



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:51 PM UTC

PDB ID : 1UNN / pdb_00001unn
Title : Complex of beta-clamp processivity factor and little finger domain of PolIV
Authors : Bunting, K.A.; Roe, S.M.; Pearl, L.H.
Deposited on : 2003-09-11
Resolution : 1.90 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

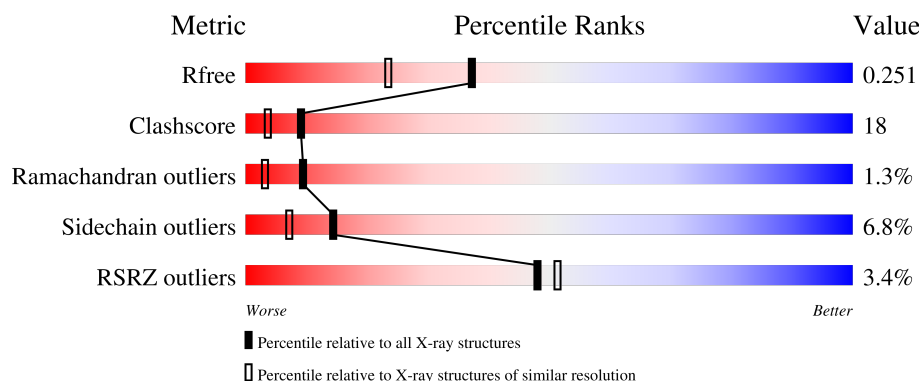
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	366	4% 63% 27% 8% .
1	B	366	4% 65% 28% 7% .
2	C	115	% 77% 17% . .
2	D	115	% 65% 23% . . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8485 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.

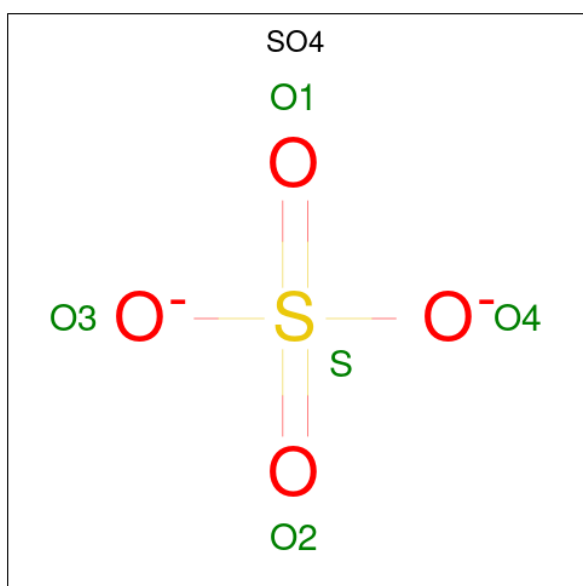
- Molecule 1 is a protein called DNA POLYMERASE III BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2844	1786	498	541	19			
1	B	366	Total	C	N	O	S	0	0	0
			2844	1786	498	541	19			

- Molecule 2 is a protein called DNA POLYMERASE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	111	Total	C	N	O	S	0	0	0
			915	576	175	161	3			
2	D	112	Total	C	N	O	S	0	0	0
			925	582	178	162	3			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

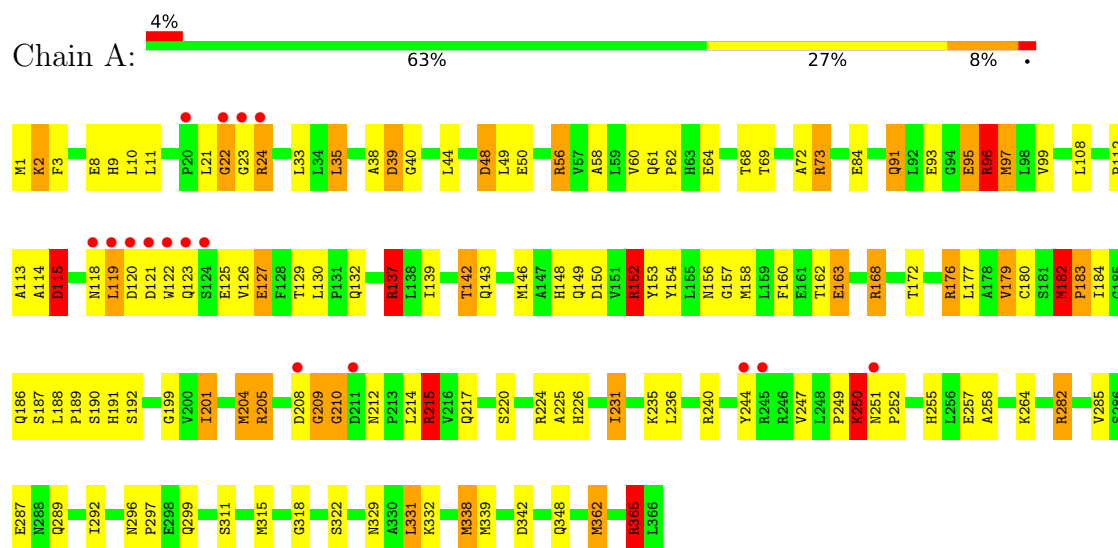
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	304	Total	O	0	0
			304	304		
4	B	375	Total	O	0	0
			375	375		
4	C	116	Total	O	0	0
			116	116		
4	D	152	Total	O	0	0
			152	152		

