



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:42 am GMT

PDB ID : 1BPD  
Title : CRYSTAL STRUCTURE OF RAT DNA POLYMERASE BETA: EVIDENCE FOR A COMMON POLYMERASE MECHANISM  
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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](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

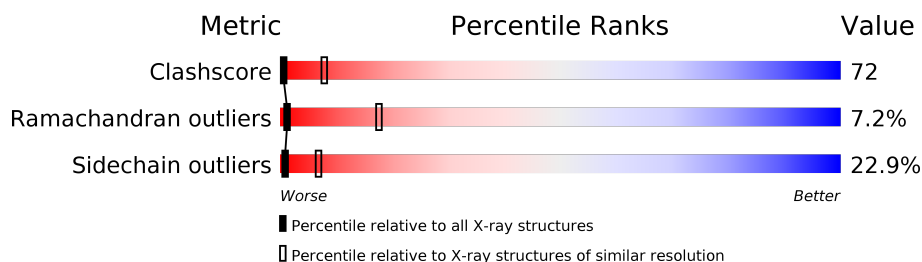
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)

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	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 (three-letter code: PO4) (formula: O<sub>4</sub>P).



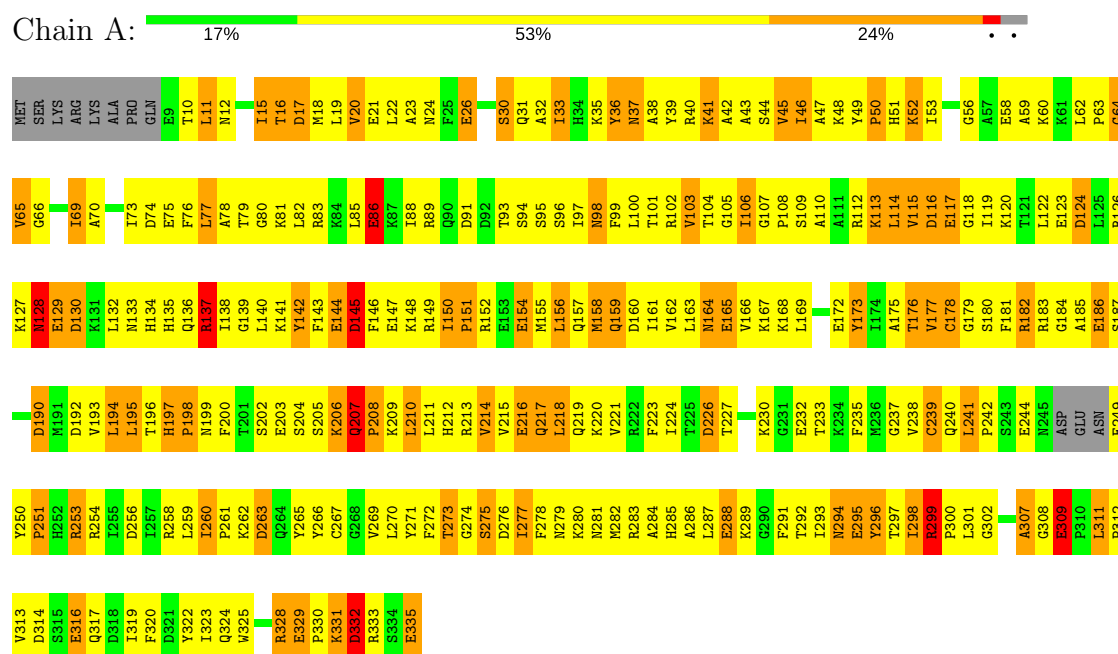
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0

