



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:51 PM UTC

PDB ID : 6AMS / pdb_00006ams
Title : Crystal structure of the DNA polymerase III subunit beta from *Pseudomonas aeruginosa*
Authors : McGrath, A.E.; Oakley, A.J.
Deposited on : 2017-08-11
Resolution : 2.39 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

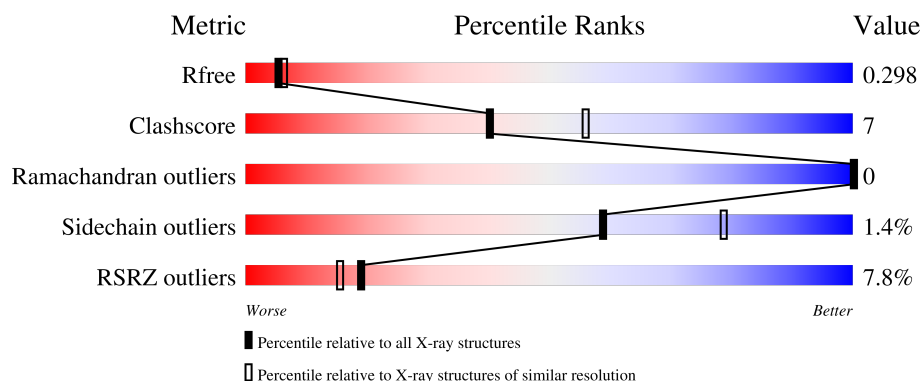
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	367	10% 81% 17% ..
1	B	367	4% 86% 12% ..
1	C	367	12% 74% 24% ..
1	D	367	6% 80% 19% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11349 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 Beta sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2812	1764	496	543	9			
1	B	363	Total	C	N	O	S	0	0	0
			2816	1765	497	545	9			
1	C	364	Total	C	N	O	S	0	0	0
			2811	1765	495	542	9			
1	D	366	Total	C	N	O	S	0	0	0
			2835	1775	506	545	9			

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



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

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

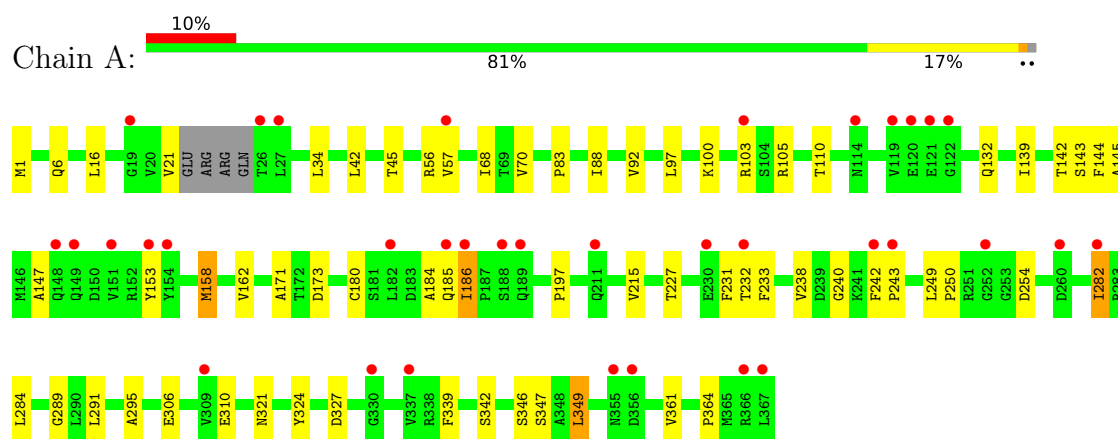
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	15	Total	O	0	0
			15	15		
3	C	15	Total	O	0	0
			15	15		
3	D	16	Total	O	0	0
			16	16		

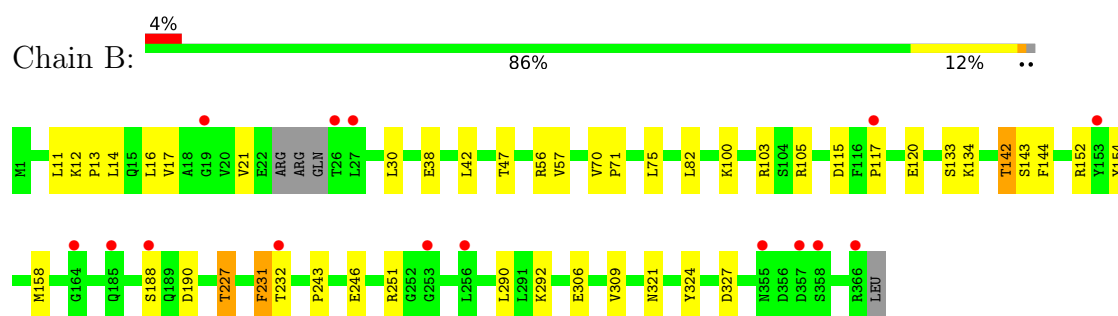
3 Residue-property plots

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 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.

