



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2020 – 01:09 pm BST

PDB ID : 2V0G  
Title : LEUCYL-TRNA SYNTHETASE FROM THERMUS THERMOPHILUS COMPLEXED WITH A tRNA(leu) transcript with 5-FLUORO-1,3-DIHYDRO-1-HYDROXY-2,1- BENZOXABOROLE (AN2690) forming an adduct to the ribose of adenosine- 76 in the enzyme editing site.  
Authors : Rock, F.; Mao, W.; Yaremchuk, A.; Tukalo, M.; Crepin, T.; Zhou, H.; Zhang, Y.; Hernandez, V.; Akama, T.; Baker, S.; Plattner, J.; Shapiro, L.; Martinis, S.A.; Benkovic, S.J.; Cusack, S.; Alley, M.R.K.  
Deposited on : 2007-05-14  
Resolution : 3.50 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

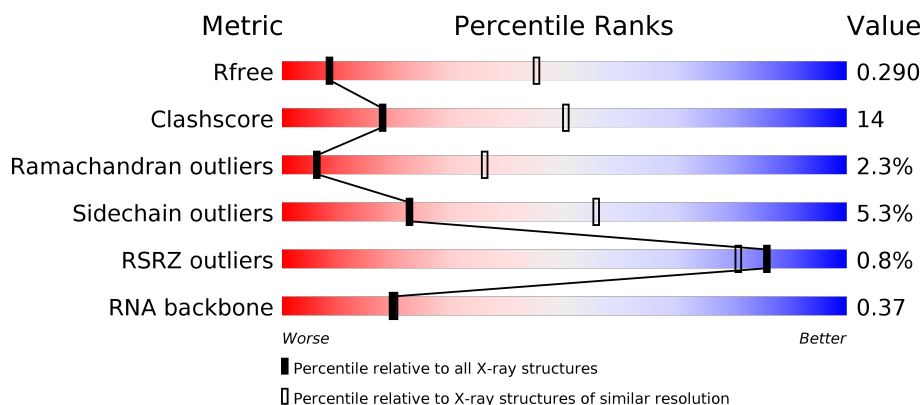
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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	
1	D	878	
2	B	83	
2	F	83	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17604 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.

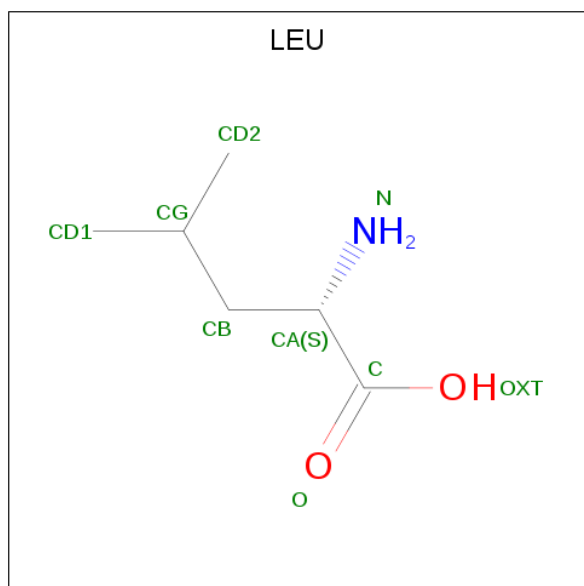
- Molecule 1 is a protein called AMINOACYL-TRNA SYNTHETASE.

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.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	B	76	Total	B	C	F	N	O	P	0	0	0
			1643	1	733	1	302	530	76			
2	F	76	Total	B	C	F	N	O	P	0	0	0
			1643	1	733	1	302	530	76			

- Molecule 3 is LEUCINE (three-letter code: LEU) (formula:  $C_6H_{13}NO_2$ ).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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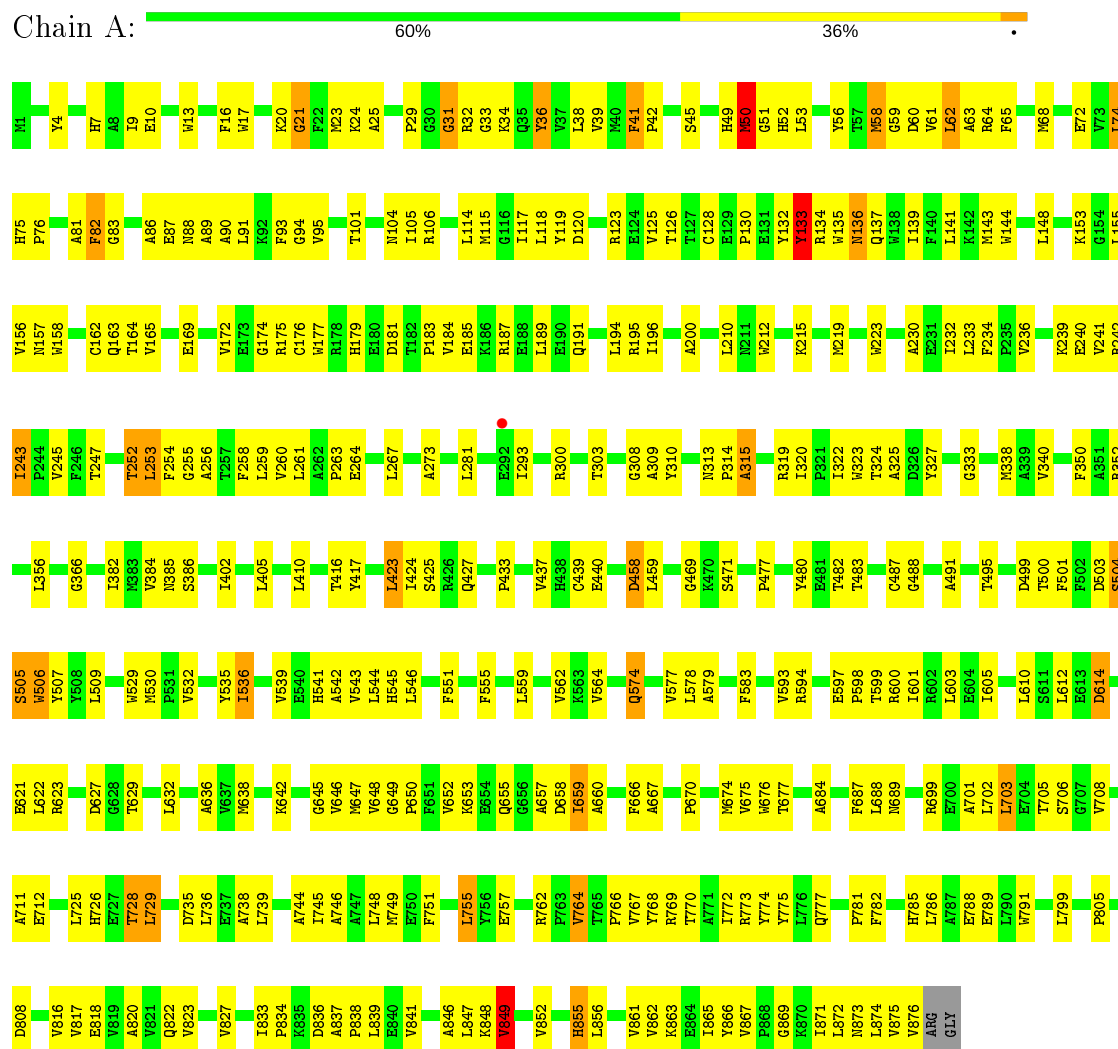
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0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