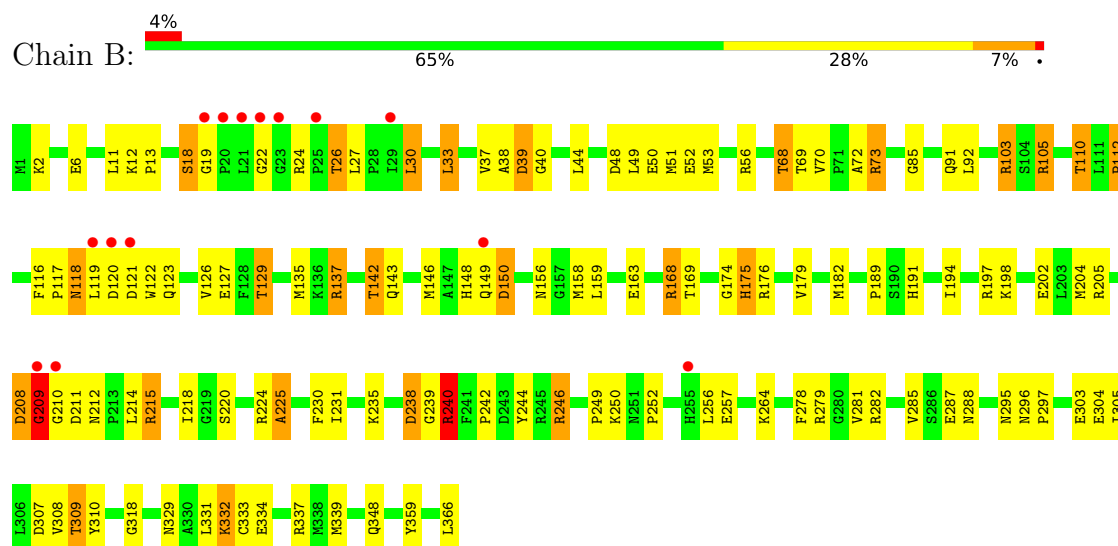
3 Residue-property plots [i](#)

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 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.

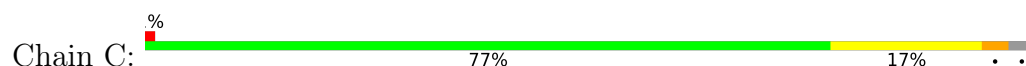
• Molecule 1: DNA POLYMERASE III BETA SUBUNIT



• Molecule 1: DNA POLYMERASE III BETA SUBUNIT

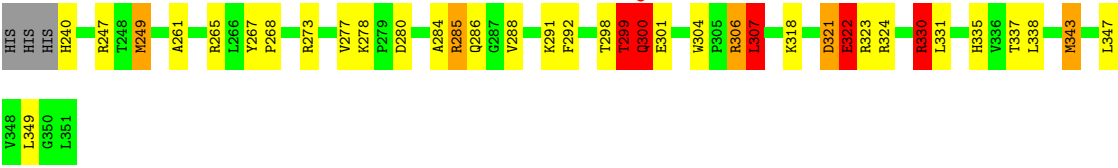


• Molecule 2: DNA POLYMERASE IV





● Molecule 2: DNA POLYMERASE IV



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	146.45Å 70.12Å 110.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.10 – 1.90 62.10 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (62.10-1.90) 96.6 (62.10-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.04 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.179 , 0.240 (Not available) , 0.251	Depositor DCC
R_{free} test set	4388 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8485	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.69	28/2893 (1.0%)	1.66	34/3915 (0.9%)
1	B	1.78	28/2893 (1.0%)	1.65	39/3915 (1.0%)
2	C	1.46	3/933 (0.3%)	1.41	3/1258 (0.2%)
2	D	2.13	17/944 (1.8%)	2.05	19/1273 (1.5%)
All	All	1.76	76/7663 (1.0%)	1.68	95/10361 (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	1	1
1	B	2	2
All	All	3	3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	307	LEU	N-CA	30.86	1.85	1.46
2	D	322	GLU	N-CA	19.01	1.70	1.46
1	A	96	ARG	N-CA	16.35	1.67	1.46
1	A	97	MET	SD-CE	-14.42	1.43	1.79
1	A	338	MET	SD-CE	13.82	2.14	1.79
1	B	148	HIS	C-O	12.60	1.38	1.23
1	B	135	MET	SD-CE	-12.23	1.49	1.79
1	A	182	MET	CG-SD	-10.30	1.55	1.80
1	B	37	VAL	CA-CB	-10.14	1.42	1.54
1	B	182	MET	CG-SD	-9.32	1.57	1.80
1	A	96	ARG	CA-C	9.14	1.65	1.52
2	D	307	LEU	CA-C	-9.13	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	247	ARG	NE-CZ	8.92	1.42	1.33
2	D	307	LEU	CA-CB	8.60	1.68	1.53
1	A	148	HIS	C-O	8.22	1.34	1.23
1	B	208	ASP	CA-C	-7.61	1.42	1.52
2	C	261	ALA	CA-CB	7.45	1.65	1.53
1	B	33	LEU	CA-C	-7.45	1.43	1.52
1	B	168	ARG	CG-CD	7.34	1.74	1.52
1	B	194	ILE	CA-CB	-7.23	1.45	1.54
1	A	152	ARG	CD-NE	-7.20	1.36	1.46
1	B	307	ASP	C-O	-7.17	1.15	1.24
1	B	18	SER	C-O	7.16	1.32	1.23
1	B	204	MET	SD-CE	-7.04	1.61	1.79
1	B	182	MET	CB-CG	6.83	1.73	1.52
2	D	247	ARG	CG-CD	6.77	1.72	1.52
1	B	279	ARG	CZ-NH1	6.73	1.42	1.32
1	A	137	ARG	NE-CZ	6.70	1.40	1.33
1	A	95	GLU	C-N	-6.67	1.24	1.33
2	D	321	ASP	C-N	-6.63	1.24	1.33
1	A	365	ARG	CG-CD	6.43	1.71	1.52
1	B	103	ARG	CD-NE	-6.28	1.37	1.46
1	A	322	SER	CA-CB	6.18	1.63	1.53
1	B	305	ILE	C-O	-6.07	1.17	1.24
1	B	70	VAL	C-O	5.96	1.28	1.24
1	B	110	THR	C-O	5.95	1.31	1.23
2	D	247	ARG	CD-NE	5.92	1.54	1.46
2	D	298	THR	N-CA	-5.91	1.38	1.46
2	C	273	ARG	NE-CZ	5.89	1.39	1.33
2	D	249	MET	SD-CE	-5.88	1.64	1.79
1	B	142	THR	CA-CB	-5.80	1.46	1.54
1	B	218	ILE	C-O	5.77	1.30	1.24
2	D	285	ARG	CZ-NH1	5.77	1.40	1.32
2	D	285	ARG	NE-CZ	5.74	1.39	1.33
1	A	322	SER	CA-C	5.70	1.60	1.52
1	A	142	THR	CA-CB	-5.66	1.45	1.54
1	B	230	PHE	CA-C	-5.59	1.46	1.52
1	B	189	PRO	C-O	5.54	1.30	1.23
1	A	91	GLN	CA-C	-5.53	1.45	1.52
2	D	288	VAL	N-CA	-5.49	1.39	1.46
1	A	108	LEU	CA-C	-5.45	1.46	1.52
1	A	183	PRO	C-O	5.41	1.29	1.23
1	A	153	TYR	C-O	-5.39	1.17	1.24
1	A	35	LEU	CA-C	-5.38	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	GLU	CA-C	5.31	1.58	1.52
2	D	299	THR	CA-CB	-5.30	1.44	1.53
1	A	180	CYS	CA-C	-5.28	1.46	1.52
1	B	197	ARG	C-O	-5.28	1.18	1.24
1	A	331	LEU	C-O	-5.23	1.17	1.24
1	B	68	THR	CA-CB	5.19	1.61	1.53
1	B	168	ARG	CD-NE	5.18	1.53	1.46
1	A	58	ALA	CA-CB	5.17	1.61	1.53
1	A	73	ARG	CB-CG	5.15	1.68	1.52
2	D	261	ALA	CA-CB	5.13	1.61	1.53
1	A	204	MET	CG-SD	-5.12	1.68	1.80
1	A	99	VAL	CA-C	-5.11	1.46	1.52
1	B	179	VAL	N-CA	-5.11	1.40	1.46
1	B	225	ALA	CA-C	-5.10	1.46	1.52
1	B	295	ASN	CA-C	-5.09	1.46	1.52
1	A	199	GLY	C-O	-5.08	1.17	1.23
2	C	272	ARG	C-O	-5.08	1.18	1.24
2	D	306	ARG	C-N	-5.06	1.26	1.33
1	B	150	ASP	C-O	5.04	1.30	1.23
1	A	258	ALA	CA-CB	5.04	1.62	1.53
1	A	3	PHE	CA-C	-5.02	1.46	1.52
2	D	338	LEU	CA-C	-5.01	1.46	1.53