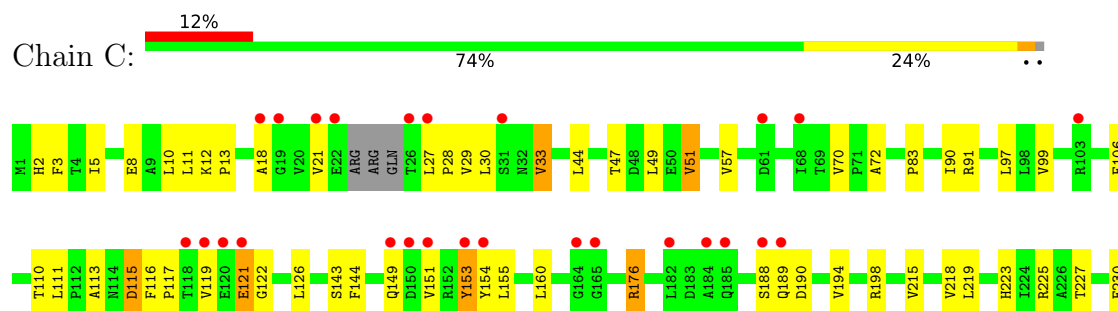
• Molecule 1: Beta sliding clamp

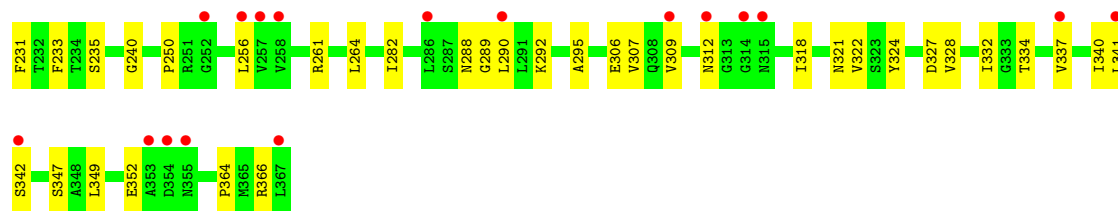


• Molecule 1: Beta sliding clamp

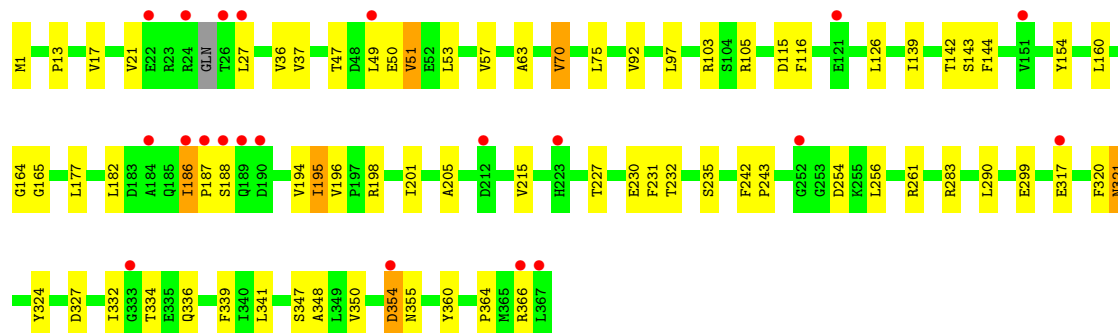
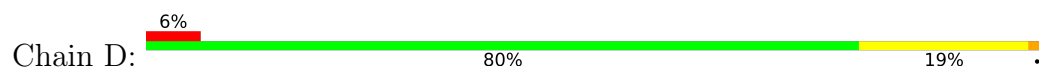


