



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:29 pm BST

PDB ID : 2BTE  
Title : Thermus thermophilus Leucyl-tRNA synthetase complexed with a tRNA<sup>Leu</sup> transcript in the post-editing conformation and a post-transfer editing substrate analogue  
Authors : Cusack, S.; Tukalo, M.; Yaremchuk, A.; Fukunaga, R.; Yokoyama, S.  
Deposited on : 2005-05-31  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

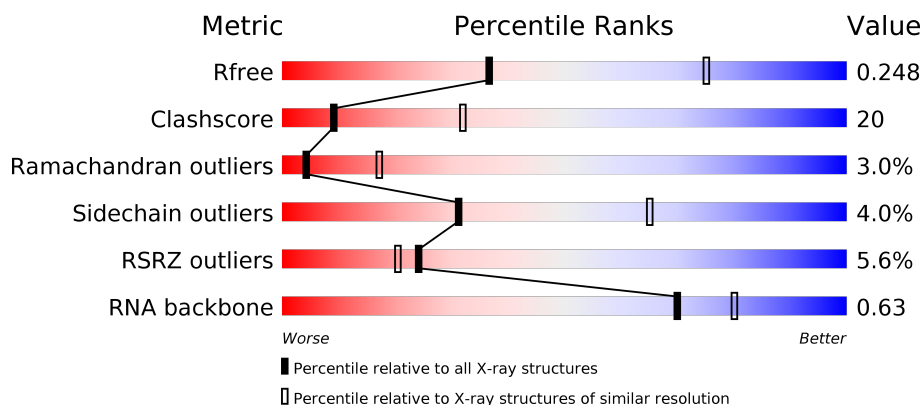
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	878	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>37%</div> <div>.</div> </div> </div>
1	D	878	<div> <div>8%</div> <div> <div></div> <div>58%</div> <div>38%</div> <div>.</div> </div> </div>
2	B	83	<div> <div>5%</div> <div> <div></div> <div>42%</div> <div>34%</div> <div>17%</div> <div>6%</div> </div> </div>
2	E	83	<div> <div>6%</div> <div> <div></div> <div>46%</div> <div>40%</div> <div>7%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17815 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AMINOACYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	876	Total	C	N	O	S	0	0	0
			7122	4593	1223	1275	31			
1	D	876	Total	C	N	O	S	0	0	0
			7122	4593	1223	1275	31			

- Molecule 2 is a RNA chain called TRNALEU TRANSCRIPT WITH ANTICODON CAG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	P	0	0	0
			1676	745	309	544	78			
2	E	78	Total	C	N	O	P	0	0	0
			1676	745	309	544	78			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		

- Molecule 4 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Hg	0	0
			1	1		
4	D	1	Total	Hg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



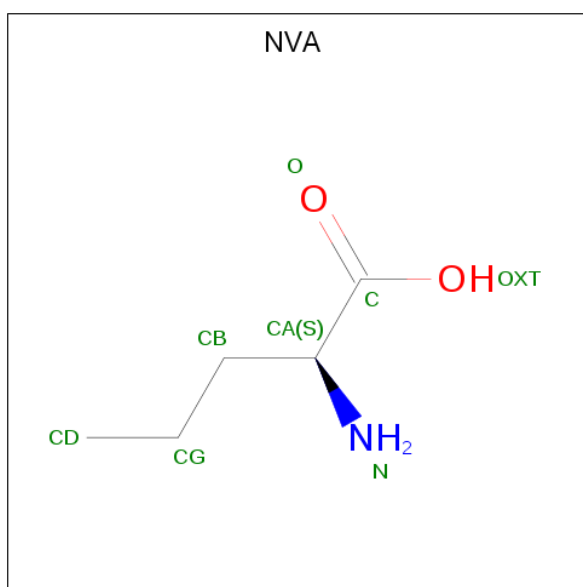
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total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

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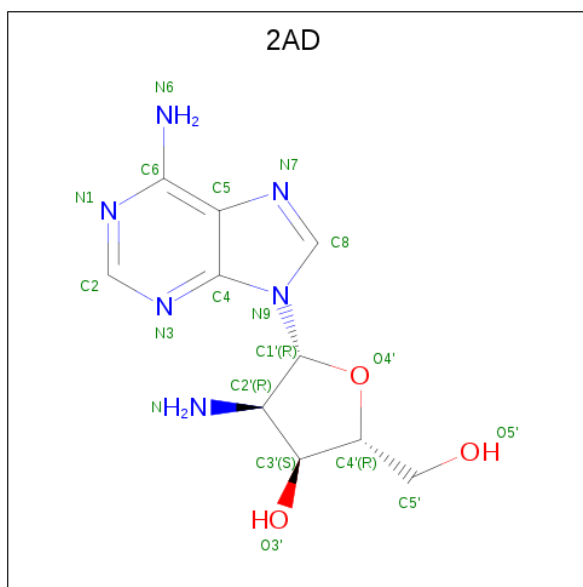
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is NORVALINE (three-letter code: NVA) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



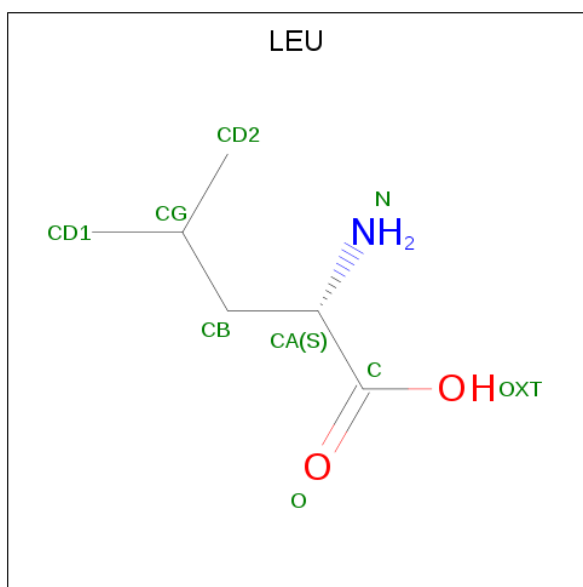
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			7	5	1	1		
6	D	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 7 is 2'-AMINO-2'-DEOXYADENOSINE (three-letter code: 2AD) (formula:  $C_{10}H_{14}N_6O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			19	10	6	3		
7	D	1	Total	C	N	O	0	0
			19	10	6	3		

- Molecule 8 is LEUCINE (three-letter code: LEU) (formula:  $C_6H_{13}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	6	1	2		
8	D	1	Total	C	N	O	0	0
			9	6	1	2		

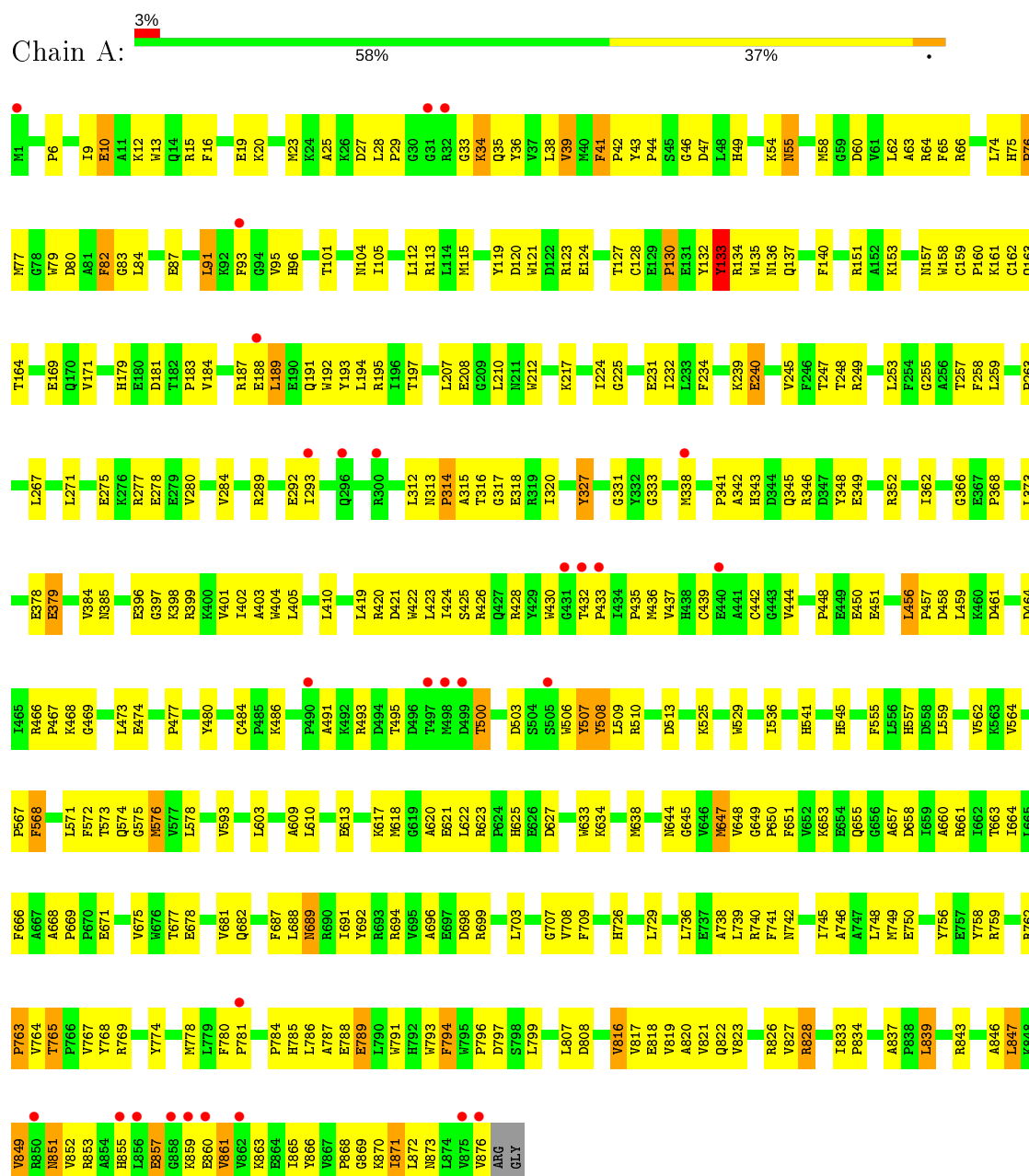
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	8	Total	O	0	0
			8	8		
9	B	5	Total	O	0	0
			5	5		
9	D	1	Total	O	0	0
			1	1		
9	E	4	Total	O	0	0
			4	4		