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	306	ARG	CA-C-N	-17.73	87.68	121.54
2	D	306	ARG	C-N-CA	-17.73	87.68	121.54
2	D	321	ASP	CA-C-N	-15.98	91.02	121.54
2	D	321	ASP	C-N-CA	-15.98	91.02	121.54
2	D	307	LEU	N-CA-CB	15.49	136.67	110.49
2	D	321	ASP	O-C-N	-13.35	107.26	123.01
1	A	95	GLU	CA-C-N	-12.14	98.34	121.54
1	A	95	GLU	C-N-CA	-12.14	98.34	121.54
1	B	279	ARG	NE-CZ-NH2	-11.93	108.47	119.20
1	A	152	ARG	NE-CZ-NH2	-11.37	108.97	119.20
1	A	250	LYS	CA-C-N	-11.30	110.76	122.74
1	A	250	LYS	C-N-CA	-11.30	110.76	122.74
1	A	96	ARG	N-CA-C	11.24	134.75	110.80
1	A	95	GLU	O-C-N	-10.69	108.38	122.59
2	D	343	MET	CG-SD-CE	-9.90	79.12	100.90
2	D	306	ARG	O-C-N	-9.86	108.85	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	322	GLU	N-CA-CB	9.59	126.70	110.49
1	B	279	ARG	NE-CZ-NH1	9.49	130.99	121.50
1	A	182	MET	CA-CB-CG	-9.44	95.23	114.10
1	B	39	ASP	CB-CA-C	-9.44	105.68	116.63
2	C	343	MET	CG-SD-CE	-9.36	80.31	100.90
1	B	18	SER	CB-CA-C	-8.42	97.09	111.41
1	B	11	LEU	N-CA-C	8.30	119.95	111.07
1	B	239	GLY	N-CA-C	-8.18	103.82	112.08
1	A	152	ARG	NE-CZ-NH1	8.16	129.66	121.50
2	D	307	LEU	CB-CG-CD2	7.69	133.76	110.70
1	B	215	ARG	NE-CZ-NH2	-7.60	112.36	119.20
1	B	339	MET	CG-SD-CE	-7.36	84.72	100.90
1	B	220	SER	CA-CB-OG	-7.25	96.60	111.10
1	B	308	VAL	CA-C-N	-7.23	113.15	122.77
1	B	308	VAL	C-N-CA	-7.23	113.15	122.77
1	B	282	ARG	NE-CZ-NH1	-7.23	114.27	121.50
2	D	247	ARG	CB-CG-CD	7.22	127.92	111.30
1	B	174	GLY	N-CA-C	-7.19	106.53	115.08
2	D	307	LEU	CB-CA-C	-7.05	96.39	110.42
2	D	349	LEU	N-CA-C	-6.90	104.33	112.89
1	A	176	ARG	NE-CZ-NH1	-6.89	114.61	121.50
1	A	125	GLU	N-CA-C	-6.83	105.50	114.31
1	B	304	GLU	CA-C-N	-6.67	113.85	123.06
1	B	304	GLU	C-N-CA	-6.67	113.85	123.06
1	A	152	ARG	CG-CD-NE	-6.62	97.44	112.00
2	D	322	GLU	CB-CG-CD	6.59	123.81	112.60
1	A	39	ASP	CB-CA-C	-6.48	107.27	116.34
1	A	322	SER	CA-CB-OG	-6.47	98.16	111.10
2	D	322	GLU	CB-CA-C	-6.38	97.72	110.42
1	A	215	ARG	CG-CD-NE	6.34	125.95	112.00
1	A	152	ARG	CD-NE-CZ	6.24	133.14	124.40
1	A	322	SER	N-CA-C	-6.21	104.62	111.82
1	B	215	ARG	NE-CZ-NH1	6.17	127.67	121.50
1	A	282	ARG	NE-CZ-NH1	-6.10	115.40	121.50
1	A	48	ASP	N-CA-C	-6.01	104.12	112.30
1	B	126	VAL	N-CA-C	-5.98	99.60	108.45
1	A	23	GLY	N-CA-C	5.92	117.11	111.67
1	A	180	CYS	CA-C-N	-5.76	112.79	122.29
1	A	180	CYS	C-N-CA	-5.76	112.79	122.29
2	C	294	ASP	N-CA-C	-5.75	105.46	112.88
1	A	50	GLU	N-CA-C	-5.71	105.43	112.90
1	B	282	ARG	CD-NE-CZ	-5.68	116.45	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	GLY	N-CA-C	-5.67	103.15	110.69
1	B	334	GLU	N-CA-C	5.66	117.26	111.14
1	B	240	ARG	N-CA-C	-5.60	99.60	108.73
1	A	292	ILE	CA-C-N	-5.54	113.89	122.59
1	A	292	ILE	C-N-CA	-5.54	113.89	122.59
2	D	343	MET	CA-C-N	-5.53	113.66	122.29
2	D	343	MET	C-N-CA	-5.53	113.66	122.29
1	A	183	PRO	CA-C-N	-5.42	115.33	122.16
1	A	183	PRO	C-N-CA	-5.42	115.33	122.16
1	B	252	PRO	CA-C-N	5.39	128.05	120.28
1	B	252	PRO	C-N-CA	5.39	128.05	120.28
1	B	281	VAL	CA-C-N	-5.37	114.88	122.94
1	B	281	VAL	C-N-CA	-5.37	114.88	122.94
1	B	142	THR	N-CA-CB	-5.37	103.76	110.90
1	B	309	THR	CB-CA-C	5.35	118.86	110.19
1	B	73	ARG	CB-CG-CD	5.35	123.60	111.30
1	B	209	GLY	O-C-N	5.34	127.58	122.99
1	B	112	PRO	CA-C-N	5.26	127.58	120.38
1	B	112	PRO	C-N-CA	5.26	127.58	120.38
1	A	236	LEU	CA-C-N	-5.24	115.62	122.37
1	A	236	LEU	C-N-CA	-5.24	115.62	122.37
1	A	362	MET	CG-SD-CE	-5.21	89.44	100.90
2	D	322	GLU	CA-CB-CG	5.20	124.51	114.10
1	B	242	PRO	CA-C-N	-5.18	115.30	122.30
1	B	242	PRO	C-N-CA	-5.18	115.30	122.30
2	D	330	ARG	N-CA-C	-5.18	107.13	113.50
1	B	282	ARG	N-CA-C	-5.17	100.97	109.40
2	C	273	ARG	CA-CB-CG	5.15	124.40	114.10
1	A	93	GLU	CB-CA-C	5.15	118.92	111.82
1	B	333	CYS	N-CA-C	-5.13	101.89	109.18
1	A	322	SER	CB-CA-C	5.12	120.50	110.67
1	A	215	ARG	CD-NE-CZ	5.11	131.55	124.40
1	B	215	ARG	CB-CG-CD	5.07	122.95	111.30
1	B	175	HIS	N-CA-C	-5.06	107.24	113.41
1	B	129	THR	CA-CB-OG1	5.05	117.18	109.60
1	B	103	ARG	CG-CD-NE	-5.03	100.93	112.00
1	B	238	ASP	N-CA-C	5.01	116.57	110.41