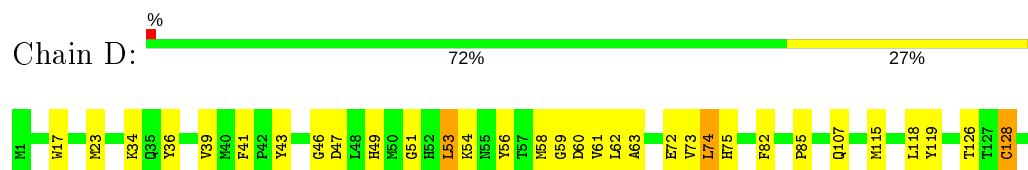
### 3 Residue-property plots

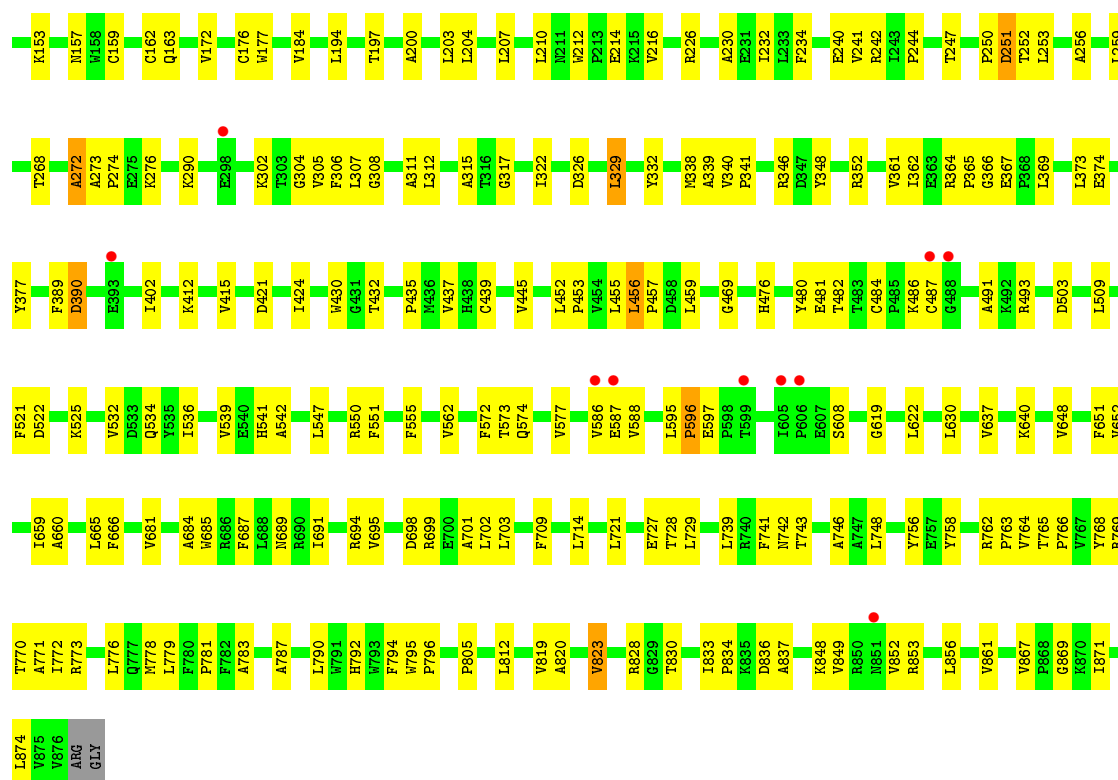
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

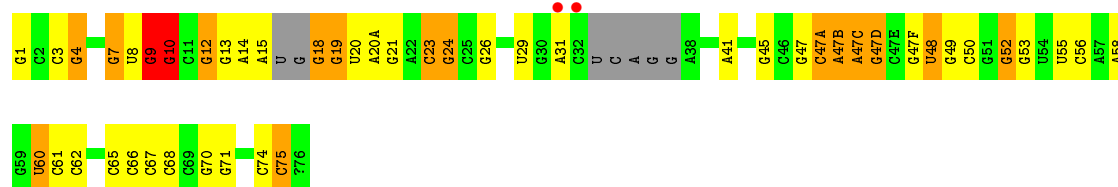


#### • Molecule 1: AMINOACYL-TRNA SYNTHETASE

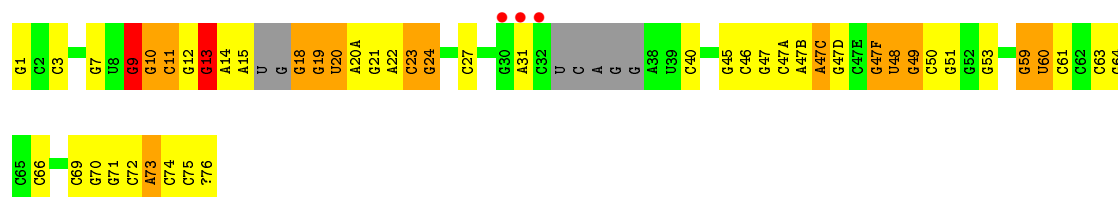




• Molecule 2: TRNALEU



• Molecule 2: TRNALEU



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.05Å 125.80Å 173.20Å 90.00° 118.71° 90.00°	Depositor
Resolution (Å)	152.50 – 3.50 44.95 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.1 (152.50-3.50) 95.1 (44.95-3.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.245 , 0.314 0.233 , 0.290	Depositor DCC
$R_{free}$ test set	2324 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.9	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	17604	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: ZN, SO4, ANZ, HG

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	0.56	0/7327	0.64	0/9945
1	D	0.45	0/7327	0.56	0/9945
2	B	0.90	1/1799 (0.1%)	1.53	23/2799 (0.8%)
2	F	0.84	1/1799 (0.1%)	1.43	16/2799 (0.6%)
All	All	0.59	2/18252 (0.0%)	0.87	39/25488 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	G	OP3-P	-10.17	1.49	1.61
2	F	1	G	OP3-P	-10.11	1.49	1.61

