



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:54 AM GMT

PDB ID : 3N2K
Title : TUBULIN-NSC 613862: RB3 Stathmin-like domain complex
Authors : Barbier, P.; Dorleans, A.; Devred, F.; Sanz, L.; Allegro, D.; Alfonso, C.;
Knossow, M.; Peyrot, V.; Andreu, J.M.
Deposited on : 2010-05-18
Resolution : 4.00 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>

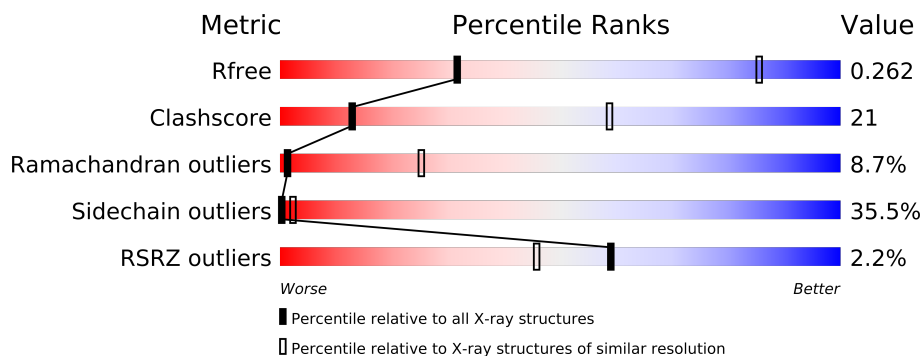
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.00 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	1035 (4.52-3.46)
Clashscore	79885	1235 (4.50-3.50)
Ramachandran outliers	78287	1170 (4.50-3.50)
Sidechain outliers	78261	1156 (4.50-3.50)
RSRZ outliers	66119	1035 (4.52-3.46)

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	451	
1	C	451	
2	B	445	
2	D	445	
3	E	142	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14225 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3300	2097	557	625	21			
1	C	429	Total	C	N	O	S	0	0	0
			3286	2084	554	627	21			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3251	2046	547	633	25			
2	D	427	Total	C	N	O	S	0	0	0
			3297	2071	559	643	24			

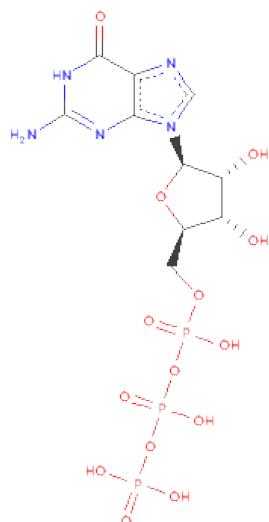
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			920	557	174	184	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	EXPRESSION TAG	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

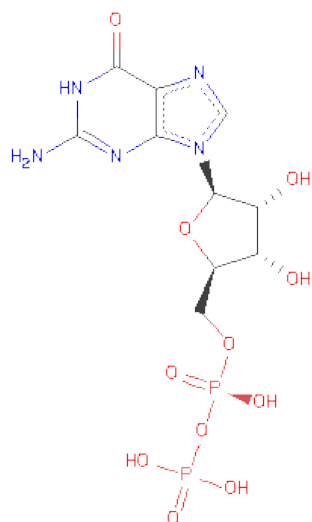


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

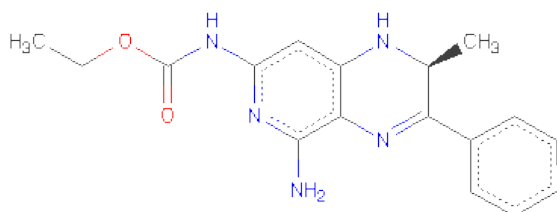
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 7 is ETHYL [(2S)-5-AMINO-2-METHYL-3-PHENYL-1,2-DIHYDROPYRIDO[3,4-B]PYRAZIN-7-YL]CARBAMATE (three-letter code: K2N) (formula: C₁₇H₁₉N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			24	17	5	2		

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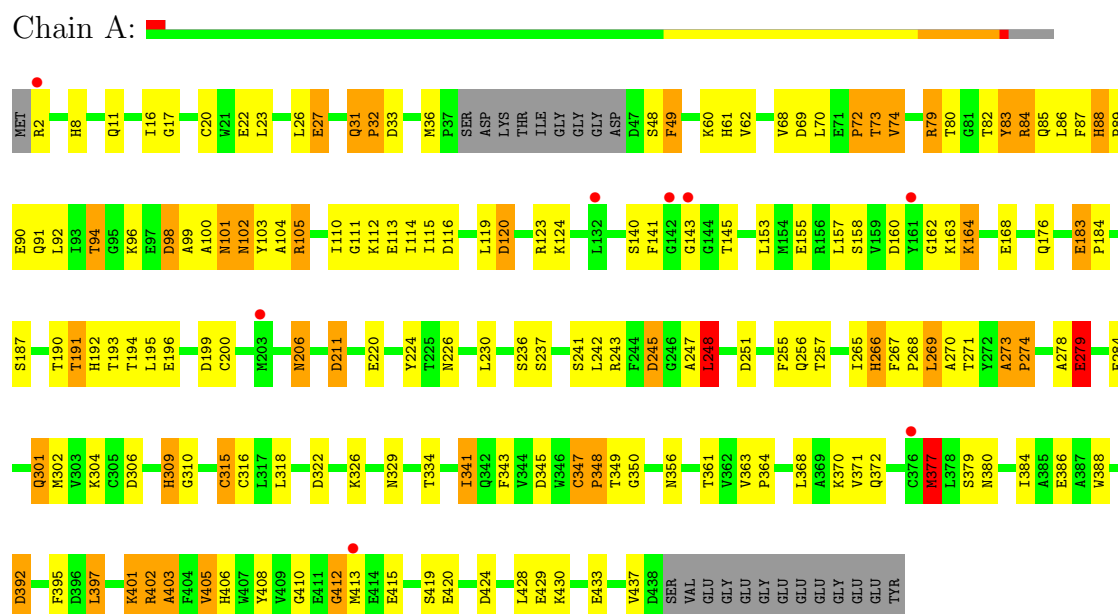
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			24	17	5	2		

