



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:40 PM GMT

PDB ID : 1UNN  
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](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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

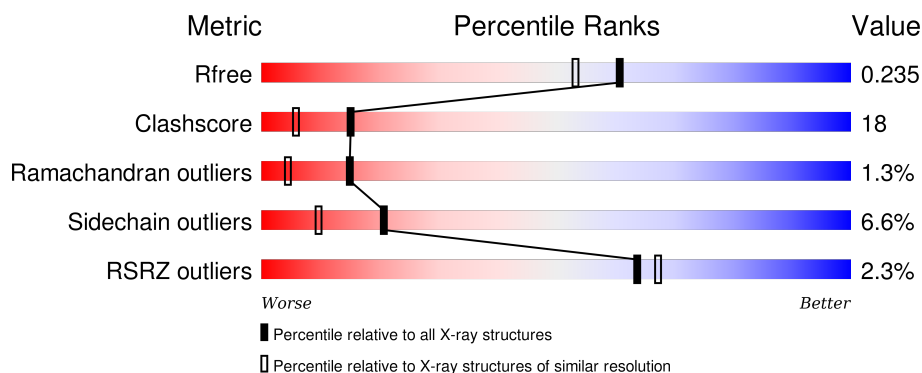
# 1 Overall quality at a glance

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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 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.

Mol	Chain	Length	Quality of chain
1	A	366	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>24%</div> <div>9%</div> <div>.</div> </div> </div>
1	B	366	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>5%</div> <div>.</div> </div> </div>
2	C	115	<div> <div></div> <div> <div></div> <div>77%</div> <div>17%</div> <div>.</div> <div>.</div> </div> </div>
2	D	115	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>23%</div> <div>.</div> <div>.</div> <div>.</div> </div> </div>

## 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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

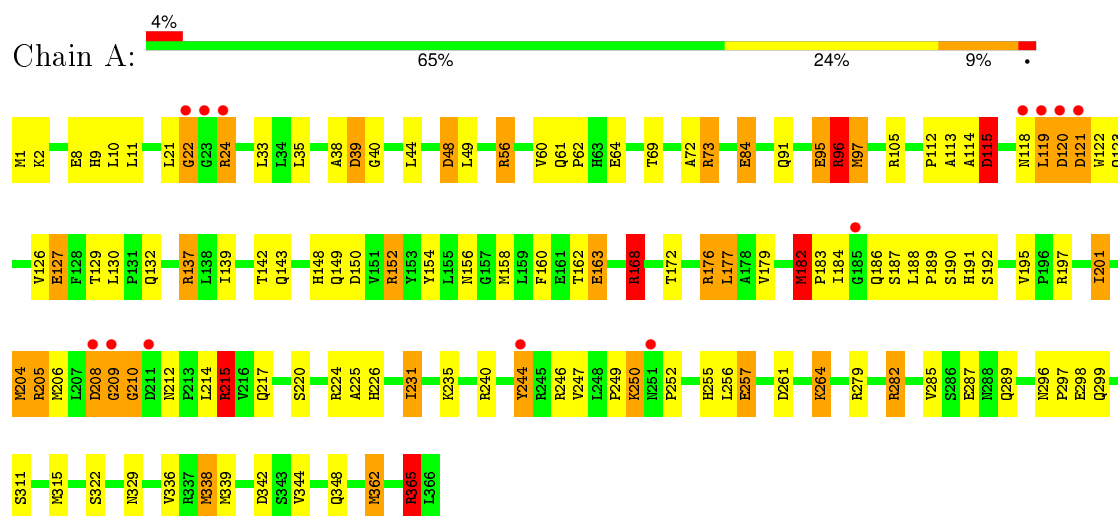
- Molecule 4 is water.