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	G	P-O3'-C3'	11.27	133.22	119.70
2	F	9	G	P-O3'-C3'	9.15	130.68	119.70
2	B	7	G	O4'-C1'-N9	7.69	114.35	108.20
2	B	12	G	N3-C4-N9	-7.06	121.77	126.00
2	F	47(F)	G	C8-N9-C4	-7.03	103.59	106.40
2	B	13	G	C5-C6-O6	-7.00	124.40	128.60
2	B	24	G	N9-C1'-C2'	-6.62	104.72	112.00
2	B	24	G	C5-C6-O6	-6.47	124.72	128.60
2	B	23	C	O4'-C1'-N1	6.44	113.35	108.20
2	B	10	G	C5-C6-O6	-6.43	124.74	128.60
2	B	10	G	N1-C6-O6	6.32	123.69	119.90
2	B	58	A	O4'-C1'-N9	-6.19	103.25	108.20
2	B	24	G	C4-C5-N7	6.13	113.25	110.80
2	F	13	G	C5-C6-O6	-6.01	124.99	128.60
2	B	18	G	P-O3'-C3'	5.99	126.89	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	15	A	C4'-C3'-C2'	-5.89	96.71	102.60
2	F	47(F)	G	N7-C8-N9	5.87	116.04	113.10
2	B	12	G	C8-N9-C1'	5.83	134.57	127.00
2	F	9	G	C2'-C3'-O3'	5.82	123.01	113.70
2	F	18	G	P-O3'-C3'	5.82	126.68	119.70
2	F	23	C	O4'-C1'-N1	5.69	112.75	108.20
2	B	15	A	C4'-C3'-C2'	-5.64	96.96	102.60
2	F	13	G	N1-C6-O6	5.64	123.29	119.90
2	B	13	G	C4-C5-N7	5.59	113.04	110.80
2	F	18	G	C3'-C2'-C1'	5.57	105.96	101.50
2	F	59	G	C5-C6-O6	-5.46	125.32	128.60
2	F	20	U	C3'-C2'-C1'	5.39	105.81	101.50
2	B	47(C)	A	O4'-C1'-N9	5.38	112.51	108.20
2	B	52	G	C8-N9-C4	-5.33	104.27	106.40
2	B	12	G	C8-N9-C4	-5.32	104.27	106.40
2	B	15	A	C8-N9-C4	-5.32	103.67	105.80
2	B	18	G	C3'-C2'-C1'	5.29	105.74	101.50
2	F	10	G	O4'-C4'-C3'	-5.28	98.72	104.00
2	B	75	C	O4'-C1'-N1	-5.28	103.98	108.20
2	B	12	G	O4'-C1'-N9	5.16	112.33	108.20
2	F	13	G	C6-C5-N7	-5.11	127.33	130.40
2	F	20	U	P-O3'-C3'	5.11	125.83	119.70
2	F	59	G	N1-C6-O6	5.06	122.94	119.90
2	B	4	G	C3'-C2'-C1'	-5.03	97.48	101.50

There are no chirality outliers.

There are no planarity outliers.

## 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	7036	250	0
1	D	7122	0	7037	158	0
2	B	1643	0	832	23	0
2	F	1643	0	832	23	0
3	A	9	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	9	0	10	1	0
4	A	2	0	0	0	0
4	D	2	0	0	1	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	35	0	0	0	0
6	D	15	0	0	0	0
All	All	17604	0	15757	446	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 14.

