



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:34 PM GMT

PDB ID : 4DPG
Title : Crystal Structure of Human LysRS: P38/AIMP2 Complex I
Authors : Fang, P.; Wang, J.; Bennett, S.P.; Guo, M.
Deposited on : 2012-02-13
Resolution : 2.84 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

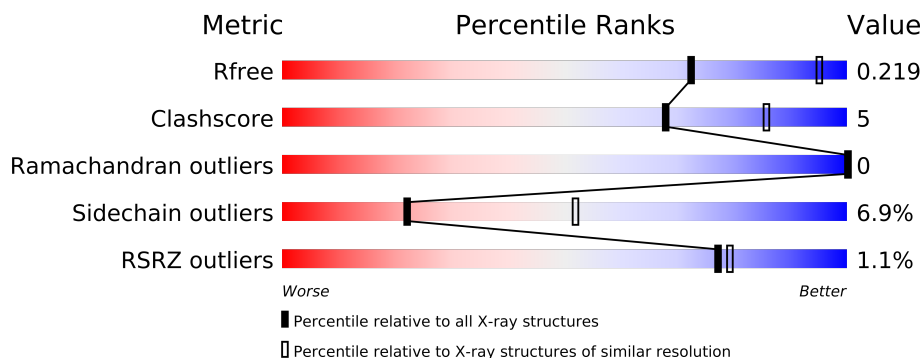
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.84 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}	66092	2270 (2.88-2.80)
Clashscore	79885	2848 (2.88-2.80)
Ramachandran outliers	78287	2786 (2.88-2.80)
Sidechain outliers	78261	2789 (2.88-2.80)
RSRZ outliers	66119	2274 (2.88-2.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	513	
1	B	513	
1	C	513	
1	D	513	
1	E	513	
1	F	513	
1	G	513	
1	H	513	
2	I	54	
2	J	54	
2	K	54	
2	L	54	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	APC	A	602	-	X
4	APC	B	602	-	X
4	APC	C	602	-	X
4	APC	D	602	-	X
4	APC	E	602	-	X
4	APC	F	602	-	X
4	APC	G	602	-	X
4	APC	H	603	-	X
5	MG	C	603	-	X
5	MG	F	604	-	X
5	MG	J	101	-	X
5	MG	L	101	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33740 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Lysine–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3932	2519	668	718	27			
1	B	506	Total	C	N	O	S	0	0	0
			4055	2596	687	744	28			
1	C	501	Total	C	N	O	S	0	0	0
			3989	2553	677	731	28			
1	D	505	Total	C	N	O	S	0	0	0
			4031	2588	685	730	28			
1	E	500	Total	C	N	O	S	0	0	0
			3969	2540	671	730	28			
1	F	505	Total	C	N	O	S	0	0	0
			4023	2580	685	730	28			
1	G	501	Total	C	N	O	S	0	0	0
			3921	2507	667	719	28			
1	H	505	Total	C	N	O	S	0	0	0
			4045	2590	685	742	28			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	MET	-	EXPRESSION TAG	UNP Q15046
B	69	MET	-	EXPRESSION TAG	UNP Q15046
C	69	MET	-	EXPRESSION TAG	UNP Q15046
D	69	MET	-	EXPRESSION TAG	UNP Q15046
E	69	MET	-	EXPRESSION TAG	UNP Q15046
F	69	MET	-	EXPRESSION TAG	UNP Q15046
G	69	MET	-	EXPRESSION TAG	UNP Q15046
H	69	MET	-	EXPRESSION TAG	UNP Q15046

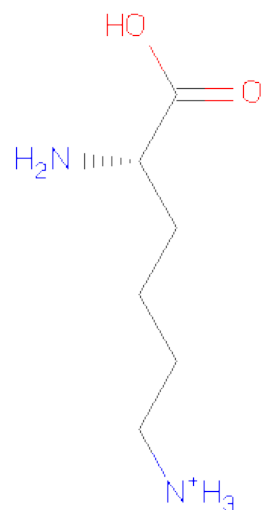
- Molecule 2 is a protein called Aminoacyl tRNA synthase complex-interacting multifunctional protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	31	Total	C	N	O	S	0	0	0
			224	144	40	37	3			
2	J	31	Total	C	N	O	S	0	0	0
			226	146	40	37	3			
2	K	31	Total	C	N	O	S	0	0	0
			224	144	40	37	3			
2	L	31	Total	C	N	O	S	0	0	0
			230	148	40	39	3			

There are 24 discrepancies between the modelled and reference sequences:

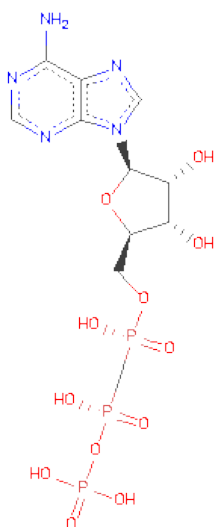
Chain	Residue	Modelled	Actual	Comment	Reference
I	49	HIS	-	EXPRESSION TAG	UNP Q13155
I	50	HIS	-	EXPRESSION TAG	UNP Q13155
I	51	HIS	-	EXPRESSION TAG	UNP Q13155
I	52	HIS	-	EXPRESSION TAG	UNP Q13155
I	53	HIS	-	EXPRESSION TAG	UNP Q13155
I	54	HIS	-	EXPRESSION TAG	UNP Q13155
J	49	HIS	-	EXPRESSION TAG	UNP Q13155
J	50	HIS	-	EXPRESSION TAG	UNP Q13155
J	51	HIS	-	EXPRESSION TAG	UNP Q13155
J	52	HIS	-	EXPRESSION TAG	UNP Q13155
J	53	HIS	-	EXPRESSION TAG	UNP Q13155
J	54	HIS	-	EXPRESSION TAG	UNP Q13155
K	49	HIS	-	EXPRESSION TAG	UNP Q13155
K	50	HIS	-	EXPRESSION TAG	UNP Q13155
K	51	HIS	-	EXPRESSION TAG	UNP Q13155
K	52	HIS	-	EXPRESSION TAG	UNP Q13155
K	53	HIS	-	EXPRESSION TAG	UNP Q13155
K	54	HIS	-	EXPRESSION TAG	UNP Q13155
L	49	HIS	-	EXPRESSION TAG	UNP Q13155
L	50	HIS	-	EXPRESSION TAG	UNP Q13155
L	51	HIS	-	EXPRESSION TAG	UNP Q13155
L	52	HIS	-	EXPRESSION TAG	UNP Q13155
L	53	HIS	-	EXPRESSION TAG	UNP Q13155
L	54	HIS	-	EXPRESSION TAG	UNP Q13155

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	2	2		
3	B	1	Total	C	N	O	0	0
			10	6	2	2		
3	C	1	Total	C	N	O	0	0
			10	6	2	2		
3	D	1	Total	C	N	O	0	0
			10	6	2	2		
3	E	1	Total	C	N	O	0	0
			10	6	2	2		
3	F	1	Total	C	N	O	0	0
			10	6	2	2		
3	G	1	Total	C	N	O	0	0
			10	6	2	2		
3	H	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONICACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	11	5	9	2		
4	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	C	1	Total	C	N	O	P	0	0
			27	11	5	9	2		
4	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	E	1	Total	C	N	O	P	0	0
			27	11	5	9	2		
4	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	G	1	Total	C	N	O	P	0	0
			27	11	5	9	2		
4	H	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

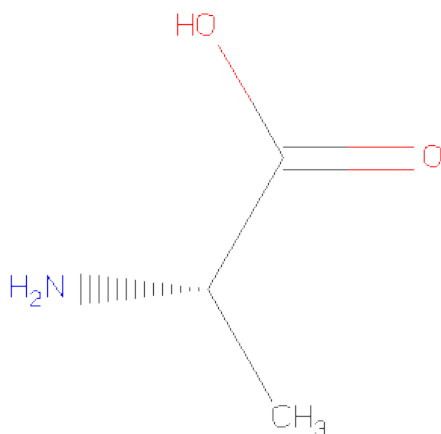
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	Mg	0	0
			2	2		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	L	1	Total	Mg	0	0
			1	1		
5	F	2	Total	Mg	0	0
			2	2		

- Molecule 6 is ALANINE (three-letter code: ALA) (formula: C₃H₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	47	Total	O	0	0
			47	47		
7	B	85	Total	O	0	0
			85	85		