• Molecule 1: Beta sliding clamp





● Molecule 1: Beta sliding clamp



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.50Å 79.73Å 86.30Å 63.43° 72.20° 87.08°	Depositor
Resolution (Å)	37.34 – 2.39 37.34 – 2.39	Depositor EDS
% Data completeness (in resolution range)	92.8 (37.34-2.39) 92.8 (37.34-2.39)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.244 , 0.283 0.256 , 0.298	Depositor DCC
R_{free} test set	2846 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11349	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1699e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.94	10/2848 (0.4%)	1.02	6/3854 (0.2%)
1	B	0.92	4/2852 (0.1%)	1.01	9/3860 (0.2%)
1	C	0.89	6/2847 (0.2%)	1.03	10/3853 (0.3%)
1	D	1.09	13/2870 (0.5%)	1.10	17/3883 (0.4%)
All	All	0.96	33/11417 (0.3%)	1.04	42/15450 (0.3%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	70	VAL	C-O	-12.61	1.15	1.24
1	A	233	PHE	C-O	-7.99	1.14	1.24
1	D	195	ILE	C-O	-6.48	1.17	1.24
1	D	196	VAL	C-O	-6.48	1.16	1.24
1	C	215	VAL	C-O	-6.44	1.17	1.24
1	C	233	PHE	C-O	-6.35	1.16	1.24
1	C	225	ARG	C-O	-5.94	1.17	1.24
1	D	194	VAL	C-O	-5.91	1.18	1.24
1	B	17	VAL	C-O	-5.82	1.17	1.24
1	A	105	ARG	C-O	-5.68	1.17	1.24
1	D	201	ILE	C-O	-5.66	1.17	1.24
1	A	349	LEU	C-O	-5.66	1.17	1.24
1	D	37	VAL	C-O	-5.61	1.18	1.24
1	B	30	LEU	C-O	-5.48	1.17	1.24
1	B	227	THR	C-O	-5.47	1.17	1.24
1	B	309	VAL	C-O	-5.41	1.17	1.23
1	A	142	THR	C-O	-5.30	1.17	1.24
1	A	158	MET	C-O	-5.27	1.17	1.24
1	A	88	ILE	C-O	-5.25	1.18	1.24
1	D	164	GLY	C-O	-5.25	1.18	1.24
1	A	339	PHE	C-O	-5.22	1.17	1.24
1	C	83	PRO	C-O	-5.18	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	ALA	C-O	-5.17	1.17	1.23
1	D	36	VAL	C-O	-5.17	1.18	1.24
1	C	218	VAL	C-O	-5.16	1.18	1.24
1	A	83	PRO	C-O	-5.15	1.17	1.23
1	C	227	THR	C-O	-5.15	1.18	1.24
1	A	180	CYS	C-O	-5.13	1.17	1.23
1	D	196	VAL	CA-C	-5.12	1.48	1.53
1	A	100	LYS	C-O	-5.09	1.17	1.24
1	D	215	VAL	C-O	-5.08	1.18	1.24
1	D	160	LEU	C-O	-5.06	1.18	1.24
1	D	75	LEU	C-O	-5.02	1.18	1.24

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	SER	N-CA-C	8.73	120.79	111.28
1	C	153	TYR	N-CA-C	8.63	121.47	111.11
1	D	354	ASP	N-CA-C	7.88	119.95	111.36
1	B	142	THR	N-CA-C	7.33	122.40	113.38
1	D	231	PHE	N-CA-C	7.29	120.25	109.24
1	C	113	ALA	N-CA-C	7.20	119.12	111.28
1	C	122	GLY	CA-C-N	7.17	127.00	119.05
1	C	122	GLY	C-N-CA	7.17	127.00	119.05
1	A	143	SER	N-CA-C	7.04	119.81	111.71
1	D	143	SER	N-CA-C	6.97	118.87	111.28
1	D	50	GLU	N-CA-C	6.80	118.78	111.36
1	D	47	THR	N-CA-C	6.79	119.17	108.79
1	C	231	PHE	N-CA-C	6.68	118.91	108.96
1	A	254	ASP	N-CA-C	6.62	118.58	111.36
1	B	231	PHE	N-CA-C	6.53	118.13	108.60
1	C	115	ASP	N-CA-C	-6.34	104.47	111.82
1	D	27	LEU	CA-C-N	6.07	125.79	119.05
1	D	27	LEU	C-N-CA	6.07	125.79	119.05
1	D	142	THR	N-CA-C	6.06	121.42	113.30
1	D	116	PHE	CA-C-N	5.95	125.89	119.76
1	D	116	PHE	C-N-CA	5.95	125.89	119.76
1	D	230	GLU	N-CA-C	5.94	117.83	111.36
1	C	230	GLU	N-CA-C	5.92	117.81	111.36
1	D	321	ASN	N-CA-C	-5.83	101.21	109.96
1	D	186	ILE	CA-C-N	5.76	125.45	119.05
1	D	186	ILE	C-N-CA	5.76	125.45	119.05
1	D	290	LEU	N-CA-C	5.69	118.72	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	ARG	N-CA-C	-5.69	99.86	108.67
1	A	68	ILE	CB-CA-C	-5.68	106.40	111.74
1	A	231	PHE	N-CA-C	5.63	117.74	109.24
1	B	227	THR	N-CA-C	5.51	118.07	108.76
1	A	142	THR	N-CA-C	5.42	121.66	114.12
1	D	355	ASN	N-CA-C	5.36	116.14	108.74
1	B	290	LEU	N-CA-C	5.33	117.86	108.75
1	B	11	LEU	N-CA-C	5.25	117.00	111.28
1	C	143	SER	N-CA-C	5.21	119.97	111.37
1	D	198	ARG	N-CA-C	5.20	117.62	111.33
1	C	11	LEU	N-CA-C	5.18	116.93	111.28
1	B	82	LEU	CA-C-N	5.11	125.02	119.76
1	B	82	LEU	C-N-CA	5.11	125.02	119.76
1	C	290	LEU	N-CA-C	5.08	117.45	108.75
1	A	186	ILE	N-CA-C	-5.06	104.28	108.63