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	142	THR	CB

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Mol	Chain	Res	Type	Atom
1	B	129	THR	CB
1	B	142	THR	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	GLY	Peptide
1	B	18	SER	Peptide
1	B	209	GLY	Peptide

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	2844	0	2861	125	0
1	B	2844	0	2861	84	1
2	C	915	0	929	19	0
2	D	925	0	936	56	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	304	0	0	25	0
4	B	375	0	0	32	2
4	C	116	0	0	6	0
4	D	152	0	0	15	1
All	All	8485	0	7587	276	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 18.

All (276) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ARG:CG	1:B:168:ARG:CD	1.74	1.63
2:D:322:GLU:N	2:D:322:GLU:CA	1.70	1.52
2:D:307:LEU:N	2:D:307:LEU:CA	1.86	1.38
2:D:321:ASP:O	2:D:322:GLU:CA	1.72	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:MET:SD	1:A:338:MET:CE	2.14	1.35
2:D:306:ARG:O	2:D:307:LEU:CA	1.75	1.34
2:D:321:ASP:O	2:D:322:GLU:CB	1.76	1.31
1:A:143:GLN:NE2	1:A:201:ILE:HD12	1.45	1.29
2:D:321:ASP:O	2:D:322:GLU:HB2	1.29	1.29
1:B:240:ARG:HD3	4:B:2271:HOH:O	1.10	1.27
1:B:39:ASP:CG	1:B:40:GLY:H	1.36	1.25
2:D:321:ASP:C	2:D:322:GLU:CA	2.12	1.22
1:B:208:ASP:HB3	4:B:2242:HOH:O	1.38	1.21
1:A:250:LYS:HE2	4:A:2190:HOH:O	1.41	1.19
1:B:246:ARG:HD3	4:B:2286:HOH:O	1.39	1.18
1:A:150:ASP:OD1	1:A:152:ARG:HD3	1.45	1.16
2:D:306:ARG:O	2:D:307:LEU:CB	1.93	1.16
2:D:306:ARG:C	2:D:307:LEU:CA	2.20	1.14
1:A:39:ASP:CG	1:A:40:GLY:H	1.53	1.12
2:D:299:THR:HG22	2:D:300:GLN:N	1.68	1.07
2:D:300:GLN:OE1	2:D:300:GLN:HA	1.47	1.07
2:D:301:GLU:OE2	2:D:335:HIS:HD2	1.37	1.06
1:B:39:ASP:CG	1:B:40:GLY:N	2.08	1.05
1:A:191:HIS:HE1	4:A:2165:HOH:O	1.43	1.00
2:D:273:ARG:HD3	4:D:2060:HOH:O	1.62	0.99
1:A:143:GLN:NE2	1:A:201:ILE:CD1	2.26	0.98
1:B:105:ARG:CZ	4:B:2144:HOH:O	2.13	0.97
1:A:143:GLN:HE21	1:A:201:ILE:CD1	1.80	0.93
2:D:322:GLU:N	2:D:322:GLU:HA	1.83	0.93
1:B:142:THR:HG23	1:B:158:MET:HE2	1.49	0.92
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.33	0.92
1:A:143:GLN:HE21	1:A:201:ILE:HD12	1.33	0.91
1:B:257:GLU:HB2	4:B:2290:HOH:O	1.71	0.90
1:A:184:ILE:CD1	1:A:186:GLN:HB3	2.02	0.90
1:A:184:ILE:HD12	1:A:186:GLN:HB3	1.55	0.88
1:A:264:LYS:CE	1:A:329:ASN:HD21	1.87	0.88
2:D:299:THR:CG2	2:D:300:GLN:N	2.35	0.87
1:A:150:ASP:OD1	1:A:152:ARG:CD	2.23	0.87
2:D:301:GLU:OE2	2:D:335:HIS:CD2	2.25	0.86
1:A:250:LYS:HE3	1:A:250:LYS:H	1.39	0.86
1:A:39:ASP:CG	1:A:40:GLY:N	2.23	0.85
2:C:317:ARG:HD3	4:C:2082:HOH:O	1.74	0.85
4:A:2249:HOH:O	1:B:103:ARG:HD3	1.76	0.84
1:A:338:MET:CE	1:A:338:MET:HB3	2.07	0.83
1:A:1:MET:HE1	1:A:97:MET:HE2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASP:OD1	1:B:40:GLY:N	2.05	0.83
2:D:330:ARG:NE	4:D:2123:HOH:O	2.05	0.83
1:A:142:THR:HG23	1:A:158:MET:HE2	1.60	0.81
1:B:52:GLU:HG2	1:B:119:LEU:HD22	1.61	0.81
1:A:1:MET:HE1	1:A:97:MET:CE	2.10	0.81
1:B:50:GLU:HA	1:B:235:LYS:HE3	1.63	0.81
1:B:163:GLU:OE1	1:B:168:ARG:NH2	2.14	0.80
1:B:129:THR:HG23	4:B:2165:HOH:O	1.82	0.79
1:A:143:GLN:HE22	1:A:201:ILE:HD12	1.48	0.78
2:C:317:ARG:HH11	2:C:317:ARG:HG3	1.50	0.77
1:B:119:LEU:HD23	4:B:2256:HOH:O	1.84	0.77
1:B:168:ARG:CD	1:B:168:ARG:CB	2.61	0.77