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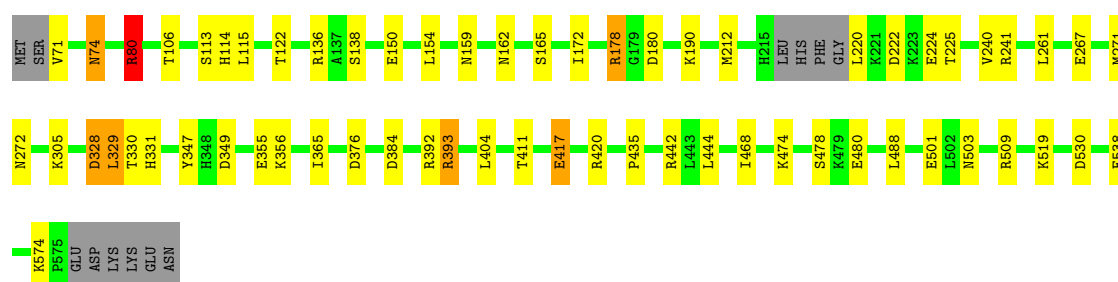
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	55	Total 55	O 55	0	0
7	D	71	Total 71	O 71	0	0
7	E	66	Total 66	O 66	0	0
7	F	81	Total 81	O 81	0	0
7	G	43	Total 43	O 43	0	0
7	H	62	Total 62	O 62	0	0
7	I	6	Total 6	O 6	0	0
7	J	3	Total 3	O 3	0	0
7	K	10	Total 10	O 10	0	0
7	L	13	Total 13	O 13	0	0

3 Residue-property plots

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

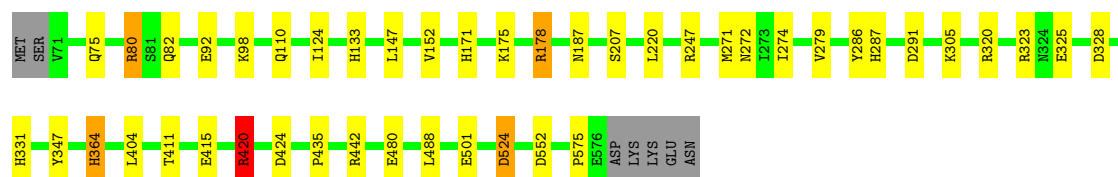
• Molecule 1: Lysine-tRNA ligase

Chain A:



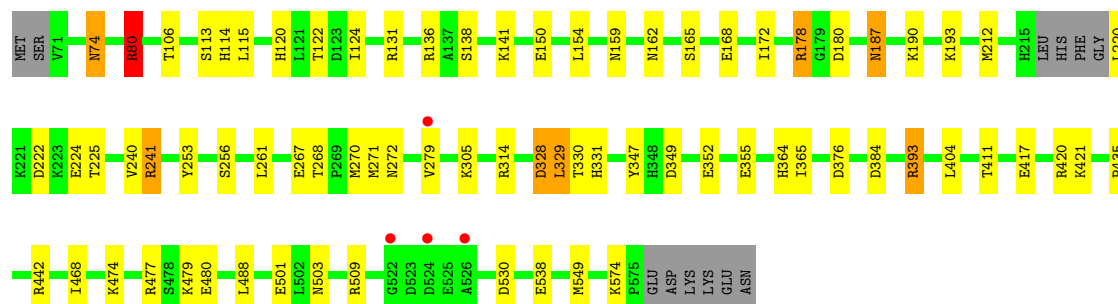
• Molecule 1: Lysine-tRNA ligase

Chain B:



• Molecule 1: Lysine-tRNA ligase

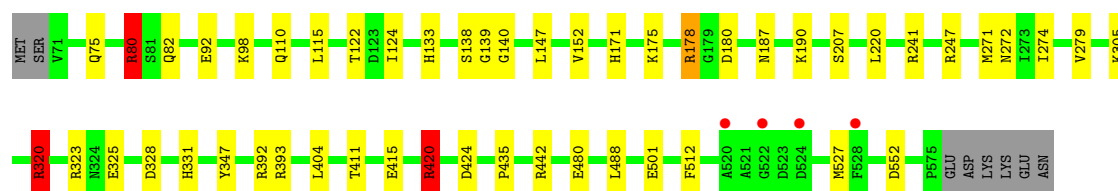
Chain C:



• Molecule 1: Lysine-tRNA ligase

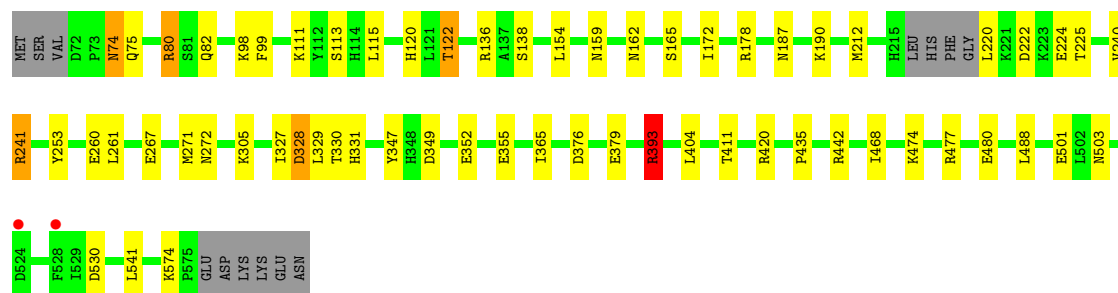
Chain D:





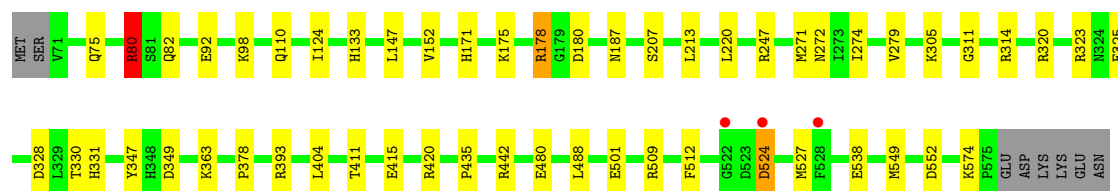
• Molecule 1: Lysine-tRNA ligase

Chain E:



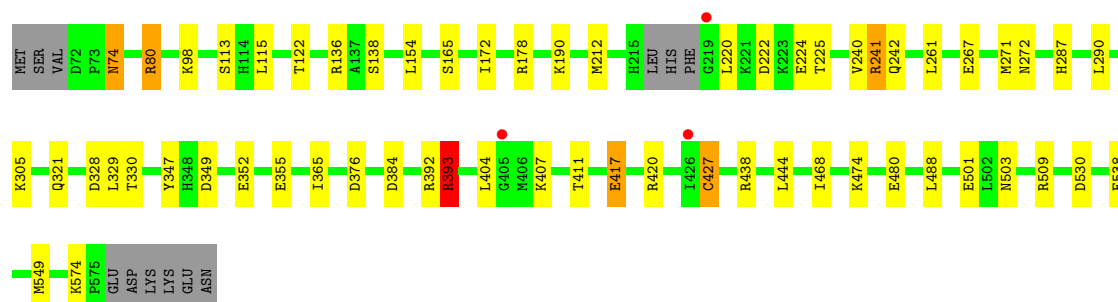
• Molecule 1: Lysine-tRNA ligase

Chain F:



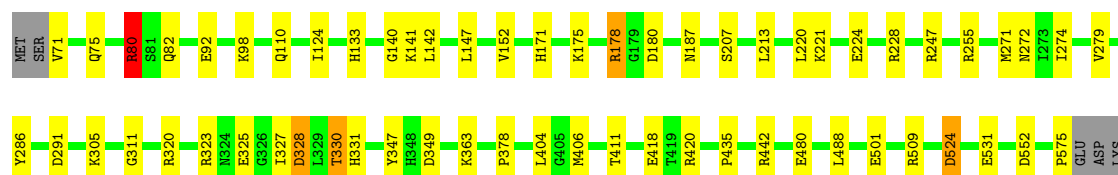
• Molecule 1: Lysine-tRNA ligase

Chain G:



• Molecule 1: Lysine-tRNA ligase

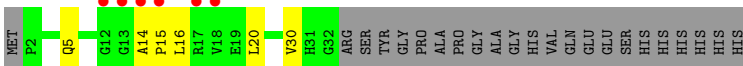
Chain H:



LYS
GLU
ASN

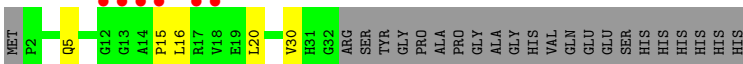
- Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2

Chain I: 



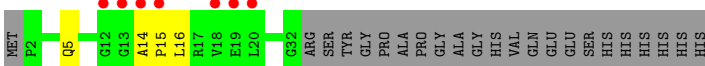
- Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2

Chain J: 



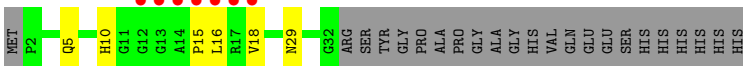
- Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2

Chain K: 



- Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.20Å 122.01Å 149.20Å 89.16° 85.58° 89.71°	Depositor
Resolution (Å)	46.84 – 2.84 47.84 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.84-2.84) 95.0 (47.84-2.84)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.185 , 0.223 0.181 , 0.219	Depositor DCC
R_{free} test set	6476 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 15.3	EDS
Estimated twinning fraction	0.339 for -h,k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 128809 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33740	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.51	0/4025	0.82	12/5457 (0.2%)
1	B	0.50	0/4152	0.75	10/5619 (0.2%)
1	C	0.48	0/4082	0.72	12/5526 (0.2%)
1	D	0.52	0/4128	0.91	14/5586 (0.3%)
1	E	0.48	0/4062	0.81	14/5503 (0.3%)
1	F	0.50	0/4120	0.73	12/5577 (0.2%)
1	G	0.49	0/4012	0.72	10/5440 (0.2%)
1	H	0.51	0/4142	0.73	10/5607 (0.2%)
2	I	0.49	0/233	0.78	0/319
2	J	0.60	0/235	0.75	0/322
2	K	0.58	0/233	0.78	0/319
2	L	0.57	0/239	0.67	0/327
All	All	0.50	0/33663	0.77	94/45602 (0.2%)

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	0	1
1	B	0	1
1	C	0	1
1	E	0	1
1	G	0	1
All	All	0	5

There are no bond length outliers.

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	320	ARG	NE-CZ-NH2	21.80	131.20	120.30
1	A	241	ARG	NE-CZ-NH2	20.63	130.61	120.30
1	D	393	ARG	NE-CZ-NH2	19.46	130.03	120.30
1	D	320	ARG	NE-CZ-NH1	-19.00	110.80	120.30
1	E	477	ARG	NE-CZ-NH1	18.84	129.72	120.30
1	A	241	ARG	NE-CZ-NH1	-18.77	110.92	120.30
1	E	477	ARG	NE-CZ-NH2	-17.75	111.42	120.30
1	D	393	ARG	NE-CZ-NH1	-17.20	111.70	120.30
1	D	178	ARG	NE-CZ-NH2	16.11	128.35	120.30
1	B	178	ARG	NE-CZ-NH2	15.24	127.92	120.30
1	D	420	ARG	NE-CZ-NH1	14.71	127.65	120.30
1	E	178	ARG	NE-CZ-NH2	14.69	127.64	120.30
1	H	420	ARG	NE-CZ-NH2	14.36	127.48	120.30
1	G	178	ARG	NE-CZ-NH2	14.33	127.46	120.30
1	G	393	ARG	NE-CZ-NH2	14.23	127.41	120.30
1	B	420	ARG	NE-CZ-NH1	14.10	127.35	120.30
1	F	420	ARG	NE-CZ-NH2	13.61	127.11	120.30
1	A	178	ARG	NE-CZ-NH1	13.55	127.07	120.30
1	C	178	ARG	NE-CZ-NH1	13.48	127.04	120.30
1	E	393	ARG	NE-CZ-NH2	13.16	126.88	120.30
1	D	420	ARG	NE-CZ-NH2	-13.05	113.77	120.30
1	C	80	ARG	NE-CZ-NH2	12.65	126.63	120.30
1	F	420	ARG	NE-CZ-NH1	-12.52	114.04	120.30
1	A	393	ARG	NE-CZ-NH1	12.31	126.45	120.30
1	C	393	ARG	NE-CZ-NH1	12.20	126.40	120.30
1	A	80	ARG	NE-CZ-NH2	12.15	126.37	120.30
1	H	420	ARG	NE-CZ-NH1	-11.96	114.32	120.30
1	B	420	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	B	178	ARG	NE-CZ-NH1	-11.75	114.43	120.30
1	F	178	ARG	NE-CZ-NH1	11.73	126.17	120.30
1	H	178	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	E	178	ARG	NE-CZ-NH1	-11.56	114.52	120.30
1	D	178	ARG	NE-CZ-NH1	-11.41	114.59	120.30
1	G	178	ARG	NE-CZ-NH1	-11.14	114.73	120.30
1	G	393	ARG	NE-CZ-NH1	-10.97	114.81	120.30
1	A	80	ARG	NE-CZ-NH1	-10.79	114.90	120.30
1	H	178	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	F	178	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	F	80	ARG	NE-CZ-NH2	10.58	125.59	120.30
1	A	178	ARG	NE-CZ-NH2	-10.49	115.06	120.30
1	H	80	ARG	NE-CZ-NH2	10.44	125.52	120.30
1	C	178	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	E	393	ARG	NE-CZ-NH1	-10.24	115.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	320	ARG	CD-NE-CZ	10.20	137.88	123.60
1	G	80	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	C	393	ARG	NE-CZ-NH2	-9.91	115.35	120.30
1	A	393	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	C	80	ARG	NE-CZ-NH1	-9.67	115.46	120.30
1	E	80	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	A	241	ARG	CD-NE-CZ	9.22	136.50	123.60
1	B	80	ARG	NE-CZ-NH1	9.05	124.82	120.30
1	D	393	ARG	CD-NE-CZ	8.40	135.36	123.60
1	E	477	ARG	CD-NE-CZ	8.32	135.24	123.60
1	G	80	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	F	80	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	G	241	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	H	320	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	H	80	ARG	NE-CZ-NH1	-7.63	116.48	120.30
1	D	80	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	B	320	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	C	241	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	H	420	ARG	CD-NE-CZ	7.14	133.59	123.60
1	E	80	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	E	241	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	H	320	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	F	420	ARG	CD-NE-CZ	6.77	133.07	123.60
1	F	178	ARG	CD-NE-CZ	6.65	132.91	123.60
1	H	178	ARG	CD-NE-CZ	6.63	132.88	123.60
1	D	178	ARG	CD-NE-CZ	6.46	132.65	123.60
1	G	178	ARG	CD-NE-CZ	6.44	132.61	123.60
1	D	420	ARG	CD-NE-CZ	6.43	132.60	123.60
1	B	178	ARG	CD-NE-CZ	6.42	132.59	123.60
1	B	420	ARG	CD-NE-CZ	6.41	132.57	123.60
1	E	178	ARG	CD-NE-CZ	6.37	132.51	123.60
1	F	320	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	G	241	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	A	178	ARG	CD-NE-CZ	5.98	131.97	123.60
1	B	320	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	E	241	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	C	178	ARG	CD-NE-CZ	5.87	131.82	123.60
1	E	393	ARG	CD-NE-CZ	5.87	131.82	123.60
1	B	80	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	C	241	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	G	393	ARG	CD-NE-CZ	5.62	131.47	123.60
1	A	393	ARG	CD-NE-CZ	5.62	131.46	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	393	ARG	CD-NE-CZ	5.43	131.20	123.60
1	F	320	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	E	477	ARG	CB-CG-CD	-5.38	97.62	111.60
1	C	80	ARG	CD-NE-CZ	5.35	131.09	123.60
1	A	80	ARG	CD-NE-CZ	5.28	131.00	123.60
1	F	393	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	D	80	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	C	477	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	F	80	ARG	CD-NE-CZ	5.03	130.64	123.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	574	LYS	Peptide
1	B	575	PRO	Peptide
1	C	574	LYS	Peptide
1	E	574	LYS	Peptide
1	G	574	LYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3932	0	0	20	0
1	B	4055	0	0	14	0
1	C	3989	0	0	32	0
1	D	4031	0	0	18	0
1	E	3969	0	0	26	0
1	F	4023	0	0	18	0
1	G	3921	0	0	19	0
1	H	4045	0	0	25	0
2	I	224	0	0	2	0
2	J	226	0	0	1	0
2	K	224	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	230	0	0	3	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
3	E	10	0	0	0	0
3	F	10	0	0	1	0
3	G	10	0	0	0	0
3	H	10	0	0	0	0
4	A	27	0	0	1	0
4	B	31	0	0	0	0
4	C	27	0	0	1	0
4	D	31	0	0	0	0
4	E	27	0	0	1	0
4	F	31	0	0	0	0
4	G	27	0	0	0	0
4	H	31	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
6	H	5	0	0	1	0
7	A	47	0	0	0	0
7	B	85	0	0	1	0
7	C	55	0	0	5	0
7	D	71	0	0	2	0
7	E	66	0	0	4	0
7	F	81	0	0	1	0
7	G	43	0	0	1	0
7	H	62	0	0	1	0
7	I	6	0	0	0	0
7	J	3	0	0	0	0
7	K	10	0	0	0	0
7	L	13	0	0	0	0
All	All	33740	0	0	164	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 5.