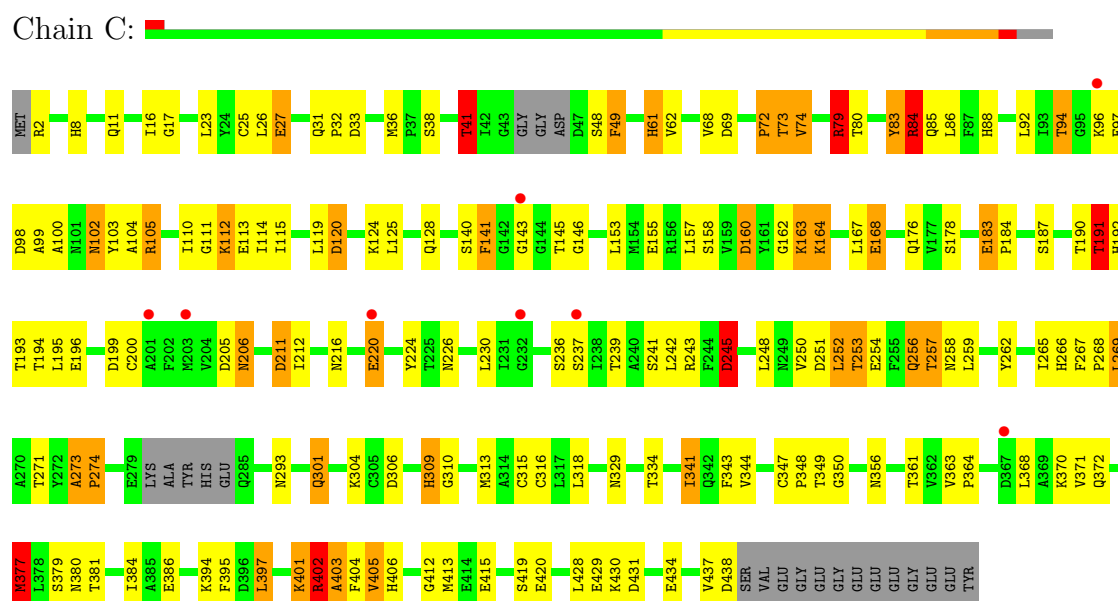
3 Residue-property plots

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: Tubulin alpha chain

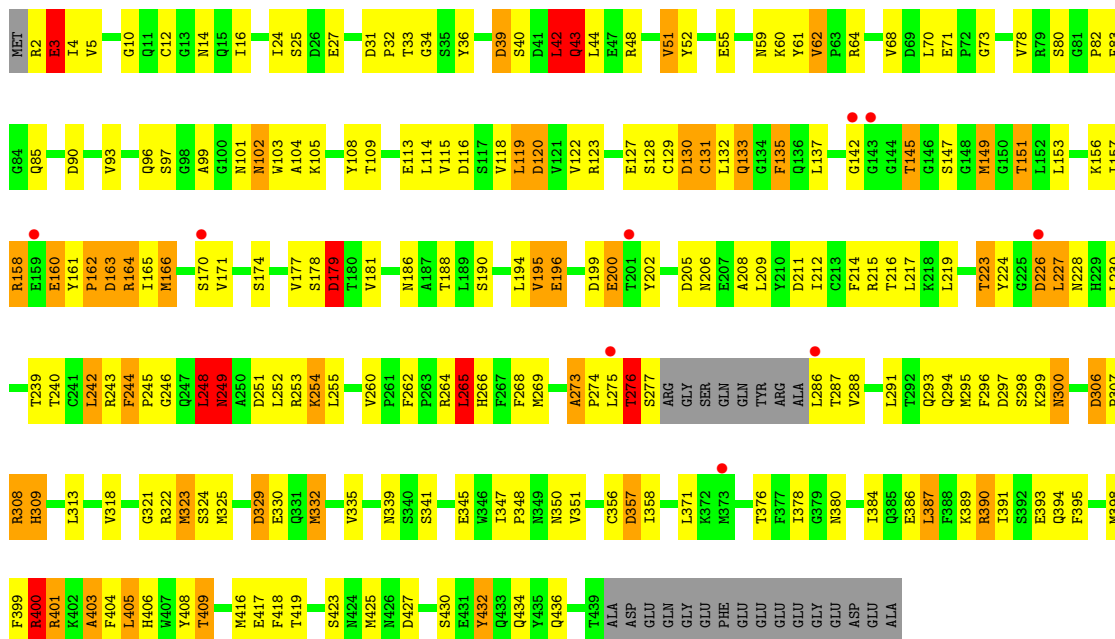


• Molecule 1: Tubulin alpha chain



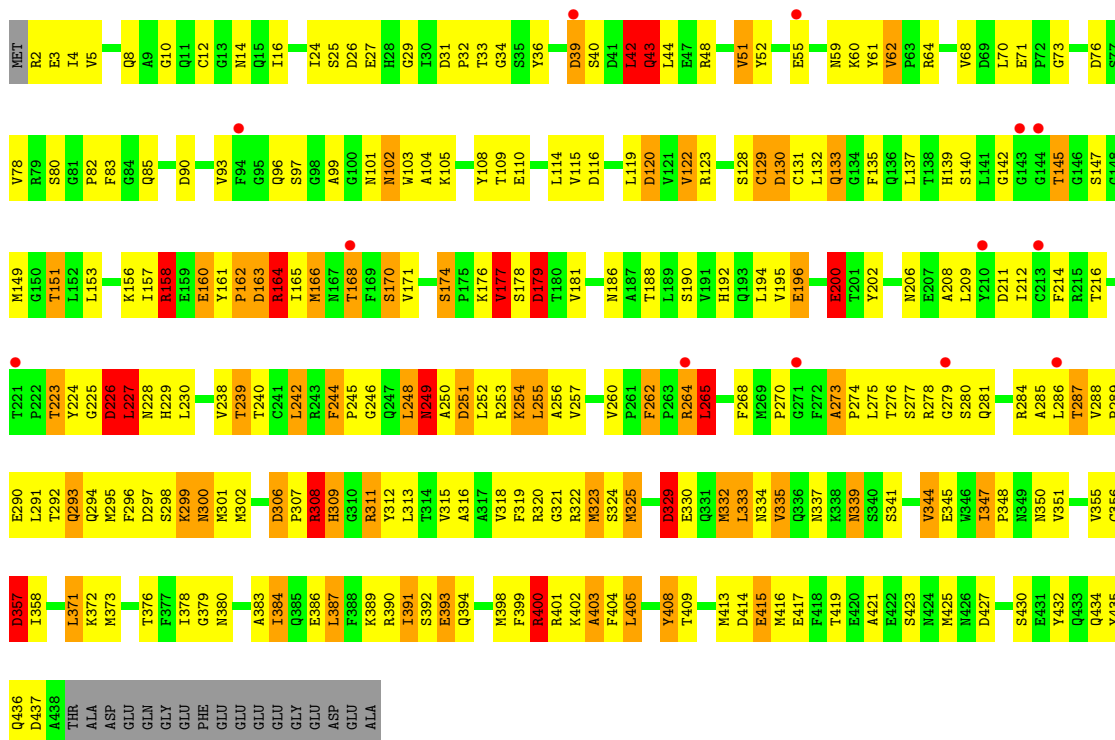
- Molecule 2: Tubulin beta chain

Chain B:



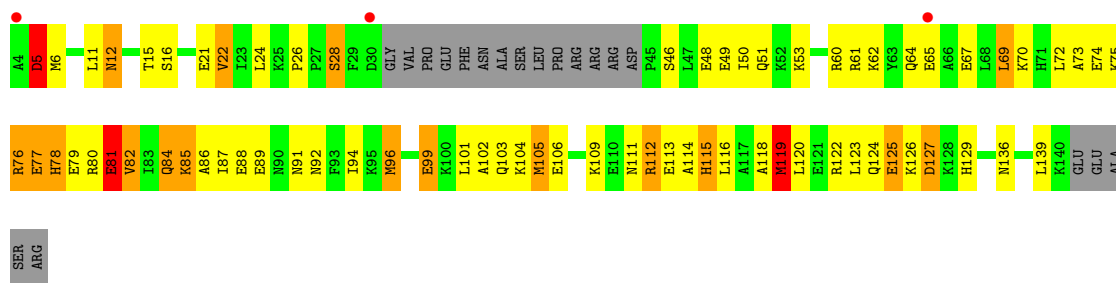
- Molecule 2: Tubulin beta chain

Chain D:



- Molecule 3: Stathmin-4

Chain E:



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	326.32Å 326.32Å 54.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.00 29.73 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-4.00) 99.6 (29.73-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.98Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.223 , 0.250 0.251 , 0.262	Depositor DCC
R_{free} test set	1433 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	162.7	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 193.3	EDS
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 28494 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14225	wwPDB-VP
Average B, all atoms (Å ²)	232.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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: GDP, GTP, MG, K2N

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	0.79	0/3377	0.96	17/4593 (0.4%)
1	C	0.71	1/3360 (0.0%)	0.95	12/4572 (0.3%)
2	B	0.78	0/3323	0.97	11/4512 (0.2%)
2	D	0.85	2/3370 (0.1%)	1.01	14/4574 (0.3%)
3	E	0.82	2/928 (0.2%)	0.94	1/1243 (0.1%)
All	All	0.79	5/14358 (0.0%)	0.97	55/19494 (0.3%)

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	C	0	2
2	B	0	4
2	D	0	4
3	E	0	1
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	200	GLU	CD-OE1	7.30	1.33	1.25
1	C	168	GLU	CD-OE1	5.61	1.31	1.25
3	E	119	MET	SD-CE	5.50	2.08	1.77
3	E	105	MET	SD-CE	5.48	2.08	1.77
2	D	177	VAL	CB-CG2	5.39	1.64	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	ASP	CB-CG-OD2	7.46	125.01	118.30
1	C	120	ASP	CB-CG-OD2	7.32	124.88	118.30
1	A	248	LEU	CA-CB-CG	7.22	131.91	115.30
1	C	397	LEU	CA-CB-CG	7.10	131.63	115.30
2	D	297	ASP	CB-CG-OD2	7.06	124.65	118.30
1	A	397	LEU	CA-CB-CG	6.97	131.32	115.30
1	A	160	ASP	CB-CG-OD2	6.96	124.57	118.30
1	C	269	LEU	CA-CB-CG	6.94	131.26	115.30
2	D	179	ASP	CB-CG-OD2	6.88	124.50	118.30
1	C	211	ASP	CB-CG-OD2	6.68	124.31	118.30
2	B	130	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	269	LEU	CA-CB-CG	6.55	130.37	115.30
2	B	306	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	322	ASP	CB-CG-OD2	6.49	124.14	118.30
1	C	245	ASP	CB-CG-OD2	6.47	124.12	118.30
2	B	39	ASP	CB-CG-OD2	6.41	124.06	118.30
2	B	120	ASP	CB-CG-OD2	6.38	124.04	118.30
2	B	199	ASP	CB-CG-OD1	6.35	124.02	118.30
1	C	33	ASP	CB-CG-OD2	6.32	123.98	118.30
1	A	211	ASP	CB-CG-OD2	6.26	123.94	118.30
1	C	69	ASP	CB-CG-OD2	6.26	123.93	118.30
2	D	308	ARG	NE-CZ-NH1	6.25	123.43	120.30
2	D	226	ASP	CB-CG-OD2	6.20	123.88	118.30
2	D	357	ASP	CB-CG-OD2	6.19	123.87	118.30
2	B	242	LEU	CA-CB-CG	6.19	129.53	115.30
2	D	242	LEU	CA-CB-CG	6.12	129.37	115.30
1	A	69	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	120	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	266	HIS	CB-CA-C	-6.03	98.34	110.40
1	A	116	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	33	ASP	CB-CG-OD2	6.00	123.70	118.30
2	B	179	ASP	CB-CG-OD2	5.93	123.64	118.30
2	D	164	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	20	CYS	CA-CB-SG	5.82	124.47	114.00
2	D	130	ASP	CB-CG-OD2	5.78	123.50	118.30
3	E	127	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	306	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	424	ASP	CB-CG-OD2	5.69	123.42	118.30
1	C	306	ASP	CB-CG-OD2	5.62	123.36	118.30
2	B	205	ASP	CB-CG-OD2	5.61	123.35	118.30
2	B	427	ASP	CB-CG-OD2	5.54	123.28	118.30
2	B	297	ASP	CB-CG-OD2	5.49	123.24	118.30
2	D	39	ASP	CB-CG-OD2	5.48	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	LEU	CA-CB-CG	5.43	127.78	115.30
2	D	427	ASP	CB-CG-OD2	5.42	123.18	118.30
2	D	306	ASP	CB-CG-OD2	5.38	123.15	118.30
2	D	120	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	205	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	98	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	431	ASP	CB-CG-OD2	5.25	123.03	118.30
2	D	329	ASP	CB-CG-OD2	5.18	122.96	118.30
2	D	379	GLY	N-CA-C	5.10	125.86	113.10
2	B	329	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	251	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	345	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLY	Peptide
2	B	162	PRO	Peptide
2	B	248	LEU	Peptide
2	B	249	ASN	Peptide
2	B	262	PHE	Peptide
1	C	143	GLY	Peptide
1	C	41	THR	Peptide
2	D	162	PRO	Peptide
2	D	248	LEU	Peptide
2	D	249	ASN	Peptide
2	D	262	PHE	Peptide
3	E	5	ASP	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	3300	0	0	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3286	0	0	48	0
2	B	3251	0	0	73	0
2	D	3297	0	0	105	0
3	E	920	0	0	29	0
4	A	32	0	12	3	0
4	C	32	0	12	6	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	6	0
6	D	28	0	12	10	0
7	B	24	0	19	3	0
7	D	24	0	19	12	0
All	All	14225	0	86	298	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 21.