2:C:273:ARG:HD2	4:C:2027:HOH:O	1.86	0.75
2:D:300:GLN:HG3	4:D:2024:HOH:O	1.87	0.75
1:A:184:ILE:HG12	1:A:188:LEU:HD11	1.67	0.74
1:A:264:LYS:HE3	1:A:329:ASN:HD21	1.53	0.73
1:B:240:ARG:NH1	4:B:2275:HOH:O	2.21	0.73
1:A:56:ARG:HD3	4:A:2019:HOH:O	1.86	0.73
2:D:306:ARG:O	2:D:307:LEU:HB3	1.86	0.72
1:B:142:THR:HG23	1:B:158:MET:CE	2.18	0.72
1:B:149:GLN:HG3	4:B:2187:HOH:O	1.90	0.72
1:B:231:ILE:HG13	4:B:2080:HOH:O	1.92	0.70
2:D:299:THR:HG22	2:D:300:GLN:CA	2.23	0.69
1:B:205:ARG:NH1	4:B:2239:HOH:O	2.26	0.69
1:A:338:MET:HB3	1:A:338:MET:HE2	1.75	0.68
1:A:150:ASP:H	1:A:156:ASN:HD21	1.42	0.68
1:B:150:ASP:H	1:B:156:ASN:HD21	1.41	0.67
2:C:300:GLN:HG2	4:C:2083:HOH:O	1.93	0.67
2:D:285:ARG:NH2	4:D:2068:HOH:O	2.26	0.67
1:B:303:GLU:OE1	4:B:2330:HOH:O	2.13	0.67
1:A:35:LEU:HD22	1:A:97:MET:HE1	1.77	0.66
1:A:264:LYS:NZ	1:A:329:ASN:HD21	1.92	0.66
1:B:210:GLY:O	4:B:2243:HOH:O	2.12	0.66
1:A:214:LEU:HD11	1:A:225:ALA:HB1	1.76	0.66
1:B:288:ASN:HB3	4:B:2316:HOH:O	1.95	0.65
2:C:291:LYS:HB2	2:C:331:LEU:HB3	1.79	0.65
1:A:250:LYS:HE3	1:A:250:LYS:N	2.10	0.65
1:A:1:MET:CE	1:A:97:MET:HE2	2.26	0.65
1:A:184:ILE:HD11	1:A:186:GLN:HB3	1.79	0.65
1:A:143:GLN:HG3	1:A:146:MET:HE2	1.80	0.64
1:A:61:GLN:HB3	1:A:62:PRO:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:300:GLN:OE1	2:D:300:GLN:CA	2.35	0.64
1:A:342:ASP:OD2	4:A:2280:HOH:O	2.15	0.63
2:D:330:ARG:CD	4:D:2123:HOH:O	2.45	0.63
1:B:191:HIS:HE1	4:B:2253:HOH:O	1.81	0.62
1:B:285:VAL:HG12	1:B:310:TYR:CE2	2.34	0.62
1:A:182:MET:HG2	1:A:183:PRO:HD2	1.81	0.62
1:A:68:THR:HG21	1:A:97:MET:HE3	1.81	0.62
1:A:121:ASP:HB3	4:A:2110:HOH:O	1.98	0.62
1:B:105:ARG:NE	4:B:2144:HOH:O	2.25	0.62
1:A:299:GLN:HE22	2:D:278:LYS:NZ	1.98	0.61
1:A:318:GLY:HA3	2:D:343:MET:HE1	1.82	0.61
1:A:139:ILE:HG22	1:A:204:MET:HE1	1.83	0.61
1:B:127:GLU:OE1	1:B:215:ARG:HD2	2.00	0.61
1:B:214:LEU:HD11	1:B:225:ALA:HB1	1.82	0.61
1:A:255:HIS:HD2	1:A:339:MET:HG2	1.67	0.60
1:A:191:HIS:CE1	4:A:2165:HOH:O	2.29	0.60
1:B:249:PRO:HD2	1:B:348:GLN:HE21	1.66	0.60
1:A:143:GLN:HE21	1:A:201:ILE:HD11	1.62	0.60
1:A:142:THR:HG23	1:A:158:MET:CE	2.31	0.60
2:D:240:HIS:N	4:D:2030:HOH:O	2.34	0.60
2:D:267:TYR:HB3	2:D:268:PRO:HD3	1.83	0.60
1:A:38:ALA:O	1:A:39:ASP:HB3	2.01	0.59
1:A:9:HIS:HD2	4:A:2005:HOH:O	1.85	0.59
2:D:318:LYS:NZ	4:D:2107:HOH:O	2.34	0.59
1:A:132:GLN:NE2	1:A:208:ASP:H	2.01	0.59
1:A:139:ILE:HG22	1:A:204:MET:CE	2.33	0.58
2:D:299:THR:HG23	2:D:335:HIS:CE1	2.39	0.57
1:A:208:ASP:O	1:A:209:GLY:C	2.47	0.57
1:A:338:MET:CE	1:A:338:MET:CB	2.81	0.57
1:B:118:ASN:OD1	1:B:118:ASN:N	2.37	0.57
1:B:105:ARG:CZ	4:B:2145:HOH:O	2.52	0.57
1:B:285:VAL:HG12	1:B:310:TYR:CD2	2.39	0.57
1:B:6:GLU:OE2	1:B:85:GLY:HA2	2.06	0.56
1:A:24:ARG:HG2	1:A:24:ARG:NH1	2.10	0.56
1:A:95:GLU:O	1:A:96:ARG:C	2.42	0.56
1:A:255:HIS:CD2	1:A:339:MET:HG2	2.40	0.56
1:A:205:ARG:HD2	4:A:2018:HOH:O	2.05	0.55
2:D:265:ARG:CZ	4:D:2051:HOH:O	2.54	0.55
1:A:215:ARG:HH11	1:A:215:ARG:HB3	1.70	0.55
1:A:226:HIS:CE1	1:A:231:ILE:HD13	2.42	0.55
2:D:278:LYS:NZ	2:D:280:ASP:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:307:LEU:N	2:D:307:LEU:C	2.59	0.55
1:A:33:LEU:HG	1:A:72:ALA:HB2	1.89	0.55
1:B:27:LEU:HB2	1:B:30:LEU:HD22	1.88	0.55
1:B:123:GLN:HG3	4:B:2158:HOH:O	2.07	0.55