All (446) 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:A:310:TYR:O	1:A:322:ILE:HD11	1.65	0.95
1:D:162:CYS:HG	4:D:1881:ZN:ZN	0.63	0.95
1:A:232:ILE:HD13	1:A:253:LEU:HD13	1.50	0.93
1:D:776:LEU:HD21	1:D:790:LEU:HD12	1.51	0.91
1:D:776:LEU:CD2	1:D:790:LEU:HD12	2.06	0.84
1:D:312:LEU:HD22	1:D:317:GLY:O	1.75	0.84
1:A:25:ALA:HB3	1:A:123:ARG:HE	1.42	0.84
1:A:574:GLN:HE22	1:A:670:PRO:HB2	1.40	0.84
1:A:324:THR:O	1:A:324:THR:HG23	1.79	0.81
1:A:7:HIS:NE2	1:A:653:LYS:O	2.14	0.81
1:A:574:GLN:HE21	1:A:574:GLN:HA	1.47	0.79
1:A:658:ASP:OD1	1:A:785:HIS:ND1	2.12	0.78
1:A:230:ALA:HB2	1:A:402:ILE:HD11	1.64	0.78
1:A:17:TRP:HB3	1:A:118:LEU:HD21	1.66	0.78
1:A:175:ARG:HE	1:A:293:ILE:HD11	1.49	0.77
1:D:194:LEU:HD12	1:D:424:ILE:HG21	1.65	0.77
1:A:157:ASN:HB3	1:A:184:VAL:HG11	1.66	0.76
1:A:509:LEU:HG	1:A:530:MET:HE2	1.67	0.76
1:D:329:LEU:HD11	2:F:75:C:C4	2.22	0.74
1:D:157:ASN:HB3	1:D:184:VAL:HG11	1.70	0.74
1:D:648:VAL:O	1:D:652:VAL:HG23	1.86	0.74
2:B:14:A:C2	2:B:21:G:H4'	2.23	0.73
1:A:191:GLN:HE22	1:A:427:GLN:HE22	1.35	0.73
1:D:833:ILE:HD13	1:D:837:ALA:HB3	1.69	0.72
1:D:256:ALA:HB2	1:D:338:MET:HE3	1.70	0.72
1:A:863:LYS:HE2	1:A:865:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:HA	1:A:338:MET:HE3	1.70	0.71
1:D:776:LEU:HD21	1:D:790:LEU:CD1	2.20	0.71
1:A:74:LEU:C	1:A:74:LEU:HD12	2.11	0.70
1:A:232:ILE:CD1	1:A:253:LEU:HD13	2.20	0.69
1:A:64:ARG:NH2	1:A:118:LEU:HD13	2.09	0.68
1:A:169:GLU:HG3	1:A:223:TRP:CZ2	2.28	0.68
1:D:482:THR:HG21	1:D:493:ARG:HG3	1.76	0.68
1:A:243:ILE:HD13	1:A:261:LEU:HD21	1.74	0.68
1:D:141:LEU:HD12	1:D:452:LEU:HD11	1.74	0.68
1:D:163:GLN:HE22	1:D:469:GLY:HA2	1.58	0.68
1:D:307:LEU:HD12	1:D:322:ILE:HG22	1.74	0.68
1:A:822:GLN:OE1	2:B:19:G:N2	2.24	0.67
1:D:23:MET:HE1	1:D:63:ALA:HB1	1.76	0.67
1:A:852:VAL:HG12	1:A:855:HIS:HB2	1.76	0.67
1:A:822:GLN:HG2	1:A:871:ILE:HD11	1.78	0.66
1:A:659:ILE:HG22	1:A:684:ALA:HB3	1.77	0.66
1:A:114:LEU:HD22	1:A:652:VAL:HG11	1.77	0.66
1:D:302:LYS:HZ3	1:D:346:ARG:HA	1.60	0.65
1:A:252:THR:O	1:A:255:GLY:N	2.29	0.65
1:D:742:ASN:OD1	1:D:743:THR:N	2.28	0.65
1:A:610:LEU:HD22	1:A:614:ASP:HB3	1.79	0.64
1:A:143:MET:HG2	1:A:555:PHE:CZ	2.33	0.64
1:A:506:TRP:O	1:A:509:LEU:N	2.31	0.63
1:D:253:LEU:HG	1:D:315:ALA:HB2	1.79	0.63
1:A:638:MET:HG3	1:A:645:GLY:HA2	1.81	0.63
1:A:83:GLY:HA3	1:A:500:THR:HB	1.80	0.62
1:D:58:MET:CE	1:D:574:GLN:HE22	2.12	0.62
1:D:833:ILE:HD12	1:D:834:PRO:O	2.00	0.62
1:A:323:TRP:CZ2	1:A:356:LEU:HD21	2.35	0.62
1:A:666:PHE:HE1	1:A:746:ALA:HB2	1.64	0.62
1:A:583:PHE:CD1	1:A:603:LEU:HD23	2.34	0.62
1:A:93:PHE:O	1:A:95:VAL:HG23	2.00	0.62
1:A:866:TYR:O	1:A:867:VAL:HG23	1.98	0.62
1:A:646:VAL:HG21	1:A:676:TRP:CD1	2.34	0.61
1:A:458:ASP:O	1:A:459:LEU:HD12	2.01	0.61
1:D:307:LEU:HD12	1:D:322:ILE:CG2	2.30	0.61
2:B:19:G:OP1	2:B:60:U:N3	2.33	0.61
1:A:130:PRO:HA	1:A:133:TYR:CE2	2.36	0.61
1:A:745:ILE:O	1:A:746:ALA:C	2.39	0.60
1:A:505:SER:O	1:A:506:TRP:HB3	2.01	0.60
1:D:779:LEU:HG	1:D:783:ALA:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:GLY:O	1:A:653:LYS:HG2	2.01	0.60
1:D:364:ARG:HG3	1:D:365:PRO:HD2	1.83	0.60
1:A:39:VAL:HA	1:A:536:ILE:HG22	1.84	0.60
1:A:875:VAL:HG12	1:A:876:VAL:H	1.67	0.60
1:A:701:ALA:O	1:A:764:VAL:HG11	2.02	0.59
1:D:539:VAL:HG22	1:D:573:THR:HB	1.84	0.59
1:A:61:VAL:HG12	1:A:62:LEU:N	2.16	0.59
1:A:659:ILE:HG22	1:A:684:ALA:CB	2.33	0.59
1:A:236:VAL:HG12	1:A:239:LYS:HB2	1.83	0.58
1:A:499:ASP:OD1	1:A:500:THR:N	2.36	0.58
1:D:216:VAL:HG13	1:D:542:ALA:HB1	1.85	0.58
1:D:361:VAL:O	1:D:362:ILE:HD13	2.03	0.58
1:A:31:GLY:O	1:A:33:GLY:N	2.37	0.58
1:D:304:GLY:O	1:D:305:VAL:HG23	2.03	0.58
1:D:588:VAL:CG2	1:D:630:LEU:HD12	2.33	0.58
1:D:727:GLU:HA	1:D:812:LEU:HD21	1.84	0.58
1:D:867:VAL:HB	1:D:871:ILE:HG22	1.85	0.58
1:A:324:THR:O	1:A:324:THR:CG2	2.51	0.58
1:A:74:LEU:HD12	1:A:75:HIS:N	2.18	0.57
1:A:627:ASP:OD2	1:A:629:THR:OG1	2.22	0.57
1:A:852:VAL:O	1:A:856:LEU:HD13	2.04	0.57
1:D:75:HIS:CE1	1:D:119:TYR:CE1	2.92	0.57
1:D:522:ASP:HB3	1:D:525:LYS:HG3	1.87	0.57
2:F:27:C:H6	2:F:27:C:O5'	1.86	0.57
1:A:23:MET:CE	1:A:63:ALA:HB1	2.34	0.57
1:D:273:ALA:HB1	1:D:274:PRO:CD	2.35	0.57
1:D:36:TYR:CE1	1:D:532:VAL:HG22	2.40	0.57
1:A:42:PRO:HB3	1:A:56:TYR:OH	2.04	0.56
1:A:751:PHE:CE2	1:A:755:LEU:HD11	2.40	0.56
1:D:251:ASP:OD1	1:D:251:ASP:N	2.35	0.56
1:D:176:CYS:SG	1:D:177:TRP:N	2.79	0.56
1:A:210:LEU:HD21	1:A:212:TRP:CE2	2.40	0.56
1:D:232:ILE:O	1:D:244:PRO:HA	2.06	0.56
2:B:4:G:H1'	2:B:70:G:N2	2.21	0.56
1:D:659:ILE:HG23	1:D:684:ALA:CB	2.36	0.56
2:B:67:C:H2'	2:B:68:C:C6	2.41	0.56
1:D:61:VAL:HG22	1:D:781:PRO:O	2.06	0.56
1:A:745:ILE:HG22	1:A:749:MET:CE	2.36	0.56
1:D:687:PHE:CE2	1:D:691:ILE:HD11	2.40	0.56
1:A:482:THR:O	1:A:491:ALA:HB3	2.06	0.56
1:A:666:PHE:CG	1:A:666:PHE:O	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:LEU:H	1:A:839:LEU:HD12	1.70	0.55
1:D:197:THR:HG23	1:D:421:ASP:OD1	2.05	0.55
1:A:579:ALA:HB2	1:A:638:MET:HE2	1.88	0.55
1:D:456:LEU:HD23	1:D:457:PRO:HD2	1.88	0.55
1:A:252:THR:CG2	1:A:340:VAL:HG11	2.36	0.55
1:A:657:ALA:O	1:A:660:ALA:N	2.39	0.55
2:B:53:G:C2	2:B:62:C:N3	2.74	0.55
1:A:191:GLN:HE22	1:A:427:GLN:NE2	2.04	0.55
1:D:39:VAL:HG21	1:D:56:TYR:HD2	1.72	0.55
1:D:210:LEU:HD21	1:D:212:TRP:CE2	2.42	0.54
1:A:252:THR:HB	1:A:340:VAL:HG21	1.88	0.54
1:A:437:VAL:HG11	1:A:491:ALA:HB1	1.90	0.54
1:D:252:THR:HB	1:D:340:VAL:HG11	1.90	0.54
1:A:82:PHE:CD1	1:A:128:CYS:HB2	2.43	0.54
1:A:820:ALA:O	1:A:871:ILE:HD12	2.06	0.54
2:B:3:C:O2	2:B:71:G:N2	2.41	0.54
1:A:655:GLN:HB3	1:A:659:ILE:HD12	1.90	0.54
1:A:241:VAL:HG22	1:A:242:ARG:N	2.22	0.54
1:A:822:GLN:O	1:A:873:ASN:HA	2.07	0.54
1:A:137:GLN:NE2	1:A:433:PRO:O	2.39	0.54
2:B:14:A:C2	2:B:21:G:C4'	2.90	0.54
1:D:665:LEU:HD22	1:D:741:PHE:HB3	1.89	0.54
1:A:702:LEU:HD22	1:A:769:ARG:HG3	1.89	0.53
1:A:141:LEU:O	1:A:144:TRP:N	2.41	0.53
1:A:646:VAL:HG21	1:A:676:TRP:NE1	2.23	0.53
2:B:8:U:H1'	2:B:48:U:H1'	1.91	0.53
1:A:123:ARG:O	1:A:125:VAL:HG23	2.08	0.53
1:D:709:PHE:CE2	1:D:714:LEU:HD11	2.43	0.53
1:D:204:LEU:HD12	1:D:204:LEU:O	2.09	0.53
1:D:685:TRP:HE3	1:D:689:ASN:HD21	1.56	0.53
1:A:132:TYR:O	1:A:134:ARG:N	2.42	0.53
1:A:846:ALA:O	1:A:849:VAL:HG13	2.08	0.53
2:F:3:C:O2	2:F:71:G:N2	2.42	0.53
1:A:477:PRO:HA	1:A:480:TYR:CE2	2.44	0.53
1:D:290:LYS:NZ	1:D:326:ASP:OD2	2.42	0.53
1:A:162:CYS:SG	1:A:179:HIS:HE1	2.32	0.52
2:F:22:A:H2'	2:F:23:C:O4'	2.09	0.52
1:A:745:ILE:O	1:A:748:LEU:N	2.42	0.52
1:A:53:LEU:CD1	1:A:115:MET:HG3	2.38	0.52
1:A:65:PHE:CG	1:A:736:LEU:HD13	2.45	0.52