### 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: DNA POLYMERASE BETA



## 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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	1.19	22/2574 (0.9%)	1.71	48/3473 (1.4%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	GLU	CD-OE2	6.52	1.32	1.25
1	A	144	GLU	CD-OE1	6.49	1.32	1.25
1	A	329	GLU	CD-OE1	6.23	1.32	1.25
1	A	30	SER	C-N	6.12	1.48	1.34
1	A	232	GLU	CD-OE1	6.12	1.32	1.25
1	A	186	GLU	CD-OE1	6.05	1.32	1.25
1	A	117	GLU	CD-OE1	5.96	1.32	1.25
1	A	249	GLU	CD-OE1	5.93	1.32	1.25
1	A	129	GLU	CD-OE1	5.85	1.32	1.25
1	A	216	GLU	CD-OE1	5.80	1.32	1.25
1	A	154	GLU	CD-OE1	5.69	1.31	1.25
1	A	58	GLU	CD-OE1	5.68	1.31	1.25
1	A	316	GLU	CD-OE2	5.68	1.31	1.25
1	A	147	GLU	CD-OE1	5.66	1.31	1.25
1	A	21	GLU	CD-OE1	5.52	1.31	1.25
1	A	203	GLU	CD-OE1	5.50	1.31	1.25
1	A	165	GLU	CD-OE1	5.38	1.31	1.25
1	A	26	GLU	CD-OE1	5.37	1.31	1.25
1	A	137	ARG	NE-CZ	5.13	1.39	1.33
1	A	172	GLU	CD-OE1	5.09	1.31	1.25
1	A	288	GLU	CD-OE1	5.09	1.31	1.25
1	A	86	GLU	CD-OE1	5.01	1.31	1.25

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ILE	C-N-CD	-19.00	78.80	120.60
1	A	137	ARG	NE-CZ-NH1	15.25	127.92	120.30
1	A	207	GLN	C-N-CD	-11.04	96.32	120.60
1	A	137	ARG	CD-NE-CZ	10.45	138.23	123.60
1	A	137	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	A	197	HIS	C-N-CD	-9.04	100.71	120.60
1	A	332	ASP	CB-CG-OD1	-9.04	110.16	118.30
1	A	263	ASP	CB-CG-OD1	-8.40	110.74	118.30
1	A	124	ASP	CB-CG-OD2	-7.85	111.23	118.30
1	A	226	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	A	309	GLU	C-N-CD	-7.24	104.68	120.60
1	A	17	ASP	CB-CG-OD1	-7.17	111.84	118.30
1	A	145	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	A	226	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	332	ASP	CB-CG-OD2	7.06	124.66	118.30
1	A	91	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	192	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	276	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	91	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	A	178	CYS	CA-CB-SG	-6.79	101.78	114.00
1	A	314	ASP	CB-CG-OD1	-6.75	112.22	118.30
1	A	253	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	116	ASP	CB-CG-OD1	-6.33	112.61	118.30
1	A	114	LEU	CA-CB-CG	-6.07	101.34	115.30
1	A	273	THR	C-N-CA	-6.00	109.69	122.30
1	A	256	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	A	314	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	17	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	112	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	190	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	52	LYS	N-CA-CB	5.80	121.04	110.60
1	A	160	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	A	116	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	24	ASN	N-CA-CB	5.76	120.97	110.60
1	A	142	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	A	195	LEU	N-CA-CB	-5.61	99.19	110.40
1	A	263	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	190	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	260	ILE	CB-CA-C	-5.44	100.72	111.60
1	A	124	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	276	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	94	SER	N-CA-CB	5.24	118.36	110.50
1	A	137	ARG	CG-CD-NE	5.20	122.72	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	THR	C-N-CA	-5.16	108.81	121.70
1	A	50	PRO	CB-CA-C	-5.15	99.12	112.00
1	A	213	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	299	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	130	ASP	N-CA-CB	-5.04	101.52	110.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2528	0	2459	359	0
2	A	5	0	0	0	0
All	All	2533	0	2459	359	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 72.