2:D:301:GLU:OE1	2:D:337:THR:OG1	2.18	0.54
2:D:331:LEU:C	2:D:331:LEU:HD23	2.34	0.53
1:B:105:ARG:NH2	4:B:2144:HOH:O	2.33	0.53
1:A:91:GLN:NE2	4:A:2077:HOH:O	2.10	0.53
2:C:317:ARG:HH11	2:C:317:ARG:CG	2.21	0.53
1:A:33:LEU:HG	1:A:72:ALA:CB	2.39	0.53
1:A:150:ASP:N	1:A:156:ASN:HD21	2.06	0.53
1:A:127:GLU:HG2	1:A:217:GLN:HG2	1.89	0.52
1:A:296:ASN:HB2	1:A:297:PRO:CD	2.39	0.52
1:A:84:GLU:OE1	4:A:2068:HOH:O	2.19	0.52
1:A:168:ARG:NH1	1:A:244:TYR:OH	2.43	0.52
1:B:2:LYS:HG2	1:B:91:GLN:HB2	1.91	0.52
1:A:249:PRO:HB2	1:A:252:PRO:HG3	1.91	0.52
1:B:288:ASN:HD22	1:B:310:TYR:H	1.57	0.52
1:B:318:GLY:HA3	2:C:343:MET:HE1	1.92	0.52
1:A:48:ASP:O	1:A:49:LEU:HB2	2.08	0.51
1:B:48:ASP:OD2	1:B:51:MET:HE3	2.11	0.51
1:A:285:VAL:CG2	1:A:315:MET:HG2	2.40	0.51
2:C:301:GLU:HG3	2:C:335:HIS:HE1	1.74	0.51
1:A:201:ILE:HD13	1:A:201:ILE:N	2.26	0.51
1:A:264:LYS:CE	1:A:329:ASN:ND2	2.68	0.51
2:D:318:LYS:O	2:D:322:GLU:HB2	2.11	0.51
1:B:143:GLN:HG2	1:B:146:MET:HE2	1.93	0.50
1:A:60:VAL:CG2	4:A:2049:HOH:O	2.59	0.50
2:D:307:LEU:N	2:D:307:LEU:HA	2.11	0.50
1:B:211:ASP:HA	4:B:2244:HOH:O	2.11	0.50
1:A:287:GLU:OE2	1:A:311:SER:HA	2.12	0.50
1:A:296:ASN:HB2	1:A:297:PRO:HD2	1.93	0.50
1:B:191:HIS:CE1	4:B:2253:HOH:O	2.62	0.50
1:A:264:LYS:NZ	1:A:329:ASN:ND2	2.59	0.49
1:A:244:TYR:CD1	1:A:244:TYR:C	2.91	0.49
1:B:264:LYS:HD2	1:B:329:ASN:ND2	2.27	0.49
1:B:38:ALA:O	1:B:39:ASP:HB3	2.11	0.49
1:B:175:HIS:HD2	4:B:2212:HOH:O	1.95	0.49
2:C:253:ILE:HD13	2:C:262:ILE:HD12	1.93	0.49
1:B:51:MET:HE1	1:B:198:LYS:HB3	1.95	0.49
2:D:306:ARG:O	2:D:307:LEU:HB2	2.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:HG22	4:A:2049:HOH:O	2.12	0.49
1:A:184:ILE:HD12	1:A:186:GLN:CB	2.34	0.49
1:B:50:GLU:HA	1:B:235:LYS:CE	2.38	0.49
2:C:317:ARG:HG3	2:C:317:ARG:NH1	2.24	0.49
1:A:235:LYS:HG2	4:A:2169:HOH:O	2.13	0.48
1:B:168:ARG:HD2	1:B:244:TYR:CE2	2.49	0.48
2:D:299:THR:HG21	4:D:2084:HOH:O	2.13	0.48
2:D:330:ARG:HD3	4:D:2123:HOH:O	2.11	0.48
1:A:35:LEU:HG	1:A:44:LEU:HD12	1.95	0.48
2:D:318:LYS:HE3	4:D:2106:HOH:O	2.13	0.48
1:B:33:LEU:HG	1:B:72:ALA:HB2	1.95	0.48
1:A:365:ARG:NH1	4:A:2301:HOH:O	2.47	0.48
1:B:331:LEU:O	1:B:332:LYS:C	2.56	0.48
2:D:318:LYS:NZ	4:D:2106:HOH:O	2.37	0.48
2:D:285:ARG:NE	4:D:2068:HOH:O	2.46	0.48
1:A:126:VAL:HG13	1:A:189:PRO:HG2	1.95	0.47
1:B:137:ARG:NH2	4:B:2174:HOH:O	2.46	0.47
1:A:160:PHE:O	1:A:192:SER:HA	2.14	0.47
1:A:2:LYS:HG3	1:A:64:GLU:HB2	1.96	0.47
1:A:8:GLU:HG2	1:A:84:GLU:OE2	2.15	0.47
1:A:220:SER:HB2	4:A:2166:HOH:O	2.14	0.47
1:B:191:HIS:HD2	4:B:2102:HOH:O	1.98	0.47
1:A:150:ASP:CG	1:A:152:ARG:HD3	2.32	0.47
1:A:137:ARG:NH1	1:A:182:MET:HE1	2.30	0.47
1:B:123:GLN:CG	4:B:2158:HOH:O	2.62	0.47
1:B:143:GLN:CG	1:B:146:MET:HE2	2.45	0.47
2:D:318:LYS:CE	4:D:2107:HOH:O	2.62	0.47
1:A:1:MET:C	1:A:2:LYS:HG2	2.40	0.47
1:A:121:ASP:HA	1:A:122:TRP:CD1	2.50	0.46
1:A:252:PRO:HB2	1:A:339:MET:HB3	1.95	0.46
1:A:250:LYS:NZ	4:A:2191:HOH:O	2.48	0.46
1:A:48:ASP:C	1:A:48:ASP:OD1	2.58	0.46
1:A:249:PRO:HD2	1:A:348:GLN:HE21	1.81	0.46
1:B:366:LEU:HD23	2:C:343:MET:CE	2.45	0.46
1:B:278:PHE:CD2	2:C:344:GLU:HG2	2.51	0.46
1:A:21:LEU:O	1:A:22:GLY:C	2.59	0.46
1:A:182:MET:CG	1:A:183:PRO:HD2	2.46	0.46
1:B:12:LYS:N	1:B:13:PRO:CD	2.78	0.46