All (298) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:96:MET:SD	3:E:96:MET:CE	2.01	1.47
3:E:105:MET:SD	3:E:105:MET:CE	2.08	1.42
3:E:119:MET:CE	3:E:119:MET:SD	2.08	1.41
2:D:252:LEU:CD1	7:D:700:K2N:HAK	1.88	1.03
2:D:252:LEU:CD1	7:D:700:K2N:CAK	2.40	0.99
2:B:403:ALA:O	2:B:405:LEU:N	2.03	0.92
7:B:700:K2N:H3	7:B:700:K2N:OAD	1.79	0.82
1:C:206:ASN:ND2	4:C:600:GTP:HN22	1.79	0.80
3:E:118:ALA:O	3:E:122:ARG:NH1	2.16	0.79
2:D:252:LEU:CD1	7:D:700:K2N:H19	2.11	0.79
2:D:273:ALA:CB	2:D:274:PRO:CD	2.61	0.79
2:D:140:SER:CB	6:D:600:GDP:H5'	2.13	0.78
2:D:312:TYR:CD2	2:D:315:VAL:CG2	2.67	0.78
2:B:2:ARG:N	2:B:133:GLN:OE1	2.17	0.78
2:D:378:ILE:CD1	7:D:700:K2N:HABA	2.14	0.77
2:B:224:TYR:O	2:B:228:ASN:ND2	2.18	0.77
2:D:224:TYR:O	2:D:228:ASN:ND2	2.19	0.76
2:B:42:LEU:O	2:B:44:LEU:N	2.19	0.76
2:B:273:ALA:CB	2:B:274:PRO:CD	2.64	0.75
2:D:403:ALA:O	2:D:405:LEU:N	2.20	0.75
2:B:142:GLY:O	6:B:600:GDP:H5'	1.86	0.75
2:D:387:LEU:O	2:D:390:ARG:CG	2.35	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:224:TYR:OH	6:D:600:GDP:H2'	1.87	0.74
2:D:42:LEU:O	2:D:44:LEU:N	2.20	0.74
2:D:306:ASP:O	2:D:308:ARG:N	2.19	0.74
2:D:2:ARG:N	2:D:133:GLN:OE1	2.21	0.73
1:A:278:ALA:O	1:A:279:GLU:CB	2.36	0.73
2:D:345:GLU:OE1	2:D:345:GLU:N	2.22	0.72
1:C:79:ARG:NH2	1:C:94:THR:CG2	2.52	0.72
2:D:114:LEU:O	2:D:116:ASP:N	2.22	0.72
7:B:700:K2N:CAA	7:B:700:K2N:OAD	2.36	0.71
2:D:192:HIS:CD2	2:D:421:ALA:CB	2.73	0.71
2:D:321:GLY:O	2:D:323:MET:N	2.24	0.71
3:E:112:ARG:O	3:E:115:HIS:N	2.24	0.70
2:B:401:ARG:NH2	1:C:434:GLU:O	2.24	0.70
2:D:265:LEU:CB	2:D:432:TYR:CE2	2.74	0.70
2:B:345:GLU:OE1	2:B:345:GLU:N	2.25	0.69
7:D:700:K2N:H3	7:D:700:K2N:OAD	1.92	0.69
2:D:179:ASP:N	2:D:179:ASP:OD1	2.25	0.69
1:A:79:ARG:NH2	1:A:94:THR:CG2	2.56	0.68
1:C:83:TYR:O	1:C:86:LEU:N	2.26	0.68
1:C:105:ARG:NH2	2:D:253:ARG:NH2	2.41	0.68
2:B:403:ALA:C	2:B:405:LEU:N	2.43	0.68
2:D:158:ARG:O	2:D:160:GLU:N	2.27	0.68
2:B:306:ASP:O	2:B:308:ARG:N	2.26	0.68
3:E:101:LEU:O	3:E:103:GLN:N	2.26	0.68
2:B:12:CYS:SG	6:B:600:GDP:C4	2.87	0.67
1:A:412:GLY:O	3:E:60:ARG:NH1	2.27	0.67
2:D:36:TYR:OH	2:D:40:SER:O	2.13	0.67
3:E:48:GLU:O	3:E:50:ILE:N	2.28	0.66
2:D:357:ASP:OD2	2:D:357:ASP:N	2.29	0.66
1:C:315:CYS:SG	1:C:377:MET:CE	2.84	0.66
2:D:298:SER:O	2:D:300:ASN:N	2.29	0.66
2:D:135:PHE:CZ	2:D:161:TYR:CD1	2.84	0.65
2:B:179:ASP:OD1	2:B:179:ASP:N	2.29	0.65
2:D:12:CYS:SG	6:D:600:GDP:C4	2.90	0.65
2:B:114:LEU:O	2:B:116:ASP:N	2.30	0.65
2:D:399:PHE:O	2:D:400:ARG:O	2.14	0.65
1:C:102:ASN:ND2	1:C:102:ASN:C	2.51	0.64
2:B:399:PHE:O	2:B:400:ARG:O	2.15	0.64
2:D:51:VAL:O	2:D:64:ARG:NH2	2.31	0.63
1:A:273:ALA:CB	1:A:274:PRO:CD	2.76	0.63
2:D:10:GLY:O	2:D:14:ASN:N	2.31	0.63
2:B:131:CYS:SG	2:B:131:CYS:O	2.56	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:147:SER:O	2:B:151:THR:OG1	2.16	0.62
2:D:142:GLY:O	6:D:600:GDP:H5"	2.00	0.62
2:B:12:CYS:SG	6:B:600:GDP:N3	2.72	0.62
3:E:81:GLU:O	3:E:82:VAL:C	2.38	0.62
1:A:83:TYR:O	1:A:86:LEU:N	2.34	0.61
2:B:408:TYR:O	2:B:409:THR:C	2.38	0.60
3:E:22:VAL:CG1	3:E:22:VAL:O	2.49	0.60
2:D:384:ILE:CG2	2:D:432:TYR:CE1	2.84	0.60
1:A:206:ASN:ND2	4:A:600:GTP:HN22	2.00	0.60
2:D:135:PHE:CB	2:D:166:MET:CE	2.81	0.59
1:C:273:ALA:CB	1:C:274:PRO:CD	2.81	0.58
1:C:256:GLN:C	1:C:258:ASN:N	2.55	0.58
3:E:74:GLU:C	3:E:76:ARG:N	2.56	0.58
1:C:206:ASN:ND2	4:C:600:GTP:N2	2.52	0.58
2:D:99:ALA:CB	2:D:145:THR:CG2	2.81	0.58
2:B:171:VAL:CG1	2:B:206:ASN:ND2	2.67	0.58
2:B:10:GLY:O	2:B:14:ASN:N	2.37	0.58
1:C:183:GLU:CB	1:C:184:PRO:CD	2.82	0.57
1:A:315:CYS:SG	1:A:377:MET:CE	2.93	0.57
2:D:208:ALA:O	2:D:211:ASP:N	2.37	0.57
2:D:200:GLU:OE2	2:D:268:PHE:CE1	2.58	0.57
2:D:309:HIS:N	2:D:309:HIS:CD2	2.73	0.57
2:B:357:ASP:OD2	2:B:357:ASP:N	2.36	0.57
1:A:72:PRO:O	1:A:74:VAL:N	2.38	0.56
1:C:8:HIS:CD2	1:C:17:GLY:CA	2.88	0.56
1:A:401:LYS:C	1:A:403:ALA:N	2.56	0.56
1:C:111:GLY:O	1:C:113:GLU:N	2.38	0.56
2:B:135:PHE:CB	2:B:166:MET:CE	2.82	0.56
1:C:83:TYR:C	1:C:85:GLN:N	2.56	0.56
2:B:135:PHE:CZ	2:B:161:TYR:CD1	2.93	0.56
2:D:229:HIS:CE1	2:D:277:SER:CB	2.88	0.56
2:B:36:TYR:OH	2:B:40:SER:O	2.24	0.56
2:B:378:ILE:CD1	7:B:700:K2N:HABA	2.36	0.55
1:C:253:THR:O	1:C:256:GLN:N	2.39	0.55
2:D:102:ASN:OD1	2:D:105:LYS:N	2.39	0.55
1:A:102:ASN:ND2	1:A:102:ASN:C	2.60	0.55
2:D:171:VAL:CG1	2:D:206:ASN:ND2	2.70	0.55
2:B:104:ALA:O	2:B:108:TYR:N	2.40	0.55
3:E:81:GLU:O	3:E:85:LYS:N	2.40	0.54
2:B:248:LEU:O	2:B:249:ASN:CB	2.55	0.54
3:E:99:GLU:C	3:E:101:LEU:N	2.60	0.54
1:A:8:HIS:CD2	1:A:17:GLY:CA	2.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:270:PRO:O	2:D:302:MET:N	2.41	0.54
1:C:100:ALA:O	1:C:102:ASN:N	2.40	0.54
2:D:147:SER:O	2:D:151:THR:OG1	2.25	0.54
2:D:224:TYR:CE2	6:D:600:GDP:C4	2.96	0.53
2:B:321:GLY:O	2:B:323:MET:N	2.41	0.53
3:E:101:LEU:O	3:E:104:LYS:N	2.42	0.53
3:E:123:LEU:C	3:E:125:GLU:N	2.62	0.52
2:D:335:VAL:O	2:D:339:ASN:N	2.42	0.52
2:D:153:LEU:O	2:D:157:ILE:N	2.42	0.52
2:D:104:ALA:O	2:D:108:TYR:N	2.42	0.52
2:B:401:ARG:O	1:C:262:TYR:OH	2.26	0.52
2:B:202:TYR:N	2:B:202:TYR:CD1	2.75	0.52
2:B:298:SER:C	2:B:300:ASN:N	2.63	0.52
2:B:102:ASN:OD1	2:B:105:LYS:N	2.41	0.52
1:A:83:TYR:C	1:A:85:GLN:N	2.61	0.52
3:E:78:HIS:CD2	3:E:78:HIS:C	2.82	0.52
1:C:48:SER:O	1:C:243:ARG:O	2.28	0.52
1:A:88:HIS:CD2	1:A:90:GLU:OE1	2.63	0.52
2:D:264:ARG:O	2:D:265:LEU:C	2.48	0.51
2:D:12:CYS:SG	6:D:600:GDP:N3	2.83	0.51
2:D:383:ALA:O	2:D:386:GLU:CB	2.58	0.51
2:B:208:ALA:O	2:B:211:ASP:N	2.43	0.51
2:D:51:VAL:CG1	2:D:52:TYR:CD1	2.94	0.51
2:D:265:LEU:CB	2:D:432:TYR:CZ	2.93	0.51
2:B:31:ASP:O	2:B:33:THR:N	2.44	0.51
2:B:149:MET:O	2:B:153:LEU:N	2.44	0.51
2:D:140:SER:CB	6:D:600:GDP:C5'	2.88	0.50
2:D:308:ARG:NH1	2:D:308:ARG:CG	2.74	0.50
2:D:311:ARG:NH2	2:D:344:VAL:CG2	2.75	0.50
2:D:276:THR:CG2	2:D:277:SER:N	2.74	0.50
1:C:402:ARG:O	1:C:403:ALA:C	2.50	0.50
1:C:309:HIS:ND1	1:C:310:GLY:N	2.60	0.50
1:C:178:SER:OG	1:C:183:GLU:OE2	2.30	0.50
2:D:262:PHE:CE1	2:D:435:TYR:CZ	3.00	0.50
1:C:401:LYS:C	1:C:403:ALA:N	2.66	0.49
3:E:81:GLU:O	3:E:84:GLN:N	2.45	0.49
1:A:401:LYS:O	1:A:403:ALA:N	2.45	0.49
2:B:51:VAL:O	2:B:64:ARG:NH2	2.44	0.49
2:D:174:SER:OG	2:D:176:LYS:O	2.31	0.49
3:E:123:LEU:O	3:E:125:GLU:N	2.46	0.49
1:A:395:PHE:CD2	1:A:395:PHE:C	2.86	0.49
2:B:298:SER:O	2:B:300:ASN:N	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:72:LEU:C	3:E:74:GLU:N	2.66	0.49
1:C:395:PHE:CD2	1:C:395:PHE:C	2.85	0.49
2:D:391:ILE:CG1	2:D:392:SER:N	2.76	0.49
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.45	0.49
2:D:226:ASP:O	2:D:227:LEU:CB	2.60	0.49