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		

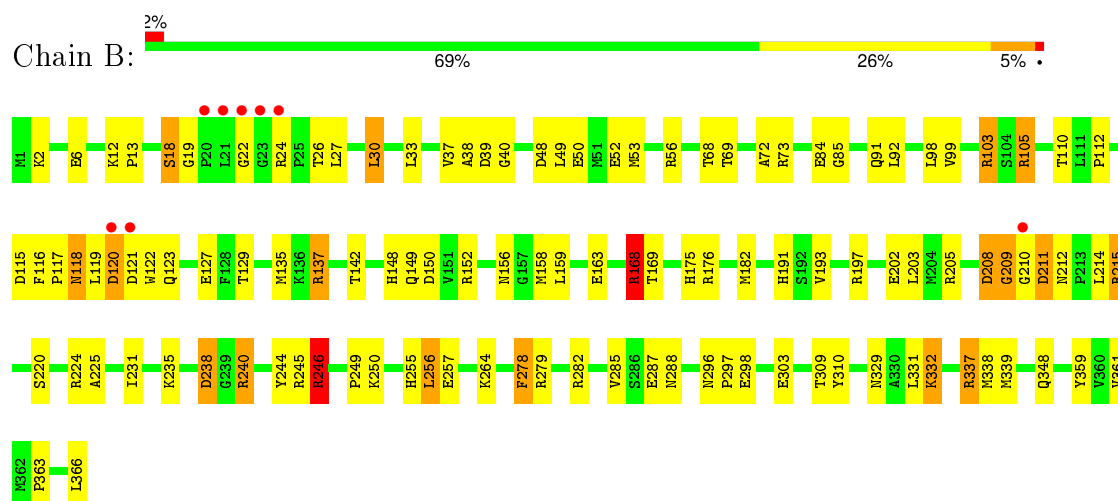
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

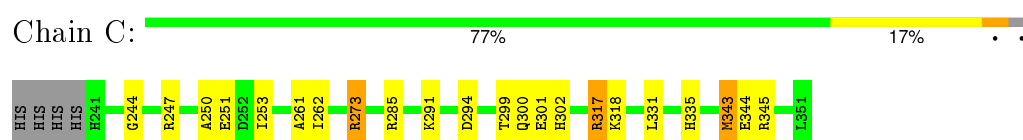
#### • Molecule 1: DNA POLYMERASE III BETA SUBUNIT



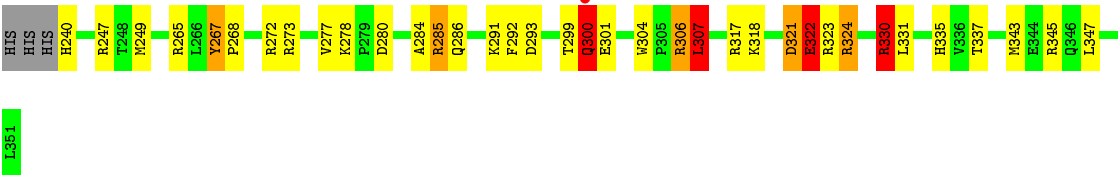
#### • Molecule 1: DNA POLYMERASE III BETA SUBUNIT



