A:328:ARG:HG2	1:A:332:ASP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:HD11	1:A:258:ARG:HD2	1.96	0.46
1:A:104:THR:O	1:A:139:GLY:HA3	2.15	0.46
1:A:11:LEU:HD23	1:A:12:ASN:N	2.21	0.46
1:A:128:ASN:N	1:A:128:ASN:ND2	2.64	0.46
1:A:103:VAL:HG12	1:A:104:THR:H	1.81	0.46
1:A:293:ILE:HG22	1:A:294:ASN:N	2.30	0.46
1:A:196:THR:HG22	1:A:265:TYR:CE1	2.51	0.46
1:A:206:LYS:HA	1:A:206:LYS:HZ3	1.79	0.46
1:A:133:ASN:ND2	1:A:135:HIS:H	2.14	0.45
1:A:193:VAL:C	1:A:194:LEU:HD12	2.40	0.45
1:A:285:HIS:HE1	1:A:289:LYS:HE3	1.81	0.45
1:A:41:LYS:HZ3	1:A:42:ALA:CA	2.29	0.45
1:A:270:LEU:HD12	1:A:270:LEU:C	2.42	0.45
1:A:18:MET:HG3	1:A:76:PHE:CG	2.50	0.45
1:A:270:LEU:CD1	1:A:333:ARG:NH1	2.80	0.45
1:A:127:LYS:C	1:A:129:GLU:H	2.24	0.45
1:A:128:ASN:ND2	1:A:128:ASN:H	2.15	0.45
1:A:145:ASP:HB3	1:A:251:PRO:HB2	1.98	0.45
1:A:196:THR:CG2	1:A:265:TYR:CD1	3.00	0.45
1:A:294:ASN:O	1:A:294:ASN:ND2	2.49	0.45
1:A:328:ARG:HH11	1:A:328:ARG:CG	2.29	0.45
1:A:227:THR:HG21	1:A:230:LYS:HB2	1.99	0.45
1:A:285:HIS:CE1	1:A:289:LYS:HE3	2.51	0.45
1:A:134:HIS:ND1	1:A:137:ARG:NH1	2.65	0.45
1:A:144:GLU:H	1:A:144:GLU:CD	2.23	0.44
1:A:287:LEU:HA	1:A:291:PHE:O	2.18	0.44
1:A:41:LYS:HD2	1:A:41:LYS:C	2.42	0.44
1:A:130:ASP:C	1:A:132:LEU:H	2.25	0.44
1:A:169:LEU:HA	1:A:169:LEU:HD23	1.57	0.44
1:A:194:LEU:N	1:A:194:LEU:CD1	2.80	0.44
1:A:11:LEU:CD1	1:A:52:LYS:N	2.81	0.44
1:A:22:LEU:CD2	1:A:39:TYR:CE1	3.00	0.44
1:A:151:PRO:O	1:A:154:GLU:HB2	2.18	0.44
1:A:148:LYS:O	1:A:253:ARG:NH1	2.50	0.44
1:A:207:GLN:HB3	1:A:210:LEU:HD12	1.99	0.43
1:A:311:LEU:HA	1:A:312:PRO:HD3	1.81	0.43
1:A:317:GLN:H	1:A:317:GLN:CD	2.24	0.43
1:A:40:ARG:O	1:A:43:ALA:HB3	2.18	0.43
1:A:107:GLY:H	1:A:110:ALA:HB3	1.84	0.43
1:A:159:GLN:HB3	1:A:159:GLN:HE21	1.57	0.43
1:A:262:LYS:O	1:A:262:LYS:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:THR:HB	1:A:301:LEU:HD13	2.00	0.43
1:A:316:GLU:HA	1:A:319:ILE:CD1	2.49	0.43
1:A:196:THR:OG1	1:A:197:HIS:N	2.52	0.43
1:A:206:LYS:N	1:A:206:LYS:HE2	2.34	0.43
1:A:294:ASN:O	1:A:296:TYR:N	2.51	0.43
1:A:278:PHE:HB2	1:A:333:ARG:O	2.17	0.43
1:A:95:SER:OG	1:A:96:SER:N	2.48	0.43
1:A:271:TYR:C	1:A:273:THR:N	2.77	0.43
1:A:287:LEU:HA	1:A:287:LEU:HD12	1.83	0.43
1:A:140:LEU:O	1:A:142:TYR:N	2.52	0.43
1:A:114:LEU:O	1:A:119:ILE:N	2.46	0.42
1:A:211:LEU:HB2	1:A:259:LEU:HB2	2.00	0.42
1:A:216:GLU:O	1:A:220:LYS:N	2.53	0.42
1:A:49:TYR:HA	1:A:50:PRO:HD3	1.88	0.42
1:A:122:LEU:HD13	1:A:126:ARG:HH11	1.84	0.42
1:A:50:PRO:HG2	1:A:51:HIS:HD2	1.82	0.42
1:A:200:PHE:HD1	1:A:204:SER:HB2	1.84	0.42
1:A:182:ARG:C	1:A:184:GLY:N	2.78	0.42
1:A:145:ASP:OD2	1:A:251:PRO:HB3	2.20	0.42
1:A:211:LEU:HD22	1:A:233:THR:O	2.20	0.41
1:A:36:TYR:CE2	1:A:37:ASN:ND2	2.88	0.41
1:A:132:LEU:HB3	1:A:136:GLN:CB	2.49	0.41
1:A:154:GLU:O	1:A:157:GLN:N	2.53	0.41
1:A:113:LYS:HG2	1:A:113:LYS:H	1.48	0.41
1:A:260:ILE:HB	1:A:265:TYR:HD1	1.86	0.41
1:A:279:ASN:C	1:A:283:ARG:HG2	2.42	0.41
1:A:90:GLN:C	1:A:92:ASP:N	2.79	0.41
1:A:317:GLN:N	1:A:317:GLN:CD	2.78	0.41
1:A:105:GLY:HA3	1:A:136:GLN:HA	2.03	0.41
1:A:150:ILE:HA	1:A:151:PRO:HD2	1.57	0.41
1:A:240:GLN:HG3	1:A:250:TYR:O	2.20	0.41
1:A:101:THR:CG2	1:A:102:ARG:N	2.79	0.41
1:A:103:VAL:CG1	1:A:104:THR:N	2.83	0.41
1:A:159:GLN:HG2	1:A:163:LEU:HD11	2.03	0.41
1:A:16:THR:HG21	1:A:47:ALA:HB2	2.02	0.41
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.86	0.41
1:A:179:GLY:C	1:A:181:PHE:N	2.78	0.41
1:A:182:ARG:C	1:A:184:GLY:H	2.28	0.41
1:A:195:LEU:HG	1:A:259:LEU:HD13	2.03	0.41
1:A:196:THR:HG22	1:A:265:TYR:CZ	2.55	0.41
1:A:197:HIS:HA	1:A:198:PRO:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.80	0.41
1:A:62:LEU:HG	1:A:63:PRO:HD2	2.00	0.40
1:A:259:LEU:HD12	1:A:259:LEU:HA	1.65	0.40
1:A:299:ARG:HB3	1:A:300:PRO:HD2	2.04	0.40
1:A:331:LYS:HG2	1:A:332:ASP:N	2.36	0.40
1:A:206:LYS:CA	1:A:206:LYS:CE	3.00	0.40
1:A:223:PHE:O	1:A:224:ILE:HD13	2.21	0.40
1:A:320:PHE:O	1:A:324:GLN:N	2.54	0.40
1:A:267:CYS:O	1:A:271:TYR:HB2	2.22	0.40
1:A:271:TYR:O	1:A:273:THR:N	2.54	0.40
1:A:285:HIS:C	1:A:288:GLU:HB3	2.45	0.40
1:A:55:SER:C	1:A:57:ALA:N	2.79	0.40
1:A:195:LEU:HD12	1:A:196:THR:H	1.86	0.40
1:A:329:GLU:CB	1:A:330:PRO:HD2	2.43	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	320/335 (96%)	244 (76%)	53 (17%)	23 (7%)	1	10