All (359) 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:NE2	1:A:317:GLN:H	1.60	0.99
1:A:299:ARG:HH11	1:A:299:ARG:HG3	1.30	0.94
1:A:11:LEU:HG	1:A:52:LYS:HA	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:163:LEU:HD23	1:A:175:ALA:HB3	1.64	0.79
1:A:62:LEU:HB3	1:A:65:VAL:HG11	1.65	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:260:ILE:HG22	1:A:261:PRO:HD2	1.65	0.76
1:A:12:ASN:HB3	1:A:46:ILE:HD12	1.67	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:NH1	1:A:254:ARG:HB3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLY:HA2	1:A:59:ALA:HB3	1.71	0.73
1:A:114:LEU:O	1:A:117:GLU:HB2	1.89	0.73
1:A:62:LEU:O	1:A:65:VAL:HG13	1.89	0.73
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: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:11:LEU:HD12	1:A:52:LYS:HB2	1.72	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
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:209:LYS:HA	1:A:212:HIS:HB2	1.73	0.69
1:A:41:LYS:O	1:A:44:SER:HB3	1.91	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:HD22	1:A:11:LEU:H	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:241:LEU:CG	1:A:242:PRO:HD2	2.25	0.67
1:A:36:TYR:OH	1:A:40:ARG:HD3	1.95	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:N	1:A:106:ILE:HD13	2.10	0.66
1:A:284:ALA:O	1:A:288:GLU:N	2.29	0.66
1:A:240:GLN:HG2	1:A:241:LEU:N	2.10	0.66
1:A:46:ILE:HD13	1:A:53:ILE:HD12	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:328:ARG:NH1	1:A:328:ARG:HG2	2.11	0.65
1:A:11:LEU:HB2	1:A:52:LYS:HG3	1.77	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:NH1	1:A:299:ARG:HG3	2.04	0.64
1:A:166:VAL:O	1:A:169:LEU:HB2	1.97	0.64
1:A:41:LYS:HD2	1:A:41:LYS:O	1.97	0.64
1:A:65:VAL:HA	1:A:69:ILE:HD12	1.79	0.64
1:A:266:TYR:O	1:A:269:VAL:N	2.30	0.64
1:A:69:ILE:HG22	1:A:73:ILE:HD11	1.80	0.64
1:A:122:LEU:HD12	1:A:123:GLU:N	2.12	0.64
1:A:215:VAL:O	1:A:219:GLN:HG3	1.98	0.64
1:A:50:PRO:HG2	1:A:51:HIS:CD2	2.33	0.64
1:A:104:THR:CG2	1:A:139:GLY:HA2	2.29	0.63
1:A:37:ASN:O	1:A:40:ARG:HB3	1.98	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:206:LYS:C	1:A:208:PRO:HD3	2.19	0.62
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:132:LEU:HA	1:A:136:GLN:NE2	2.14	0.62
1:A:35:LYS:O	1:A:38:ALA:HB3	2.00	0.62
1:A:144:GLU:N	1:A:144:GLU:OE1	2.29	0.62
1:A:62:LEU:C	1:A:65:VAL:HG13	2.20	0.62
1:A:302:GLY:HA3	1:A:307:ALA:CB	2.29	0.62
1:A:42:ALA:O	1:A:45:VAL:HG12	1.99	0.62
1:A:159:GLN:HG3	1:A:177:VAL:HG11	1.82	0.61
1:A:44:SER:O	1:A:48:LYS:HG3	1.99	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:H	1:A:311:LEU:HD22	1.64	0.60
1:A:11:LEU:HB2	1:A:52:LYS:HB2	1.83	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:66:GLY:N	1:A:69:ILE:HD12	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:NZ	1:A:206:LYS:HA	2.17	0.60
1:A:143:PHE:HB3	1:A:144:GLU:OE1	2.02	0.59
1:A:62:LEU:HB3	1:A:65:VAL:CG1	2.32	0.59
1:A:145:ASP:HA	1:A:148:LYS:HD2	1.83	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:110:ALA:HA	1:A:113:LYS:HZ2	1.67	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
1:A:161:ILE:O	1:A:165:GLU:HG2	2.04	0.58
1:A:254:ARG:HH11	1:A:254:ARG:HB3	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:HH11	1:A:328:ARG:HG2	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:63:PRO:C	1:A:65:VAL:H	2.07	0.57
1:A:195:LEU:HB3	1:A:258:ARG:O	2.05	0.57
1:A:143:PHE:O	1:A:146:PHE:HB2	2.05	0.57
1:A:79:THR:O	1:A:81:LYS:N	2.29	0.57
1:A:56:GLY:C	1:A:59:ALA:HB3	2.25	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:HA	1:A:217:GLN:HE21	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:CD2	1:A:11:LEU:H	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:152:ARG:NH2	1:A:181:PHE:O	2.39	0.55
1:A:86:GLU:HG2	1:A:86:GLU:O	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:NZ	1:A:168:LYS:HB3	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: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:214:VAL:O	1:A:217:GLN:HB3	2.06	0.54
1:A:196:THR:HG21	1:A:265:TYR:CG	2.42	0.54
1:A:132:LEU:HB3	1:A:136:GLN:HB2	1.88	0.54
1:A:159:GLN:O	1:A:163:LEU:HD12	2.08	0.54
1:A:152:ARG:NE	1:A:185:ALA:O	2.41	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
1:A:82:LEU:O	1:A:85:LEU:HB3	2.09	0.53
1:A:278:PHE:CE2	1:A:333:ARG:HD3	2.43	0.53
1:A:70:ALA:CA	1:A:73:ILE:HD12	2.33	0.53