All (164) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:270:MET:CE	7:C:739:HOH:O	2.23	0.86
1:G:427:CYS:SG	1:G:438:ARG:NH1	2.51	0.84
2:J:15:PRO:O	2:J:16:LEU:CB	2.35	0.73
2:I:15:PRO:O	2:I:16:LEU:CB	2.37	0.71
1:B:435:PRO:O	1:B:442:ARG:NH2	2.24	0.70
1:E:328:ASP:OD1	1:E:328:ASP:C	2.30	0.69
1:D:435:PRO:O	1:D:442:ARG:NH2	2.27	0.68
1:B:524:ASP:OD2	1:B:524:ASP:N	2.26	0.68
1:G:113:SER:O	1:G:190:LYS:NZ	2.27	0.66
1:D:241:ARG:NH2	7:D:727:HOH:O	2.29	0.66
1:F:524:ASP:OD2	1:F:524:ASP:N	2.29	0.66
1:E:328:ASP:OD1	1:E:330:THR:N	2.29	0.66
1:G:328:ASP:OD1	1:G:329:LEU:N	2.30	0.65
2:K:15:PRO:O	2:K:16:LEU:CB	2.42	0.65
1:A:328:ASP:OD1	1:A:330:THR:N	2.30	0.65
1:H:575:PRO:C	6:H:601:ALA:N	2.50	0.65
1:F:435:PRO:O	1:F:442:ARG:NH2	2.30	0.65
1:E:328:ASP:OD1	1:E:329:LEU:N	2.30	0.64
1:C:328:ASP:OD1	1:C:329:LEU:N	2.29	0.64
1:A:328:ASP:OD2	1:A:331:HIS:ND1	2.30	0.64
1:C:328:ASP:OD1	1:C:330:THR:N	2.30	0.64
1:A:114:HIS:NE2	1:H:378:PRO:O	2.31	0.64
1:G:74:ASN:N	1:G:74:ASN:OD1	2.30	0.64
1:A:328:ASP:OD1	1:A:329:LEU:N	2.30	0.64
1:E:113:SER:O	1:E:190:LYS:NZ	2.31	0.64
1:H:328:ASP:OD1	1:H:331:HIS:ND1	2.30	0.64
1:C:74:ASN:N	1:C:74:ASN:OD1	2.31	0.63
1:H:524:ASP:N	1:H:524:ASP:OD2	2.28	0.63
1:H:435:PRO:O	1:H:442:ARG:NH2	2.32	0.63
1:A:74:ASN:N	1:A:74:ASN:OD1	2.31	0.62
1:A:113:SER:O	1:A:190:LYS:NZ	2.33	0.62
1:E:420:ARG:NE	7:E:717:HOH:O	2.33	0.62
1:H:328:ASP:OD1	1:H:331:HIS:CG	2.53	0.62
1:C:80:ARG:NH1	1:C:180:ASP:OD2	2.33	0.61
1:E:74:ASN:OD1	1:E:74:ASN:N	2.33	0.61
1:C:113:SER:O	1:C:190:LYS:NZ	2.34	0.60
1:H:286:TYR:OH	1:H:291:ASP:OD1	2.20	0.59
1:F:80:ARG:NH1	1:F:180:ASP:OD1	2.36	0.59
1:A:80:ARG:NH1	1:A:180:ASP:OD2	2.34	0.59
1:H:323:ARG:NH1	1:H:325:GLU:OE2	2.36	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:323:ARG:NH1	1:F:325:GLU:OE2	2.37	0.58
1:B:286:TYR:OH	1:B:291:ASP:OD1	2.21	0.58
1:F:305:LYS:NZ	1:F:501:GLU:OE1	2.37	0.58
1:C:268:THR:O	1:D:320:ARG:NH1	2.36	0.58
1:H:305:LYS:NZ	1:H:501:GLU:OE1	2.37	0.57
1:B:305:LYS:NZ	1:B:501:GLU:OE1	2.38	0.57
1:B:323:ARG:NH1	1:B:325:GLU:OE2	2.37	0.56
1:G:328:ASP:OD1	1:G:330:THR:N	2.39	0.56
1:D:323:ARG:NH1	1:D:325:GLU:OE2	2.38	0.56
1:E:99:PHE:N	7:E:727:HOH:O	2.39	0.55
1:C:328:ASP:OD2	1:C:331:HIS:ND1	2.40	0.55
1:C:120:HIS:NE2	1:C:187:ASN:OD1	2.40	0.55
1:G:267:GLU:OE2	1:H:247:ARG:NH2	2.40	0.54
1:D:305:LYS:NZ	1:D:501:GLU:OE1	2.40	0.54
1:H:80:ARG:NH1	1:H:180:ASP:OD1	2.40	0.54
1:B:364:HIS:ND1	1:B:364:HIS:O	2.41	0.54
1:B:364:HIS:ND1	1:B:364:HIS:C	2.62	0.53
1:H:124:ILE:O	1:H:187:ASN:ND2	2.42	0.53
1:C:305:LYS:NZ	1:C:501:GLU:OE1	2.42	0.53
1:C:479:LYS:NZ	7:C:703:HOH:O	2.41	0.52
1:E:541:LEU:N	7:E:716:HOH:O	2.42	0.52
1:D:139:GLY:CA	1:D:140:GLY:C	2.75	0.52
1:A:222:ASP:OD1	1:A:225:THR:OG1	2.27	0.52
1:G:417:GLU:OE2	1:G:420:ARG:NE	2.42	0.52
1:A:417:GLU:OE2	1:A:420:ARG:NE	2.43	0.52
1:C:417:GLU:OE2	1:C:420:ARG:NE	2.43	0.52
1:E:222:ASP:OD1	1:E:225:THR:OG1	2.27	0.51
1:E:435:PRO:O	1:E:442:ARG:NH2	2.43	0.51
1:D:92:GLU:OE1	1:D:171:HIS:NE2	2.42	0.51
1:G:222:ASP:OD1	1:G:225:THR:OG1	2.28	0.51
1:B:92:GLU:OE1	1:B:171:HIS:NE2	2.43	0.51
7:B:776:HOH:O	2:I:14:ALA:CB	2.59	0.51
1:G:242:GLN:NE2	7:G:713:HOH:O	2.43	0.51
1:E:253:TYR:CD1	2:L:15:PRO:CB	2.94	0.50
1:G:474:LYS:NZ	1:G:503:ASN:OD1	2.44	0.50
1:A:474:LYS:NZ	1:A:503:ASN:OD1	2.44	0.50
1:C:114:HIS:NE2	1:F:378:PRO:O	2.44	0.50
1:E:267:GLU:OE2	1:F:247:ARG:NH2	2.45	0.50
1:H:92:GLU:OE1	1:H:171:HIS:NE2	2.45	0.50
1:C:124:ILE:O	1:C:187:ASN:CB	2.59	0.50
1:E:330:THR:OG1	1:E:330:THR:O	2.30	0.49
1:C:330:THR:O	1:C:330:THR:OG1	2.30	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:92:GLU:OE1	1:F:171:HIS:NE2	2.45	0.49
1:E:120:HIS:CD2	1:E:122:THR:CG2	2.95	0.49
1:C:474:LYS:NZ	1:C:503:ASN:OD1	2.46	0.49
1:C:222:ASP:OD1	1:C:225:THR:OG1	2.30	0.49
1:C:253:TYR:CD1	2:K:15:PRO:CB	2.96	0.49
1:A:435:PRO:O	1:A:442:ARG:NH2	2.46	0.48
1:B:124:ILE:O	1:B:187:ASN:ND2	2.47	0.48
1:H:140:GLY:O	1:H:141:LYS:CB	2.60	0.48
1:C:435:PRO:O	1:C:442:ARG:NH2	2.46	0.48
1:D:124:ILE:O	1:D:187:ASN:ND2	2.47	0.47
1:E:474:LYS:NZ	1:E:503:ASN:OD1	2.47	0.47
1:A:305:LYS:NZ	1:A:501:GLU:OE1	2.47	0.47
1:G:305:LYS:NZ	1:G:501:GLU:OE1	2.47	0.47
1:G:355:GLU:OE2	1:G:393:ARG:NH2	2.47	0.47