1:A:38:LEU:HD23	1:A:535:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:SER:O	1:A:545:HIS:ND1	2.40	0.52
1:A:51:GLY:HA2	1:A:577:VAL:HB	1.92	0.52
1:D:702:LEU:HD23	1:D:769:ARG:HG3	1.92	0.52
1:A:838:PRO:HD2	1:A:841:VAL:HG23	1.92	0.52
1:A:215:LYS:CE	1:A:539:VAL:HG11	2.40	0.51
1:A:254:PHE:CZ	1:A:315:ALA:HB1	2.44	0.51
1:A:817:VAL:HG12	1:A:818:GLU:N	2.25	0.51
1:D:58:MET:HE2	1:D:574:GLN:HE22	1.74	0.51
1:A:243:ILE:CD1	1:A:261:LEU:HD21	2.39	0.51
1:A:253:LEU:HA	1:A:338:MET:CE	2.39	0.51
1:A:253:LEU:HD23	1:A:315:ALA:HB2	1.92	0.51
1:D:622:LEU:HB3	1:D:630:LEU:HD22	1.92	0.51
1:A:823:VAL:HG22	1:A:874:LEU:HB2	1.92	0.51
1:D:820:ALA:HA	1:D:830:THR:HG22	1.92	0.51
2:F:48:U:C2	2:F:59:G:O4'	2.63	0.51
1:A:64:ARG:NH2	1:A:118:LEU:CD1	2.74	0.51
1:A:65:PHE:CD1	1:A:736:LEU:HD13	2.46	0.51
1:D:348:TYR:OH	1:D:374:GLU:HA	2.11	0.51
1:A:81:ALA:HB1	1:A:101:THR:HG21	1.93	0.51
1:A:439:CYS:SG	1:A:440:GLU:N	2.84	0.51
1:A:254:PHE:CD2	1:A:386:SER:HA	2.46	0.51
1:D:770:THR:O	1:D:773:ARG:HB3	2.11	0.51
1:A:657:ALA:O	1:A:660:ALA:HB3	2.11	0.51
1:D:834:PRO:HD2	1:D:837:ALA:HB2	1.93	0.51
1:A:41:PHE:CE2	1:A:507:TYR:CG	2.99	0.50
1:A:51:GLY:HA2	1:A:577:VAL:CG2	2.41	0.50
1:A:215:LYS:NZ	1:A:539:VAL:HG11	2.26	0.50
2:B:9:G:O2'	2:B:10:G:OP1	2.29	0.50
2:B:47(A):C:H2'	2:B:47(B):A:O4'	2.11	0.50
1:D:216:VAL:HG13	1:D:542:ALA:CB	2.41	0.50
2:B:66:C:C1'	2:F:47(C):A:H1'	2.41	0.50
1:A:49:HIS:O	1:A:51:GLY:N	2.44	0.50
1:A:60:ASP:OD2	1:A:117:ILE:HA	2.10	0.50
1:D:200:ALA:HA	1:D:203:LEU:HD12	1.93	0.50
2:F:23:C:H2'	2:F:24:G:O4'	2.12	0.50
1:D:241:VAL:HG22	1:D:242:ARG:O	2.12	0.49
1:A:10:GLU:OE1	1:A:657:ALA:N	2.31	0.49
1:A:148:LEU:CD2	1:A:195:ARG:HB3	2.43	0.49
1:A:319:ARG:O	1:A:320:ILE:HG23	2.11	0.49
1:A:405:LEU:HD22	1:A:410:LEU:HB2	1.94	0.49
1:A:9:ILE:HG21	1:A:789:GLU:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:TRP:CE3	1:A:799:LEU:HD21	2.47	0.49
1:D:141:LEU:HD21	1:D:435:PRO:O	2.12	0.49
1:D:701:ALA:HB3	1:D:764:VAL:HG21	1.93	0.49
1:A:258:PHE:CZ	1:A:356:LEU:HD12	2.48	0.49
2:B:7:G:H4'	2:B:8:U:OP2	2.12	0.49
1:D:268:THR:HG23	1:D:307:LEU:HD21	1.94	0.49
1:D:699:ARG:O	1:D:703:LEU:HD12	2.12	0.49
2:F:51:G:C6	2:F:64:G:N1	2.81	0.49
1:A:148:LEU:HD23	1:A:195:ARG:HB3	1.94	0.49
1:A:17:TRP:CB	1:A:118:LEU:HD21	2.41	0.49
1:A:156:VAL:HG11	1:A:191:GLN:HG3	1.95	0.49
1:A:687:PHE:CE1	1:A:749:MET:HG2	2.47	0.49
1:D:341:PRO:O	1:D:348:TYR:HB2	2.13	0.49
1:D:364:ARG:HD3	1:D:377:TYR:CE1	2.48	0.49
1:D:768:TYR:O	1:D:771:ALA:HB3	2.12	0.49
1:A:157:ASN:HB3	1:A:184:VAL:CG1	2.40	0.49
1:A:53:LEU:HG	1:A:115:MET:HE3	1.95	0.49
1:D:272:ALA:HB2	1:D:307:LEU:HD22	1.94	0.49
2:F:49:G:N2	2:F:50:C:C2	2.81	0.49
1:A:49:HIS:O	1:A:50:MET:C	2.52	0.48
1:A:667:ALA:HB3	1:A:674:MET:HE3	1.95	0.48
2:B:14:A:H2	2:B:21:G:H4'	1.77	0.48
2:F:45:G:H2'	2:F:46:C:H6	1.77	0.48
2:B:66:C:O4'	2:F:47(C):A:H1'	2.13	0.48
1:A:23:MET:HE2	1:A:63:ALA:HB1	1.95	0.48
1:D:721:LEU:HD22	1:D:758:TYR:CG	2.49	0.48
2:B:23:C:H2'	2:B:24:G:O4'	2.13	0.48
1:A:115:MET:O	1:A:657:ALA:HB1	2.14	0.48
1:A:49:HIS:HA	1:A:648:VAL:HG23	1.94	0.48
1:A:543:VAL:HG23	1:A:543:VAL:O	2.14	0.48
1:D:51:GLY:HA2	1:D:577:VAL:HB	1.95	0.48
1:A:219:MET:CE	1:A:542:ALA:HB3	2.44	0.48
1:A:555:PHE:CE1	1:A:559:LEU:HD21	2.49	0.48
2:B:12:G:C4	2:B:24:G:N2	2.82	0.48
1:D:23:MET:HE1	1:D:73:VAL:HG11	1.94	0.48
1:D:833:ILE:CD1	1:D:837:ALA:HB3	2.41	0.48
1:A:41:PHE:HD1	1:A:41:PHE:O	1.96	0.48
1:D:172:VAL:HG13	2:F:72:C:OP1	2.14	0.48
1:D:259:LEU:HD23	1:D:338:MET:HA	1.95	0.48
1:D:509:LEU:HD13	1:D:521:PHE:CZ	2.49	0.48
1:A:38:LEU:HD23	1:A:535:TYR:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:MET:CG	1:A:645:GLY:HA2	2.42	0.48
1:A:786:LEU:HD12	1:A:786:LEU:O	2.13	0.48
1:A:471:SER:OG	1:A:495:THR:O	2.25	0.48
1:D:369:LEU:HD13	1:D:373:LEU:HD21	1.95	0.48
1:A:24:LYS:HA	1:A:120:ASP:OD1	2.14	0.47
1:D:54:LYS:O	1:D:58:MET:HG2	2.13	0.47
1:A:58:MET:HE3	1:A:670:PRO:CB	2.43	0.47
1:A:772:ILE:O	1:A:773:ARG:C	2.51	0.47
1:D:437:VAL:CG1	1:D:491:ALA:HB1	2.45	0.47
1:D:748:LEU:HD21	1:D:778:MET:HB3	1.96	0.47
1:D:779:LEU:HD23	1:D:787:ALA:HB2	1.95	0.47
2:B:8:U:H2'	2:B:8:U:O2	2.14	0.47
1:D:61:VAL:HG13	1:D:781:PRO:CB	2.45	0.47
2:F:9:G:H3'	2:F:11:C:OP2	2.15	0.47
1:D:361:VAL:HG23	1:D:362:ILE:HG12	1.97	0.47
1:D:588:VAL:HG21	1:D:630:LEU:HD12	1.96	0.47
1:D:701:ALA:CB	1:D:764:VAL:HG21	2.44	0.47
1:D:764:VAL:HG12	1:D:764:VAL:O	2.15	0.47
1:A:252:THR:HG22	1:A:340:VAL:HG11	1.95	0.47
1:A:725:LEU:O	1:A:728:THR:N	2.48	0.47
1:D:136:ASN:HB2	1:D:432:THR:HG21	1.96	0.46
1:A:833:ILE:HD13	1:A:837:ALA:HB3	1.96	0.46
1:D:23:MET:CE	1:D:63:ALA:HB1	2.45	0.46
1:D:306:PHE:CE2	1:D:308:GLY:HA2	2.50	0.46
1:D:729:LEU:HD21	1:D:805:PRO:HB2	1.98	0.46
1:D:536:ILE:N	1:D:536:ILE:HD12	2.31	0.46
1:D:49:HIS:O	1:D:53:LEU:HD23	2.15	0.46
1:D:770:THR:O	1:D:771:ALA:C	2.53	0.46
1:A:219:MET:HE2	1:A:542:ALA:HB3	1.98	0.46
2:B:20(A):A:H2'	2:B:21:G:O4'	2.15	0.46
1:D:823:VAL:HG13	1:D:874:LEU:HB2	1.97	0.46
1:A:245:VAL:HG23	1:A:245:VAL:O	2.15	0.46
1:A:61:VAL:HG22	1:A:781:PRO:O	2.16	0.46
1:D:453:PRO:HG2	1:D:455:LEU:HD12	1.98	0.46
1:A:90:ALA:HB1	1:A:95:VAL:O	2.16	0.46
2:B:66:C:H1'	2:F:47(C):A:N3	2.30	0.46
2:F:45:G:H2'	2:F:46:C:C6	2.51	0.46
1:A:487:CYS:SG	1:A:488:GLY:N	2.89	0.46
1:A:725:LEU:HD13	1:A:751:PHE:CE2	2.50	0.46
1:A:745:ILE:HG22	1:A:749:MET:HE3	1.98	0.46
1:D:276:LYS:HG3	1:D:308:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:823:VAL:HG23	1:D:828:ARG:CG	2.46	0.46
1:A:735:ASP:HB3	1:A:744:ALA:HB2	1.98	0.45
1:D:311:ALA:HB2	1:D:322:ILE:HD11	1.97	0.45
1:D:659:ILE:HG23	1:D:684:ALA:HB3	1.96	0.45
1:D:43:TYR:CE1	1:D:85:PRO:HG2	2.51	0.45
1:D:159:CYS:O	1:D:163:GLN:N	2.42	0.45
1:A:325:ALA:HB2	1:A:350:PHE:CE2	2.51	0.45
1:A:384:VAL:HG22	1:A:385:ASN:N	2.31	0.45
1:D:39:VAL:HG11	1:D:56:TYR:HA	1.98	0.45
2:F:12:G:C6	2:F:13:G:H1'	2.51	0.45
1:A:49:HIS:O	1:A:52:HIS:N	2.45	0.45
1:D:273:ALA:HB1	1:D:274:PRO:HD2	1.98	0.45
1:D:364:ARG:CG	1:D:365:PRO:HD2	2.47	0.45
1:D:819:VAL:HG13	1:D:871:ILE:N	2.31	0.45
1:A:702:LEU:O	1:A:705:THR:N	2.49	0.45
1:D:143:MET:HG2	1:D:555:PHE:CE2	2.52	0.45
1:D:17:TRP:HB3	1:D:118:LEU:HD21	1.99	0.45
1:D:651:PHE:CE2	1:D:660:ALA:HB2	2.52	0.45
1:A:313:ASN:O	1:A:314:PRO:C	2.52	0.45
1:A:260:VAL:HG13	1:A:325:ALA:H	1.82	0.45
1:A:822:GLN:CG	1:A:871:ILE:HD11	2.44	0.45
1:A:236:VAL:HB	1:A:241:VAL:HG13	1.99	0.44
1:A:234:PHE:CE2	1:A:259:LEU:HD21	2.52	0.44
1:D:194:LEU:CD1	1:D:424:ILE:HD13	2.47	0.44
1:A:158:TRP:N	1:A:185:GLU:O	2.43	0.44
1:D:256:ALA:HA	1:D:339:ALA:O	2.17	0.44
1:A:163:GLN:NE2	1:A:469:GLY:HA2	2.32	0.44
1:A:501:PHE:CZ	1:A:544:LEU:HD13	2.53	0.44
1:A:621:GLU:OE2	1:A:623:ARG:NE	2.50	0.44