2:D:287:THR:CG2	2:D:290:GLU:CB	2.91	0.49
1:A:405:VAL:CG1	1:A:406:HIS:N	2.76	0.48
2:D:168:THR:OG1	2:D:170:SER:OG	2.31	0.48
2:B:51:VAL:CG1	2:B:52:TYR:N	2.75	0.48
2:D:250:ALA:O	2:D:252:LEU:N	2.46	0.48
2:D:51:VAL:CG1	2:D:52:TYR:N	2.77	0.48
1:A:98:ASP:OD1	1:A:99:ALA:N	2.47	0.48
2:B:224:TYR:OH	6:B:600:GDP:H2'	2.14	0.48
2:B:99:ALA:CB	2:B:145:THR:CG2	2.91	0.48
1:A:105:ARG:NH2	2:B:253:ARG:NH2	2.62	0.48
2:D:52:TYR:OH	2:D:239:THR:CG2	2.62	0.48
1:A:100:ALA:O	1:A:102:ASN:N	2.46	0.48
3:E:76:ARG:O	3:E:79:GLU:N	2.47	0.47
2:D:325:MET:O	2:D:329:ASP:OD2	2.32	0.47
2:B:158:ARG:O	2:B:160:GLU:N	2.47	0.47
2:B:308:ARG:NH1	2:B:308:ARG:CG	2.76	0.47
4:C:600:GTP:O3G	2:D:254:LYS:NZ	2.48	0.47
3:E:76:ARG:O	3:E:79:GLU:CB	2.63	0.47
1:A:88:HIS:O	1:A:91:GLN:N	2.48	0.47
2:B:399:PHE:O	2:B:400:ARG:C	2.52	0.47
2:B:51:VAL:CG1	2:B:52:TYR:CD1	2.97	0.47
3:E:11:LEU:O	3:E:12:ASN:CB	2.62	0.47
2:D:389:LYS:O	2:D:393:GLU:CB	2.63	0.47
2:D:202:TYR:OH	7:D:700:K2N:CAU	2.63	0.47
2:B:253:ARG:O	2:B:254:LYS:C	2.52	0.46
1:A:111:GLY:O	1:A:113:GLU:N	2.48	0.46
2:D:408:TYR:CD1	2:D:408:TYR:N	2.82	0.46
1:A:309:HIS:ND1	1:A:310:GLY:N	2.63	0.46
2:B:224:TYR:CE2	6:B:600:GDP:C4	3.03	0.46
2:D:306:ASP:C	2:D:308:ARG:N	2.69	0.46
1:C:405:VAL:CG1	1:C:406:HIS:N	2.77	0.46
1:C:111:GLY:O	1:C:112:LYS:C	2.52	0.46
2:D:223:THR:CB	2:D:225:GLY:N	2.79	0.46
2:D:238:VAL:CG1	7:D:700:K2N:CAJ	2.93	0.46
1:A:408:TYR:C	1:A:410:GLY:N	2.67	0.46
1:C:72:PRO:O	1:C:74:VAL:N	2.48	0.46
2:D:202:TYR:CD1	2:D:202:TYR:N	2.84	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:27:GLU:OE2	1:C:243:ARG:NH2	2.48	0.46
2:D:298:SER:C	2:D:300:ASN:N	2.68	0.46
2:B:395:PHE:C	2:B:395:PHE:CD2	2.89	0.46
2:D:316:ALA:CB	7:D:700:K2N:CAI	2.94	0.46
1:A:266:HIS:O	1:A:268:PRO:CD	2.63	0.46
2:D:122:VAL:CG2	2:D:123:ARG:N	2.79	0.46
2:B:133:GLN:NE2	2:B:252:LEU:CD2	2.79	0.45
1:C:266:HIS:O	1:C:268:PRO:CD	2.64	0.45
1:C:224:TYR:CD2	4:C:600:GTP:C6	3.04	0.45
2:B:31:ASP:C	2:B:33:THR:N	2.68	0.45
2:B:401:ARG:NH1	2:B:401:ARG:CG	2.79	0.45
2:D:256:ALA:O	2:D:257:VAL:C	2.55	0.45
2:D:26:ASP:O	2:D:29:GLY:N	2.50	0.45
2:B:265:LEU:CB	2:B:432:TYR:CE2	2.99	0.45
1:C:98:ASP:OD1	1:C:99:ALA:N	2.49	0.45
3:E:84:GLN:C	3:E:86:ALA:N	2.70	0.45
3:E:116:LEU:O	3:E:119:MET:CB	2.64	0.45
1:A:82:THR:O	1:A:83:TYR:CG	2.70	0.45
2:D:292:THR:O	2:D:294:GLN:N	2.49	0.45
1:A:102:ASN:ND2	1:A:104:ALA:N	2.65	0.45
3:E:69:LEU:O	3:E:73:ALA:N	2.50	0.45
2:D:177:VAL:CG1	2:D:177:VAL:O	2.64	0.45
2:D:42:LEU:O	2:D:43:GLN:C	2.55	0.44
2:B:118:VAL:O	2:B:119:LEU:C	2.55	0.44
2:B:194:LEU:O	2:B:196:GLU:N	2.51	0.44
2:D:226:ASP:N	2:D:226:ASP:OD1	2.51	0.44
2:B:102:ASN:OD1	2:B:102:ASN:O	2.36	0.44
1:C:428:LEU:C	1:C:430:LYS:N	2.71	0.44
2:D:164:ARG:CA	2:D:164:ARG:NE	2.80	0.44
2:B:309:HIS:CD2	2:B:386:GLU:OE2	2.71	0.44
1:C:41:THR:CG2	1:C:61:HIS:CE1	3.01	0.44
1:A:224:TYR:CE2	4:A:600:GTP:C4	3.05	0.44
1:C:163:LYS:O	1:C:164:LYS:C	2.56	0.44
2:B:42:LEU:O	2:B:43:GLN:C	2.55	0.44
3:E:74:GLU:O	3:E:76:ARG:N	2.50	0.44
1:A:103:TYR:O	1:A:104:ALA:C	2.56	0.44
1:A:100:ALA:O	1:A:101:ASN:C	2.56	0.44
2:B:387:LEU:O	2:B:390:ARG:CG	2.66	0.44
1:C:125:LEU:CD2	1:C:128:GLN:NE2	2.81	0.44
2:B:103:TRP:N	2:B:186:ASN:OD1	2.51	0.43
7:D:700:K2N:CAA	7:D:700:K2N:OAD	2.62	0.43
1:C:190:THR:CG2	1:C:191:THR:N	2.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:103:TYR:O	1:C:104:ALA:C	2.54	0.43
1:C:267:PHE:CD1	1:C:267:PHE:N	2.86	0.43
2:D:202:TYR:OH	7:D:700:K2N:NAM	2.52	0.43
3:E:84:GLN:O	3:E:88:GLU:N	2.52	0.43
2:B:102:ASN:OD1	2:B:102:ASN:C	2.56	0.43
2:D:296:PHE:CE1	2:D:332:MET:CE	3.01	0.43
2:B:223:THR:OG1	2:B:226:ASP:OD1	2.36	0.43
1:A:270:ALA:O	1:A:302:MET:CB	2.67	0.43
2:D:238:VAL:CG1	7:D:700:K2N:HAJ	2.49	0.43
1:A:31:GLN:O	1:A:32:PRO:C	2.56	0.43
2:B:123:ARG:O	2:B:127:GLU:CB	2.66	0.43
1:C:83:TYR:O	1:C:84:ARG:C	2.57	0.43
1:A:83:TYR:O	1:A:85:GLN:N	2.51	0.43
2:D:268:PHE:N	2:D:268:PHE:CD2	2.83	0.43
1:A:428:LEU:C	1:A:430:LYS:N	2.72	0.43
2:D:8:GLN:OE1	2:D:14:ASN:ND2	2.52	0.43
1:A:88:HIS:O	1:A:89:PRO:C	2.56	0.43
1:A:388:TRP:O	1:A:392:ASP:CG	2.57	0.43
1:A:49:PHE:CD2	1:A:49:PHE:C	2.93	0.43
2:D:224:TYR:CD2	6:D:600:GDP:C5	3.06	0.42
2:D:158:ARG:C	2:D:160:GLU:N	2.71	0.42
3:E:112:ARG:O	3:E:114:ALA:N	2.51	0.42
1:C:212:ILE:O	1:C:216:ASN:N	2.52	0.42
2:D:31:ASP:C	2:D:33:THR:N	2.72	0.42
6:D:600:GDP:O2B	6:D:600:GDP:O1A	2.37	0.42
2:D:253:ARG:O	2:D:254:LYS:C	2.58	0.42
2:D:224:TYR:CE2	6:D:600:GDP:C5	3.07	0.42
1:C:239:THR:OG1	1:C:243:ARG:NH1	2.53	0.42
2:B:153:LEU:O	2:B:157:ILE:N	2.53	0.42
1:C:190:THR:O	1:C:192:HIS:N	2.53	0.42
2:D:133:GLN:NE2	2:D:252:LEU:CD2	2.83	0.42
1:A:183:GLU:CB	1:A:184:PRO:CD	2.98	0.42
1:A:190:THR:O	1:A:192:HIS:N	2.53	0.42
1:C:404:PHE:CE1	2:D:347:ILE:CG2	3.03	0.42
2:D:255:LEU:CD1	7:D:700:K2N:HAH	2.50	0.41
1:C:97:GLU:OE1	2:D:164:ARG:NH2	2.51	0.41
2:D:31:ASP:O	2:D:33:THR:N	2.53	0.41
1:C:256:GLN:O	1:C:259:LEU:N	2.52	0.41
1:A:87:PHE:N	1:A:87:PHE:CD2	2.88	0.41
2:B:200:GLU:OE2	2:B:268:PHE:CE1	2.73	0.41
1:C:224:TYR:CE2	4:C:600:GTP:C5	3.08	0.41
2:B:224:TYR:CD2	6:B:600:GDP:C5	3.09	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:298:SER:O	2:D:301:MET:N	2.53	0.41
1:C:49:PHE:CD2	1:C:49:PHE:C	2.94	0.41
2:B:296:PHE:CE1	2:B:332:MET:CE	3.03	0.41
1:A:309:HIS:C	1:A:309:HIS:ND1	2.73	0.41
2:D:192:HIS:C	2:D:192:HIS:ND1	2.74	0.41
1:A:224:TYR:CE2	4:A:600:GTP:C5	3.08	0.41
2:D:333:LEU:O	2:D:334:ASN:C	2.59	0.41
2:D:103:TRP:N	2:D:186:ASN:OD1	2.54	0.41
1:C:146:GLY:N	4:C:600:GTP:O1B	2.54	0.41
2:B:3:GLU:O	2:B:133:GLN:N	2.53	0.41
1:C:102:ASN:ND2	1:C:104:ALA:N	2.69	0.41
2:B:399:PHE:CE1	2:B:418:PHE:CB	3.03	0.41
2:D:414:ASP:OD1	2:D:415:GLU:N	2.54	0.41
2:B:164:ARG:CA	2:B:164:ARG:NE	2.83	0.41
2:D:194:LEU:O	2:D:196:GLU:N	2.54	0.41
1:A:267:PHE:CD1	1:A:267:PHE:N	2.89	0.41
1:A:347:CYS:O	1:A:348:PRO:C	2.59	0.41
3:E:123:LEU:O	3:E:127:ASP:N	2.54	0.40
2:D:319:PHE:CB	2:D:355:VAL:CG1	2.99	0.40
2:B:306:ASP:C	2:B:308:ARG:N	2.74	0.40
2:B:276:THR:CG2	2:B:277:SER:N	2.84	0.40
1:A:88:HIS:O	1:A:90:GLU:N	2.54	0.40
2:B:226:ASP:OD1	2:B:226:ASP:N	2.54	0.40
2:B:240:THR:O	2:B:243:ARG:N	2.54	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	424/451 (94%)	327 (77%)	65 (15%)	32 (8%)	2	30
1	C	423/451 (94%)	331 (78%)	62 (15%)	30 (7%)	2	32
2	B	416/445 (94%)	306 (74%)	74 (18%)	36 (9%)	1	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	425/445 (96%)	295 (69%)	84 (20%)	46 (11%)	1	17
3	E	119/142 (84%)	80 (67%)	25 (21%)	14 (12%)	1	14
All	All	1807/1934 (93%)	1339 (74%)	310 (17%)	158 (9%)	1	25