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	2812	0	2857	30	2
1	B	2816	0	2858	30	1
1	C	2811	0	2851	63	1
1	D	2835	0	2884	39	2
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	9	0	0	0	0
3	B	15	0	0	0	0
3	C	15	0	0	1	0
3	D	16	0	0	0	0
All	All	11349	0	11450	151	3

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 7.

All (151) 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:C:18:ALA:O	1:C:21:VAL:HG12	1.40	1.21
1:D:70:VAL:HG11	1:D:97:LEU:HD22	1.26	1.12
1:C:18:ALA:O	1:C:21:VAL:CG1	2.10	0.99
1:B:133:SER:OG	1:D:366:ARG:HG3	1.64	0.95
1:A:197:PRO:HD3	1:A:238:VAL:HG23	1.48	0.95
1:B:133:SER:OG	1:D:366:ARG:CG	2.16	0.94
1:C:70:VAL:HG11	1:C:97:LEU:HD22	1.50	0.93
1:A:70:VAL:HG11	1:A:97:LEU:HD22	1.59	0.85
1:A:289:GLY:HA3	1:C:151:VAL:HG13	1.60	0.81
1:C:332:ILE:HG21	1:C:337:VAL:HG22	1.61	0.80
1:C:292:LYS:HE2	1:C:306:GLU:OE2	1.81	0.79
1:C:318:ILE:HD13	1:C:341:LEU:HD21	1.63	0.79
1:C:29:VAL:HG11	1:C:116:PHE:HA	1.65	0.77
1:C:282:ILE:CD1	1:C:295:ALA:HB2	2.15	0.76
1:C:12:LYS:HB3	1:C:13:PRO:HD3	1.67	0.76
1:C:18:ALA:C	1:C:21:VAL:HG12	2.10	0.75
1:A:153:TYR:HE1	1:A:240:GLY:HA3	1.53	0.74
1:D:70:VAL:HG11	1:D:97:LEU:CD2	2.15	0.72
1:B:133:SER:OG	1:D:366:ARG:CD	2.39	0.71
1:B:133:SER:OG	1:D:366:ARG:HD2	1.90	0.71
1:C:12:LYS:HB3	1:C:13:PRO:CD	2.21	0.70
1:C:292:LYS:CE	1:C:306:GLU:OE2	2.41	0.69
1:C:121:GLU:OE2	1:C:223:HIS:HB3	1.92	0.69
1:B:70:VAL:CG2	1:B:71:PRO:HD2	2.23	0.69
1:A:147:ALA:HB2	1:A:173:ASP:HA	1.74	0.68
1:C:189:GLN:O	1:C:190:ASP:OD1	2.12	0.68
1:C:289:GLY:HA2	1:C:309:VAL:O	1.96	0.66
1:D:261:ARG:HD2	1:D:332:ILE:HB	1.78	0.65
1:B:227:THR:HG23	1:B:232:THR:HG22	1.79	0.65
1:A:184:ALA:HB3	1:A:186:ILE:HD12	1.79	0.64
1:A:242:PHE:CD2	1:A:243:PRO:HD2	2.32	0.64
1:C:261:ARG:HB2	1:C:337:VAL:HG23	1.81	0.63
1:B:133:SER:HG	1:D:366:ARG:HG3	1.63	0.63
1:D:51:VAL:HG22	1:D:235:SER:HB2	1.80	0.63
1:C:288:ASN:OD1	1:C:312:ASN:OD1	2.19	0.61
1:B:292:LYS:HG2	1:B:306:GLU:HG2	1.84	0.60
1:B:12:LYS:HB3	1:B:13:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:VAL:HG22	1:B:71:PRO:HD2	1.84	0.58
1:A:70:VAL:HG12	1:A:110:THR:HG22	1.86	0.58
1:C:334:THR:HG23	1:C:352:GLU:HG2	1.85	0.58
1:A:242:PHE:CG	1:A:243:PRO:HD2	2.39	0.58
1:D:339:PHE:HB3	1:D:341:LEU:HD11	1.86	0.57
1:D:242:PHE:CG	1:D:243:PRO:HD2	2.40	0.56
1:A:347:SER:HA	1:A:364:PRO:HD3	1.87	0.56
1:B:142:THR:HG22	1:B:158:MET:HE2	1.87	0.56
1:D:17:VAL:HG12	1:D:53:LEU:HD12	1.88	0.56