#### • Molecule 2: DNA POLYMERASE IV



● Molecule 2: DNA POLYMERASE IV



L351

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.45Å 70.12Å 110.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.10 – 1.90 61.11 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (62.10-1.90) 96.6 (61.11-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.04 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.179 , 0.240 0.178 , 0.235	Depositor DCC
$R_{free}$ test set	4388 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 87611 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8485	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.37	21/2893 (0.7%)	1.47	32/3915 (0.8%)
1	B	1.45	17/2893 (0.6%)	1.53	27/3915 (0.7%)
2	C	1.18	2/933 (0.2%)	1.28	5/1258 (0.4%)
2	D	1.64	10/944 (1.1%)	1.83	25/1273 (2.0%)
All	All	1.41	50/7663 (0.7%)	1.52	89/10361 (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 (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	307	LEU	N-CA	19.82	1.85	1.46
2	D	322	GLU	N-CA	12.18	1.70	1.46
1	A	96	ARG	N-CA	10.47	1.67	1.46
1	A	182	MET	CG-SD	-10.05	1.55	1.81
1	B	182	MET	CG-SD	-9.11	1.57	1.81
1	B	168	ARG	CG-CD	9.00	1.74	1.51
2	D	247	ARG	CG-CD	8.33	1.72	1.51
1	B	148	HIS	C-O	8.04	1.38	1.23
1	A	365	ARG	CG-CD	7.92	1.71	1.51
2	D	247	ARG	NE-CZ	7.55	1.42	1.33
1	A	322	SER	CA-CB	7.07	1.63	1.52
1	B	279	ARG	CZ-NH1	7.01	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	MET	CB-CG	6.75	1.73	1.51
1	B	37	VAL	CB-CG2	6.48	1.66	1.52
1	A	338	MET	SD-CE	6.47	2.14	1.77
1	B	99	VAL	CB-CG1	6.21	1.66	1.52
2	D	307	LEU	CA-CB	6.19	1.68	1.53
1	A	344	VAL	CB-CG2	6.17	1.65	1.52
1	A	97	MET	SD-CE	-6.13	1.43	1.77
1	A	148	HIS	C-O	6.13	1.34	1.23
1	B	193	VAL	CB-CG1	6.10	1.65	1.52
1	A	336	VAL	CB-CG1	-6.06	1.40	1.52
1	A	152	ARG	CD-NE	-6.05	1.36	1.46
2	C	261	ALA	CA-CB	6.04	1.65	1.52
1	B	298	GLU	CD-OE2	6.02	1.32	1.25
1	A	298	GLU	CD-OE1	5.99	1.32	1.25
2	D	285	ARG	CZ-NH1	5.98	1.40	1.33
1	B	37	VAL	CA-CB	-5.95	1.42	1.54
2	D	272	ARG	CG-CD	5.79	1.66	1.51
1	A	73	ARG	CB-CG	5.69	1.68	1.52
1	A	137	ARG	NE-CZ	5.67	1.40	1.33
1	A	163	GLU	CG-CD	5.62	1.60	1.51
1	A	197	ARG	CG-CD	5.62	1.66	1.51
1	A	163	GLU	CD-OE2	5.38	1.31	1.25
2	D	247	ARG	CB-CG	5.35	1.67	1.52
1	A	257	GLU	CD-OE1	5.30	1.31	1.25
1	B	103	ARG	CD-NE	-5.29	1.37	1.46
1	B	197	ARG	CG-CD	5.21	1.65	1.51
2	D	267	TYR	CG-CD1	5.20	1.46	1.39
1	A	261	ASP	CB-CG	5.19	1.62	1.51
1	B	278	PHE	CD1-CE1	5.19	1.49	1.39
1	B	361	VAL	CB-CG2	5.19	1.63	1.52
1	B	84	GLU	CD-OE1	5.18	1.31	1.25
2	D	322	GLU	CG-CD	5.16	1.59	1.51
1	B	135	MET	SD-CE	-5.15	1.49	1.77
1	A	195	VAL	CB-CG2	5.13	1.63	1.52
1	A	264	LYS	CD-CE	5.11	1.64	1.51
2	C	273	ARG	CG-CD	5.11	1.64	1.51
1	A	204	MET	CG-SD	-5.08	1.68	1.81
1	B	363	PRO	CG-CD	5.05	1.67	1.50