1:A:729:LEU:HD21	1:A:805:PRO:HB2	1.99	0.44
1:D:74:LEU:C	1:D:74:LEU:HD12	2.37	0.44
1:D:332:TYR:OH	2:F:76:ANZ:O1P	2.31	0.44
1:D:480:TYR:O	1:D:482:THR:HG22	2.17	0.44
1:A:20:LYS:O	1:A:21:GLY:C	2.55	0.44
1:A:87:GLU:O	1:A:88:ASN:C	2.55	0.44
1:D:509:LEU:HD11	1:D:562:VAL:HG21	1.99	0.44
1:A:155:LEU:HD11	1:A:264:GLU:HG2	1.99	0.44
1:A:657:ALA:O	1:A:658:ASP:C	2.55	0.44
1:A:699:ARG:O	1:A:703:LEU:HD12	2.18	0.44
1:A:156:VAL:HG22	1:A:187:ARG:O	2.18	0.44
1:A:838:PRO:HD2	1:A:841:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:PHE:O	1:A:559:LEU:HG	2.18	0.44
1:A:711:ALA:HB3	1:A:712:GLU:OE1	2.18	0.44
1:D:226:ARG:NH1	1:D:415:VAL:HG11	2.32	0.44
2:F:19:G:OP1	2:F:60:U:N3	2.51	0.44
1:A:143:MET:HG2	1:A:555:PHE:CE2	2.53	0.43
1:D:58:MET:HE3	1:D:574:GLN:HE22	1.82	0.43
1:A:636:ALA:HB1	1:A:642:LYS:HE2	2.00	0.43
1:A:74:LEU:HD11	1:A:76:PRO:HB3	2.00	0.43
1:D:203:LEU:O	1:D:207:LEU:HB2	2.18	0.43
1:D:46:GLY:HA3	1:D:640:LYS:NZ	2.32	0.43
1:A:176:CYS:SG	1:A:179:HIS:ND1	2.87	0.43
1:A:241:VAL:CG2	1:A:242:ARG:N	2.82	0.43
1:A:325:ALA:HB1	1:A:327:TYR:HD2	1.84	0.43
1:A:578:LEU:O	1:A:675:VAL:HA	2.18	0.43
1:A:674:MET:HB2	1:A:674:MET:HE3	1.82	0.43
1:D:128:CYS:HB2	1:D:430:TRP:CZ2	2.52	0.43
1:D:763:PRO:O	1:D:765:THR:HG23	2.18	0.43
1:A:252:THR:HG21	1:A:340:VAL:HG11	2.00	0.43
1:A:647:MET:HB3	1:A:650:PRO:HD2	2.00	0.43
1:D:728:THR:O	1:D:729:LEU:C	2.55	0.43
1:D:572:PHE:HB2	1:D:739:LEU:HD23	2.01	0.43
1:A:273:ALA:HB2	1:A:308:GLY:O	2.18	0.43
1:A:645:GLY:O	1:A:647:MET:HE2	2.18	0.43
1:D:765:THR:HB	1:D:766:PRO:CD	2.49	0.43
2:F:12:G:C5	2:F:13:G:H1'	2.54	0.43
2:F:69:C:H2'	2:F:70:G:H8	1.83	0.43
1:A:105:ILE:O	1:A:106:ARG:C	2.57	0.43
1:A:230:ALA:HB2	1:A:402:ILE:CD1	2.41	0.43
1:A:748:LEU:HD22	1:A:775:TYR:CE2	2.54	0.43
1:D:194:LEU:HD12	1:D:424:ILE:CG2	2.44	0.43
1:D:729:LEU:CD2	1:D:805:PRO:HB2	2.48	0.43
1:D:695:VAL:O	1:D:695:VAL:HG12	2.18	0.43
1:A:135:TRP:O	1:A:137:GLN:N	2.52	0.43
1:A:667:ALA:CB	1:A:674:MET:HE3	2.49	0.43
2:B:26:G:H8	2:B:26:G:O5'	2.01	0.43
1:D:143:MET:HE1	1:D:551:PHE:CZ	2.54	0.43
1:D:648:VAL:HG12	1:D:652:VAL:CG2	2.49	0.43
1:A:56:TYR:HB3	1:A:117:ILE:HD13	2.01	0.43
1:D:681:VAL:O	1:D:684:ALA:HB3	2.19	0.43
1:A:688:LEU:HD22	1:A:786:LEU:HD23	2.00	0.42
1:D:234:PHE:CG	1:D:259:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:687:PHE:CZ	1:D:691:ILE:HD11	2.53	0.42
1:A:10:GLU:OE1	1:A:657:ALA:HB3	2.20	0.42
1:A:215:LYS:HZ3	1:A:539:VAL:HG11	1.84	0.42
1:A:867:VAL:O	1:A:867:VAL:HG12	2.17	0.42
1:D:230:ALA:HB2	1:D:402:ILE:CD1	2.49	0.42
1:D:698:ASP:O	1:D:702:LEU:HD13	2.19	0.42
1:A:53:LEU:HD12	1:A:115:MET:HG3	2.00	0.42
1:A:132:TYR:CE1	1:A:136:ASN:ND2	2.87	0.42
1:A:260:VAL:HG11	1:A:325:ALA:HB3	2.01	0.42
1:A:597:GLU:N	1:A:598:PRO:CD	2.82	0.42
1:A:676:TRP:C	1:A:677:THR:HG23	2.40	0.42
2:F:47(A):C:H2'	2:F:47(B):A:O4'	2.20	0.42
2:F:73:A:H5''	2:F:73:A:H8	1.84	0.42
1:D:389:PHE:O	1:D:390:ASP:C	2.57	0.42
1:D:595:LEU:HD23	1:D:596:PRO:N	2.34	0.42
1:A:183:PRO:HB3	1:A:293:ILE:HD12	2.02	0.42
1:A:256:ALA:HB2	1:A:338:MET:HE3	2.01	0.42
1:A:702:LEU:O	1:A:703:LEU:C	2.58	0.42
1:D:541:HIS:CE1	3:D:1883:LEU:HD22	2.54	0.42
1:D:828:ARG:HB3	1:D:853:ARG:HG2	2.01	0.42
1:A:143:MET:HE2	1:A:555:PHE:CE2	2.55	0.42
1:A:86:ALA:O	1:A:87:GLU:C	2.58	0.42
1:D:547:LEU:O	1:D:550:ARG:N	2.48	0.42
1:A:86:ALA:O	1:A:89:ALA:N	2.53	0.42
1:D:765:THR:CB	1:D:766:PRO:CD	2.97	0.42
1:A:135:TRP:C	1:A:137:GLN:N	2.73	0.42
1:A:223:TRP:CD1	1:A:223:TRP:C	2.92	0.42
1:A:599:THR:HG22	1:A:599:THR:O	2.19	0.42
1:D:794:PHE:HB2	1:D:795:TRP:CE3	2.55	0.42
1:A:333:GLY:HA2	1:A:416:THR:HG21	2.02	0.41
1:A:58:MET:HE3	1:A:670:PRO:HB3	2.02	0.41
1:A:728:THR:HG22	1:A:729:LEU:N	2.35	0.41
1:A:309:ALA:O	1:A:310:TYR:CD1	2.73	0.41
1:A:4:TYR:HB3	1:A:689:ASN:OD1	2.20	0.41
1:A:36:TYR:CE2	1:A:532:VAL:HG22	2.55	0.41
1:D:373:LEU:H	1:D:373:LEU:HD12	1.84	0.41
1:D:695:VAL:CG1	1:D:772:ILE:HG21	2.49	0.41
2:B:66:C:H1'	2:F:47(C):A:H1'	2.03	0.41
1:A:382:ILE:HD13	1:A:382:ILE:N	2.36	0.41
1:A:667:ALA:HB3	1:A:674:MET:CE	2.51	0.41
1:A:194:LEU:HD21	1:A:424:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ILE:HG13	1:A:551:PHE:CG	2.55	0.41
1:A:39:VAL:HG21	1:A:56:TYR:HA	2.01	0.41
1:A:172:VAL:C	1:A:174:GLY:H	2.24	0.41
1:A:29:PRO:HG3	1:A:529:TRP:CZ2	2.56	0.41
1:A:726:HIS:CD2	1:A:808:ASP:H	2.38	0.41
1:D:23:MET:HE1	1:D:73:VAL:CG1	2.51	0.41
1:A:164:THR:OG1	1:A:165:VAL:N	2.53	0.41
1:A:232:ILE:HG22	1:A:233:LEU:N	2.35	0.41
1:A:82:PHE:CE1	1:A:128:CYS:HB2	2.55	0.41
1:A:833:ILE:HD12	1:A:834:PRO:O	2.21	0.41
1:A:139:ILE:HG23	1:A:143:MET:HE2	2.02	0.41
1:A:162:CYS:SG	1:A:179:HIS:CE1	3.14	0.41
1:A:200:ALA:HB3	1:A:417:TYR:CD2	2.56	0.41
1:A:509:LEU:CD2	1:A:562:VAL:HG21	2.50	0.41
1:A:593:VAL:CG2	1:A:612:LEU:HD23	2.50	0.41
1:A:725:LEU:HD13	1:A:751:PHE:CZ	2.55	0.41
1:A:866:TYR:HD1	1:A:872:LEU:HD13	1.85	0.41
1:D:445:VAL:HG11	1:D:484:CYS:SG	2.60	0.41
1:A:36:TYR:CD1	1:A:74:LEU:HG	2.56	0.41
1:D:234:PHE:CE1	1:D:259:LEU:HD21	2.56	0.41
1:D:666:PHE:HE1	1:D:746:ALA:HB2	1.86	0.41
1:A:725:LEU:HD21	1:A:774:TYR:CD2	2.56	0.41
1:D:53:LEU:HD12	1:D:115:MET:HG3	2.02	0.41
1:D:247:THR:HG23	1:D:250:PRO:HB3	2.03	0.41
1:D:701:ALA:HB1	1:D:764:VAL:HB	2.02	0.41
1:A:256:ALA:N	1:A:340:VAL:HG22	2.36	0.41
1:A:738:ALA:O	1:A:739:LEU:HB2	2.21	0.41
1:A:745:ILE:HG22	1:A:749:MET:HE2	2.01	0.41
1:A:117:ILE:CG2	1:A:119:TYR:CE2	3.04	0.40
1:A:156:VAL:HG12	1:A:423:LEU:HD11	2.03	0.40
1:A:622:LEU:HD23	1:A:632:LEU:HA	2.03	0.40
1:A:817:VAL:HG12	1:A:818:GLU:H	1.86	0.40
2:B:47:G:N2	2:B:47(D):G:C4	2.89	0.40
1:D:47:ASP:OD2	1:D:107:GLN:HB3	2.21	0.40
1:D:59:GLY:O	1:D:60:ASP:C	2.60	0.40
1:D:694:ARG:HB2	1:D:756:TYR:CE1	2.56	0.40
1:A:13:TRP:O	1:A:16:PHE:HB3	2.21	0.40
1:A:259:LEU:CD2	1:A:338:MET:HA	2.51	0.40
1:A:541:HIS:C	1:A:546:LEU:HD12	2.42	0.40
1:A:766:PRO:O	1:A:767:VAL:C	2.59	0.40
1:A:767:VAL:HG13	1:A:768:TYR:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:665:LEU:HD22	1:D:741:PHE:CB	2.51	0.40
1:A:130:PRO:HA	1:A:133:TYR:CZ	2.56	0.40
1:D:141:LEU:CD1	1:D:452:LEU:HD11	2.45	0.40
1:D:459:LEU:HD21	1:D:476:HIS:CD2	2.56	0.40
1:D:702:LEU:HD12	1:D:764:VAL:HG11	2.04	0.40
1:A:68:MET:HE1	1:A:777:GLN:HB3	2.03	0.40
1:A:846:ALA:O	1:A:848:LYS:N	2.54	0.40
1:D:852:VAL:O	1:D:856:LEU:HD13	2.21	0.40
1:A:852:VAL:C	1:A:856:LEU:HD13	2.42	0.40
1:D:762:ARG:HG3	1:D:763:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	874/878 (100%)	728 (83%)	119 (14%)	27 (3%)	4	30
1	D	874/878 (100%)	750 (86%)	110 (13%)	14 (2%)	9	43
All	All	1748/1756 (100%)	1478 (85%)	229 (13%)	41 (2%)	6	36