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	PRO
1	A	73	THR
1	A	112	LYS
1	A	265	ILE
1	A	341	ILE
1	A	348	PRO
1	A	377	MET
1	A	403	ALA
2	B	43	GLN
2	B	62	VAL
2	B	73	GLY
2	B	82	PRO
2	B	162	PRO
2	B	163	ASP
2	B	245	PRO
2	B	249	ASN
2	B	288	VAL
2	B	299	LYS
2	B	348	PRO
2	B	371	LEU
2	B	400	ARG
2	B	404	PHE
1	C	72	PRO
1	C	73	THR
1	C	112	LYS
1	C	257	THR
1	C	265	ILE
1	C	341	ILE
1	C	348	PRO
1	C	377	MET
1	C	403	ALA
1	C	437	VAL
2	D	43	GLN
2	D	62	VAL

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Mol	Chain	Res	Type
2	D	73	GLY
2	D	82	PRO
2	D	163	ASP
2	D	249	ASN
2	D	251	ASP
2	D	285	ALA
2	D	288	VAL
2	D	299	LYS
2	D	322	ARG
2	D	371	LEU
2	D	400	ARG
3	E	26	PRO
3	E	28	SER
3	E	49	GLU
3	E	82	VAL
3	E	102	ALA
1	A	83	TYR
1	A	84	ARG
1	A	162	GLY
1	A	164	LYS
1	A	247	ALA
1	A	284	GLU
1	A	350	GLY
1	A	392	ASP
1	A	402	ARG
1	A	429	GLU
1	A	437	VAL
2	B	3	GLU
2	B	34	GLY
2	B	42	LEU
2	B	60	LYS
2	B	115	VAL
2	B	226	ASP
2	B	227	LEU
2	B	264	ARG
2	B	273	ALA
2	B	276	THR
1	C	83	TYR
1	C	162	GLY
1	C	164	LYS
1	C	183	GLU
1	C	191	THR