All (89) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	ARG	NE-CZ-NH2	-23.66	108.47	120.30
1	A	152	ARG	NE-CZ-NH2	-22.66	108.97	120.30
1	B	279	ARG	NE-CZ-NH1	21.37	130.99	120.30
1	A	152	ARG	NE-CZ-NH1	18.71	129.66	120.30
1	B	215	ARG	NE-CZ-NH2	-15.88	112.36	120.30
1	B	215	ARG	NE-CZ-NH1	14.73	127.67	120.30
2	D	306	ARG	C-N-CA	-13.61	87.68	121.70
2	D	307	LEU	CB-CG-CD2	13.39	133.76	111.00
2	D	343	MET	CG-SD-CE	-13.18	79.12	100.20
2	D	307	LEU	N-CA-CB	13.13	136.67	110.40
2	C	343	MET	CG-SD-CE	-12.43	80.31	100.20
2	D	247	ARG	NE-CZ-NH1	12.36	126.48	120.30
2	D	321	ASP	C-N-CA	-12.27	91.02	121.70
1	B	282	ARG	NE-CZ-NH1	-12.06	114.27	120.30
2	D	285	ARG	NE-CZ-NH1	11.84	126.22	120.30
1	A	176	ARG	NE-CZ-NH1	-11.39	114.61	120.30
1	A	182	MET	CA-CB-CG	-10.63	95.23	113.30
2	D	285	ARG	NE-CZ-NH2	-10.45	115.07	120.30
2	C	273	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	A	137	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	A	282	ARG	NE-CZ-NH1	-9.80	115.40	120.30
1	B	339	MET	CG-SD-CE	-9.68	84.72	100.20
2	D	321	ASP	O-C-N	-9.65	107.26	122.70
1	A	95	GLU	C-N-CA	-9.34	98.34	121.70
1	A	95	GLU	O-C-N	-8.95	108.38	122.70
2	D	322	GLU	N-CA-CB	8.94	126.70	110.60
1	A	96	ARG	N-CA-C	8.80	134.75	111.00
2	D	306	ARG	O-C-N	-8.66	108.85	122.70
2	D	317	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	B	103	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	B	197	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	B	337	ARG	NE-CZ-NH2	-8.20	116.20	120.30
2	D	330	ARG	NE-CZ-NH2	-7.72	116.44	120.30
2	C	273	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	256	LEU	CA-CB-CG	7.53	132.61	115.30
1	A	215	ARG	NE-CZ-NH1	7.47	124.03	120.30
2	D	307	LEU	CB-CA-C	-7.27	96.39	110.20
1	A	279	ARG	NE-CZ-NH2	-7.12	116.74	120.30
2	D	330	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	B	246	ARG	NE-CZ-NH1	6.98	123.79	120.30
2	D	317	ARG	NE-CZ-NH1	6.98	123.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	B	18	SER	CB-CA-C	-6.85	97.09	110.10
1	A	152	ARG	CG-CD-NE	-6.84	97.44	111.80
1	A	152	ARG	CD-NE-CZ	6.82	133.14	123.60
1	A	215	ARG	CG-CD-NE	6.74	125.95	111.80
1	A	362	MET	CG-SD-CE	-6.72	89.44	100.20
1	B	245	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	B	238	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	A	177	LEU	CB-CG-CD2	-6.45	100.03	111.00
2	D	322	GLU	CB-CA-C	-6.34	97.72	110.40
1	A	197	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	D	322	GLU	OE1-CD-OE2	-6.29	115.75	123.30
2	D	306	ARG	NE-CZ-NH2	-6.29	117.16	120.30
2	D	247	ARG	CB-CG-CD	6.28	127.92	111.60
1	A	39	ASP	CB-CG-OD2	6.25	123.92	118.30
2	C	294	ASP	CB-CG-OD1	6.25	123.92	118.30
1	B	211	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	282	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	A	247	VAL	CG1-CB-CG2	6.03	120.54	110.90
1	A	208	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	256	LEU	CB-CG-CD1	-5.83	101.10	111.00
1	A	48	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	168	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	115	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	215	ARG	CD-NE-CZ	5.68	131.55	123.60
1	B	256	LEU	CB-CG-CD1	5.63	120.57	111.00
2	C	345	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	206	MET	CG-SD-CE	-5.56	91.30	100.20
2	D	324	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	96	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	322	SER	CB-CA-C	5.47	120.50	110.10
2	D	293	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	220	SER	CA-CB-OG	-5.41	96.60	111.20
2	D	272	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	B	256	LEU	CB-CG-CD2	-5.36	101.88	111.00
1	B	203	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	A	105	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	282	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	A	121	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	103	ARG	CG-CD-NE	-5.17	100.93	111.80
1	B	208	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	84	GLU	OE1-CD-OE2	-5.16	117.11	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	282	ARG	CD-NE-CZ	-5.11	116.45	123.60
1	B	98	LEU	CB-CG-CD1	-5.09	102.34	111.00
1	B	337	ARG	CG-CD-NE	-5.09	101.12	111.80
2	D	322	GLU	CA-CB-CG	5.05	124.51	113.40
2	D	345	ARG	CG-CD-NE	-5.02	101.25	111.80