### 3 Residue-property plots

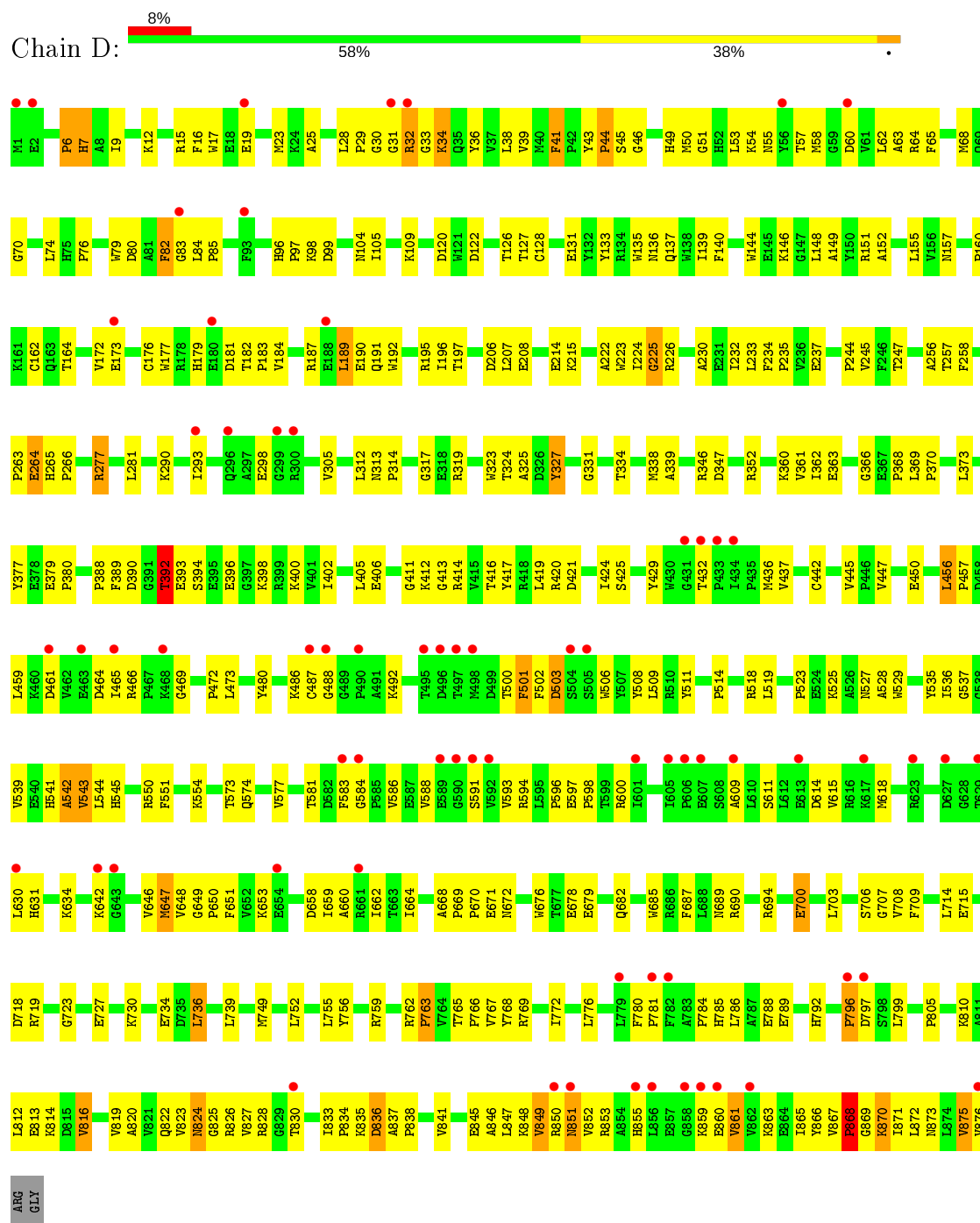
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

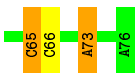
#### • Molecule 1: AMINOACYL-TRNA SYNTHETASE



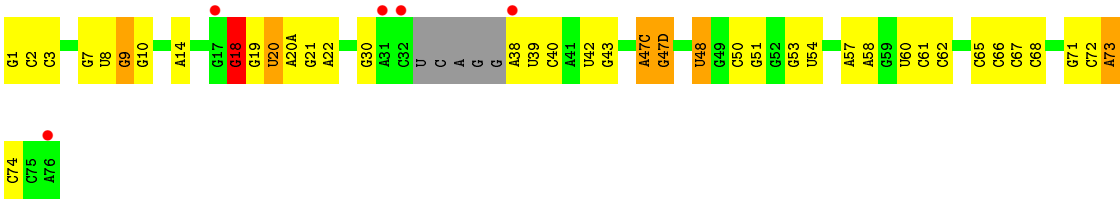


• Molecule 1: AMINOACYL-TRNA SYNTHETASE





● Molecule 2: TRNALEU TRANSCRIPT WITH ANTICODON CAG



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.12Å 125.70Å 175.43Å 90.00° 120.86° 90.00°	Depositor
Resolution (Å)	24.89 – 2.90 24.89 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.6 (24.89-2.90) 93.7 (24.89-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.217 , 0.253 0.218 , 0.248	Depositor DCC
$R_{free}$ test set	2369 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 81.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HG, 2AD, ZN, NVA, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.48	0/7327	0.65	0/9945
1	D	0.38	0/7327	0.54	0/9945
2	B	0.63	1/1873 (0.1%)	0.83	5/2917 (0.2%)
2	E	0.58	1/1873 (0.1%)	0.76	3/2917 (0.1%)
All	All	0.48	2/18400 (0.0%)	0.65	8/25724 (0.0%)

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	2
2	B	0	4
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	G	OP3-P	-7.19	1.52	1.61
2	E	1	G	OP3-P	-6.97	1.52	1.61