1:A:113:ALA:O	1:A:115:ASP:N	2.49	0.46
1:A:163:GLU:O	4:A:2145:HOH:O	2.21	0.45
2:D:284:ALA:C	2:D:285:ARG:HG3	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:O	1:B:69:THR:HA	2.15	0.45
1:A:244:TYR:HD2	4:A:2186:HOH:O	2.00	0.45
1:A:130:LEU:N	1:A:130:LEU:HD23	2.32	0.45
2:D:323:ARG:HA	2:D:323:ARG:HD2	1.88	0.45
1:A:68:THR:CG2	1:A:97:MET:HE3	2.46	0.45
1:A:162:THR:O	1:A:190:SER:HA	2.18	0.44
1:A:215:ARG:HH11	1:A:215:ARG:CB	2.31	0.44
1:B:48:ASP:O	1:B:49:LEU:HB2	2.17	0.44
1:B:116:PHE:HA	1:B:117:PRO:HD3	1.79	0.44
1:B:212:ASN:HB3	4:B:2248:HOH:O	2.17	0.44
2:D:277:VAL:O	2:D:277:VAL:HG22	2.17	0.44
1:A:33:LEU:O	1:A:69:THR:HA	2.18	0.44
1:A:139:ILE:CG2	1:A:204:MET:CE	2.96	0.44
1:A:61:GLN:HB2	4:A:2003:HOH:O	2.17	0.44
2:D:304:TRP:HD1	2:D:307:LEU:H	1.63	0.44
2:D:318:LYS:CE	4:D:2106:HOH:O	2.64	0.44
2:D:291:LYS:HB3	2:D:331:LEU:HB3	1.99	0.44
1:B:33:LEU:HG	1:B:72:ALA:CB	2.47	0.44
1:B:69:THR:O	1:B:110:THR:HA	2.17	0.44
1:A:112:PRO:O	1:A:115:ASP:HB2	2.18	0.44
1:B:150:ASP:N	1:B:156:ASN:HD21	2.11	0.44
2:D:286:GLN:OE1	2:D:307:LEU:HA	2.18	0.44
1:A:126:VAL:HG13	1:A:189:PRO:CG	2.47	0.43
2:C:249:MET:HE2	2:C:249:MET:HB2	1.82	0.43
1:A:217:GLN:HB2	1:A:224:ARG:HB3	2.00	0.43
1:B:235:LYS:HG3	4:B:2072:HOH:O	2.17	0.43
1:B:224:ARG:HD2	4:B:2250:HOH:O	2.18	0.43
2:C:244:GLY:H	2:C:273:ARG:NH1	2.17	0.43
1:A:182:MET:HG3	4:A:2151:HOH:O	2.18	0.43
1:A:168:ARG:HD3	1:A:179:VAL:CG2	2.49	0.43
1:B:288:ASN:ND2	1:B:310:TYR:H	2.15	0.43
2:D:292:PHE:CE2	2:D:324:ARG:HA	2.53	0.43
1:B:366:LEU:HD23	2:C:343:MET:HE3	2.01	0.43
1:A:285:VAL:HG22	1:A:315:MET:HG3	2.00	0.43
1:B:348:GLN:HA	1:B:359:TYR:O	2.19	0.42
1:A:152:ARG:HB3	1:A:154:TYR:CZ	2.55	0.42
2:C:318:LYS:HD3	4:C:2017:HOH:O	2.19	0.42
1:A:118:ASN:O	1:A:120:ASP:N	2.52	0.42
1:A:257:GLU:HG3	4:A:2278:HOH:O	2.19	0.42
2:D:249:MET:HB2	2:D:249:MET:HE2	1.88	0.42
1:A:331:LEU:O	1:A:332:LYS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:MET:CE	1:B:202:GLU:OE2	2.67	0.42
2:D:299:THR:HG22	2:D:300:GLN:C	2.44	0.42
1:A:129:THR:HA	1:A:214:LEU:O	2.19	0.42
1:B:296:ASN:HB2	1:B:297:PRO:CD	2.50	0.42
2:C:250:ALA:HB2	4:C:2031:HOH:O	2.20	0.42
1:A:172:THR:HB	1:A:177:LEU:HD12	2.01	0.41
1:B:50:GLU:HB3	4:B:2074:HOH:O	2.20	0.41
2:C:285:ARG:HD2	4:C:2018:HOH:O	2.19	0.41
1:A:285:VAL:CG2	1:A:315:MET:CG	2.99	0.41
1:A:289:GLN:NE2	4:A:2235:HOH:O	2.16	0.41
1:A:282:ARG:HH11	1:A:282:ARG:HD3	1.48	0.41
1:B:12:LYS:N	1:B:13:PRO:HD2	2.36	0.41
1:B:26:THR:C	4:B:2035:HOH:O	2.63	0.41
1:B:337:ARG:NE	4:B:2353:HOH:O	2.53	0.41
1:B:129:THR:HG22	1:B:215:ARG:HA	2.03	0.41
1:A:35:LEU:HD12	1:A:35:LEU:N	2.35	0.41
1:B:68:THR:HB	1:B:92:LEU:HD22	2.03	0.41
1:A:226:HIS:CE1	4:A:2170:HOH:O	2.73	0.41
1:B:159:LEU:O	1:B:169:THR:HA	2.21	0.41
1:B:120:ASP:O	1:B:122:TRP:HD1	2.04	0.41
2:C:317:ARG:CG	2:C:317:ARG:NH1	2.80	0.40
2:D:249:MET:SD	2:D:249:MET:N	2.94	0.40
1:A:362:MET:HG3	2:D:347:LEU:HB2	2.03	0.40
1:A:249:PRO:HB3	4:A:2287:HOH:O	2.21	0.40
1:A:299:GLN:HE22	2:D:278:LYS:HZ1	1.68	0.40
1:B:123:GLN:HB2	4:B:2067:HOH:O	2.21	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:209:GLY:CA	1:B:209:GLY:CA[2_665]	2.14	0.06
4:B:2018:HOH:O	4:D:2028:HOH:O[2_655]	2.19	0.01
4:B:2114:HOH:O	4:B:2168:HOH:O[2_665]	2.19	0.01