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	142	THR	CB
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

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	121	0
1	B	2844	0	2861	80	1
2	C	915	0	929	17	0
2	D	925	0	936	53	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	304	0	0	24	0
4	B	375	0	0	31	2
4	C	116	0	0	6	0
4	D	152	0	0	15	1
All	All	8485	0	7587	265	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 (265) 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
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:208:ASP:HB3	4:B:2242:HOH:O	1.38	1.21
1:B:39:ASP:CG	1:B:40:GLY:H	1.36	1.20
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
2:D:321:ASP:C	2:D:322:GLU:CA	2.12	1.17
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	1.09
2:D:299:THR:HG22	2:D:300:GLN:N	1.68	1.07
1:A:39:ASP:CG	1:A:40:GLY:H	1.53	1.07
2:D:300:GLN:HA	2:D:300:GLN:OE1	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	1.01
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: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:A:39:ASP:CG	1:A:40:GLY:N	2.23	0.90
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:B:39:ASP:OD1	1:B:40:GLY:N	2.05	0.89
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HB3	1:A:338:MET:CE	2.07	0.83
2:D:330:ARG:NE	4:D:2123:HOH:O	2.05	0.83
1:B:52:GLU:HG2	1:B:119:LEU:HD22	1.61	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:HG3	2:C:317:ARG:HH11	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:B:240:ARG:NH1	4:B:2275:HOH:O	2.21	0.73
1:A:264:LYS:HE3	1:A:329:ASN:HD21	1.53	0.73
1:B:142:THR:HG23	1:B:158:MET:CE	2.18	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: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
1:A:1:MET:HE3	1:A:97:MET:HE1	1.75	0.69
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:150:ASP:H	1:A:156:ASN:HD21	1.42	0.68
2:C:300:GLN:HG2	4:C:2083:HOH:O	1.93	0.67
1:B:150:ASP:H	1:B:156:ASN:HD21	1.41	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: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:B:366:LEU:HD23	2:C:343:MET:HE1	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ILE:HD11	1:A:186:GLN:HB3	1.79	0.65
2:D:300:GLN:CA	2:D:300:GLN:OE1	2.35	0.64
1:A:61:GLN:HB3	1:A:62:PRO:HD2	1.80	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:285:VAL:HG12	1:B:310:TYR:CE2	2.34	0.62
1:B:191:HIS:HE1	4:B:2253:HOH:O	1.81	0.62
1:A:182:MET:HG2	1:A:183:PRO:HD2	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:B:127:GLU:OE1	1:B:215:ARG:HD2	2.00	0.61
1:B:142:THR:HG23	1:B:158:MET:HE2	1.83	0.61
1:B:214:LEU:HD11	1:B:225:ALA:HB1	1.82	0.61
1:A:142:THR:HG23	1:A:158:MET:CE	2.31	0.60
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