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	G	N9-C1'-C2'	10.60	127.78	114.00
2	B	48	U	C5'-C4'-C3'	-7.96	103.26	116.00
2	B	65	C	O4'-C1'-N1	6.01	113.01	108.20
2	E	21	G	N9-C1'-C2'	5.82	121.57	114.00
2	E	18	G	C2'-C3'-O3'	5.34	122.25	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47(F)	G	OP2-P-O3'	5.22	116.69	105.20
2	E	9	G	N9-C1'-C2'	5.17	120.73	114.00
2	B	53	G	O4'-C1'-N9	5.14	112.32	108.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	TYR	Sidechain
1	A	507	TYR	Sidechain
2	B	14	A	Sidechain
2	B	21	G	Sidechain
2	B	24	G	Sidechain
2	B	47(D)	G	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7122	0	7031	317	0
1	D	7122	0	7031	290	0
2	B	1676	0	849	34	0
2	E	1676	0	849	38	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	60	0	0	0	0
5	D	65	0	0	0	0
6	A	7	0	10	2	0
6	D	7	0	10	0	0
7	A	19	0	12	3	0
7	D	19	0	12	1	0
8	A	9	0	10	0	0
8	D	9	0	10	1	0
9	A	8	0	0	1	0
9	B	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	1	0	0	0	0
9	E	4	0	0	0	0
All	All	17815	0	15824	672	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (672) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:826:ARG:HB2	1:D:828:ARG:HH21	1.12	1.08
1:D:826:ARG:HB2	1:D:828:ARG:NH2	1.80	0.96
1:D:851:ASN:HD22	1:D:853:ARG:HG3	1.30	0.94
1:D:62:LEU:HD11	1:D:739:LEU:HD11	1.47	0.93
1:A:839:LEU:H	1:A:839:LEU:HD12	1.33	0.92
1:A:687:PHE:O	1:A:691:ILE:HG13	1.72	0.89
1:A:821:VAL:HG13	1:A:872:LEU:HD23	1.56	0.88
1:D:870:LYS:O	1:D:871:ILE:HD12	1.75	0.87
1:A:688:LEU:HA	1:A:691:ILE:HD12	1.57	0.86
1:D:852:VAL:HG12	1:D:855:HIS:HB2	1.57	0.86
1:D:679:GLU:HA	1:D:682:GLN:HE21	1.40	0.86
1:D:649:GLY:O	1:D:653:LYS:HG2	1.74	0.86
1:A:183:PRO:HB3	1:A:293:ILE:HD12	1.60	0.83
1:D:277:ARG:HH11	1:D:277:ARG:HB2	1.45	0.80
1:D:581:THR:HG21	1:D:642:LYS:HD2	1.62	0.79
1:D:824:ASN:HD21	1:D:876:VAL:HB	1.46	0.79
2:B:47(C):A:H5'	2:B:47(D):G:OP2	1.84	0.78
1:D:39:VAL:HG12	1:D:536:ILE:HB	1.65	0.78
1:D:34:LYS:HD2	1:D:34:LYS:C	2.04	0.78
1:A:726:HIS:HD2	1:A:808:ASP:H	1.28	0.78
1:A:823:VAL:HG23	1:A:828:ARG:HG3	1.65	0.77
1:D:189:LEU:HD22	1:D:191:GLN:HE21	1.49	0.77
1:D:224:ILE:HA	1:D:419:LEU:HB2	1.67	0.77
2:E:14:A:H1'	2:E:22:A:N7	2.01	0.76
1:A:331:GLY:HA3	1:A:420:ARG:HH22	1.50	0.76
1:A:726:HIS:CD2	1:A:808:ASP:H	2.03	0.76
1:D:83:GLY:HA3	1:D:500:THR:HB	1.67	0.75
1:A:823:VAL:HB	1:A:828:ARG:HD2	1.67	0.75
1:A:248:THR:HG23	7:A:1893:2AD:H5'1	1.67	0.75
1:A:82:PHE:CD2	1:A:128:CYS:HA	2.22	0.74
1:D:189:LEU:HD23	1:D:190:GLU:H	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:GLU:H	1:D:450:GLU:CD	1.91	0.74
1:D:687:PHE:CE1	1:D:749:MET:HG2	2.23	0.74
1:A:817:VAL:CG1	1:A:870:LYS:HE2	2.19	0.73
1:A:439:CYS:HB2	1:A:484:CYS:HB2	1.70	0.73
1:D:647:MET:HB3	1:D:650:PRO:HD2	1.69	0.73
1:A:774:TYR:O	1:A:778:MET:HG3	1.89	0.72
1:A:474:GLU:OE2	1:A:495:THR:HG21	1.88	0.72
2:E:7:G:H3'	2:E:8:U:H5'	1.69	0.72
1:D:863:LYS:HE2	1:D:865:ILE:HD11	1.72	0.72
1:A:780:PHE:HB3	1:A:781:PRO:HD3	1.69	0.72
1:A:765:THR:OG1	1:A:767:VAL:HG12	1.91	0.71
2:E:18:G:N2	2:E:57:A:H2'	2.05	0.71
1:A:822:GLN:HB3	1:A:827:VAL:HA	1.71	0.71
7:D:1895:2AD:H5'1	2:E:74:C:H5''	1.72	0.71
1:A:457:PRO:HG2	1:A:473:LEU:HD22	1.72	0.71
1:A:819:VAL:HG22	1:A:870:LYS:HA	1.70	0.71
1:A:852:VAL:HG12	1:A:855:HIS:HB2	1.72	0.70
1:D:700:GLU:HA	1:D:703:LEU:HD12	1.73	0.70
1:A:187:ARG:HH11	1:A:187:ARG:HG3	1.55	0.70
1:D:406:GLU:HG2	1:D:412:LYS:HA	1.72	0.70
1:A:677:THR:O	1:A:681:VAL:HG23	1.92	0.70
1:A:823:VAL:CG2	1:A:828:ARG:HG3	2.21	0.70
1:D:823:VAL:CG2	1:D:828:ARG:HD2	2.22	0.69
1:D:537:GLY:O	1:D:573:THR:HA	1.93	0.69
2:E:66:C:H2'	2:E:67:C:H6	1.57	0.69
1:A:817:VAL:HG12	1:A:818:GLU:H	1.58	0.69
1:D:851:ASN:HD22	1:D:853:ARG:CG	2.05	0.69
1:A:647:MET:HB3	1:A:650:PRO:HD2	1.75	0.68
1:A:189:LEU:HD22	1:A:191:GLN:NE2	2.08	0.68
1:A:609:ALA:O	1:A:610:LEU:HD23	1.92	0.68
1:A:823:VAL:HB	1:A:828:ARG:CD	2.24	0.68
1:D:392:THR:HG22	1:D:393:GLU:H	1.58	0.67
1:A:658:ASP:OD2	1:A:785:HIS:HB2	1.94	0.67
1:A:456:LEU:HD23	1:A:457:PRO:HD2	1.77	0.67
1:D:849:VAL:HG23	1:D:852:VAL:HA	1.75	0.67
1:A:846:ALA:O	1:A:849:VAL:HG13	1.94	0.67
1:A:870:LYS:O	1:A:871:ILE:HD12	1.95	0.67
1:D:709:PHE:CE2	1:D:714:LEU:HD11	2.30	0.67
1:D:860:GLU:HB2	1:D:876:VAL:HG13	1.77	0.67
1:D:338:MET:O	1:D:338:MET:HG3	1.94	0.66
1:D:851:ASN:ND2	1:D:853:ARG:HG3	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:GLU:H	1:A:240:GLU:CD	1.99	0.66
1:D:823:VAL:HG23	1:D:828:ARG:HD2	1.78	0.66
1:A:249:ARG:HG3	6:A:1892:NVA:HD1	1.78	0.66
1:A:450:GLU:H	1:A:450:GLU:CD	1.98	0.66
1:D:55:ASN:ND2	1:D:574:GLN:HG3	2.10	0.66
1:A:41:PHE:HD1	1:A:41:PHE:O	1.79	0.66
1:A:194:LEU:HD11	1:A:424:ILE:HD13	1.78	0.65
1:A:331:GLY:HA3	1:A:420:ARG:NH2	2.10	0.65
1:D:851:ASN:HB2	1:D:853:ARG:HG3	1.78	0.65
1:D:9:ILE:O	1:D:12:LYS:HB3	1.97	0.65
1:A:75:HIS:NE2	9:A:2003:HOH:O	2.26	0.65
1:D:861:VAL:HA	1:D:876:VAL:HA	1.79	0.65
2:E:66:C:H2'	2:E:67:C:C6	2.32	0.65
1:A:192:TRP:HB2	1:A:425:SER:HB3	1.79	0.65
1:D:816:VAL:HA	1:D:834:PRO:HA	1.79	0.65
1:A:507:TYR:O	1:A:510:ARG:N	2.30	0.64
1:A:572:PHE:CD1	1:A:573:THR:N	2.65	0.64
1:A:839:LEU:HD12	1:A:839:LEU:N	2.08	0.64
1:A:823:VAL:CB	1:A:828:ARG:HG3	2.28	0.64
1:A:466:ARG:HD3	1:A:468:LYS:NZ	2.13	0.64
1:A:162:CYS:HB3	1:A:164:THR:HG22	1.80	0.63
1:D:523:PRO:O	1:D:527:ASN:ND2	2.31	0.63
1:A:649:GLY:O	1:A:653:LYS:HG2	1.99	0.63
1:D:752:LEU:HA	1:D:755:LEU:HD12	1.79	0.63
1:D:105:ILE:O	1:D:109:LYS:HB2	1.99	0.63
1:D:814:LYS:O	1:D:835:LYS:HE3	1.98	0.63
1:A:750:GLU:OE1	2:B:23:C:H5'	1.99	0.63
1:D:162:CYS:SG	1:D:179:HIS:HE1	2.21	0.63
1:D:660:ALA:O	1:D:664:ILE:HG13	1.99	0.63
1:A:82:PHE:HE2	1:A:133:TYR:CD1	2.17	0.63
1:D:195:ARG:HA	1:D:421:ASP:OD1	1.99	0.63
1:A:623:ARG:HD2	1:A:633:TRP:CD1	2.34	0.62
1:D:574:GLN:HE21	1:D:574:GLN:HA	1.65	0.62
1:D:588:VAL:HG22	1:D:593:VAL:HG13	1.81	0.62
1:A:83:GLY:HA3	1:A:500:THR:HB	1.82	0.62
1:A:833:ILE:HD13	1:A:837:ALA:HB3	1.81	0.62
1:A:38:LEU:HD12	1:A:39:VAL:N	2.15	0.62
1:A:745:ILE:HG22	1:A:749:MET:HE3	1.80	0.62
1:A:819:VAL:HG13	1:A:870:LYS:C	2.20	0.62
1:D:263:PRO:HD3	1:D:325:ALA:O	2.01	0.61
2:E:20:U:O2'	2:E:20(A):A:H5'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:833:ILE:HD13	1:D:837:ALA:HB3	1.81	0.61
1:A:29:PRO:HG3	1:A:529:TRP:CZ2	2.34	0.61
1:D:23:MET:CE	1:D:63:ALA:HB1	2.30	0.61
1:D:709:PHE:HE2	1:D:714:LEU:HD11	1.63	0.61
1:A:157:ASN:HB3	1:A:184:VAL:HG11	1.82	0.61
1:A:169:GLU:OE1	1:A:169:GLU:N	2.32	0.61
1:D:759:ARG:HD3	1:D:768:TYR:CE1	2.36	0.61
1:D:456:LEU:HD23	1:D:457:PRO:HD2	1.83	0.60
1:D:394:SER:O	1:D:398:LYS:HG3	2.00	0.60
1:A:41:PHE:CE1	1:A:80:ASP:HB2	2.37	0.60
1:A:668:ALA:HB1	1:A:669:PRO:CD	2.31	0.60
2:E:47(C):A:H5'	2:E:47(D):G:OP2	2.01	0.60
1:D:136:ASN:HD21	1:D:506:TRP:HE1	1.49	0.60
1:D:28:LEU:HD21	1:D:525:LYS:HG2	1.81	0.60
1:D:55:ASN:HD21	1:D:574:GLN:HB2	1.66	0.60
1:A:263:PRO:O	1:A:284:VAL:HG13	2.02	0.60
1:D:668:ALA:HB1	1:D:669:PRO:CD	2.32	0.59
1:A:255:GLY:O	1:A:257:THR:HG23	2.01	0.59
1:D:678:GLU:O	1:D:682:GLN:HG3	2.02	0.59
1:D:780:PHE:HB3	1:D:781:PRO:HD3	1.84	0.59
1:A:484:CYS:SG	1:A:486:LYS:HB3	2.42	0.59
1:D:277:ARG:NH1	1:D:277:ARG:HB2	2.16	0.59
2:E:50:C:H2'	2:E:51:G:H8	1.67	0.59
2:E:65:C:O2'	2:E:66:C:H5'	2.02	0.59
1:A:43:TYR:CE1	1:A:80:ASP:OD2	2.56	0.59
1:A:707:GLY:N	1:A:769:ARG:HD3	2.17	0.59
1:D:694:ARG:HD2	1:D:756:TYR:CE1	2.38	0.59
2:E:14:A:H1'	2:E:22:A:C5	2.37	0.59
1:A:764:VAL:O	1:A:764:VAL:HG12	2.03	0.58
1:D:82:PHE:CD2	1:D:128:CYS:HA	2.37	0.58
1:D:668:ALA:HB1	1:D:669:PRO:HD2	1.85	0.58
1:D:816:VAL:HG22	1:D:834:PRO:HG3	1.84	0.58
1:A:9:ILE:HG21	1:A:789:GLU:HG2	1.85	0.58
1:A:863:LYS:HE2	1:A:865:ILE:HD11	1.85	0.58
1:A:817:VAL:HG11	1:A:870:LYS:HE2	1.84	0.58