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Mol	Chain	Res	Type
1	C	253	THR
1	C	429	GLU
2	D	3	GLU
2	D	34	GLY
2	D	42	LEU
2	D	115	VAL
2	D	162	PRO
2	D	227	LEU
2	D	244	PHE
2	D	245	PRO
2	D	264	ARG
2	D	402	LYS
2	D	404	PHE
3	E	12	ASN
3	E	75	LYS
3	E	81	GLU
3	E	124	GLN
1	A	32	PRO
1	A	48	SER
1	A	191	THR
1	A	273	ALA
1	A	279	GLU
2	B	244	PHE
2	B	307	PRO
2	B	322	ARG
2	B	403	ALA
1	C	32	PRO
1	C	245	ASP
1	C	273	ALA
1	C	301	GLN
2	D	158	ARG
2	D	195	VAL
2	D	265	LEU
2	D	278	ARG
2	D	293	GLN
2	D	348	PRO
2	D	403	ALA
2	D	437	ASP
3	E	5	ASP
3	E	46	SER
1	A	245	ASP
1	A	301	GLN

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Mol	Chain	Res	Type
1	A	364	PRO
1	C	84	ARG
1	C	141	PHE
1	C	220	GLU
2	D	59	ASN
2	D	60	LYS
2	D	129	CYS
2	D	226	ASP
2	D	273	ALA
2	D	409	THR
3	E	85	LYS
1	A	101	ASN
1	A	183	GLU
1	A	248	LEU
2	B	59	ASN
2	B	217	LEU
2	B	265	LEU
2	B	409	THR
1	C	402	ARG
2	D	240	THR
2	D	246	GLY
2	D	279	GLY
2	D	307	PRO
3	E	139	LEU
2	B	246	GLY
1	C	79	ARG
1	C	274	PRO
1	C	364	PRO
1	C	412	GLY
2	D	139	HIS
3	E	77	GLU
1	A	274	PRO
2	B	32	PRO
2	B	195	VAL
2	D	289	PRO
1	A	412	GLY
1	C	350	GLY
2	D	32	PRO
2	B	177	VAL
2	D	177	VAL

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	346/378 (92%)	243 (70%)	103 (30%)	0	5
1	C	344/378 (91%)	236 (69%)	108 (31%)	0	4
2	B	350/383 (91%)	217 (62%)	133 (38%)	0	1
2	D	353/383 (92%)	216 (61%)	137 (39%)	0	1
3	E	82/126 (65%)	40 (49%)	42 (51%)	0	0
All	All	1475/1648 (90%)	952 (64%)	523 (36%)	0	2

All (523) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	11	GLN
1	A	16	ILE
1	A	22	GLU
1	A	23	LEU
1	A	26	LEU
1	A	27	GLU
1	A	31	GLN
1	A	36	MET
1	A	49	PHE
1	A	60	LYS
1	A	61	HIS
1	A	62	VAL
1	A	68	VAL
1	A	70	LEU
1	A	73	THR
1	A	74	VAL
1	A	79	ARG
1	A	80	THR
1	A	84	ARG
1	A	88	HIS
1	A	92	LEU
1	A	94	THR
1	A	96	LYS
1	A	102	ASN

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Mol	Chain	Res	Type
1	A	105	ARG
1	A	110	ILE
1	A	114	ILE
1	A	115	ILE
1	A	119	LEU
1	A	120	ASP
1	A	123	ARG
1	A	124	LYS
1	A	140	SER
1	A	141	PHE
1	A	145	THR
1	A	153	LEU
1	A	155	GLU
1	A	157	LEU
1	A	158	SER
1	A	163	LYS
1	A	164	LYS
1	A	168	GLU
1	A	176	GLN
1	A	187	SER
1	A	191	THR
1	A	193	THR
1	A	194	THR
1	A	195	LEU
1	A	196	GLU
1	A	199	ASP
1	A	200	CYS
1	A	206	ASN
1	A	211	ASP
1	A	220	GLU
1	A	226	ASN
1	A	230	LEU
1	A	236	SER
1	A	237	SER
1	A	241	SER
1	A	242	LEU
1	A	245	ASP
1	A	248	LEU
1	A	255	PHE
1	A	256	GLN
1	A	257	THR
1	A	269	LEU

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Mol	Chain	Res	Type
1	A	271	THR
1	A	279	GLU
1	A	301	GLN
1	A	304	LYS
1	A	309	HIS
1	A	315	CYS
1	A	316	CYS
1	A	318	LEU
1	A	326	LYS
1	A	329	ASN
1	A	334	THR
1	A	341	ILE
1	A	343	PHE
1	A	347	CYS
1	A	349	THR
1	A	356	ASN
1	A	361	THR
1	A	363	VAL
1	A	368	LEU
1	A	370	LYS
1	A	371	VAL
1	A	372	GLN
1	A	377	MET
1	A	379	SER
1	A	380	ASN
1	A	384	ILE
1	A	386	GLU
1	A	397	LEU
1	A	401	LYS
1	A	402	ARG
1	A	405	VAL
1	A	413	MET
1	A	415	GLU
1	A	419	SER
1	A	420	GLU
1	A	433	GLU
2	B	3	GLU
2	B	4	ILE
2	B	5	VAL
2	B	16	ILE
2	B	24	ILE
2	B	25	SER

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Mol	Chain	Res	Type
2	B	27	GLU
2	B	39	ASP
2	B	42	LEU
2	B	43	GLN
2	B	48	ARG
2	B	51	VAL
2	B	55	GLU
2	B	61	TYR
2	B	62	VAL
2	B	68	VAL
2	B	70	LEU
2	B	71	GLU
2	B	78	VAL
2	B	80	SER
2	B	83	PHE
2	B	85	GLN
2	B	90	ASP
2	B	93	VAL
2	B	96	GLN
2	B	97	SER
2	B	101	ASN
2	B	102	ASN
2	B	109	THR
2	B	113	GLU
2	B	119	LEU
2	B	120	ASP
2	B	122	VAL
2	B	128	SER
2	B	129	CYS
2	B	130	ASP
2	B	131	CYS
2	B	132	LEU
2	B	133	GLN
2	B	135	PHE
2	B	137	LEU
2	B	145	THR
2	B	149	MET
2	B	151	THR
2	B	156	LYS
2	B	158	ARG
2	B	160	GLU
2	B	163	ASP

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Mol	Chain	Res	Type
2	B	164	ARG
2	B	165	ILE
2	B	166	MET
2	B	170	SER
2	B	174	SER
2	B	178	SER
2	B	179	ASP
2	B	181	VAL
2	B	188	THR
2	B	190	SER
2	B	195	VAL
2	B	196	GLU
2	B	200	GLU
2	B	209	LEU
2	B	212	ILE
2	B	214	PHE
2	B	215	ARG
2	B	216	THR
2	B	219	LEU
2	B	223	THR
2	B	227	LEU
2	B	230	LEU
2	B	239	THR
2	B	242	LEU
2	B	244	PHE
2	B	248	LEU
2	B	249	ASN
2	B	251	ASP
2	B	254	LYS
2	B	255	LEU
2	B	260	VAL
2	B	265	LEU
2	B	266	HIS
2	B	269	MET
2	B	275	LEU
2	B	276	THR
2	B	286	LEU
2	B	287	THR
2	B	291	LEU
2	B	293	GLN
2	B	294	GLN
2	B	295	MET