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
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:338:MET:CB	1:A:338:MET:CE	2.81	0.57
1:B:118:ASN:N	1:B:118:ASN:OD1	2.37	0.57
2:D:318:LYS:NZ	4:D:2106:HOH:O	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:NH1	1:A:24:ARG:HG2	2.10	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
2:D:278:LYS:NZ	2:D:280:ASP:OD1	2.39	0.55
1:A:226:HIS:CE1	1:A:231:ILE:HD13	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLN:HG3	4:B:2158:HOH:O	2.07	0.55
1:A:1:MET:CE	1:A:97:MET:HE1	2.37	0.54
1:B:142:THR:HG23	1:B:158:MET:HE1	1.90	0.53
1:B:105:ARG:NH2	4:B:2144:HOH:O	2.33	0.53
2:C:317:ARG:CG	2:C:317:ARG:HH11	2.21	0.53
1:A:91:GLN:NE2	4:A:2077:HOH:O	2.10	0.53
1:A:150:ASP:N	1:A:156:ASN:HD21	2.06	0.53
1:A:33:LEU:HG	1:A:72:ALA:CB	2.39	0.53
1:A:208:ASP:O	1:A:209:GLY:C	2.47	0.53
2:D:318:LYS:NZ	4:D:2107:HOH:O	2.34	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:B:2:LYS:HG2	1:B:91:GLN:HB2	1.91	0.52
1:A:168:ARG:NH1	1:A:244:TYR:OH	2.43	0.52
1:B:288:ASN:HD22	1:B:310:TYR:H	1.57	0.52
1:A:249:PRO:HB2	1:A:252:PRO:HG3	1.91	0.52
1:A:48:ASP:O	1:A:49:LEU:HB2	2.08	0.51
1:A:338:MET:HB3	1:A:338:MET:HE2	1.88	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:N	1:A:201:ILE:HD13	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
2:D:307:LEU:N	2:D:307:LEU:HA	2.11	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:C	2.59	0.50
1:A:142:THR:HG23	1:A:158:MET:HE2	1.92	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:139:ILE:HG22	1:A:204:MET:HE1	1.94	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
2:D:306:ARG:O	2:D:307:LEU:HB2	2.00	0.49
1:A:184:ILE:HD12	1:A:186:GLN:CB	2.34	0.49
2:C:317:ARG:HG3	2:C:317:ARG:NH1	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:GLU:HA	1:B:235:LYS:CE	2.38	0.49
1:A:60:VAL:HG22	4:A:2049:HOH:O	2.12	0.49
2:D:331:LEU:HD23	2:D:331:LEU:C	2.34	0.49
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
1:A:235:LYS:HG2	4:A:2169:HOH:O	2.13	0.48
2:D:330:ARG:HD3	4:D:2123:HOH:O	2.11	0.48
2:D:318:LYS:HE3	4:D:2106:HOH:O	2.13	0.48
1:A:35:LEU:HG	1:A:44:LEU:HD12	1.95	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
2:D:285:ARG:NE	4:D:2068:HOH:O	2.46	0.48
1:B:137:ARG:NH2	4:B:2174:HOH:O	2.46	0.47
1:A:126:VAL:HG13	1:A:189:PRO:HG2	1.95	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:139:ILE:HG22	1:A:204:MET:HE2	1.94	0.47
1:B:191:HIS:HD2	4:B:2102:HOH:O	1.98	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
2:D:318:LYS:CE	4:D:2107:HOH:O	2.62	0.47
1:B:123:GLN:CG	4:B:2158:HOH:O	2.62	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:249:PRO:HD2	1:A:348:GLN:HE21	1.81	0.46
1:B:278:PHE:CD2	2:C:344:GLU:HG2	2.51	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