1:G:241:ARG:NH2	1:H:311:GLY:O	2.48	0.47
1:G:411:THR:OG1	1:G:480:GLU:O	2.32	0.47
1:C:115:LEU:O	1:C:190:LYS:NZ	2.48	0.47
1:E:355:GLU:OE2	1:E:393:ARG:NH2	2.49	0.46
1:G:349:ASP:OD2	1:H:98:LYS:NZ	2.48	0.46
1:A:411:THR:OG1	1:A:480:GLU:O	2.34	0.46
1:E:328:ASP:OD2	1:E:331:HIS:ND1	2.49	0.46
1:D:420:ARG:NH2	1:D:424:ASP:OD1	2.49	0.46
1:E:260:GLU:OE2	2:L:29:ASN:ND2	2.49	0.46
1:E:349:ASP:OD2	1:F:98:LYS:NZ	2.48	0.46
1:B:328:ASP:OD1	1:B:331:HIS:ND1	2.49	0.46
1:D:328:ASP:OD1	1:D:331:HIS:ND1	2.48	0.46
1:A:115:LEU:O	1:A:190:LYS:NZ	2.49	0.46
1:F:328:ASP:OD1	1:F:331:HIS:ND1	2.48	0.46
1:B:411:THR:OG1	1:B:480:GLU:O	2.34	0.45
1:F:124:ILE:O	1:F:187:ASN:ND2	2.49	0.45
1:F:314:ARG:NE	7:F:758:HOH:O	2.50	0.45
1:E:411:THR:OG1	1:E:480:GLU:O	2.35	0.44
1:D:392:ARG:NH2	7:D:771:HOH:O	2.49	0.44
1:D:115:LEU:O	1:D:190:LYS:NZ	2.50	0.44
1:G:115:LEU:O	1:G:190:LYS:NZ	2.50	0.44
1:C:349:ASP:OD2	1:D:98:LYS:NZ	2.50	0.44
1:H:330:THR:O	1:H:331:HIS:CD2	2.71	0.44
1:A:355:GLU:OE2	1:A:393:ARG:NH2	2.51	0.44
1:H:255:ARG:NH2	7:H:716:HOH:O	2.49	0.44
1:E:241:ARG:NH2	1:F:311:GLY:O	2.51	0.43
1:F:411:THR:OG1	1:F:480:GLU:O	2.35	0.43
1:A:267:GLU:OE2	1:B:247:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:115:LEU:O	1:E:190:LYS:NZ	2.51	0.43
1:G:98:LYS:NZ	1:H:349:ASP:OD2	2.51	0.43
1:C:411:THR:OG1	1:C:480:GLU:O	2.36	0.43
1:C:355:GLU:OE2	1:C:393:ARG:NH2	2.52	0.43
1:E:305:LYS:NZ	1:E:501:GLU:OE1	2.52	0.43
1:A:159:ASN:ND2	1:A:162:ASN:OD1	2.51	0.43
1:C:241:ARG:NH1	7:C:715:HOH:O	2.51	0.43
1:E:503:ASN:ND2	7:E:761:HOH:O	2.52	0.42
1:H:178:ARG:NH1	1:H:213:LEU:O	2.52	0.42
1:H:224:GLU:OE1	1:H:228:ARG:NE	2.53	0.42
1:C:256:SER:CB	2:K:15:PRO:O	2.67	0.42
1:C:256:SER:OG	2:K:14:ALA:CB	2.67	0.42
1:E:159:ASN:ND2	1:E:162:ASN:OD1	2.52	0.42
1:C:131:ARG:NE	7:C:754:HOH:O	2.52	0.42
1:C:267:GLU:OE2	1:D:247:ARG:NH2	2.52	0.42
1:B:420:ARG:NH2	1:B:424:ASP:OD1	2.53	0.42
4:A:602:APC:O3B	4:A:602:APC:O2A	2.38	0.42
1:C:314:ARG:NE	7:C:714:HOH:O	2.53	0.42
1:G:509:ARG:NH2	1:G:538:GLU:OE2	2.52	0.42
1:D:122:THR:O	1:H:406:MET:SD	2.77	0.42
1:D:501:GLU:OE2	3:D:601:LYS:NZ	2.54	0.41
1:A:349:ASP:OD2	1:B:98:LYS:NZ	2.52	0.41
1:D:411:THR:OG1	1:D:480:GLU:O	2.38	0.41
1:H:411:THR:OG1	1:H:480:GLU:O	2.38	0.41
1:H:418:GLU:OE1	1:H:418:GLU:N	2.53	0.41
1:F:509:ARG:NH2	1:F:538:GLU:OE2	2.54	0.41
1:F:501:GLU:OE2	3:F:601:LYS:NZ	2.53	0.41
4:E:602:APC:O2A	4:E:602:APC:O3B	2.39	0.41
1:C:106:THR:OG1	1:C:150:GLU:OE2	2.37	0.41
1:H:509:ARG:NE	1:H:531:GLU:OE2	2.54	0.41
2:L:15:PRO:O	2:L:16:LEU:CB	2.69	0.41
4:C:602:APC:O3B	4:C:602:APC:O2A	2.38	0.41
1:E:98:LYS:NZ	1:F:349:ASP:OD2	2.53	0.41
1:A:509:ARG:NH2	1:A:538:GLU:OE2	2.54	0.41
1:A:106:THR:OG1	1:A:150:GLU:OE2	2.39	0.40
1:D:80:ARG:NH1	1:D:180:ASP:OD1	2.55	0.40
1:F:178:ARG:NH1	1:F:213:LEU:O	2.55	0.40
1:C:509:ARG:NH2	1:C:538:GLU:OE2	2.55	0.40
1:C:159:ASN:ND2	1:C:162:ASN:OD1	2.54	0.40
1:G:287:HIS:CD2	1:G:290:LEU:CG	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/513 (97%)	477 (96%)	20 (4%)	0	100	100
1	B	504/513 (98%)	495 (98%)	9 (2%)	0	100	100
1	C	497/513 (97%)	479 (96%)	18 (4%)	0	100	100
1	D	503/513 (98%)	493 (98%)	10 (2%)	0	100	100
1	E	496/513 (97%)	478 (96%)	18 (4%)	0	100	100
1	F	503/513 (98%)	495 (98%)	8 (2%)	0	100	100
1	G	497/513 (97%)	477 (96%)	20 (4%)	0	100	100
1	H	503/513 (98%)	493 (98%)	10 (2%)	0	100	100
2	I	29/54 (54%)	25 (86%)	4 (14%)	0	100	100
2	J	29/54 (54%)	24 (83%)	5 (17%)	0	100	100
2	K	29/54 (54%)	23 (79%)	6 (21%)	0	100	100
2	L	29/54 (54%)	26 (90%)	3 (10%)	0	100	100
All	All	4116/4320 (95%)	3985 (97%)	131 (3%)	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	409/455 (90%)	376 (92%)	33 (8%)	17	42
1	B	435/455 (96%)	411 (94%)	24 (6%)	30	64
1	C	425/455 (93%)	390 (92%)	35 (8%)	17	42
1	D	430/455 (94%)	405 (94%)	25 (6%)	28	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	422/455 (93%)	391 (93%)	31 (7%)	20	48
1	F	430/455 (94%)	404 (94%)	26 (6%)	27	60
1	G	410/455 (90%)	378 (92%)	32 (8%)	18	44
1	H	436/455 (96%)	410 (94%)	26 (6%)	27	60
2	I	21/44 (48%)	18 (86%)	3 (14%)	5	13
2	J	22/44 (50%)	19 (86%)	3 (14%)	5	15
2	K	21/44 (48%)	20 (95%)	1 (5%)	35	71
2	L	23/44 (52%)	20 (87%)	3 (13%)	6	16
All	All	3484/3816 (91%)	3242 (93%)	242 (7%)	22	52