1:C:51:VAL:HG22	1:C:235:SER:HB2	1.88	0.56
1:D:126:LEU:HD13	1:D:188:SER:HB3	1.87	0.55
1:B:154:TYR:CD2	1:B:243:PRO:HD3	2.41	0.55
1:C:328:VAL:O	1:C:332:ILE:HG12	2.06	0.55
1:D:332:ILE:HG22	1:D:334:THR:H	1.71	0.54
1:C:8:GLU:OE2	1:C:8:GLU:N	2.38	0.54
1:B:12:LYS:HB3	1:B:13:PRO:CD	2.37	0.54
1:B:100:LYS:HG2	1:B:105:ARG:HD3	1.91	0.53
1:D:187:PRO:O	1:D:188:SER:C	2.52	0.53
1:A:321:ASN:HB3	1:A:324:TYR:CD2	2.43	0.53
1:B:47:THR:HG21	1:B:117:PRO:HG2	1.90	0.53
1:D:49:LEU:H	1:D:49:LEU:HD22	1.74	0.52
1:C:99:VAL:HB	1:C:106:PHE:HB2	1.92	0.52
1:C:176:ARG:HD3	3:C:512:HOH:O	2.09	0.52
1:A:42:LEU:HB3	1:A:57:VAL:HG13	1.91	0.51
1:C:341:LEU:HD12	1:C:342:SER:H	1.74	0.51
1:C:29:VAL:HG11	1:C:116:PHE:CA	2.40	0.51
1:C:282:ILE:HD11	1:C:295:ALA:HB2	1.93	0.51
1:C:44:LEU:N	1:C:44:LEU:HD12	2.26	0.51
1:C:160:LEU:HB2	1:C:194:VAL:HG23	1.92	0.51
1:A:153:TYR:CE1	1:A:240:GLY:HA3	2.41	0.50
1:A:56:ARG:HH22	1:A:232:THR:HG23	1.76	0.50
1:C:33:VAL:HG23	1:C:72:ALA:HB2	1.93	0.50
1:D:347:SER:HA	1:D:364:PRO:HD3	1.94	0.50
1:C:321:ASN:HB3	1:C:324:TYR:CD2	2.47	0.50
1:A:1:MET:HE2	1:A:92:VAL:HG23	1.95	0.49
1:B:188:SER:OG	1:B:190:ASP:O	2.30	0.49
1:D:227:THR:HG22	1:D:232:THR:HG23	1.94	0.49
1:C:5:ILE:HD13	1:C:10:LEU:HB2	1.92	0.49
1:C:149:GLN:HG3	1:C:151:VAL:HG23	1.94	0.49
1:D:13:PRO:HG3	1:D:57:VAL:CG2	2.42	0.49
1:D:283:ARG:HH21	1:D:317:GLU:CD	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:VAL:HG21	1:C:115:ASP:HB3	1.94	0.48
1:C:292:LYS:HG2	1:C:306:GLU:HG2	1.96	0.48
1:B:56:ARG:HH12	1:B:232:THR:HG23	1.78	0.48
1:D:139:ILE:HG21	1:D:205:ALA:HB2	1.96	0.48
1:C:155:LEU:N	1:C:155:LEU:HD23	2.29	0.47
1:A:284:LEU:HG	1:A:291:LEU:HD11	1.95	0.47
1:C:30:LEU:HD11	1:C:49:LEU:HD11	1.95	0.47
1:C:119:VAL:O	1:C:119:VAL:HG13	2.14	0.47
1:A:227:THR:HG22	1:A:232:THR:HG22	1.97	0.47
1:C:160:LEU:HB2	1:C:194:VAL:CG2	2.44	0.47
1:A:342:SER:OG	1:A:346:SER:HB2	2.15	0.47
1:B:21:VAL:O	1:B:21:VAL:HG23	2.15	0.47
1:A:139:ILE:HG23	1:A:158:MET:HE1	1.97	0.46
1:A:250:PRO:HG2	1:A:349:LEU:HB2	1.98	0.46
1:C:126:LEU:HD13	1:C:188:SER:HB3	1.98	0.46
1:C:111:LEU:HD23	1:C:111:LEU:HA	1.80	0.46
1:C:282:ILE:CG1	1:C:322:VAL:HB	2.46	0.46
1:B:42:LEU:HB3	1:B:57:VAL:CG1	2.45	0.46
1:A:162:VAL:HG11	1:A:186:ILE:HG21	1.98	0.46
1:B:70:VAL:HG23	1:B:71:PRO:HD2	1.97	0.46
1:A:144:PHE:CD2	1:A:327:ASP:HB3	2.51	0.45
1:C:154:TYR:CE1	1:C:240:GLY:HA3	2.51	0.45