1:A:269:VAL:O	1:A:273:THR:OG1	2.27	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: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:106:ILE:H	1:A:106:ILE:HD13	1.73	0.53
1:A:134:HIS:HA	1:A:137:ARG:HH12	1.74	0.53
1:A:11:LEU:CD1	1:A:52:LYS:HB2	2.39	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:134:HIS:O	1:A:138:ILE:HG12	2.10	0.52
1:A:49:TYR:CD1	1:A:50:PRO:HD2	2.44	0.52
1:A:129:GLU:O	1:A:132:LEU:HB2	2.10	0.52
1:A:289:LYS:HZ2	1:A:324:GLN:HB2	1.75	0.52
1:A:283:ARG:HH21	1:A:294:ASN:HA	1.74	0.52
1:A:134:HIS:CE1	1:A:137:ARG:HH22	2.27	0.52
1:A:33:ILE:O	1:A:37:ASN:HB2	2.09	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ALA:HA	1:A:113:LYS:HZ1	1.76	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: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: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:11:LEU:CG	1:A:52:LYS:HB2	2.41	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:37:ASN:C	1:A:40:ARG:HB3	2.32	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
1:A:23:ALA:HB2	1:A:39:TYR:HB3	1.94	0.49
1:A:298:ILE:O	1:A:298:ILE:HG23	2.12	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: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:N	1:A:11:LEU:CD2	2.76	0.48
1:A:163:LEU:O	1:A:166:VAL:HG22	2.13	0.48
1:A:65:VAL:HA	1:A:69:ILE:CD1	2.43	0.48
1:A:12:ASN:HD21	1:A:52:LYS:HA	1.79	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: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:60:LYS:HA	1:A:65:VAL:HG22	1.95	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:223:PHE:C	1:A:224:ILE:HD13	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:157:GLN:O	1:A:161:ILE:HG13	2.14	0.47
1:A:17:ASP:N	1:A:17:ASP:OD1	2.48	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
1:A:79:THR:C	1:A:81:LYS:H	2.15	0.46
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:101:THR:CG2	1:A:102:ARG:N	2.79	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:HZ1	1:A:206:LYS:HA	1.79	0.46
1:A:133:ASN:ND2	1:A:135:HIS:H	2.14	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: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:128:ASN:H	1:A:128:ASN:ND2	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:ND2	1:A:294:ASN:O	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:289:LYS:HZ3	1:A:324:GLN:HB2	1.82	0.45
1:A:109:SER:C	1:A:113:LYS:HE3	2.37	0.44
1:A:287:LEU:HA	1:A:291:PHE:O	2.18	0.44
1:A:169:LEU:HD23	1:A:169:LEU:HA	1.57	0.44
1:A:194:LEU:CD1	1:A:194:LEU:N	2.80	0.44
1:A:11:LEU:CD1	1:A:52:LYS:N	2.81	0.44
1:A:151:PRO:O	1:A:154:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:CD2	1:A:39:TYR:CE1	3.00	0.44
1:A:119:ILE:HA	1:A:124:ASP:CG	2.39	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:107:GLY:H	1:A:110:ALA:HB3	1.84	0.43
1:A:159:GLN:HE21	1:A:159:GLN:HB3	1.57	0.43
1:A:262:LYS:O	1:A:262:LYS:HG2	2.17	0.43
1:A:292:THR:HB	1:A:301:LEU:HD13	2.00	0.43
1:A:40:ARG:O	1:A:43:ALA:HB3	2.18	0.43
1:A:211:LEU:C	1:A:211:LEU:HD12	2.38	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:HE2	1:A:206:LYS:N	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:287:LEU:HA	1:A:287:LEU:HD12	1.83	0.43
1:A:95:SER:OG	1:A:96:SER:N	2.48	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:193:VAL:C	1:A:194:LEU:HD12	2.40	0.42
1:A:216:GLU:O	1:A:220:LYS:N	2.53	0.42
1:A:211:LEU:HB2	1:A:259:LEU:HB2	2.00	0.42
1:A:70:ALA:C	1:A:73:ILE:HB	2.40	0.42
1:A:122:LEU:HD13	1:A:126:ARG:HH11	1.84	0.42
1:A:49:TYR:HA	1:A:50:PRO:HD3	1.88	0.42
1:A:200:PHE:HD1	1:A:204:SER:HB2	1.84	0.42
1:A:50:PRO:HG2	1:A:51:HIS:HD2	1.82	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: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: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: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:195:LEU:HG	1:A:259:LEU:HD13	2.03	0.41
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.86	0.41
1:A:196:THR:HG22	1:A:265:TYR:CZ	2.55	0.41
1:A:16:THR:HG21	1:A:47:ALA:HB2	2.02	0.41
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.80	0.41
1:A:270:LEU:HD12	1:A:270:LEU:C	2.42	0.41
1:A:127:LYS:C	1:A:129:GLU:H	2.24	0.40
1:A:259:LEU:HA	1:A:259:LEU:HD12	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:62:LEU:HG	1:A:63:PRO:HD2	2.00	0.40
1:A:206:LYS:CE	1:A:206:LYS:CA	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: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