All (242) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
1	A	74	ASN
1	A	80	ARG
1	A	122	THR
1	A	136	ARG
1	A	138	SER
1	A	154	LEU
1	A	165	SER
1	A	172	ILE
1	A	178	ARG
1	A	212	MET
1	A	220	LEU
1	A	224	GLU
1	A	240	VAL
1	A	261	LEU
1	A	271	MET
1	A	272	ASN
1	A	328	ASP
1	A	329	LEU
1	A	347	TYR
1	A	356	LYS
1	A	365	ILE
1	A	376	ASP
1	A	384	ASP
1	A	392	ARG
1	A	404	LEU

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Mol	Chain	Res	Type
1	A	417	GLU
1	A	444	LEU
1	A	468	ILE
1	A	478	SER
1	A	488	LEU
1	A	519	LYS
1	A	530	ASP
1	B	75	GLN
1	B	80	ARG
1	B	82	GLN
1	B	110	GLN
1	B	133	HIS
1	B	147	LEU
1	B	152	VAL
1	B	175	LYS
1	B	178	ARG
1	B	207	SER
1	B	220	LEU
1	B	271	MET
1	B	272	ASN
1	B	274	ILE
1	B	279	VAL
1	B	287	HIS
1	B	347	TYR
1	B	364	HIS
1	B	404	LEU
1	B	415	GLU
1	B	420	ARG
1	B	488	LEU
1	B	524	ASP
1	B	552	ASP
1	C	74	ASN
1	C	80	ARG
1	C	122	THR
1	C	136	ARG
1	C	138	SER
1	C	141	LYS
1	C	154	LEU
1	C	165	SER
1	C	168	GLU
1	C	172	ILE
1	C	178	ARG

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Mol	Chain	Res	Type
1	C	187	ASN
1	C	193	LYS
1	C	212	MET
1	C	220	LEU
1	C	224	GLU
1	C	240	VAL
1	C	261	LEU
1	C	271	MET
1	C	272	ASN
1	C	279	VAL
1	C	328	ASP
1	C	329	LEU
1	C	347	TYR
1	C	352	GLU
1	C	364	HIS
1	C	365	ILE
1	C	376	ASP
1	C	384	ASP
1	C	404	LEU
1	C	421	LYS
1	C	468	ILE
1	C	488	LEU
1	C	530	ASP
1	C	549	MET
1	D	75	GLN
1	D	80	ARG
1	D	82	GLN
1	D	110	GLN
1	D	133	HIS
1	D	138	SER
1	D	147	LEU
1	D	152	VAL
1	D	175	LYS
1	D	178	ARG
1	D	207	SER
1	D	220	LEU
1	D	271	MET
1	D	272	ASN
1	D	274	ILE
1	D	279	VAL
1	D	320	ARG
1	D	347	TYR

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Mol	Chain	Res	Type
1	D	404	LEU
1	D	415	GLU
1	D	420	ARG
1	D	488	LEU
1	D	512	PHE
1	D	527	MET
1	D	552	ASP
1	E	74	ASN
1	E	75	GLN
1	E	80	ARG
1	E	82	GLN
1	E	111	LYS
1	E	122	THR
1	E	136	ARG
1	E	138	SER
1	E	154	LEU
1	E	165	SER
1	E	172	ILE
1	E	187	ASN
1	E	212	MET
1	E	220	LEU
1	E	224	GLU
1	E	240	VAL
1	E	261	LEU
1	E	271	MET
1	E	272	ASN
1	E	327	ILE
1	E	328	ASP
1	E	347	TYR
1	E	352	GLU
1	E	365	ILE
1	E	376	ASP
1	E	379	GLU
1	E	393	ARG
1	E	404	LEU
1	E	468	ILE
1	E	488	LEU
1	E	530	ASP
1	F	75	GLN
1	F	80	ARG
1	F	82	GLN
1	F	110	GLN

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Mol	Chain	Res	Type
1	F	133	HIS
1	F	147	LEU
1	F	152	VAL
1	F	175	LYS
1	F	207	SER
1	F	220	LEU
1	F	271	MET
1	F	272	ASN
1	F	274	ILE
1	F	279	VAL
1	F	330	THR
1	F	347	TYR
1	F	363	LYS
1	F	404	LEU
1	F	415	GLU
1	F	488	LEU
1	F	512	PHE
1	F	524	ASP
1	F	527	MET
1	F	549	MET
1	F	552	ASP
1	F	574	LYS
1	G	74	ASN
1	G	80	ARG
1	G	122	THR
1	G	136	ARG
1	G	138	SER
1	G	154	LEU
1	G	165	SER
1	G	172	ILE
1	G	212	MET
1	G	220	LEU
1	G	224	GLU
1	G	240	VAL
1	G	261	LEU
1	G	271	MET
1	G	272	ASN
1	G	321	GLN
1	G	347	TYR
1	G	352	GLU
1	G	365	ILE
1	G	376	ASP

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Mol	Chain	Res	Type
1	G	384	ASP
1	G	392	ARG
1	G	393	ARG
1	G	404	LEU
1	G	407	LYS
1	G	417	GLU
1	G	427	CYS
1	G	444	LEU
1	G	468	ILE
1	G	488	LEU
1	G	530	ASP
1	G	549	MET
1	H	71	VAL
1	H	75	GLN
1	H	80	ARG
1	H	82	GLN
1	H	110	GLN
1	H	133	HIS
1	H	142	LEU
1	H	147	LEU
1	H	152	VAL
1	H	175	LYS
1	H	207	SER
1	H	220	LEU
1	H	221	LYS
1	H	271	MET
1	H	272	ASN
1	H	274	ILE
1	H	279	VAL
1	H	327	ILE
1	H	328	ASP
1	H	330	THR
1	H	347	TYR
1	H	363	LYS
1	H	404	LEU
1	H	488	LEU
1	H	524	ASP
1	H	552	ASP
2	I	5	GLN
2	I	20	LEU
2	I	30	VAL
2	J	5	GLN

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Mol	Chain	Res	Type
2	J	20	LEU
2	J	30	VAL
2	K	5	GLN
2	L	5	GLN
2	L	10	HIS
2	L	18	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 29 ligands modelled in this entry, 12 are monoatomic - leaving 17 for Mogul analysis.

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	LYS	A	601	-	9,9,9	0.65	0	10,10,10	1.40	2 (20%)
4	APC	A	602	-	29,29,33	1.55	4 (13%)	45,45,52	2.12	12 (26%)
3	LYS	B	601	-	9,9,9	0.66	0	10,10,10	1.28	2 (20%)
4	APC	B	602	5	33,33,33	1.36	5 (15%)	52,52,52	1.85	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LYS	C	601	-	9,9,9	0.67	0	10,10,10	1.57	3 (30%)
4	APC	C	602	-	29,29,33	1.50	4 (13%)	45,45,52	2.16	12 (26%)
3	LYS	D	601	-	9,9,9	0.74	0	10,10,10	1.29	1 (10%)
4	APC	D	602	5	33,33,33	1.39	5 (15%)	52,52,52	1.86	9 (17%)
3	LYS	E	601	-	9,9,9	0.72	0	10,10,10	1.53	3 (30%)
4	APC	E	602	-	29,29,33	1.53	4 (13%)	45,45,52	2.17	12 (26%)
3	LYS	F	601	-	9,9,9	0.66	0	10,10,10	1.25	1 (10%)
4	APC	F	602	5	33,33,33	1.43	5 (15%)	52,52,52	1.91	10 (19%)
3	LYS	G	601	-	9,9,9	0.69	0	10,10,10	1.31	2 (20%)
4	APC	G	602	-	29,29,33	1.58	4 (13%)	45,45,52	2.10	13 (28%)
6	ALA	H	601	-	4,4,5	9.68	2 (50%)	3,4,6	16.82	2 (66%)
3	LYS	H	602	-	9,9,9	0.71	0	10,10,10	1.26	1 (10%)
4	APC	H	603	5	33,33,33	1.35	6 (18%)	52,52,52	1.91	9 (17%)