1:D:321:ASN:HB3	1:D:324:TYR:CD2	2.51	0.45
1:D:154:TYR:CD2	1:D:243:PRO:HD3	2.51	0.45
1:D:195:ILE:HD11	1:D:242:PHE:HB2	1.98	0.45
1:C:29:VAL:CG1	1:C:116:PHE:HA	2.41	0.45
1:D:144:PHE:CD1	1:D:327:ASP:HB3	2.52	0.45
1:D:186:ILE:HA	1:D:187:PRO:HD3	1.81	0.45
1:C:27:LEU:HD12	1:C:28:PRO:CD	2.48	0.44
1:C:194:VAL:HG21	1:C:219:LEU:HD22	1.98	0.44
1:D:49:LEU:HD22	1:D:49:LEU:N	2.31	0.44
1:A:103:ARG:HD3	1:B:306:GLU:HB2	1.99	0.44
1:A:132:GLN:HG2	1:A:215:VAL:HB	1.99	0.44
1:B:134:LYS:HE3	1:D:366:ARG:NH2	2.32	0.44
1:D:53:LEU:C	1:D:53:LEU:HD13	2.43	0.44
1:B:144:PHE:CD1	1:B:327:ASP:HB3	2.52	0.44
1:A:249:LEU:HD23	1:A:361:VAL:HG21	1.99	0.43
1:B:16:LEU:HD23	1:B:16:LEU:HA	1.78	0.43
1:C:256:LEU:HD23	1:C:340:ILE:HG12	2.00	0.43
1:C:347:SER:HA	1:C:364:PRO:HD3	1.99	0.43
1:C:282:ILE:HD13	1:C:295:ALA:HB2	1.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:HB3	1:A:45:THR:HB	2.01	0.43
1:B:134:LYS:HE3	1:D:366:ARG:HH22	1.83	0.43
1:D:1:MET:HE2	1:D:92:VAL:HG23	2.01	0.43
1:B:231:PHE:C	1:B:231:PHE:CD1	2.95	0.43
1:C:264:LEU:HD23	1:C:307:VAL:HG11	2.01	0.42
1:A:310:GLU:HB3	1:C:153:TYR:HA	2.00	0.42
1:C:250:PRO:HG2	1:C:349:LEU:HB2	2.02	0.42
1:C:256:LEU:CD2	1:C:340:ILE:HG12	2.49	0.42
1:A:145:ALA:HB3	1:A:171:ALA:HB3	2.01	0.42
1:B:14:LEU:HD21	1:B:75:LEU:HG	2.01	0.42
1:B:321:ASN:HB3	1:B:324:TYR:CD2	2.55	0.42
1:D:103:ARG:HA	1:D:105:ARG:HH12	1.84	0.42
1:D:320:PHE:CZ	1:D:348:ALA:HB2	2.54	0.42
1:C:2:HIS:HD2	1:C:91:ARG:HB2	1.84	0.42
1:C:47:THR:HG21	1:C:117:PRO:HG2	2.02	0.42
1:C:292:LYS:HE3	1:C:306:GLU:OE2	2.18	0.41
1:D:332:ILE:HD13	1:D:332:ILE:HA	1.88	0.41
1:C:27:LEU:HD12	1:C:28:PRO:HD3	2.01	0.41
1:D:283:ARG:NH2	1:D:317:GLU:OE2	2.44	0.41
1:D:350:VAL:HB	1:D:360:TYR:HB2	2.02	0.41
1:A:282:ILE:CD1	1:A:295:ALA:HB2	2.51	0.41
1:D:165:GLY:HA2	1:D:186:ILE:O	2.21	0.41
1:C:144:PHE:CD1	1:C:327:ASP:HB3	2.56	0.41
1:D:177:LEU:C	1:D:177:LEU:HD23	2.46	0.40
1:C:282:ILE:HG13	1:C:322:VAL:HB	2.04	0.40
1:B:246:GLU:O	1:B:251:ARG:NH1	2.52	0.40
1:C:12:LYS:N	1:C:13:PRO:HD2	2.37	0.40
1:C:13:PRO:HG3	1:C:57:VAL:CG2	2.52	0.40
1:C:3:PHE:CZ	1:C:90:ILE:HD12	2.57	0.40
1:D:341:LEU:HD12	1:D:341:LEU:N	2.36	0.40
1:A:306:GLU:HB2	1:B:103:ARG:HD2	2.03	0.40
1:C:70:VAL:HG12	1:C:110:THR:HG22	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ASP:OD2	1:D:354:ASP:OD2[1_455]	1.68	0.52
1:A:6:GLN:NE2	1:C:366:ARG:NH1[1_546]	1.91	0.29
1:A:185:GLN:NE2	1:D:115:ASP:O[1_545]	1.94	0.26