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Mol	Chain	Res	Type
2	B	300	ASN
2	B	308	ARG
2	B	309	HIS
2	B	313	LEU
2	B	318	VAL
2	B	323	MET
2	B	324	SER
2	B	325	MET
2	B	329	ASP
2	B	330	GLU
2	B	332	MET
2	B	335	VAL
2	B	339	ASN
2	B	341	SER
2	B	347	ILE
2	B	350	ASN
2	B	351	VAL
2	B	356	CYS
2	B	357	ASP
2	B	358	ILE
2	B	376	THR
2	B	380	ASN
2	B	384	ILE
2	B	387	LEU
2	B	389	LYS
2	B	390	ARG
2	B	391	ILE
2	B	393	GLU
2	B	394	GLN
2	B	398	MET
2	B	400	ARG
2	B	401	ARG
2	B	405	LEU
2	B	406	HIS
2	B	416	MET
2	B	417	GLU
2	B	419	THR
2	B	423	SER
2	B	425	MET
2	B	430	SER
2	B	432	TYR
2	B	434	GLN

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Mol	Chain	Res	Type
2	B	436	GLN
1	C	2	ARG
1	C	11	GLN
1	C	16	ILE
1	C	23	LEU
1	C	25	CYS
1	C	26	LEU
1	C	27	GLU
1	C	31	GLN
1	C	36	MET
1	C	38	SER
1	C	41	THR
1	C	49	PHE
1	C	61	HIS
1	C	62	VAL
1	C	68	VAL
1	C	73	THR
1	C	74	VAL
1	C	79	ARG
1	C	80	THR
1	C	84	ARG
1	C	88	HIS
1	C	92	LEU
1	C	94	THR
1	C	96	LYS
1	C	102	ASN
1	C	105	ARG
1	C	110	ILE
1	C	114	ILE
1	C	115	ILE
1	C	119	LEU
1	C	120	ASP
1	C	124	LYS
1	C	140	SER
1	C	141	PHE
1	C	145	THR
1	C	153	LEU
1	C	155	GLU
1	C	157	LEU
1	C	158	SER
1	C	160	ASP
1	C	163	LYS

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Mol	Chain	Res	Type
1	C	167	LEU
1	C	168	GLU
1	C	176	GLN
1	C	187	SER
1	C	191	THR
1	C	193	THR
1	C	194	THR
1	C	195	LEU
1	C	196	GLU
1	C	199	ASP
1	C	200	CYS
1	C	206	ASN
1	C	211	ASP
1	C	220	GLU
1	C	226	ASN
1	C	230	LEU
1	C	236	SER
1	C	237	SER
1	C	241	SER
1	C	242	LEU
1	C	245	ASP
1	C	248	LEU
1	C	250	VAL
1	C	251	ASP
1	C	252	LEU
1	C	254	GLU
1	C	256	GLN
1	C	257	THR
1	C	269	LEU
1	C	271	THR
1	C	293	ASN
1	C	301	GLN
1	C	304	LYS
1	C	309	HIS
1	C	313	MET
1	C	316	CYS
1	C	318	LEU
1	C	329	ASN
1	C	334	THR
1	C	341	ILE
1	C	343	PHE
1	C	344	VAL

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Mol	Chain	Res	Type
1	C	347	CYS
1	C	349	THR
1	C	356	ASN
1	C	361	THR
1	C	363	VAL
1	C	368	LEU
1	C	370	LYS
1	C	371	VAL
1	C	372	GLN
1	C	377	MET
1	C	379	SER
1	C	380	ASN
1	C	381	THR
1	C	384	ILE
1	C	386	GLU
1	C	394	LYS
1	C	397	LEU
1	C	401	LYS
1	C	402	ARG
1	C	405	VAL
1	C	413	MET
1	C	415	GLU
1	C	419	SER
1	C	420	GLU
1	C	438	ASP
2	D	4	ILE
2	D	5	VAL
2	D	16	ILE
2	D	24	ILE
2	D	25	SER
2	D	27	GLU
2	D	39	ASP
2	D	42	LEU
2	D	43	GLN
2	D	48	ARG
2	D	51	VAL
2	D	55	GLU
2	D	61	TYR
2	D	62	VAL
2	D	68	VAL
2	D	70	LEU
2	D	71	GLU

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Mol	Chain	Res	Type
2	D	76	ASP
2	D	78	VAL
2	D	80	SER
2	D	83	PHE
2	D	85	GLN
2	D	90	ASP
2	D	93	VAL
2	D	96	GLN
2	D	97	SER
2	D	101	ASN
2	D	102	ASN
2	D	109	THR
2	D	110	GLU
2	D	119	LEU
2	D	120	ASP
2	D	122	VAL
2	D	128	SER
2	D	129	CYS
2	D	130	ASP
2	D	131	CYS
2	D	132	LEU
2	D	133	GLN
2	D	137	LEU
2	D	145	THR
2	D	149	MET
2	D	151	THR
2	D	156	LYS
2	D	158	ARG
2	D	160	GLU
2	D	163	ASP
2	D	164	ARG
2	D	165	ILE
2	D	166	MET
2	D	168	THR
2	D	170	SER
2	D	174	SER
2	D	178	SER
2	D	179	ASP
2	D	181	VAL
2	D	188	THR
2	D	190	SER
2	D	196	GLU

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Mol	Chain	Res	Type
2	D	200	GLU
2	D	209	LEU
2	D	212	ILE
2	D	214	PHE
2	D	216	THR
2	D	223	THR
2	D	227	LEU
2	D	230	LEU
2	D	239	THR
2	D	242	LEU
2	D	244	PHE
2	D	248	LEU
2	D	249	ASN
2	D	251	ASP
2	D	254	LYS
2	D	255	LEU
2	D	260	VAL
2	D	265	LEU
2	D	275	LEU
2	D	280	SER
2	D	281	GLN
2	D	284	ARG
2	D	286	LEU
2	D	287	THR
2	D	291	LEU
2	D	293	GLN
2	D	295	MET
2	D	299	LYS
2	D	300	ASN
2	D	308	ARG
2	D	309	HIS
2	D	311	ARG
2	D	313	LEU
2	D	318	VAL
2	D	320	ARG
2	D	323	MET
2	D	324	SER
2	D	325	MET
2	D	329	ASP
2	D	330	GLU
2	D	332	MET
2	D	333	LEU

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Mol	Chain	Res	Type
2	D	335	VAL
2	D	337	ASN
2	D	339	ASN
2	D	341	SER
2	D	344	VAL
2	D	347	ILE
2	D	350	ASN
2	D	351	VAL
2	D	356	CYS
2	D	357	ASP
2	D	358	ILE
2	D	371	LEU
2	D	372	LYS
2	D	373	MET
2	D	376	THR
2	D	380	ASN
2	D	384	ILE
2	D	387	LEU
2	D	391	ILE
2	D	393	GLU
2	D	394	GLN
2	D	398	MET
2	D	400	ARG
2	D	401	ARG
2	D	405	LEU
2	D	408	TYR
2	D	413	MET
2	D	415	GLU
2	D	416	MET
2	D	417	GLU
2	D	419	THR
2	D	423	SER
2	D	425	MET
2	D	430	SER
2	D	434	GLN
2	D	436	GLN
3	E	5	ASP
3	E	6	MET
3	E	15	THR
3	E	16	SER
3	E	21	GLU
3	E	22	VAL

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Mol	Chain	Res	Type
3	E	24	LEU
3	E	28	SER
3	E	51	GLN
3	E	53	LYS
3	E	61	ARG
3	E	62	LYS
3	E	64	GLN
3	E	65	GLU
3	E	67	GLU
3	E	69	LEU
3	E	70	LYS
3	E	76	ARG
3	E	77	GLU
3	E	78	HIS
3	E	80	ARG
3	E	81	GLU
3	E	84	GLN
3	E	87	ILE
3	E	89	GLU
3	E	91	ASN
3	E	92	ASN
3	E	94	ILE
3	E	96	MET
3	E	99	GLU
3	E	106	GLU
3	E	109	LYS
3	E	111	ASN
3	E	112	ARG
3	E	113	GLU
3	E	115	HIS
3	E	119	MET
3	E	120	LEU
3	E	125	GLU
3	E	126	LYS
3	E	129	HIS
3	E	136	ASN

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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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$
4	GTP	A	600	5	34,34,34	0.99	1 (2%)	51,54,54	2.57	11 (21%)
6	GDP	B	600	-	30,30,30	1.04	1 (3%)	44,47,47	2.17	10 (22%)
7	K2N	B	700	-	26,26,26	1.57	2 (7%)	36,36,36	2.65	11 (30%)
4	GTP	C	600	5	34,34,34	1.17	1 (2%)	51,54,54	1.91	14 (27%)
6	GDP	D	600	-	30,30,30	1.08	1 (3%)	44,47,47	3.15	13 (29%)
7	K2N	D	700	-	26,26,26	1.82	4 (15%)	36,36,36	2.45	10 (27%)