1:A:1:MET:CE	1:A:97:MET:CE	2.95	0.45
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:HD23	1:A:130:LEU:N	2.32	0.45
2:D:323:ARG:HD2	2:D:323:ARG:HA	1.88	0.45
1:A:244:TYR:C	1:A:244:TYR:CD1	2.91	0.44
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
2:D:277:VAL:HG22	2:D:277:VAL:O	2.17	0.44
1:B:116:PHE:HA	1:B:117:PRO:HD3	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ASN:HB3	4:B:2248:HOH:O	2.17	0.44
1:A:139:ILE:CG2	1:A:204:MET:CE	2.96	0.44
1:A:33:LEU:O	1:A:69:THR:HA	2.18	0.44
2:D:318:LYS:CE	4:D:2106:HOH:O	2.64	0.44
2:D:304:TRP:HD1	2:D:307:LEU:H	1.63	0.44
1:A:61:GLN:HB2	4:A:2003:HOH:O	2.17	0.44
2:D:291:LYS:HB3	2:D:331:LEU:HB3	1.99	0.44
1:B:69:THR:O	1:B:110:THR:HA	2.17	0.44
1:B:33:LEU:HG	1:B:72:ALA:CB	2.47	0.44
1:A:95:GLU:O	1:A:96:ARG:C	2.42	0.44
2:D:286:GLN:OE1	2:D:307:LEU:HA	2.18	0.44
1:B:150:ASP:N	1:B:156:ASN:HD21	2.11	0.44
1:A:112:PRO:O	1:A:115:ASP:HB2	2.18	0.44
1:A:126:VAL:HG13	1:A:189:PRO:CG	2.47	0.43
1:B:235:LYS:HG3	4:B:2072:HOH:O	2.17	0.43
1:A:217:GLN:HB2	1:A:224:ARG:HB3	2.00	0.43
2:C:244:GLY:H	2:C:273:ARG:NH1	2.17	0.43
1:B:224:ARG:HD2	4:B:2250:HOH:O	2.18	0.43
1:A:182:MET:HG3	4:A:2151:HOH:O	2.18	0.43
1:B:288:ASN:ND2	1:B:310:TYR:H	2.15	0.43
1:A:168:ARG:HD3	1:A:179:VAL:CG2	2.49	0.43
2:D:292:PHE:CE2	2:D:324:ARG:HA	2.53	0.43
1:B:331:LEU:O	1:B:332:LYS:C	2.56	0.43
1:A:285:VAL:HG22	1:A:315:MET:HG3	2.00	0.43
1:A:338:MET:HB3	1:A:338:MET:HE3	1.97	0.42
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:150:ASP:CG	1:A:152:ARG:HD3	2.32	0.42
1:B:366:LEU:HD23	2:C:343:MET:CE	2.45	0.42
1:A:257:GLU:HG3	4:A:2278:HOH:O	2.19	0.42
1:A:118:ASN:O	1:A:120:ASP:N	2.52	0.42
1:B:53:MET:CE	1:B:202:GLU:OE2	2.67	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
1:A:1:MET:C	1:A:2:LYS:HG2	2.40	0.42
2:C:250:ALA:HB2	4:C:2031:HOH:O	2.20	0.42
1:B:338:MET:HE3	1:B:338:MET:HB3	1.80	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:172:THR:HB	1:A:177:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE1	1:A:97:MET:CE	2.49	0.41
1:A:48:ASP:OD1	1:A:48:ASP:C	2.58	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:B:12:LYS:N	1:B:13:PRO:HD2	2.36	0.41
1:A:282:ARG:HH11	1:A:282:ARG:HD3	1.48	0.41
1:A:21:LEU:O	1:A:22:GLY:C	2.59	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
2:D:284:ALA:C	2:D:285:ARG:HG3	2.41	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:NH1	2:C:317:ARG:CG	2.80	0.40
2:D:249:MET:SD	2:D:249:MET:N	2.94	0.40
1:A:139:ILE:CG2	1:A:204:MET:HE2	2.51	0.40
1:A:362:MET:HG3	2:D:347:LEU:HB2	2.03	0.40
2:D:301:GLU:OE1	2:D:337:THR:OG1	2.18	0.40
1:A:299:GLN:HE22	2:D:278:LYS:HZ1	1.68	0.40
1:A:249:PRO:HB3	4:A:2287:HOH:O	2.21	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