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	359/367 (98%)	351 (98%)	8 (2%)	0	100	100
1	B	359/367 (98%)	353 (98%)	6 (2%)	0	100	100
1	C	360/367 (98%)	355 (99%)	5 (1%)	0	100	100
1	D	362/367 (99%)	356 (98%)	6 (2%)	0	100	100
All	All	1440/1468 (98%)	1415 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	311/317 (98%)	308 (99%)	3 (1%)	68	84
1	B	312/317 (98%)	310 (99%)	2 (1%)	78	89
1	C	309/317 (98%)	304 (98%)	5 (2%)	55	76
1	D	313/317 (99%)	306 (98%)	7 (2%)	45	67
All	All	1245/1268 (98%)	1228 (99%)	17 (1%)	59	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	21	VAL

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Mol	Chain	Res	Type
1	A	282	ILE
1	B	38	GLU
1	B	120	GLU
1	C	33	VAL
1	C	51	VAL
1	C	121	GLU
1	C	176	ARG
1	C	198	ARG
1	D	21	VAL
1	D	51	VAL
1	D	182	LEU
1	D	254	ASP
1	D	256	LEU
1	D	299	GLU
1	D	336	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	149	GLN
1	A	294	GLN
1	A	296	ASN
1	B	132	GLN
1	B	294	GLN
1	B	296	ASN
1	B	300	GLN
1	C	294	GLN
1	C	296	ASN
1	C	300	GLN
1	D	175	HIS
1	D	222	HIS
1	D	294	GLN
1	D	296	ASN
1	D	308	GLN

5.3.3 RNA ⓘ

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	C	401	-	4,4,4	1.17	0	6,6,6	0.59	0
2	PO4	A	401	-	4,4,4	1.17	0	6,6,6	0.53	0
2	PO4	D	401	-	4,4,4	0.94	0	6,6,6	1.36	1 (16%)
2	PO4	B	401	-	4,4,4	0.87	0	6,6,6	1.08	1 (16%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	PO4	O3-P-O2	2.07	114.37	107.91
2	D	401	PO4	O4-P-O3	2.03	114.24	107.91