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	320/335 (96%)	244 (76%)	53 (17%)	23 (7%)	<b>1</b> <b>17</b>

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	32	ALA
1	A	128	ASN

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Mol	Chain	Res	Type
1	A	180	SER
1	A	198	PRO
1	A	275	SER
1	A	295	GLU
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%)	<b>1</b> <b>7</b>

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

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	31	GLN
1	A	33	ILE
1	A	36	TYR
1	A	37	ASN
1	A	41	LYS
1	A	45	VAL
1	A	46	ILE
1	A	65	VAL
1	A	77	LEU
1	A	83	ARG
1	A	88	ILE
1	A	89	ARG
1	A	93	THR
1	A	98	ASN
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	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	214	VAL
1	A	217	GLN
1	A	218	LEU
1	A	226	ASP
1	A	239	CYS
1	A	241	LEU

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Mol	Chain	Res	Type
1	A	277	ILE
1	A	294	ASN
1	A	296	TYR
1	A	297	THR
1	A	298	ILE
1	A	299	ARG
1	A	311	LEU
1	A	313	VAL
1	A	325	TRP
1	A	328	ARG
1	A	331	LYS
1	A	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	31	GLN
1	A	37	ASN
1	A	51	HIS
1	A	128	ASN
1	A	135	HIS
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 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	PO4	A	337	-	4,4,4	4.81	3 (75%)	6,6,6	0.87	0

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	PO4	A	337	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	337	PO4	P-O3	4.27	1.69	1.54
2	A	337	PO4	P-O1	5.80	1.63	1.50
2	A	337	PO4	P-O4	6.39	1.76	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

### 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.