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	LYS	A	601	-	-	0/9/9/9	0/0/0/0
4	APC	A	602	-	-	0/16/32/38	0/1/3/3
3	LYS	B	601	-	-	0/9/9/9	0/0/0/0
4	APC	B	602	5	-	0/20/38/38	0/1/3/3
3	LYS	C	601	-	-	0/9/9/9	0/0/0/0
4	APC	C	602	-	-	0/16/32/38	0/1/3/3
3	LYS	D	601	-	-	0/9/9/9	0/0/0/0
4	APC	D	602	5	-	0/20/38/38	0/1/3/3
3	LYS	E	601	-	-	0/9/9/9	0/0/0/0
4	APC	E	602	-	-	0/16/32/38	0/1/3/3
3	LYS	F	601	-	-	0/9/9/9	0/0/0/0
4	APC	F	602	5	-	0/20/38/38	0/1/3/3
3	LYS	G	601	-	-	0/9/9/9	0/0/0/0
4	APC	G	602	-	-	0/16/32/38	0/1/3/3
6	ALA	H	601	-	-	0/0/2/4	0/0/0/0
3	LYS	H	602	-	-	0/9/9/9	0/0/0/0
4	APC	H	603	5	-	0/20/38/38	0/1/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	601	ALA	O-C	19.13	1.24	1.11
4	G	602	APC	PB-O3B	5.61	1.62	1.51
4	A	602	APC	PB-O3B	5.57	1.62	1.51
4	E	602	APC	PB-O3B	5.36	1.61	1.51
4	C	602	APC	PB-O3B	5.21	1.61	1.51
4	F	602	APC	PA-C3A	3.40	1.82	1.79
4	F	602	APC	PB-C3A	3.26	1.82	1.79
4	D	602	APC	PG-O1G	3.15	1.61	1.51
4	B	602	APC	PG-O1G	3.09	1.61	1.51
4	F	602	APC	PG-O1G	3.08	1.61	1.51
4	D	602	APC	PA-C3A	3.07	1.82	1.79
4	G	602	APC	PA-C3A	3.05	1.82	1.79
4	H	603	APC	PG-O1G	3.03	1.61	1.51
4	A	602	APC	PA-C3A	3.01	1.82	1.79
4	E	602	APC	PA-C3A	3.00	1.82	1.79
4	H	603	APC	PA-C3A	2.98	1.82	1.79
6	H	601	ALA	CA-C	2.93	1.53	1.48
4	D	602	APC	PB-C3A	2.90	1.82	1.79
4	B	602	APC	PA-C3A	2.84	1.82	1.79
4	B	602	APC	PB-C3A	2.65	1.82	1.79
4	C	602	APC	PA-C3A	2.65	1.82	1.79
4	G	602	APC	PB-O2B	2.58	1.62	1.56
4	C	602	APC	PA-O2A	2.41	1.62	1.56
4	H	603	APC	PB-C3A	2.40	1.81	1.79
4	G	602	APC	PA-O2A	2.39	1.62	1.56
4	A	602	APC	PA-O2A	2.39	1.62	1.56
4	E	602	APC	PA-O2A	2.38	1.61	1.56
4	D	602	APC	PB-O2B	2.30	1.61	1.56
4	A	602	APC	PB-O2B	2.27	1.61	1.56
4	C	602	APC	PB-O2B	2.27	1.61	1.56
4	F	602	APC	PB-O2B	2.21	1.61	1.56
4	B	602	APC	PB-O2B	2.20	1.61	1.56
4	E	602	APC	PB-O2B	2.19	1.61	1.56
4	H	603	APC	PA-O2A	2.15	1.61	1.56
4	B	602	APC	PA-O2A	2.12	1.61	1.56
4	D	602	APC	PA-O2A	2.11	1.61	1.56
4	H	603	APC	PB-O2B	2.11	1.61	1.56
4	F	602	APC	PA-O2A	2.04	1.61	1.56
4	H	603	APC	O4'-C1'	2.01	1.44	1.41