2:E:42:U:H2'	2:E:43:G:H8	1.69	0.58
1:A:466:ARG:HH11	1:A:468:LYS:HZ1	1.52	0.58
1:D:869:GLY:C	1:D:870:LYS:HD3	2.24	0.58
1:A:663:THR:HG22	1:A:663:THR:O	2.03	0.58
2:B:47(D):G:O2'	2:B:47(E):C:H5'	2.03	0.58
1:A:816:VAL:H	1:A:834:PRO:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:511:TYR:O	1:D:514:PRO:HD3	2.02	0.57
2:E:7:G:H3'	2:E:8:U:C5'	2.33	0.57
1:A:79:TRP:CE2	1:A:105:ILE:HG23	2.39	0.57
1:A:817:VAL:HG12	1:A:870:LYS:HE2	1.87	0.57
1:A:826:ARG:HD3	1:A:828:ARG:HH21	1.69	0.57
1:D:51:GLY:HA2	1:D:577:VAL:HB	1.85	0.57
1:D:823:VAL:HB	1:D:828:ARG:CZ	2.33	0.57
1:A:46:GLY:N	1:A:104:ASN:HD21	2.03	0.57
1:A:651:PHE:CZ	1:A:655:GLN:HG3	2.40	0.57
1:A:426:ARG:HG2	1:A:426:ARG:HH11	1.69	0.57
1:A:826:ARG:HD3	1:A:828:ARG:NH2	2.20	0.57
1:A:93:PHE:O	1:A:95:VAL:HG23	2.04	0.57
1:D:327:TYR:CE1	1:D:346:ARG:HD3	2.40	0.57
1:D:256:ALA:HB2	1:D:338:MET:HE3	1.85	0.56
1:A:437:VAL:HG12	1:A:491:ALA:HB1	1.86	0.56
1:A:195:ARG:HA	1:A:421:ASP:OD1	2.06	0.56
1:D:172:VAL:HG12	1:D:173:GLU:HG3	1.88	0.56
1:A:112:LEU:HD13	1:A:119:TYR:HE2	1.70	0.56
1:A:258:PHE:HA	1:A:320:ILE:HB	1.86	0.56
1:A:338:MET:HG3	1:A:338:MET:O	2.05	0.56
1:D:847:LEU:O	1:D:852:VAL:HG13	2.06	0.56
1:A:187:ARG:NH1	1:A:187:ARG:HG3	2.21	0.56
1:A:541:HIS:HB3	1:A:545:HIS:HB3	1.86	0.56
1:A:823:VAL:HB	1:A:828:ARG:HG3	1.88	0.56
1:D:29:PRO:HD2	1:D:528:ALA:HB1	1.87	0.56
1:A:54:LYS:O	1:A:58:MET:HG3	2.06	0.56
1:D:215:LYS:HE2	1:D:539:VAL:HG11	1.87	0.56
1:D:232:ILE:HG12	1:D:405:LEU:HD13	1.87	0.56
1:A:726:HIS:CD2	1:A:808:ASP:N	2.74	0.55
1:A:707:GLY:CA	1:A:769:ARG:HD3	2.36	0.55
1:A:726:HIS:HD2	1:A:808:ASP:N	2.02	0.55
1:A:669:PRO:HA	1:A:742:ASN:ND2	2.21	0.55
1:A:74:LEU:CD1	1:A:76:PRO:HD3	2.35	0.55
1:A:823:VAL:H	1:A:828:ARG:CG	2.19	0.55
1:D:290:LYS:HE3	1:D:298:GLU:OE2	2.06	0.55
1:D:96:HIS:HB3	1:D:99:ASP:OD2	2.06	0.55
1:A:657:ALA:O	1:A:660:ALA:N	2.39	0.55
1:A:153:LYS:HG2	1:A:188:GLU:OE2	2.05	0.55
1:A:843:ARG:O	1:A:847:LEU:HG	2.07	0.55
1:A:866:TYR:O	1:A:868:PRO:HD3	2.06	0.55
1:A:423:LEU:HD23	1:A:423:LEU:C	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:TRP:O	1:A:509:LEU:HB2	2.07	0.55
1:D:245:VAL:HA	1:D:334:THR:OG1	2.07	0.55
1:D:187:ARG:HH11	1:D:187:ARG:HG3	1.71	0.55
1:D:331:GLY:HA3	1:D:420:ARG:NH2	2.22	0.55
2:E:53:G:O2'	2:E:54:U:H5'	2.07	0.55
1:D:586:VAL:HG22	1:D:630:LEU:O	2.07	0.55
1:A:493:ARG:HH11	1:A:493:ARG:HG2	1.72	0.55
2:E:61:C:O2'	2:E:62:C:H5'	2.07	0.54
1:A:239:LYS:HD2	1:A:239:LYS:N	2.22	0.54
1:D:225:GLY:HA2	2:E:73:A:N3	2.23	0.54
1:A:234:PHE:CE2	1:A:259:LEU:HD21	2.42	0.54
1:D:852:VAL:HG12	1:D:855:HIS:CB	2.35	0.54
1:A:248:THR:CG2	7:A:1893:2AD:H5'1	2.36	0.54
1:A:54:LYS:HG2	1:A:58:MET:HE3	1.89	0.54
1:A:823:VAL:HB	1:A:828:ARG:CG	2.37	0.54
2:B:42:U:O2'	2:B:43:G:H5'	2.08	0.54
1:D:370:PRO:O	1:D:373:LEU:HD12	2.06	0.54
1:A:694:ARG:HD2	1:A:756:TYR:CE1	2.42	0.54
1:D:820:ALA:HA	1:D:830:THR:HG22	1.89	0.54
1:D:870:LYS:HD3	1:D:870:LYS:N	2.21	0.54
1:D:658:ASP:OD2	1:D:785:HIS:HB2	2.08	0.54
1:D:257:THR:HG1	1:D:258:PHE:HD1	1.56	0.54
1:D:136:ASN:OD1	1:D:503:ASP:HB3	2.08	0.53
1:A:43:TYR:HE1	1:A:80:ASP:OD2	1.90	0.53
2:B:38:A:O2'	2:B:39:U:H5'	2.07	0.53
2:B:47(A):C:H2'	2:B:47(B):A:O4'	2.08	0.53
1:D:772:ILE:O	1:D:776:LEU:HG	2.08	0.53
1:D:398:LYS:O	1:D:402:ILE:HG13	2.08	0.53
1:D:501:PHE:CE2	1:D:544:LEU:HD22	2.43	0.53
1:D:574:GLN:NE2	1:D:574:GLN:HA	2.22	0.53
2:E:65:C:H2'	2:E:66:C:H6	1.74	0.53
1:A:610:LEU:HD13	1:A:618:MET:CE	2.39	0.53
1:D:55:ASN:HD21	1:D:574:GLN:CB	2.22	0.53
1:D:870:LYS:C	1:D:871:ILE:HD12	2.29	0.53
1:A:396:GLU:HA	1:A:399:ARG:HE	1.73	0.53
1:D:256:ALA:HB2	1:D:338:MET:CE	2.39	0.53
1:D:84:LEU:HB2	1:D:85:PRO:HD3	1.89	0.53
2:B:18:G:N2	2:B:57:A:H2'	2.24	0.53
2:B:1:G:H2'	2:B:2:C:C6	2.44	0.53
1:D:380:PRO:HB3	1:D:394:SER:HB2	1.91	0.53
1:D:845:GLU:HA	1:D:848:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:863:LYS:HB3	1:D:875:VAL:HB	1.89	0.53
1:A:267:LEU:HB3	1:A:271:LEU:HD12	1.90	0.53
1:A:568:PHE:N	1:A:568:PHE:CD1	2.74	0.53
1:A:623:ARG:HD2	1:A:633:TRP:NE1	2.23	0.53
1:D:396:GLU:HG2	1:D:400:LYS:HE3	1.91	0.53
1:A:833:ILE:HD12	1:A:834:PRO:O	2.09	0.53
1:D:65:PHE:CG	1:D:736:LEU:HD13	2.44	0.53
1:D:841:VAL:O	1:D:845:GLU:HB2	2.08	0.53
1:A:745:ILE:CG2	1:A:749:MET:HE3	2.39	0.52
1:D:866:TYR:O	1:D:868:PRO:HD3	2.09	0.52
1:A:694:ARG:HH21	1:A:698:ASP:CG	2.12	0.52
2:B:1:G:H2'	2:B:2:C:H6	1.74	0.52
1:D:136:ASN:ND2	1:D:506:TRP:HE1	2.07	0.52
1:D:863:LYS:HE2	1:D:865:ILE:CD1	2.39	0.52
1:A:64:ARG:HG2	1:A:64:ARG:HH11	1.73	0.52
1:A:15:ARG:HB3	1:A:19:GLU:OE2	2.10	0.52
1:A:852:VAL:HG12	1:A:855:HIS:CB	2.38	0.52
2:E:50:C:H2'	2:E:51:G:C8	2.45	0.52
1:A:696:ALA:HA	1:A:793:TRP:HZ3	1.75	0.52
1:A:793:TRP:HB2	1:A:794:PHE:CE2	2.44	0.52
2:E:18:G:H5'	2:E:18:G:H8	1.74	0.52
1:A:780:PHE:CD1	1:A:784:PRO:HA	2.45	0.52
1:D:43:TYR:O	1:D:45:SER:N	2.43	0.52
1:D:583:PHE:HE2	1:D:634:LYS:HB3	1.75	0.52
1:D:352:ARG:HG3	1:D:352:ARG:HH11	1.75	0.52
1:A:666:PHE:HE1	1:A:746:ALA:HB2	1.75	0.52
1:A:13:TRP:CE3	1:A:788:GLU:HG2	2.45	0.51
1:D:226:ARG:HH11	1:D:226:ARG:HG3	1.75	0.51
1:D:277:ARG:HD2	1:D:281:LEU:CD1	2.40	0.51
1:A:133:TYR:HB2	1:A:432:THR:HG23	1.91	0.51
1:A:823:VAL:H	1:A:828:ARG:HG2	1.74	0.51
1:D:715:GLU:HA	1:D:719:ARG:HB2	1.91	0.51
2:E:18:G:H21	2:E:57:A:H2'	1.73	0.51
1:A:137:GLN:NE2	1:A:433:PRO:O	2.37	0.51
1:A:442:CYS:SG	1:A:486:LYS:HD3	2.51	0.51
1:D:133:TYR:O	1:D:137:GLN:HG3	2.10	0.51
1:D:594:ARG:HA	1:D:609:ALA:HA	1.91	0.51
1:D:162:CYS:HB3	1:D:164:THR:HG22	1.90	0.51
1:A:275:GLU:H	1:A:275:GLU:CD	2.13	0.51
1:D:327:TYR:CD1	1:D:327:TYR:C	2.84	0.51
1:A:341:PRO:HB3	1:A:348:TYR:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:ILE:O	1:A:748:LEU:N	2.37	0.51
2:B:7:G:H3'	2:B:8:U:H5'	1.91	0.51
1:A:25:ALA:N	1:A:120:ASP:OD2	2.42	0.51
1:A:46:GLY:H	1:A:104:ASN:HD21	1.59	0.51
1:D:50:MET:HE2	1:D:648:VAL:HG22	1.93	0.51
1:D:706:SER:O	1:D:766:PRO:HB3	2.11	0.51
2:B:47(D):G:C2'	2:B:47(E):C:H5'	2.41	0.51
1:D:687:PHE:CD1	1:D:749:MET:HG2	2.46	0.51
1:A:327:TYR:CE1	1:A:346:ARG:HD3	2.46	0.50
1:A:557:HIS:HD2	1:A:562:VAL:O	1.94	0.50
1:A:625:HIS:ND1	1:A:627:ASP:OD2	2.44	0.50
1:D:366:GLY:O	1:D:368:PRO:HD3	2.11	0.50
1:D:369:LEU:HD11	1:D:377:TYR:CD2	2.46	0.50
1:A:267:LEU:HB3	1:A:271:LEU:CD1	2.41	0.50
1:D:133:TYR:HB2	1:D:432:THR:HG23	1.94	0.50
1:A:253:LEU:HA	1:A:338:MET:HE3	1.92	0.50
1:A:638:MET:HA	1:A:644:ASN:OD1	2.11	0.50
1:D:16:PHE:HA	1:D:19:GLU:OE1	2.11	0.50
1:D:34:LYS:HD2	1:D:34:LYS:O	2.11	0.50
1:D:96:HIS:CD2	1:D:98:LYS:HB3	2.47	0.50
1:D:277:ARG:CB	1:D:277:ARG:HH11	2.19	0.50
1:D:140:PHE:HE2	1:D:424:ILE:HD11	1.76	0.50
1:D:647:MET:HB3	1:D:650:PRO:CD	2.40	0.50
1:A:121:TRP:C	1:A:123:ARG:H	2.14	0.50
1:A:280:VAL:O	1:A:284:VAL:HG23	2.12	0.50
1:A:826:ARG:CD	1:A:828:ARG:HH21	2.24	0.50
1:A:9:ILE:CG2	1:A:789:GLU:OE1	2.59	0.50
1:D:816:VAL:CA	1:D:834:PRO:HA	2.40	0.50
1:A:34:LYS:C	1:A:34:LYS:HD2	2.32	0.50
1:A:55:ASN:HD22	1:A:55:ASN:N	2.10	0.50
1:A:9:ILE:HG22	1:A:789:GLU:OE1	2.11	0.50
1:D:312:LEU:HD12	1:D:317:GLY:O	2.12	0.50
1:D:312:LEU:HD11	1:D:319:ARG:HG3	1.93	0.50
1:D:388:PRO:HG2	1:D:389:PHE:CD2	2.47	0.50
1:D:50:MET:CE	1:D:648:VAL:HG22	2.42	0.50
1:D:679:GLU:HA	1:D:682:GLN:NE2	2.20	0.50
1:A:312:LEU:HD12	1:A:317:GLY:O	2.11	0.49
1:A:823:VAL:HG11	1:A:857:GLU:HB3	1.93	0.49
1:D:414:ARG:HH21	1:D:416:THR:CG2	2.25	0.49
1:D:597:GLU:HB2	1:D:598:PRO:HD3	1.94	0.49
1:D:723:GLY:O	1:D:727:GLU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:867:VAL:O	1:D:867:VAL:HG12	2.12	0.49
1:D:588:VAL:HG13	1:D:593:VAL:HG22	1.94	0.49
1:D:671:GLU:HG2	1:D:672:ASN:N	2.28	0.49
2:E:8:U:H1'	2:E:48:U:H1'	1.94	0.49
1:A:189:LEU:HD22	1:A:191:GLN:HE21	1.75	0.49