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
4	GTP	A	600	5	-	0/22/38/38	0/1/3/3
6	GDP	B	600	-	-	0/16/32/32	0/1/3/3
7	K2N	B	700	-	-	0/11/23/23	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	C	600	5	-	0/22/38/38	0/1/3/3
6	GDP	D	600	-	-	0/16/32/32	0/1/3/3
7	K2N	D	700	-	-	0/11/23/23	0/1/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	700	K2N	CAS-CAR	-6.41	1.38	1.48
7	B	700	K2N	CAS-CAR	-6.04	1.38	1.48
6	D	600	GDP	C2-N3	4.21	1.38	1.33
4	C	600	GTP	C2-N3	4.19	1.38	1.33
6	B	600	GDP	C2-N3	3.51	1.37	1.33
7	D	700	K2N	CAR-NAL	3.22	1.35	1.30
7	B	700	K2N	CAU-NAN	-2.57	1.35	1.40
7	D	700	K2N	CAU-NAM	2.24	1.38	1.34
7	D	700	K2N	CAT-NAM	2.21	1.38	1.35
4	A	600	GTP	O4'-C4'	-2.21	1.39	1.45

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	600	GDP	C6-C5-N7	-17.10	131.84	134.14
4	A	600	GTP	C6-C5-N7	-12.97	132.39	134.14
7	B	700	K2N	CAK-OAP-CAQ	-7.85	100.84	116.09
7	D	700	K2N	CAK-OAP-CAQ	-7.38	101.74	116.09
6	B	600	GDP	C6-C5-N7	-7.19	133.17	134.14
7	B	700	K2N	OAP-CAQ-NAN	6.87	122.47	109.37
4	C	600	GTP	PB-O3B-PG	-6.40	112.93	131.68
4	C	600	GTP	C6-C5-N7	-5.77	133.36	134.14
7	D	700	K2N	NAN-CAU-NAM	5.66	126.27	113.21
6	B	600	GDP	O4'-C1'-N9	5.54	113.59	108.44
4	A	600	GTP	O4'-C1'-N9	5.38	113.44	108.44
7	D	700	K2N	NAC-CAT-NAM	4.98	124.11	116.88
4	A	600	GTP	PB-O3B-PG	-4.83	117.51	131.68
7	B	700	K2N	CAB-CAX-NAO	-4.76	104.47	110.22
7	B	700	K2N	OAP-CAQ-OAD	-4.56	114.21	124.19
4	A	600	GTP	C5-C4-N3	-4.50	119.42	125.94
6	B	600	GDP	N2-C2-N3	-4.49	114.21	120.30
6	D	600	GDP	PA-O3A-PB	-4.45	118.64	131.68
6	D	600	GDP	N3-C4-N9	4.39	133.35	126.91
4	A	600	GTP	C2-N3-C4	4.38	121.24	115.09
6	D	600	GDP	C2-N3-C4	4.18	120.96	115.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	600	GDP	C5-C4-N3	-4.11	119.98	125.94
7	D	700	K2N	CAH-CAS-CAR	-4.07	115.92	120.74
7	B	700	K2N	NAC-CAT-NAM	4.04	122.74	116.88
6	B	600	GDP	C5-C4-N3	-3.96	120.20	125.94
4	A	600	GTP	N2-C2-N1	3.93	122.19	117.86
6	B	600	GDP	C2-N3-C4	3.88	120.54	115.09
4	C	600	GTP	C2-N3-C4	3.85	120.50	115.09
7	B	700	K2N	CAW-CAT-NAC	-3.65	116.11	123.52
7	B	700	K2N	CAI-CAS-CAR	3.46	124.84	120.74
7	D	700	K2N	CAJ-CAU-NAM	-3.39	115.49	123.41
4	A	600	GTP	N3-C4-N9	3.39	131.88	126.91
4	C	600	GTP	N3-C4-N9	3.34	131.81	126.91
7	B	700	K2N	CAH-CAS-CAR	-3.30	116.83	120.74
6	B	600	GDP	N3-C4-N9	3.22	131.63	126.91
7	D	700	K2N	CAW-CAT-NAC	-3.20	117.02	123.52
6	B	600	GDP	PA-O3A-PB	-3.13	122.51	131.68
7	D	700	K2N	OAP-CAQ-NAN	3.11	115.32	109.37
4	C	600	GTP	C5-C4-N3	-3.08	121.47	125.94
4	C	600	GTP	C4'-O4'-C1'	-3.06	106.42	109.75
7	B	700	K2N	CAJ-CAU-NAM	-2.88	116.68	123.41
6	B	600	GDP	C4-C5-N7	-2.87	107.06	109.52
4	C	600	GTP	C8-N9-C4	2.86	109.08	106.90
4	A	600	GTP	PA-O3A-PB	-2.82	123.42	131.68
4	A	600	GTP	C4-C5-N7	-2.80	107.12	109.52
6	D	600	GDP	O4'-C1'-N9	-2.61	106.01	108.44
4	C	600	GTP	N7-C8-N9	-2.54	107.18	114.36
4	C	600	GTP	N2-C2-N1	2.53	120.65	117.86
6	B	600	GDP	C3'-C2'-C1'	2.53	104.86	100.91
6	D	600	GDP	N7-C8-N9	-2.51	107.26	114.36
6	D	600	GDP	C4-C5-N7	-2.43	107.44	109.52
7	D	700	K2N	CAU-NAM-CAT	2.40	124.95	118.25
6	D	600	GDP	N2-C2-N3	-2.37	117.09	120.30
4	A	600	GTP	N2-C2-N3	-2.34	117.13	120.30
4	C	600	GTP	C1'-N9-C4	-2.33	122.60	126.64
7	D	700	K2N	CAU-NAN-CAQ	2.29	133.60	127.47
4	C	600	GTP	N1-C2-N3	-2.28	118.58	121.78
6	D	600	GDP	N1-C2-N3	-2.24	118.64	121.78
4	C	600	GTP	C3'-C2'-C1'	-2.22	97.43	100.91
7	D	700	K2N	CAB-CAX-NAO	-2.20	107.56	110.22
6	D	600	GDP	C8-N9-C4	2.13	108.53	106.90
4	C	600	GTP	C4-C5-N7	-2.12	107.71	109.52
6	D	600	GDP	C8-N7-C5	2.10	110.09	103.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	GTP	N7-C8-N9	-2.09	108.45	114.36
4	C	600	GTP	PA-O3A-PB	-2.09	125.56	131.68
7	B	700	K2N	CAU-NAM-CAT	2.07	124.02	118.25
6	B	600	GDP	N7-C8-N9	-2.05	108.56	114.36
7	B	700	K2N	CAU-NAN-CAQ	2.05	132.95	127.47
6	D	600	GDP	C2'-C1'-N9	-2.01	108.11	113.27

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(Å ²)	Q<0.9
1	A	428/451 (94%)	0.22	8 (1%) 64 49	173, 213, 260, 322	0
1	C	429/451 (95%)	0.23	8 (1%) 64 49	190, 236, 318, 350	0
2	B	420/445 (94%)	0.22	9 (2%) 60 47	176, 220, 277, 315	0
2	D	427/445 (95%)	0.29	13 (3%) 48 38	189, 246, 315, 389	0
3	E	123/142 (86%)	0.45	3 (2%) 56 43	216, 250, 323, 363	0
All	All	1827/1934 (94%)	0.26	41 (2%) 59 46	173, 229, 306, 389	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	30	ASP	3.3
2	D	210	TYR	3.3
2	D	143	GLY	3.2
1	C	367	ASP	3.2
1	C	143	GLY	3.1
2	B	286	LEU	3.0
2	D	55	GLU	2.9
3	E	4	ALA	2.8
2	D	39	ASP	2.8
2	D	144	GLY	2.8
2	B	373	MET	2.8
1	A	413	MET	2.6
1	A	132	LEU	2.6
2	B	143	GLY	2.5
1	C	201	ALA	2.5
2	D	94	PHE	2.5
1	C	220	GLU	2.5
2	D	286	LEU	2.5
1	A	142	GLY	2.5
1	C	232	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	264	ARG	2.4
1	A	161	TYR	2.4
2	B	159	GLU	2.3
1	C	203	MET	2.3
1	A	376	CYS	2.3
3	E	65	GLU	2.2
1	C	96	LYS	2.2
2	D	279	GLY	2.2
2	D	213	CYS	2.2
1	A	203	MET	2.2
2	B	226	ASP	2.2
1	A	143	GLY	2.2
2	B	201	THR	2.1
2	D	271	GLY	2.1
1	C	237	SER	2.1
2	B	142	GLY	2.1
2	B	275	LEU	2.0
1	A	2	ARG	2.0
2	B	170	SER	2.0
2	D	168	THR	2.0
2	D	221	THR	2.0

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
5	MG	B	601	1/1	0.46	1.98	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	K2N	B	700	24/24	0.38	1.17	61,64,68,71	0
7	K2N	D	700	24/24	0.31	-0.05	71,74,80,81	0
6	GDP	D	600	28/28	0.30	-0.29	64,67,68,69	0
6	GDP	B	600	28/28	0.24	-0.71	64,67,68,68	0
4	GTP	C	600	32/32	0.21	-0.75	55,64,66,66	0
4	GTP	A	600	32/32	0.17	-0.97	61,65,66,66	0
5	MG	C	601	1/1	0.09	-1.31	43,43,43,43	0
5	MG	A	601	1/1	0.05	-1.99	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.