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	32	ALA
1	A	128	ASN
1	A	180	SER
1	A	198	PRO
1	A	275	SER
1	A	295	GLU

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Mol	Chain	Res	Type
1	A	309	GLU
1	A	86	GLU
1	A	141	LYS
1	A	151	PRO
1	A	332	ASP
1	A	80	GLY
1	A	108	PRO
1	A	208	PRO
1	A	244	GLU
1	A	69	ILE
1	A	210	LEU
1	A	251	PRO
1	A	307	ALA
1	A	207	GLN
1	A	272	PHE
1	A	64	GLY

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	262/296 (88%)	202 (77%)	60 (23%)	1 6

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	15	ILE
1	A	16	THR
1	A	20	VAL
1	A	26	GLU
1	A	30	SER
1	A	31	GLN
1	A	33	ILE
1	A	36	TYR
1	A	37	ASN

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Mol	Chain	Res	Type
1	A	41	LYS
1	A	45	VAL
1	A	46	ILE
1	A	65	VAL
1	A	77	LEU
1	A	88	ILE
1	A	93	THR
1	A	97	ILE
1	A	100	LEU
1	A	103	VAL
1	A	106	ILE
1	A	113	LYS
1	A	115	VAL
1	A	116	ASP
1	A	128	ASN
1	A	130	ASP
1	A	137	ARG
1	A	145	ASP
1	A	156	LEU
1	A	158	MET
1	A	159	GLN
1	A	164	ASN
1	A	168	LYS
1	A	173	TYR
1	A	177	VAL
1	A	182	ARG
1	A	186	GLU
1	A	190	ASP
1	A	194	LEU
1	A	202	SER
1	A	206	LYS
1	A	211	LEU
1	A	214	VAL
1	A	217	GLN
1	A	218	LEU
1	A	226	ASP
1	A	239	CYS
1	A	241	LEU
1	A	260	ILE
1	A	277	ILE
1	A	294	ASN
1	A	297	THR

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Mol	Chain	Res	Type
1	A	298	ILE
1	A	299	ARG
1	A	311	LEU
1	A	313	VAL
1	A	323	ILE
1	A	328	ARG
1	A	331	LYS
1	A	335	GLU

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	12	ASN
1	A	37	ASN
1	A	51	HIS
1	A	128	ASN
1	A	136	GLN
1	A	159	GLN
1	A	212	HIS
1	A	217	GLN
1	A	252	HIS
1	A	279	ASN
1	A	285	HIS
1	A	294	ASN
1	A	317	GLN

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 [i](#)

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	PO4	A	337	-	4,4,4	5.32	3 (75%)	6,6,6	1.04	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	337	PO4	P-O4	7.66	1.76	1.54
2	A	337	PO4	P-O1	5.37	1.63	1.50
2	A	337	PO4	P-O3	5.09	1.69	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.