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	601	ALA	C-CA-N	-28.08	110.09	113.27
4	C	602	APC	N3-C2-N1	-9.29	120.94	128.71
4	E	602	APC	N3-C2-N1	-9.27	120.96	128.71
4	A	602	APC	N3-C2-N1	-9.10	121.11	128.71
4	G	602	APC	N3-C2-N1	-9.08	121.12	128.71
4	H	603	APC	N3-C2-N1	-9.01	121.17	128.71
4	F	602	APC	N3-C2-N1	-8.94	121.24	128.71
4	B	602	APC	N3-C2-N1	-8.39	121.69	128.71
4	D	602	APC	N3-C2-N1	-8.20	121.85	128.71
6	H	601	ALA	CB-CA-C	7.68	111.88	108.46
4	E	602	APC	N3-C4-N9	4.43	133.43	125.43
4	C	602	APC	N3-C4-N9	4.36	133.31	125.43
4	A	602	APC	N3-C4-N9	4.34	133.26	125.43
4	G	602	APC	N3-C4-N9	4.31	133.21	125.43
4	F	602	APC	N3-C4-N9	4.18	132.98	125.43
4	D	602	APC	N3-C4-N9	4.17	132.97	125.43
4	B	602	APC	N3-C4-N9	4.11	132.85	125.43
4	H	603	APC	N3-C4-N9	4.03	132.71	125.43
4	A	602	APC	PA-C3A-PB	-3.90	112.01	117.62
4	C	602	APC	PA-C3A-PB	-3.80	112.15	117.62
4	E	602	APC	PA-C3A-PB	-3.69	112.31	117.62
4	G	602	APC	PA-C3A-PB	-3.44	112.67	117.62
3	E	601	LYS	OXT-C-O	-3.37	116.44	124.07
4	H	603	APC	PA-C3A-PB	-3.34	112.82	117.62
3	C	601	LYS	OXT-C-O	-3.30	116.61	124.07
4	E	602	APC	C3'-C2'-C1'	3.29	106.06	100.91
4	G	602	APC	C3'-C2'-C1'	3.29	106.06	100.91
4	A	602	APC	C3'-C2'-C1'	3.29	106.05	100.91
4	B	602	APC	PA-C3A-PB	-3.24	112.96	117.62
4	C	602	APC	C3'-C2'-C1'	3.16	105.85	100.91
4	C	602	APC	O2B-PB-C3A	3.03	110.70	104.74
4	H	603	APC	C3'-C2'-C1'	2.99	105.59	100.91
4	E	602	APC	C5-C4-N3	-2.98	119.21	125.70
3	D	601	LYS	OXT-C-O	-2.95	117.40	124.07
4	F	602	APC	C3'-C2'-C1'	2.94	105.52	100.91
4	D	602	APC	C3'-C2'-C1'	2.93	105.50	100.91
4	D	602	APC	PA-C3A-PB	-2.91	113.43	117.62
4	C	602	APC	C5-C4-N3	-2.91	119.36	125.70
4	D	602	APC	C5-C4-N3	-2.89	119.40	125.70
4	A	602	APC	C5-C4-N3	-2.89	119.41	125.70
4	H	603	APC	PG-O3B-PB	-2.88	121.97	131.81
4	G	602	APC	C5-C4-N3	-2.85	119.48	125.70
4	D	602	APC	C4-C5-N7	-2.85	107.08	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	APC	PG-O3B-PB	-2.84	122.11	131.81
4	D	602	APC	O4'-C1'-N9	2.83	111.07	108.44
3	A	601	LYS	OXT-C-O	-2.82	117.69	124.07
4	E	602	APC	O2B-PB-C3A	2.81	110.27	104.74
4	F	602	APC	PG-O3B-PB	-2.81	122.20	131.81
3	H	602	LYS	OXT-C-O	-2.80	117.74	124.07
4	F	602	APC	O4'-C1'-N9	2.79	111.04	108.44
4	B	602	APC	PG-O3B-PB	-2.79	122.27	131.81
3	F	601	LYS	OXT-C-O	-2.77	117.82	124.07
4	B	602	APC	C3'-C2'-C1'	2.76	105.22	100.91
4	B	602	APC	C5-C4-N3	-2.76	119.69	125.70
4	F	602	APC	C5-C4-N3	-2.76	119.70	125.70
4	B	602	APC	C4-C5-N7	-2.74	107.17	109.52
4	G	602	APC	O2B-PB-C3A	2.66	109.96	104.74
4	A	602	APC	O2B-PB-C3A	2.65	109.94	104.74
4	E	602	APC	O3B-PB-O1B	-2.65	108.94	115.59
4	H	603	APC	C5-C4-N3	-2.64	119.96	125.70
4	C	602	APC	O3B-PB-O1B	-2.61	109.04	115.59
3	C	601	LYS	C-CA-N	2.59	113.66	109.36
3	G	601	LYS	C-CA-N	2.58	113.63	109.36
4	G	602	APC	O3B-PB-O1B	-2.57	109.13	115.59
3	A	601	LYS	C-CA-N	2.56	113.60	109.36
4	C	602	APC	C4-C5-N7	-2.56	107.33	109.52
4	F	602	APC	PA-C3A-PB	-2.53	113.97	117.62
4	E	602	APC	O4'-C1'-N9	2.52	110.78	108.44
4	A	602	APC	O3B-PB-O1B	-2.50	109.31	115.59
3	G	601	LYS	OXT-C-O	-2.49	118.44	124.07
4	G	602	APC	O5'-PA-O1A	-2.47	108.05	114.21
4	G	602	APC	O4'-C1'-N9	2.43	110.70	108.44
4	F	602	APC	C4-C5-N7	-2.42	107.45	109.52
4	E	602	APC	O5'-PA-O1A	-2.42	108.16	114.21
4	E	602	APC	C4-C5-N7	-2.41	107.46	109.52
3	B	601	LYS	C-CA-N	2.40	113.33	109.36
4	H	603	APC	C4-C5-N7	-2.39	107.47	109.52
4	C	602	APC	O4'-C1'-N9	2.39	110.67	108.44
3	E	601	LYS	C-CA-N	2.33	113.23	109.36
4	A	602	APC	O5'-PA-O1A	-2.33	108.39	114.21
4	A	602	APC	C4-C5-N7	-2.32	107.53	109.52
4	C	602	APC	O5'-PA-O1A	-2.31	108.45	114.21
3	B	601	LYS	OXT-C-O	-2.30	118.86	124.07
4	H	603	APC	O4'-C1'-N9	2.29	110.57	108.44
4	E	602	APC	C2-N3-C4	2.24	120.39	114.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	APC	O4'-C1'-N9	2.20	110.48	108.44
4	B	602	APC	O4'-C1'-N9	2.19	110.48	108.44
4	H	603	APC	O5'-PA-C3A	2.18	109.39	103.97
4	C	602	APC	C2-N3-C4	2.18	120.20	114.01
4	C	602	APC	O5'-PA-C3A	2.17	109.36	103.97
3	C	601	LYS	OXT-C-CA	2.16	121.74	116.88
4	A	602	APC	C2-N3-C4	2.16	120.15	114.01
4	G	602	APC	C2-N3-C4	2.15	120.13	114.01
4	B	602	APC	O5'-PA-C3A	2.14	109.27	103.97
4	E	602	APC	O5'-PA-C3A	2.12	109.23	103.97
4	B	602	APC	C2'-C3'-C4'	2.08	106.79	102.65
4	A	602	APC	O5'-PA-C3A	2.07	109.12	103.97
4	G	602	APC	C4-C5-N7	-2.05	107.77	109.52
4	G	602	APC	O5'-PA-C3A	2.04	109.04	103.97
4	D	602	APC	O5'-PA-C3A	2.03	109.02	103.97
4	F	602	APC	C2'-C3'-C4'	2.03	106.70	102.65
4	F	602	APC	C2-N3-C4	2.03	119.79	114.01
4	G	602	APC	C4'-O4'-C1'	2.01	111.94	109.75
3	E	601	LYS	OXT-C-CA	2.01	121.40	116.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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(Å²)	Q<0.9	
1	A	501/513 (97%)	-0.26	0	100	100	17, 49, 84, 100	0
1	B	506/513 (98%)	-0.48	0	100	100	17, 33, 66, 82	0
1	C	501/513 (97%)	-0.39	4 (0%)	83	84	16, 40, 74, 97	0
1	D	505/513 (98%)	-0.41	4 (0%)	83	84	16, 34, 70, 112	0
1	E	500/513 (97%)	-0.42	2 (0%)	90	92	16, 39, 75, 114	0
1	F	505/513 (98%)	-0.45	3 (0%)	86	88	16, 33, 72, 117	0
1	G	501/513 (97%)	-0.27	3 (0%)	86	88	19, 49, 83, 108	0
1	H	505/513 (98%)	-0.38	0	100	100	18, 33, 65, 91	0
2	I	31/54 (57%)	0.72	6 (19%)	2	1	23, 50, 114, 118	0
2	J	31/54 (57%)	0.93	6 (19%)	2	1	21, 53, 115, 125	0
2	K	31/54 (57%)	1.03	7 (22%)	1	1	21, 53, 113, 118	0
2	L	31/54 (57%)	1.15	7 (22%)	1	1	20, 49, 114, 116	0
All	All	4148/4320 (96%)	-0.34	42 (1%)	77	81	16, 37, 79, 125	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	14	ALA	9.3
2	L	12	GLY	9.0
2	L	13	GLY	8.7
1	D	524	ASP	7.1
2	I	14	ALA	7.1
2	J	12	GLY	6.9
2	K	14	ALA	6.8
2	K	18	VAL	6.7
2	J	18	VAL	6.5
2	L	18	VAL	6.2
2	L	14	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
2	K	13	GLY	5.9
1	F	524	ASP	5.5
2	I	12	GLY	5.3
2	K	15	PRO	4.9
1	D	522	GLY	4.8
2	J	15	PRO	4.7
2	I	13	GLY	4.4
2	L	15	PRO	4.2
2	K	12	GLY	3.9
2	J	17	ARG	3.7
2	J	13	GLY	3.5
1	E	524	ASP	3.5
2	L	17	ARG	3.3
1	C	524	ASP	3.3
2	K	20	LEU	3.2
1	F	522	GLY	3.2
1	C	526	ALA	3.1
2	K	19	GLU	3.0
2	I	18	VAL	2.9
2	I	17	ARG	2.8
2	L	16	LEU	2.7
1	G	405	GLY	2.7
2	I	15	PRO	2.7
1	D	528	PHE	2.5
1	C	522	GLY	2.5
1	D	520	ALA	2.4
1	E	528	PHE	2.4
1	G	426	ILE	2.3
1	C	279	VAL	2.3
1	G	219	GLY	2.1
1	F	528	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	APC	A	602	27/31	0.42	7.28	73,101,138,154	0
5	MG	J	101	1/1	0.27	6.33	21,21,21,21	0
4	APC	G	602	27/31	0.41	6.15	83,111,142,148	0
5	MG	L	101	1/1	0.30	5.17	20,20,20,20	0
4	APC	B	602	31/31	0.29	4.87	57,101,132,156	0
4	APC	H	603	31/31	0.29	4.35	56,105,139,158	0
4	APC	E	602	27/31	0.28	4.02	74,99,127,160	0
5	MG	C	603	1/1	0.16	3.43	59,59,59,59	0
5	MG	F	604	1/1	0.21	2.96	12,12,12,12	0
4	APC	C	602	27/31	0.34	2.78	72,101,131,155	0
4	APC	F	602	31/31	0.29	2.78	61,107,145,155	0
4	APC	D	602	31/31	0.27	2.18	60,108,149,152	0
6	ALA	H	601	5/6	0.20	1.89	69,76,79,80	0
5	MG	H	605	1/1	0.26	1.80	13,13,13,13	0
3	LYS	C	601	10/10	0.20	1.18	15,19,42,44	0
3	LYS	A	601	10/10	0.19	0.99	16,24,46,61	0
3	LYS	G	601	10/10	0.18	0.58	17,33,43,52	0
3	LYS	B	601	10/10	0.15	0.50	15,24,32,35	0
3	LYS	H	602	10/10	0.17	0.48	18,22,30,32	0
5	MG	B	603	1/1	0.18	0.41	63,63,63,63	0
3	LYS	D	601	10/10	0.16	0.27	15,31,36,38	0
3	LYS	F	601	10/10	0.15	-0.22	17,30,36,39	0
3	LYS	E	601	10/10	0.14	-0.72	15,22,45,49	0
5	MG	D	603	1/1	0.12	-1.51	68,68,68,68	0
5	MG	G	603	1/1	0.12	-1.63	55,55,55,55	0
5	MG	H	604	1/1	0.09	-2.42	66,66,66,66	0
5	MG	A	603	1/1	0.09	-2.76	53,53,53,53	0
5	MG	F	603	1/1	0.09	-3.09	59,59,59,59	0
5	MG	E	603	1/1	0.09	-5.29	53,53,53,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.