1:A:197:THR:HG23	1:A:421:ASP:OD1	2.12	0.49
1:A:477:PRO:HG3	1:A:480:TYR:OH	2.12	0.49
1:D:54:LYS:O	1:D:58:MET:HG3	2.12	0.49
1:A:397:GLY:O	1:A:401:VAL:HG23	2.11	0.49
1:A:668:ALA:HB1	1:A:669:PRO:HD3	1.94	0.49
1:D:659:ILE:HD12	1:D:659:ILE:N	2.27	0.49
1:A:136:ASN:ND2	1:A:506:TRP:HE1	2.10	0.49
1:A:699:ARG:O	1:A:703:LEU:HD12	2.13	0.49
1:A:822:GLN:O	1:A:873:ASN:HA	2.13	0.49
1:D:339:ALA:HA	1:D:347:ASP:OD2	2.12	0.49
1:D:207:LEU:HD21	1:D:550:ARG:NH1	2.28	0.49
1:D:363:GLU:OE2	1:D:368:PRO:HB3	2.13	0.49
1:A:638:MET:HG3	1:A:645:GLY:HA2	1.95	0.49
1:D:152:ALA:O	1:D:190:GLU:HA	2.13	0.49
1:A:101:THR:O	1:A:105:ILE:HG13	2.13	0.49
1:A:27:ASP:O	1:A:28:LEU:HD23	2.12	0.49
1:A:253:LEU:HG	1:A:315:ALA:HB2	1.94	0.49
1:D:313:ASN:O	1:D:317:GLY:N	2.41	0.49
1:A:593:VAL:HG12	1:A:593:VAL:O	2.13	0.48
1:A:758:TYR:OH	1:A:765:THR:HG21	2.12	0.48
1:D:135:TRP:O	1:D:139:ILE:HG13	2.13	0.48
1:D:38:LEU:HD23	1:D:535:TYR:CE1	2.48	0.48
1:D:49:HIS:HB2	1:D:646:VAL:O	2.13	0.48
1:D:442:CYS:SG	1:D:486:LYS:HD3	2.52	0.48
1:A:42:PRO:HD3	1:A:77:MET:HE1	1.95	0.48
2:B:14:A:H1'	2:B:22:A:C5	2.48	0.48
2:E:42:U:H2'	2:E:43:G:C8	2.48	0.48
1:A:423:LEU:CD2	1:A:423:LEU:C	2.81	0.48
1:A:507:TYR:O	1:A:509:LEU:N	2.46	0.48
1:A:651:PHE:CE1	1:A:655:GLN:HG3	2.48	0.48
1:A:678:GLU:HG2	1:A:682:GLN:HE21	1.77	0.48
1:D:694:ARG:NH1	1:D:759:ARG:HG3	2.28	0.48
1:A:194:LEU:HD12	1:A:424:ILE:HG21	1.96	0.48
1:A:480:TYR:HA	1:A:493:ARG:HB2	1.96	0.48
1:A:791:TRP:CD2	1:A:799:LEU:HD21	2.49	0.48
1:A:671:GLU:CD	1:A:671:GLU:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47(C):A:C8	2:B:47(D):G:H1'	2.48	0.48
1:D:222:ALA:HA	2:E:73:A:C5	2.48	0.48
1:A:458:ASP:C	1:A:459:LEU:HD12	2.34	0.48
1:A:785:HIS:O	1:A:787:ALA:N	2.46	0.48
1:D:402:ILE:O	1:D:406:GLU:HG3	2.13	0.48
1:D:465:ILE:HG13	1:D:466:ARG:N	2.28	0.48
1:D:796:PRO:HG2	1:D:797:ASP:H	1.78	0.48
1:D:46:GLY:H	1:D:104:ASN:ND2	2.12	0.48
1:A:58:MET:SD	1:A:574:GLN:OE1	2.72	0.48
2:B:53:G:O2'	2:B:54:U:H5'	2.13	0.48
1:D:151:ARG:HG3	1:D:192:TRP:CZ3	2.49	0.48
1:D:206:ASP:OD2	1:D:554:LYS:HE3	2.13	0.48
1:A:620:ALA:HB1	1:A:633:TRP:O	2.14	0.47
1:A:729:LEU:HD23	1:A:807:LEU:HA	1.96	0.47
1:D:237:GLU:HB2	1:D:312:LEU:HD21	1.95	0.47
1:A:194:LEU:CD1	1:A:424:ILE:HG21	2.44	0.47
1:D:574:GLN:CA	1:D:574:GLN:NE2	2.77	0.47
1:D:730:LYS:O	1:D:734:GLU:HG3	2.14	0.47
1:D:687:PHE:HE1	1:D:749:MET:HA	1.79	0.47
1:A:555:PHE:CE2	1:A:559:LEU:HD11	2.49	0.47
1:A:758:TYR:OH	1:A:765:THR:CG2	2.63	0.47
2:B:24:G:O2'	2:B:25:C:H5'	2.14	0.47
1:D:148:LEU:HD23	1:D:195:ARG:HB3	1.96	0.47
1:D:690:ARG:HH21	1:D:756:TYR:HD2	1.60	0.47
1:A:316:THR:OG1	1:A:318:GLU:HG2	2.15	0.47
1:A:578:LEU:HB2	1:A:675:VAL:HG22	1.96	0.47
1:A:571:LEU:HG	1:A:571:LEU:O	2.14	0.47
1:A:851:ASN:ND2	1:A:851:ASN:H	2.12	0.47
1:A:420:ARG:NH1	1:A:420:ARG:HG2	2.28	0.47
1:A:428:ARG:NH1	1:A:467:PRO:HG3	2.30	0.47
1:A:861:VAL:HA	1:A:876:VAL:HA	1.96	0.47
2:B:19:G:OP1	2:B:60:U:N3	2.47	0.47
1:A:851:ASN:CG	1:A:853:ARG:HB2	2.35	0.47
2:B:7:G:H3'	2:B:8:U:C5'	2.45	0.47
2:B:20:U:H6	2:B:20:U:H5'	1.79	0.47
1:D:226:ARG:HG3	1:D:417:TYR:HE1	1.79	0.47
1:D:583:PHE:CE2	1:D:634:LYS:HB3	2.49	0.47
2:E:60:U:C5'	2:E:61:C:H5	2.27	0.47
1:D:361:VAL:HG23	1:D:362:ILE:HG12	1.97	0.47
1:D:406:GLU:HA	1:D:411:GLY:O	2.15	0.47
1:D:17:TRP:CH2	1:D:784:PRO:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:HG13	1:A:184:VAL:HG21	1.96	0.47
1:A:16:PHE:CE1	1:A:20:LYS:HG3	2.50	0.47
1:A:210:LEU:HG	1:A:212:TRP:CD1	2.50	0.46
1:A:466:ARG:HD3	1:A:468:LYS:HZ2	1.79	0.46
1:A:663:THR:O	1:A:663:THR:CG2	2.62	0.46
1:D:518:ARG:O	1:D:519:LEU:HG	2.14	0.46
2:B:60:U:H5''	2:B:61:C:H5	1.80	0.46
1:D:822:GLN:HB3	1:D:827:VAL:HA	1.96	0.46
1:A:121:TRP:C	1:A:123:ARG:N	2.68	0.46
1:A:373:LEU:HD12	1:A:373:LEU:N	2.30	0.46
1:D:312:LEU:HD13	1:D:319:ARG:HA	1.96	0.46
1:D:866:TYR:HD1	1:D:872:LEU:HD13	1.80	0.46
1:D:819:VAL:HG22	1:D:870:LYS:HA	1.96	0.46
2:E:18:G:C8	2:E:18:G:H5'	2.50	0.46
1:A:183:PRO:CB	1:A:293:ILE:HD12	2.39	0.46
2:E:2:C:H2'	2:E:3:C:H6	1.81	0.46
1:A:29:PRO:CG	1:A:529:TRP:CZ2	2.99	0.46
1:D:508:TYR:CD1	1:D:509:LEU:HG	2.51	0.46
1:A:161:LYS:HD3	1:A:179:HIS:CD2	2.50	0.46
1:A:513:ASP:OD2	1:A:525:LYS:HD2	2.16	0.46
1:D:157:ASN:HB3	1:D:184:VAL:HG11	1.98	0.46
1:D:55:ASN:ND2	1:D:574:GLN:CG	2.79	0.46
2:E:38:A:O2'	2:E:39:U:H5'	2.16	0.46
1:A:240:GLU:N	1:A:240:GLU:CD	2.68	0.46
1:A:748:LEU:HD21	1:A:778:MET:CE	2.45	0.46
1:A:313:ASN:O	1:A:315:ALA:N	2.48	0.46
1:A:60:ASP:OD1	1:A:661:ARG:NH2	2.40	0.46
1:D:826:ARG:HG3	1:D:826:ARG:HH11	1.79	0.46
1:D:38:LEU:CD1	1:D:76:PRO:HG2	2.46	0.45
1:D:41:PHE:CE1	8:D:1893:LEU:HG	2.50	0.45
1:D:851:ASN:HB2	1:D:853:ARG:CG	2.45	0.45
2:E:67:C:O2'	2:E:68:C:H5'	2.15	0.45
1:A:623:ARG:HD2	1:A:633:TRP:CE2	2.51	0.45
1:D:189:LEU:CD2	1:D:190:GLU:H	2.24	0.45
1:D:480:TYR:HB2	1:D:492:LYS:HG3	1.97	0.45
1:D:823:VAL:C	1:D:825:GLY:H	2.20	0.45
1:A:159:CYS:HB3	1:A:162:CYS:HB2	1.97	0.45
1:A:853:ARG:O	1:A:857:GLU:HB2	2.17	0.45
1:D:196:ILE:HG13	1:D:551:PHE:CG	2.52	0.45
1:D:183:PRO:HG3	1:D:293:ILE:HD12	1.97	0.45
1:D:824:ASN:ND2	1:D:876:VAL:HB	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:ALA:HB1	1:A:740:ARG:HH12	1.82	0.45
2:B:65:C:H2'	2:B:66:C:H6	1.81	0.45
1:D:96:HIS:ND1	1:D:97:PRO:HD2	2.32	0.45
2:E:71:G:O2'	2:E:72:C:H5'	2.16	0.45
1:A:163:GLN:NE2	1:A:469:GLY:HA2	2.32	0.45
1:A:95:VAL:HG12	1:A:96:HIS:N	2.32	0.45
2:B:60:U:C5'	2:B:61:C:H5	2.30	0.45
1:D:144:TRP:HA	1:D:149:ALA:HB3	1.98	0.45
1:D:38:LEU:HD13	1:D:76:PRO:HG2	1.98	0.45
1:A:366:GLY:O	1:A:368:PRO:HD3	2.17	0.45
1:D:79:TRP:CE2	1:D:105:ILE:HG23	2.52	0.45
1:D:816:VAL:HA	1:D:833:ILE:O	2.17	0.45
1:A:507:TYR:O	1:A:508:TYR:C	2.54	0.45
1:A:780:PHE:HB3	1:A:781:PRO:CD	2.44	0.45
1:A:849:VAL:HG23	1:A:852:VAL:H	1.81	0.45
1:A:859:LYS:HB2	1:A:860:GLU:OE2	2.16	0.45
1:D:457:PRO:O	1:D:459:LEU:HD13	2.17	0.45
1:D:867:VAL:O	1:D:869:GLY:N	2.50	0.45
1:A:826:ARG:O	1:A:828:ARG:HG2	2.16	0.45
1:D:176:CYS:HB3	1:D:179:HIS:HB2	1.98	0.45
1:D:819:VAL:HG13	1:D:870:LYS:C	2.37	0.45
1:D:181:ASP:O	1:D:183:PRO:HD3	2.17	0.44
1:A:689:ASN:O	1:A:692:TYR:N	2.50	0.44
1:A:74:LEU:HD12	1:A:76:PRO:HD3	1.98	0.44
1:A:249:ARG:HG3	1:A:249:ARG:HH11	1.82	0.44
1:D:690:ARG:NH2	1:D:756:TYR:HD2	2.16	0.44
2:E:2:C:O2'	2:E:3:C:H5'	2.17	0.44
2:B:65:C:H2'	2:B:66:C:C6	2.53	0.44
1:A:232:ILE:HG12	1:A:405:LEU:HD13	1.99	0.44
1:A:426:ARG:HG2	1:A:426:ARG:NH1	2.32	0.44
2:B:3:C:H2'	2:B:4:G:H8	1.82	0.44
1:A:157:ASN:HB3	1:A:184:VAL:CG1	2.47	0.44
1:A:193:TYR:HA	1:A:422:TRP:O	2.16	0.44
1:A:555:PHE:CZ	1:A:559:LEU:HD11	2.53	0.44
1:D:57:THR:O	1:D:60:ASP:N	2.51	0.44
1:A:104:ASN:O	1:A:105:ILE:C	2.56	0.44
1:A:575:GLY:O	1:A:576:MET:O	2.36	0.44
1:D:152:ALA:O	1:D:190:GLU:HG3	2.17	0.44
1:D:836:ASP:O	1:D:837:ALA:C	2.56	0.44
1:A:84:LEU:HD22	1:A:162:CYS:SG	2.58	0.44
1:D:25:ALA:HB2	1:D:74:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TYR:CD2	1:A:133:TYR:C	2.90	0.44
1:D:191:GLN:HB3	1:D:425:SER:OG	2.18	0.44
1:A:507:TYR:CD2	1:A:508:TYR:N	2.85	0.43
1:D:323:TRP:HB3	1:D:324:THR:H	1.71	0.43
1:D:31:GLY:C	1:D:33:GLY:H	2.21	0.43
1:A:179:HIS:C	1:A:181:ASP:H	2.22	0.43
1:A:345:GLN:HG3	1:A:349:GLU:OE2	2.18	0.43
1:A:759:ARG:NH2	1:A:764:VAL:HG23	2.34	0.43
1:A:748:LEU:HD21	1:A:778:MET:HE2	1.99	0.43
1:D:600:ARG:NH1	1:D:600:ARG:HG2	2.33	0.43
1:D:833:ILE:HG13	1:D:833:ILE:H	1.71	0.43
1:D:846:ALA:O	1:D:849:VAL:HG13	2.17	0.43
1:D:445:VAL:HG11	1:D:486:LYS:HB2	2.00	0.43
1:D:664:ILE:HG12	1:D:676:TRP:HZ3	1.83	0.43
1:D:822:GLN:HG3	1:D:873:ASN:OD1	2.19	0.43
1:A:647:MET:H	1:A:647:MET:HE1	1.82	0.43
1:A:817:VAL:HG12	1:A:818:GLU:N	2.29	0.43
1:D:429:TYR:CE1	1:D:456:LEU:HD22	2.54	0.43