### 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	364/366 (100%)	349 (96%)	8 (2%)	7 (2%)	10	2
1	B	364/366 (100%)	355 (98%)	7 (2%)	2 (0%)	34	21
2	C	109/115 (95%)	108 (99%)	1 (1%)	0	100	100
2	D	110/115 (96%)	103 (94%)	4 (4%)	3 (3%)	6	1
All	All	947/962 (98%)	915 (97%)	20 (2%)	12 (1%)	15	4

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 ⓘ

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%)	288 (92%)	25 (8%)	15	6
1	B	313/313 (100%)	291 (93%)	22 (7%)	19	8
2	C	97/101 (96%)	92 (95%)	5 (5%)	29	17
2	D	98/101 (97%)	96 (98%)	2 (2%)	63	57
All	All	821/828 (99%)	767 (93%)	54 (7%)	21	10

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	168	ARG
1	A	176	ARG
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	244	TYR
1	A	246	ARG
1	A	250	LYS
1	A	365	ARG
1	B	24	ARG
1	B	26	THR
1	B	30	LEU
1	B	56	ARG
1	B	73	ARG
1	B	105	ARG
1	B	112	PRO
1	B	118	ASN
1	B	120	ASP
1	B	121	ASP
1	B	137	ARG
1	B	168	ARG
1	B	176	ARG
1	B	238	ASP
1	B	240	ARG
1	B	246	ARG
1	B	250	LYS

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Mol	Chain	Res	Type
1	B	255	HIS
1	B	256	LEU
1	B	287	GLU
1	B	309	THR
1	B	332	LYS
2	C	247	ARG
2	C	251	GLU
2	C	299	THR
2	C	302	HIS
2	C	317	ARG
2	D	300	GLN
2	D	330	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) 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	9	HIS
1	B	132	GLN
1	B	156	ASN
1	B	191	HIS
1	B	217	GLN
1	B	288	ASN
1	B	329	ASN
1	B	348	GLN
2	C	335	HIS
2	D	335	HIS
2	D	346	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 ⓘ

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	0.07	0	6,6,6	0.29	0
3	SO4	D	1352	-	4,4,4	0.18	0	6,6,6	0.33	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
3	SO4	C	1352	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1352	-	-	0/0/0/0	0/0/0/0

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	366/366 (100%)	0.18	13 (3%) 46 50	5, 20, 40, 69	0
1	B	366/366 (100%)	-0.03	8 (2%) 65 68	5, 15, 36, 70	0
2	C	111/115 (96%)	-0.07	0 100 100	8, 21, 34, 40	0
2	D	112/115 (97%)	-0.25	1 (0%) 85 87	7, 14, 26, 36	0
All	All	955/962 (99%)	0.02	22 (2%) 64 67	5, 17, 37, 70	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	GLY	11.0
1	A	22	GLY	5.4
1	A	23	GLY	4.7
1	A	119	LEU	4.2
1	A	211	ASP	4.2
1	B	120	ASP	4.1
1	B	22	GLY	4.0
1	A	118	ASN	3.8
1	A	121	ASP	3.8
1	B	20	PRO	3.5
1	A	208	ASP	3.3
1	A	24	ARG	3.3
2	D	300	GLN	3.0
1	B	24	ARG	2.9
1	A	120	ASP	2.9
1	A	251	ASN	2.9
1	A	244	TYR	2.6
1	A	209	GLY	2.5
1	B	21	LEU	2.4
1	A	185	GLY	2.4
1	B	210	GLY	2.2
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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	C	1352	5/5	0.85	0.18	-	91,93,93,94	0
3	SO4	D	1352	5/5	0.90	0.18	-	79,80,82,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.