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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	363/367 (98%)	0.79	35 (9%)	13	10	19, 35, 63, 81	4 (1%)
1	B	363/367 (98%)	0.49	15 (4%)	41	37	18, 33, 56, 75	2 (0%)
1	C	364/367 (99%)	0.93	43 (11%)	9	6	21, 38, 67, 105	6 (1%)
1	D	366/367 (99%)	0.58	21 (5%)	29	25	16, 32, 57, 78	4 (1%)
All	All	1456/1468 (99%)	0.70	114 (7%)	19	15	16, 34, 62, 105	16 (1%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	TYR	5.1
1	D	189	GLN	5.1
1	A	185	GLN	4.8
1	C	185	GLN	4.5
1	D	354	ASP	4.5
1	D	367	LEU	4.3
1	A	337	VAL	4.1
1	D	188	SER	4.0
1	C	150	ASP	4.0
1	C	309	VAL	3.9
1	C	367	LEU	3.9
1	A	151	VAL	3.9
1	C	26	THR	3.9
1	C	153	TYR	3.9
1	C	182	LEU	3.7
1	C	337	VAL	3.7
1	C	189	GLN	3.6
1	C	314	GLY	3.6
1	C	341	LEU	3.6
1	C	256	LEU	3.6
1	B	27	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	164	GLY	3.5
1	D	24	ARG	3.5
1	A	189	GLN	3.4
1	B	366	ARG	3.4
1	C	120	GLU	3.4
1	A	121	GLU	3.4
1	B	26	THR	3.2
1	C	149	GLN	3.2
1	A	182	LEU	3.2
1	C	188	SER	3.2
1	B	153	TYR	3.1
1	C	154	TYR	3.0
1	A	119	VAL	3.0
1	D	26	THR	3.0
1	B	355	ASN	3.0
1	C	164	GLY	2.9
1	C	119	VAL	2.9
1	C	27	LEU	2.9
1	C	184	ALA	2.9
1	D	366	ARG	2.9
1	A	355	ASN	2.9
1	A	356	ASP	2.8
1	C	19	GLY	2.8
1	C	353	ALA	2.8
1	C	286	LEU	2.8
1	A	211	GLN	2.8
1	D	121	GLU	2.8
1	C	21	VAL	2.8
1	A	120	GLU	2.7
1	C	22	GLU	2.7
1	A	148	GLN	2.7
1	A	188	SER	2.7
1	C	103	ARG	2.7
1	A	154	TYR	2.6
1	D	151	VAL	2.6
1	D	187	PRO	2.6
1	A	242	PHE	2.6
1	C	61	ASP	2.6
1	A	122	GLY	2.6
1	C	290	LEU	2.6
1	A	19	GLY	2.6
1	A	252	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	186	ILE	2.6
1	C	257	VAL	2.6
1	C	258	VAL	2.6
1	D	252	GLY	2.5
1	C	151	VAL	2.5
1	D	27	LEU	2.5
1	C	312	ASN	2.5
1	D	212	ASP	2.5
1	C	165	GLY	2.5
1	D	333	GLY	2.5
1	B	185	GLN	2.5
1	C	354	ASP	2.5
1	A	232	THR	2.5
1	A	367	LEU	2.4
1	A	103	ARG	2.4
1	B	253	GLY	2.4
1	A	57	VAL	2.4
1	A	27	LEU	2.4
1	C	355	ASN	2.4
1	B	232	THR	2.4
1	C	342	SER	2.4
1	B	19	GLY	2.3
1	A	243	PRO	2.3
1	C	68	ILE	2.3
1	D	190	ASP	2.3
1	B	358	SER	2.3
1	A	114	ASN	2.2
1	D	317	GLU	2.2
1	A	260	ASP	2.2
1	C	315	ASN	2.2
1	C	118	THR	2.2
1	A	149	GLN	2.2
1	A	26	THR	2.2
1	A	309	VAL	2.2
1	D	49	LEU	2.1
1	A	230	GLU	2.1
1	C	252	GLY	2.1
1	C	18	ALA	2.1
1	C	31	SER	2.1
1	D	184	ALA	2.1
1	A	282	ILE	2.1
1	D	22	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	256	LEU	2.1
1	B	357	ASP	2.1
1	D	223	HIS	2.1
1	B	188	SER	2.0
1	A	366	ARG	2.0
1	A	330	GLY	2.0
1	C	121	GLU	2.0
1	B	117	PRO	2.0
1	D	186	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	B	401	5/5	0.77	0.15	62,64,74,77	0
2	PO4	C	401	5/5	0.84	0.11	56,59,62,67	0
2	PO4	A	401	5/5	0.85	0.11	70,72,73,77	0
2	PO4	D	401	5/5	0.86	0.18	54,71,77,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.