1:D:83:GLY:CA	1:D:500:THR:HB	2.44	0.43
1:D:762:ARG:HA	1:D:763:PRO:HD3	1.83	0.43
1:A:851:ASN:N	1:A:851:ASN:HD22	2.16	0.43
1:D:183:PRO:HB3	1:D:293:ILE:HD12	1.99	0.43
1:D:541:HIS:HB3	1:D:545:HIS:HB3	2.01	0.43
1:D:43:TYR:CE1	1:D:80:ASP:OD2	2.71	0.43
1:D:44:PRO:HD2	1:D:80:ASP:O	2.18	0.43
1:D:810:LYS:HA	1:D:813:GLU:OE1	2.17	0.43
1:D:819:VAL:HG21	1:D:833:ILE:HD11	2.00	0.43
1:A:79:TRP:CD2	1:A:105:ILE:HG23	2.54	0.43
1:A:234:PHE:CD2	1:A:259:LEU:HD21	2.54	0.43
2:B:28:A:P	9:B:2002:HOH:O	2.75	0.43
1:D:234:PHE:HA	1:D:235:PRO:HD3	1.87	0.43
1:D:541:HIS:O	1:D:542:ALA:C	2.57	0.43
1:D:651:PHE:CE1	1:D:676:TRP:HZ2	2.36	0.43
1:D:658:ASP:O	1:D:662:ILE:HG12	2.19	0.43
1:D:845:GLU:HA	1:D:848:LYS:CE	2.48	0.43
1:A:120:ASP:C	1:A:120:ASP:OD1	2.56	0.43
1:A:127:THR:HA	1:A:132:TYR:CD1	2.53	0.43
1:A:133:TYR:O	1:A:134:ARG:C	2.57	0.43
1:D:136:ASN:HA	1:D:136:ASN:HD22	1.63	0.43
1:D:29:PRO:HG3	1:D:529:TRP:CZ2	2.53	0.43
1:D:32:ARG:HG2	1:D:70:GLY:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:HG22	1:A:403:ALA:N	2.33	0.43
1:A:9:ILE:O	1:A:12:LYS:HB3	2.19	0.43
1:D:15:ARG:O	1:D:19:GLU:HG3	2.19	0.43
1:D:838:PRO:HD2	1:D:841:VAL:CG2	2.49	0.43
1:A:133:TYR:HB2	1:A:432:THR:CG2	2.49	0.43
1:A:738:ALA:HB1	1:A:740:ARG:NH1	2.33	0.43
1:A:767:VAL:HG13	1:A:768:TYR:N	2.34	0.43
1:A:799:LEU:HD23	1:A:799:LEU:HA	1.80	0.43
1:A:225:GLY:HA2	2:B:73:A:N3	2.34	0.43
1:D:360:LYS:HE2	1:D:360:LYS:HB3	1.90	0.43
2:B:50:C:O4'	2:E:47(C):A:C2	2.71	0.43
1:A:75:HIS:O	1:A:119:TYR:HD1	2.02	0.42
2:B:45:G:H2'	2:B:46:C:H6	1.84	0.42
1:D:393:GLU:O	1:D:394:SER:C	2.57	0.42
1:A:741:PHE:O	1:A:742:ASN:C	2.55	0.42
1:A:745:ILE:O	1:A:748:LEU:HB2	2.19	0.42
1:A:823:VAL:N	1:A:828:ARG:HG3	2.34	0.42
1:D:277:ARG:HD2	1:D:281:LEU:HD11	2.01	0.42
1:D:671:GLU:HG2	1:D:672:ASN:H	1.83	0.42
1:A:140:PHE:CD1	1:A:140:PHE:C	2.93	0.42
1:A:207:LEU:O	1:A:217:LYS:HE2	2.19	0.42
1:A:373:LEU:H	1:A:373:LEU:HD12	1.83	0.42
1:A:507:TYR:C	1:A:509:LEU:N	2.71	0.42
1:A:742:ASN:OD1	1:A:742:ASN:N	2.49	0.42
2:B:47(B):A:C6	2:B:47(C):A:N1	2.87	0.42
2:B:47:G:N2	2:B:47(C):A:OP2	2.48	0.42
1:D:131:GLU:CD	1:D:131:GLU:H	2.23	0.42
1:D:788:GLU:OE2	1:D:799:LEU:HB2	2.18	0.42
1:A:135:TRP:O	1:A:136:ASN:C	2.58	0.42
1:A:158:TRP:HZ2	1:A:163:GLN:NE2	2.17	0.42
1:A:160:PRO:O	1:A:163:GLN:HG2	2.20	0.42
1:A:507:TYR:CG	1:A:508:TYR:N	2.87	0.42
1:A:621:GLU:O	1:A:622:LEU:HD23	2.20	0.42
1:A:762:ARG:HA	1:A:763:PRO:HD3	1.87	0.42
1:A:849:VAL:HG23	1:A:852:VAL:N	2.34	0.42
2:B:28:A:H8	9:B:2002:HOH:O	2.01	0.42
1:D:707:GLY:N	1:D:769:ARG:HD3	2.35	0.42
1:A:79:TRP:NE1	1:A:124:GLU:OE2	2.42	0.42
1:A:239:LYS:N	1:A:239:LYS:CD	2.82	0.42
1:A:613:GLU:O	1:A:617:LYS:HG3	2.20	0.42
1:D:120:ASP:OD1	1:D:122:ASP:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:PRO:HG2	1:D:182:THR:CG2	2.49	0.42
1:D:457:PRO:HG2	1:D:473:LEU:HD22	2.01	0.42
1:D:461:ASP:OD1	1:D:464:ASP:HB2	2.20	0.42
1:D:465:ILE:O	1:D:472:PRO:HG2	2.19	0.42
1:D:859:LYS:C	1:D:860:GLU:OE2	2.58	0.42
1:A:35:GLN:HG3	1:A:66:ARG:HD2	2.01	0.42
1:A:675:VAL:HG12	1:A:677:THR:HG23	2.01	0.42
1:A:758:TYR:CZ	1:A:762:ARG:HG2	2.54	0.42
1:D:226:ARG:HG3	1:D:226:ARG:NH1	2.33	0.42
1:D:500:THR:C	1:D:502:PHE:H	2.23	0.42
1:D:64:ARG:O	1:D:68:MET:HG3	2.19	0.42
1:A:55:ASN:ND2	1:A:574:GLN:HG3	2.35	0.42
1:A:620:ALA:HB2	1:A:634:LYS:HB2	2.01	0.42
1:D:226:ARG:HA	1:D:417:TYR:HD1	1.84	0.42
1:D:233:LEU:CD2	1:D:244:PRO:HB3	2.49	0.42
1:D:727:GLU:HA	1:D:812:LEU:HD22	2.02	0.42
2:E:30:G:H1	2:E:40:C:H42	1.66	0.42
1:A:791:TRP:CE3	1:A:799:LEU:HD21	2.54	0.42
1:D:146:LYS:O	1:D:146:LYS:HG2	2.19	0.42
1:A:819:VAL:HG12	1:A:820:ALA:N	2.35	0.42
1:A:231:GLU:HA	1:A:245:VAL:O	2.20	0.41
1:A:384:VAL:HG22	1:A:385:ASN:N	2.35	0.41
1:A:477:PRO:HG3	1:A:480:TYR:CZ	2.55	0.41
1:D:133:TYR:HB2	1:D:432:THR:CG2	2.49	0.41
1:D:234:PHE:CE2	1:D:314:PRO:HD2	2.55	0.41
1:D:223:TRP:HB2	1:D:543:VAL:HG11	2.02	0.41
1:D:225:GLY:HA2	2:E:73:A:C2	2.55	0.41
1:A:401:VAL:O	1:A:404:TRP:HB3	2.20	0.41
1:D:41:PHE:N	1:D:41:PHE:CD1	2.88	0.41
1:A:249:ARG:CG	6:A:1892:NVA:HD1	2.48	0.41
1:A:23:MET:HE1	1:A:63:ALA:HB1	2.02	0.41
1:A:343:HIS:CE1	1:A:362:ILE:HB	2.56	0.41
1:D:151:ARG:HG3	1:D:192:TRP:CE3	2.55	0.41
1:A:192:TRP:CH2	1:A:436:MET:HG3	2.55	0.41
1:A:466:ARG:NH1	1:A:468:LYS:HE3	2.35	0.41
1:A:493:ARG:NH1	1:A:493:ARG:HG2	2.34	0.41
1:D:312:LEU:CD1	1:D:319:ARG:HG3	2.49	0.41
1:D:480:TYR:O	1:D:492:LYS:HA	2.19	0.41
1:D:487:CYS:SG	1:D:488:GLY:N	2.93	0.41
1:D:687:PHE:CE1	1:D:749:MET:HA	2.55	0.41
1:D:836:ASP:N	1:D:836:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ALA:O	1:A:658:ASP:C	2.58	0.41
1:A:762:ARG:HG3	1:A:763:PRO:HD2	2.01	0.41
1:D:265:HIS:ND1	1:D:266:PRO:HD2	2.35	0.41
1:D:388:PRO:HG2	1:D:389:PHE:H	1.84	0.41
1:D:614:ASP:O	1:D:618:MET:HG2	2.20	0.41
1:D:685:TRP:O	1:D:689:ASN:HB2	2.21	0.41
1:A:436:MET:HE3	1:A:444:VAL:HG12	2.02	0.41
1:A:567:PRO:HB2	1:A:568:PHE:CE1	2.56	0.41
1:A:621:GLU:C	1:A:622:LEU:HD23	2.41	0.41
1:A:678:GLU:HG2	1:A:682:GLN:NE2	2.36	0.41
1:D:584:GLY:O	1:D:631:HIS:HA	2.20	0.41
1:D:823:VAL:HB	1:D:828:ARG:NH1	2.36	0.41
2:E:14:A:H1'	2:E:22:A:C8	2.54	0.41
1:A:461:ASP:OD1	1:A:464:ASP:HB2	2.21	0.41
2:B:55:U:H2'	2:B:57:A:OP2	2.19	0.41
1:D:230:ALA:HA	1:D:413:GLY:HA2	2.03	0.41
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.86	0.41
1:D:305:VAL:O	1:D:324:THR:HG22	2.20	0.41
1:D:49:HIS:O	1:D:50:MET:C	2.59	0.41
1:D:58:MET:CE	1:D:670:PRO:HB3	2.51	0.41
1:D:786:LEU:O	1:D:789:GLU:HB3	2.21	0.41
1:A:41:PHE:CE1	1:A:80:ASP:CB	3.03	0.41
1:A:536:ILE:HD12	1:A:536:ILE:N	2.35	0.41
1:A:610:LEU:HD13	1:A:618:MET:HE1	2.03	0.41
1:D:58:MET:HE1	1:D:670:PRO:HB3	2.02	0.41
1:D:765:THR:O	1:D:768:TYR:HB3	2.20	0.41
2:B:47(C):A:N3	2:E:66:C:H1'	2.35	0.41
1:A:253:LEU:O	1:A:253:LEU:HD12	2.21	0.41
1:A:378:GLU:O	1:A:379:GLU:O	2.39	0.41
1:A:739:LEU:N	1:A:739:LEU:HD12	2.36	0.41
1:A:87:GLU:HG2	1:A:91:LEU:HD22	2.03	0.41
1:A:448:PRO:HD2	1:A:451:GLU:OE1	2.21	0.41
1:D:126:THR:O	1:D:128:CYS:N	2.54	0.41
1:D:177:TRP:HD1	1:D:177:TRP:H	1.66	0.41
1:D:767:VAL:HG13	1:D:768:TYR:N	2.34	0.41
2:E:58:A:C2	2:E:60:U:H2'	2.56	0.41
1:A:133:TYR:HD2	1:A:133:TYR:C	2.24	0.40
1:A:708:VAL:O	1:A:709:PHE:HB3	2.21	0.40
1:D:144:TRP:CE3	1:D:436:MET:HE2	2.56	0.40
1:D:155:LEU:HD12	1:D:264:GLU:HG2	2.02	0.40
1:D:392:THR:HG22	1:D:393:GLU:N	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:591:SER:O	1:D:611:SER:HA	2.21	0.40
1:D:708:VAL:O	1:D:709:PHE:HB3	2.21	0.40
1:D:816:VAL:H	1:D:834:PRO:HA	1.86	0.40
2:E:66:C:C2	2:E:67:C:C5	3.09	0.40
1:A:115:MET:CE	1:A:648:VAL:HG13	2.51	0.40
1:A:224:ILE:HA	1:A:419:LEU:HB2	2.02	0.40
1:A:342:ALA:O	1:A:343:HIS:ND1	2.55	0.40
1:D:611:SER:O	1:D:615:VAL:HG23	2.21	0.40
1:A:247:THR:HA	7:A:1893:2AD:H3'	2.03	0.40
1:A:314:PRO:HB2	1:A:410:LEU:HD22	2.02	0.40
1:A:625:HIS:HB3	1:A:627:ASP:OD2	2.21	0.40
1:A:65:PHE:CG	1:A:736:LEU:HD13	2.56	0.40
1:D:600:ARG:HH11	1:D:600:ARG:HG2	1.86	0.40
1:D:6:PRO:O	1:D:7:HIS:C	2.60	0.40
2:E:60:U:H5'	2:E:61:C:H5	1.85	0.40
1:A:64:ARG:NH1	1:A:64:ARG:HG2	2.36	0.40
1:A:826:ARG:HB2	1:A:828:ARG:HH21	1.87	0.40
2:B:18:G:H21	2:B:57:A:H2'	1.87	0.40
1:D:437:VAL:HG23	1:D:447:VAL:HG22	2.04	0.40
1:A:130:PRO:HA	1:A:133:TYR:CE2	2.56	0.40
1:A:457:PRO:O	1:A:459:LEU:HD13	2.22	0.40
1:A:603:LEU:HD23	1:A:603:LEU:HA	1.87	0.40
1:A:740:ARG:HG3	1:A:740:ARG:HH11	1.86	0.40
1:A:82:PHE:HE2	1:A:133:TYR:HD1	1.66	0.40
2:B:27:C:O2'	2:B:28:A:H5'	2.21	0.40
1:D:816:VAL:N	1:D:834:PRO:HA	2.36	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	874/878 (100%)	728 (83%)	120 (14%)	26 (3%)	4	17
1	D	874/878 (100%)	735 (84%)	113 (13%)	26 (3%)	4	17
All	All	1748/1756 (100%)	1463 (84%)	233 (13%)	52 (3%)	4	17