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	364/366 (100%)	349 (96%)	8 (2%)	7 (2%)	6	1
1	B	364/366 (100%)	355 (98%)	7 (2%)	2 (0%)	24	16
2	C	109/115 (95%)	108 (99%)	1 (1%)	0	100	100
2	D	110/115 (96%)	103 (94%)	4 (4%)	3 (3%)	4	1
All	All	947/962 (98%)	915 (97%)	20 (2%)	12 (1%)	9	3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	ALA
1	A	115	ASP
2	D	322	GLU
1	A	22	GLY
1	A	119	LEU
1	A	210	GLY
2	D	307	LEU
1	A	96	ARG
1	B	22	GLY
2	D	300	GLN
1	B	19	GLY
1	A	209	GLY

5.3.2 Protein sidechains [i](#)

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	313/313 (100%)	285 (91%)	28 (9%)	9	4
1	B	313/313 (100%)	293 (94%)	20 (6%)	16	8
2	C	97/101 (96%)	92 (95%)	5 (5%)	21	13
2	D	98/101 (97%)	95 (97%)	3 (3%)	35	29
All	All	821/828 (99%)	765 (93%)	56 (7%)	14	7

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	10	LEU
1	A	11	LEU
1	A	24	ARG
1	A	56	ARG
1	A	73	ARG
1	A	115	ASP
1	A	119	LEU
1	A	123	GLN
1	A	127	GLU
1	A	137	ARG
1	A	149	GLN
1	A	152	ARG
1	A	168	ARG
1	A	176	ARG
1	A	179	VAL
1	A	182	MET
1	A	187	SER
1	A	201	ILE
1	A	205	ARG
1	A	212	ASN
1	A	215	ARG
1	A	231	ILE
1	A	240	ARG
1	A	247	VAL
1	A	250	LYS
1	A	251	ASN
1	A	365	ARG
1	B	24	ARG
1	B	26	THR
1	B	30	LEU
1	B	44	LEU
1	B	56	ARG

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Mol	Chain	Res	Type
1	B	73	ARG
1	B	105	ARG
1	B	112	PRO
1	B	118	ASN
1	B	121	ASP
1	B	137	ARG
1	B	176	ARG
1	B	238	ASP
1	B	240	ARG
1	B	246	ARG
1	B	250	LYS
1	B	256	LEU
1	B	287	GLU
1	B	309	THR
1	B	332	LYS
2	C	247	ARG
2	C	248	THR
2	C	251	GLU
2	C	299	THR
2	C	317	ARG
2	D	299	THR
2	D	300	GLN
2	D	330	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	143	GLN
1	A	148	HIS
1	A	149	GLN
1	A	156	ASN
1	A	191	HIS
1	A	217	GLN
1	A	255	HIS
1	A	299	GLN
1	A	329	ASN
1	A	348	GLN
1	B	91	GLN
1	B	132	GLN
1	B	156	ASN
1	B	175	HIS

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Mol	Chain	Res	Type
1	B	191	HIS
1	B	221	ASN
1	B	222	ASN
1	B	288	ASN
1	B	329	ASN
1	B	348	GLN
2	C	254	HIS
2	C	300	GLN
2	C	335	HIS
2	D	254	HIS
2	D	335	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](#)

2 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	$\# Z > 2$
3	SO4	C	1352	-	4,4,4	0.28	0	6,6,6	0.18	0
3	SO4	D	1352	-	4,4,4	0.29	0	6,6,6	0.38	0

There are no bond length outliers.

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

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	366/366 (100%)	0.20	16 (4%) 39 41	5, 20, 40, 68	0
1	B	366/366 (100%)	0.04	14 (3%) 44 47	5, 14, 36, 70	0
2	C	111/115 (96%)	0.03	1 (0%) 81 83	8, 21, 34, 40	0
2	D	112/115 (97%)	-0.12	1 (0%) 81 83	6, 14, 26, 36	0
All	All	955/962 (99%)	0.08	32 (3%) 48 51	5, 17, 37, 70	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	210	GLY	4.7
1	B	20	PRO	4.4
1	A	23	GLY	4.3
1	A	121	ASP	4.0
1	B	23	GLY	3.8
1	A	119	LEU	3.7
1	A	22	GLY	3.7
1	A	244	TYR	3.5
1	B	21	LEU	3.4
1	A	251	ASN	3.4
1	B	209	GLY	3.3
1	A	124	SER	3.1
1	B	22	GLY	3.0
1	A	118	ASN	3.0
1	A	211	ASP	2.9
1	A	208	ASP	2.8
1	A	24	ARG	2.7
1	B	120	ASP	2.5
1	B	19	GLY	2.5
2	C	250	ALA	2.4
1	B	149	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	300	GLN	2.4
1	B	255	HIS	2.4
1	B	25	PRO	2.3
1	A	123	GLN	2.2
1	A	120	ASP	2.2
1	B	29	ILE	2.2
1	A	245	ARG	2.2
1	A	122	TRP	2.1
1	A	20	PRO	2.1
1	B	119	LEU	2.1
1	B	121	ASP	2.1

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
3	SO4	C	1352	5/5	0.66	0.16	91,93,93,94	0
3	SO4	D	1352	5/5	0.79	0.14	79,80,82,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.