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	GLY
1	A	32	ARG
1	A	50	MET
1	A	153	LYS
1	A	506	TRP
1	D	153	LYS
1	D	848	LYS
1	D	861	VAL

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Mol	Chain	Res	Type
1	A	45	SER
1	A	58	MET
1	A	94	GLY
1	A	136	ASN
1	A	847	LEU
1	A	861	VAL
1	D	366	GLY
1	D	481	GLU
1	D	637	VAL
1	A	564	VAL
1	A	253	LEU
1	A	764	VAL
1	A	133	TYR
1	A	181	ASP
1	A	315	ALA
1	A	505	SER
1	D	486	LYS
1	A	31	GLY
1	D	272	ALA
1	D	597	GLU
1	A	263	PRO
1	A	366	GLY
1	A	816	VAL
1	D	619	GLY
1	D	796	PRO
1	D	849	VAL
1	A	827	VAL
1	A	849	VAL
1	D	869	GLY
1	A	59	GLY
1	A	869	GLY
1	D	596	PRO
1	A	862	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%)	690 (93%)	51 (7%)	15	47
1	D	741/742 (100%)	713 (96%)	28 (4%)	33	65
All	All	1482/1484 (100%)	1403 (95%)	79 (5%)	22	55

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	36	TYR
1	A	41	PHE
1	A	50	MET
1	A	62	LEU
1	A	72	GLU
1	A	74	LEU
1	A	82	PHE
1	A	91	LEU
1	A	104	ASN
1	A	126	THR
1	A	133	TYR
1	A	177	TRP
1	A	189	LEU
1	A	240	GLU
1	A	243	ILE
1	A	247	THR
1	A	252	THR
1	A	267	LEU
1	A	281	LEU
1	A	300	ARG
1	A	303	THR
1	A	352	ARG
1	A	423	LEU
1	A	425	SER
1	A	458	ASP
1	A	483	THR
1	A	503	ASP
1	A	504	SER
1	A	536	ILE
1	A	574	GLN
1	A	594	ARG
1	A	600	ARG
1	A	601	ILE
1	A	605	ILE