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	576	MET
1	A	796	PRO
1	D	208	GLU
1	D	542	ALA
1	D	861	VAL
1	A	430	TRP
1	A	763	PRO
1	A	786	LEU
1	A	861	VAL
1	D	53	LEU
1	D	127	THR
1	D	225	GLY
1	D	390	ASP
1	D	392	THR
1	D	501	PHE
1	D	850	ARG
1	A	398	LYS
1	A	789	GLU
1	A	797	ASP
1	D	6	PRO
1	D	596	PRO
1	D	868	PRO
1	A	10	GLU
1	A	208	GLU
1	A	333	GLY
1	A	847	LEU
1	D	7	HIS
1	D	30	GLY
1	D	32	ARG
1	D	44	PRO
1	A	277	ARG
1	A	508	TYR
1	D	792	HIS
1	D	796	PRO
1	D	824	ASN

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Mol	Chain	Res	Type
1	A	6	PRO
1	A	689	ASN
1	A	869	GLY
1	D	469	GLY
1	D	543	VAL
1	D	875	VAL
1	A	379	GLU
1	A	33	GLY
1	A	314	PRO
1	A	435	PRO
1	A	564	VAL
1	D	763	PRO
1	D	805	PRO
1	A	44	PRO
1	A	816	VAL
1	A	849	VAL
1	D	816	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	741/742 (100%)	706 (95%)	35 (5%)	26	59
1	D	741/742 (100%)	717 (97%)	24 (3%)	39	73
All	All	1482/1484 (100%)	1423 (96%)	59 (4%)	31	65

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	34	LYS
1	A	36	TYR
1	A	39	VAL
1	A	41	PHE
1	A	47	ASP

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Mol	Chain	Res	Type
1	A	49	HIS
1	A	55	ASN
1	A	62	LEU
1	A	76	PRO
1	A	82	PHE
1	A	91	LEU
1	A	113	ARG
1	A	130	PRO
1	A	133	TYR
1	A	189	LEU
1	A	240	GLU
1	A	278	GLU
1	A	289	ARG
1	A	292	GLU
1	A	327	TYR
1	A	352	ARG
1	A	456	LEU
1	A	500	THR
1	A	503	ASP
1	A	568	PHE
1	A	647	MET
1	A	664	ILE
1	A	765	THR
1	A	794	PHE
1	A	828	ARG
1	A	839	LEU
1	A	851	ASN
1	A	857	GLU
1	A	871	ILE
1	D	34	LYS
1	D	36	TYR
1	D	41	PHE
1	D	82	PHE
1	D	189	LEU
1	D	197	THR
1	D	214	GLU
1	D	247	THR
1	D	264	GLU
1	D	277	ARG
1	D	327	TYR
1	D	379	GLU
1	D	392	THR

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Mol	Chain	Res	Type
1	D	456	LEU
1	D	503	ASP
1	D	647	MET
1	D	700	GLU
1	D	718	ASP
1	D	736	LEU
1	D	836	ASP
1	D	849	VAL
1	D	851	ASN
1	D	868	PRO
1	D	870	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	104	ASN
1	A	107	GLN
1	A	163	GLN
1	A	179	HIS
1	A	557	HIS
1	A	574	GLN
1	A	682	GLN
1	A	726	HIS
1	A	822	GLN
1	A	851	ASN
1	D	5	ASN
1	D	55	ASN
1	D	104	ASN
1	D	136	ASN
1	D	163	GLN
1	D	515	HIS
1	D	655	GLN
1	D	682	GLN
1	D	726	HIS
1	D	824	ASN
1	D	851	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	76/83 (91%)	10 (13%)	2 (2%)
2	E	76/83 (91%)	8 (10%)	2 (2%)
All	All	152/166 (91%)	18 (11%)	4 (2%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	7	G
2	B	8	U
2	B	10	G
2	B	18	G
2	B	19	G
2	B	20	U
2	B	47(C)	A
2	B	47(D)	G
2	B	48	U
2	B	73	A
2	E	10	G
2	E	18	G
2	E	19	G
2	E	20	U
2	E	47(C)	A
2	E	47(D)	G
2	E	48	U
2	E	73	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	18	G
2	E	9	G
2	E	18	G

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 37 ligands modelled in this entry, 6 are monoatomic - leaving 31 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	$\# Z  > 2$
5	SO4	A	1881	-	4,4,4	0.25	0	6,6,6	0.16	0
5	SO4	D	1887	-	4,4,4	0.26	0	6,6,6	0.09	0
5	SO4	D	1880	-	4,4,4	0.25	0	6,6,6	0.07	0
5	SO4	D	1884	-	4,4,4	0.27	0	6,6,6	0.05	0
5	SO4	A	1890	-	4,4,4	0.27	0	6,6,6	0.07	0
5	SO4	A	1884	-	4,4,4	0.27	0	6,6,6	0.09	0
5	SO4	D	1888	-	4,4,4	0.25	0	6,6,6	0.06	0
5	SO4	D	1890	-	4,4,4	0.26	0	6,6,6	0.08	0
7	2AD	A	1893	6	18,21,21	0.69	0	15,31,31	0.81	0
5	SO4	A	1880	-	4,4,4	0.28	0	6,6,6	0.10	0
6	NVA	D	1894	7	5,6,7	0.46	0	2,6,8	0.32	0
5	SO4	A	1889	-	4,4,4	0.27	0	6,6,6	0.06	0
5	SO4	A	1887	-	4,4,4	0.27	0	6,6,6	0.08	0
5	SO4	D	1885	-	4,4,4	0.27	0	6,6,6	0.07	0
5	SO4	D	1891	-	4,4,4	0.26	0	6,6,6	0.08	0
5	SO4	A	1886	-	4,4,4	0.25	0	6,6,6	0.08	0
5	SO4	D	1892	-	4,4,4	0.27	0	6,6,6	0.08	0
5	SO4	A	1882	-	4,4,4	0.26	0	6,6,6	0.09	0
5	SO4	A	1885	-	4,4,4	0.28	0	6,6,6	0.05	0
7	2AD	D	1895	6	18,21,21	0.65	0	15,31,31	0.89	0
5	SO4	A	1888	-	4,4,4	0.27	0	6,6,6	0.06	0
5	SO4	A	1883	-	4,4,4	0.28	0	6,6,6	0.09	0
6	NVA	A	1892	7	5,6,7	0.52	0	2,6,8	0.33	0
5	SO4	D	1883	-	4,4,4	0.25	0	6,6,6	0.08	0
5	SO4	D	1889	-	4,4,4	0.27	0	6,6,6	0.07	0
5	SO4	D	1882	-	4,4,4	0.27	0	6,6,6	0.06	0
5	SO4	D	1886	-	4,4,4	0.25	0	6,6,6	0.10	0
5	SO4	D	1881	-	4,4,4	0.27	0	6,6,6	0.08	0
5	SO4	A	1891	-	4,4,4	0.25	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	2AD	D	1895	6	-	0/2/22/22	0/3/3/3
6	NVA	D	1894	7	-	0/4/5/7	-
6	NVA	A	1892	7	-	1/4/5/7	-
7	2AD	A	1893	6	-	0/2/22/22	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1892	NVA	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1893	2AD	3	0
7	D	1895	2AD	1	0
6	A	1892	NVA	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	876/878 (99%)	0.08	28 (3%) 47 43	25, 67, 104, 136	0
1	D	876/878 (99%)	0.41	69 (7%) 12 10	57, 93, 139, 161	0
2	B	78/83 (93%)	0.27	4 (5%) 28 24	35, 70, 150, 186	0
2	E	78/83 (93%)	0.31	5 (6%) 19 15	50, 79, 157, 189	0
All	All	1908/1922 (99%)	0.25	106 (5%) 24 20	25, 79, 130, 189	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	6.6
2	B	17	G	6.3
2	E	17	G	6.2
1	A	858	GLY	5.8
1	D	591	SER	5.1
1	D	432	THR	4.9
1	D	858	GLY	4.8
1	D	855	HIS	4.8
1	D	497	THR	4.6
1	D	431	GLY	4.5
2	B	32	C	4.5
1	D	583	PHE	4.3
1	D	584	GLY	4.3
1	D	487	CYS	4.2
1	D	498	MET	4.1
1	D	627	ASP	3.8
1	D	629	THR	3.8
1	A	855	HIS	3.8
1	D	433	PRO	3.8
1	D	300	ARG	3.8
1	D	32	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	31	A	3.7
1	D	642	LYS	3.7
1	D	505	SER	3.6
2	E	32	C	3.6
1	D	797	ASP	3.5
1	D	590	GLY	3.4
1	A	497	THR	3.4
2	E	31	A	3.3
1	D	496	ASP	3.3
1	D	180	GLU	3.3
1	D	605	ILE	3.3
1	D	589	GLU	3.3
1	D	856	LEU	3.2
1	D	630	LEU	3.2
1	A	440	GLU	3.1
1	D	850	ARG	3.1
1	A	1	MET	3.1
1	A	490	PRO	3.1
1	D	606	PRO	3.1
1	D	876	VAL	3.1
1	D	862	VAL	3.0
1	D	488	GLY	3.0
1	D	2	GLU	3.0
1	D	851	ASN	2.9
1	A	850	ARG	2.9
1	A	431	GLY	2.9
1	A	432	THR	2.9
1	D	173	GLU	2.8
1	A	433	PRO	2.8
1	A	338	MET	2.8
1	A	31	GLY	2.8
1	D	504	SER	2.8
1	D	860	GLU	2.8
1	D	617	LYS	2.7
1	A	876	VAL	2.7
1	A	862	VAL	2.7
1	A	860	GLU	2.7
1	D	296	GLN	2.6
2	E	76	A	2.6
1	A	498	MET	2.6
1	D	592	VAL	2.6
1	A	781	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	623	ARG	2.5
1	D	607	GLU	2.5
1	A	505	SER	2.5
1	D	654	GLU	2.4
1	D	781	PRO	2.4
2	E	38	A	2.4
1	D	31	GLY	2.4
1	D	299	GLY	2.4
1	D	60	ASP	2.4
1	D	83	GLY	2.3
1	D	93	PHE	2.3
1	D	643	GLY	2.3
1	D	461	ASP	2.3
1	D	490	PRO	2.3
1	D	434	ILE	2.3
1	D	830	THR	2.2
1	A	32	ARG	2.2
2	B	38	A	2.2
1	D	601	ILE	2.2
1	A	188	GLU	2.2
1	D	495	THR	2.2
1	D	779	LEU	2.2
1	A	296	GLN	2.1
1	D	188	GLU	2.1
1	A	499	ASP	2.1
1	A	859	LYS	2.1
1	D	859	LYS	2.1
1	D	56	TYR	2.1
1	D	19	GLU	2.1
1	D	465	ILE	2.1
1	D	463	GLU	2.1
1	A	93	PHE	2.1
1	D	293	ILE	2.1
1	A	875	VAL	2.1
1	D	468	LYS	2.1
1	A	300	ARG	2.0
1	D	613	GLU	2.0
1	D	782	PHE	2.0
1	A	293	ILE	2.0
1	D	609	ALA	2.0
1	D	661	ARG	2.0
1	A	856	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	796	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	D	1885	5/5	0.79	0.24	143,145,146,146	0
3	ZN	A	1877	1/1	0.81	0.06	117,117,117,117	0
5	SO4	D	1882	5/5	0.83	0.21	153,154,155,155	0
5	SO4	A	1890	5/5	0.83	0.35	148,150,150,151	0
5	SO4	A	1891	5/5	0.83	0.27	143,144,145,145	0
5	SO4	D	1886	5/5	0.86	0.21	133,135,136,136	0
5	SO4	A	1880	5/5	0.87	0.30	148,148,149,149	0
5	SO4	D	1890	5/5	0.87	0.40	153,153,154,155	0
5	SO4	D	1883	5/5	0.89	0.19	140,140,141,142	0
5	SO4	A	1886	5/5	0.89	0.26	144,144,145,146	0
5	SO4	D	1892	5/5	0.91	0.20	135,136,138,138	0
5	SO4	D	1889	5/5	0.92	0.21	136,137,138,139	0
5	SO4	A	1888	5/5	0.92	0.23	146,147,147,148	0
5	SO4	D	1880	5/5	0.92	0.28	152,152,153,153	0
6	NVA	A	1892	7/8	0.92	0.28	75,77,81,84	0
5	SO4	A	1883	5/5	0.93	0.11	132,133,134,134	0
8	LEU	D	1893	9/9	0.93	0.27	91,94,95,95	0
5	SO4	D	1888	5/5	0.94	0.14	153,154,154,154	0
5	SO4	A	1889	5/5	0.94	0.13	117,117,119,120	0
5	SO4	A	1885	5/5	0.94	0.12	122,122,123,123	0
3	ZN	D	1877	1/1	0.95	0.11	142,142,142,142	0
5	SO4	D	1891	5/5	0.95	0.10	112,113,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	1884	5/5	0.95	0.13	95,96,98,98	0
6	NVA	D	1894	7/8	0.95	0.23	58,61,66,67	0
5	SO4	A	1882	5/5	0.96	0.09	86,89,92,93	0
7	2AD	A	1893	19/19	0.96	0.21	50,58,75,76	0
5	SO4	A	1887	5/5	0.96	0.13	113,114,115,116	0
5	SO4	D	1881	5/5	0.96	0.10	101,101,103,104	0
5	SO4	D	1887	5/5	0.96	0.12	103,104,105,106	0
5	SO4	D	1884	5/5	0.97	0.08	119,119,121,121	0
3	ZN	D	1878	1/1	0.97	0.15	97,97,97,97	0
8	LEU	A	1894	9/9	0.97	0.16	41,50,58,60	0
7	2AD	D	1895	19/19	0.97	0.20	59,66,71,71	0
3	ZN	A	1878	1/1	0.97	0.17	68,68,68,68	0
5	SO4	A	1881	5/5	0.98	0.11	69,75,76,76	0
4	HG	D	1879	1/1	0.99	0.14	156,156,156,156	0
4	HG	A	1879	1/1	0.99	0.14	109,109,109,109	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.