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Mol	Chain	Res	Type
1	A	614	ASP
1	A	659	ILE
1	A	703	LEU
1	A	706	SER
1	A	708	VAL
1	A	728	THR
1	A	729	LEU
1	A	755	LEU
1	A	757	GLU
1	A	762	ARG
1	A	770	THR
1	A	782	PHE
1	A	788	GLU
1	A	836	ASP
1	A	849	VAL
1	A	855	HIS
1	D	34	LYS
1	D	41	PHE
1	D	53	LEU
1	D	62	LEU
1	D	72	GLU
1	D	74	LEU
1	D	82	PHE
1	D	126	THR
1	D	128	CYS
1	D	214	GLU
1	D	240	GLU
1	D	251	ASP
1	D	329	LEU
1	D	352	ARG
1	D	367	GLU
1	D	390	ASP
1	D	412	LYS
1	D	439	CYS
1	D	456	LEU
1	D	487	CYS
1	D	503	ASP
1	D	534	GLN
1	D	586	VAL
1	D	587	GLU
1	D	608	SER
1	D	792	HIS

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Mol	Chain	Res	Type
1	D	823	VAL
1	D	836	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	163	GLN
1	A	191	GLN
1	A	557	HIS
1	A	574	GLN
1	A	726	HIS
1	A	824	ASN
1	D	52	HIS
1	D	55	ASN
1	D	104	ASN
1	D	163	GLN
1	D	541	HIS
1	D	574	GLN
1	D	689	ASN
1	D	726	HIS
1	D	777	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	73/83 (87%)	22 (30%)	7 (9%)
2	F	73/83 (87%)	24 (32%)	7 (9%)
All	All	146/166 (87%)	46 (31%)	14 (9%)

All (46) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	10	G
2	B	19	G
2	B	20	U
2	B	29	U
2	B	41	A
2	B	45	G
2	B	47(A)	C

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Mol	Chain	Res	Type
2	B	47(B)	A
2	B	47(C)	A
2	B	47(D)	G
2	B	47(F)	G
2	B	48	U
2	B	49	G
2	B	50	C
2	B	52	G
2	B	55	U
2	B	56	C
2	B	60	U
2	B	61	C
2	B	65	C
2	B	74	C
2	B	75	C
2	F	9	G
2	F	10	G
2	F	11	C
2	F	13	G
2	F	14	A
2	F	19	G
2	F	20	U
2	F	20(A)	A
2	F	21	G
2	F	24	G
2	F	31	A
2	F	40	C
2	F	47(C)	A
2	F	47(D)	G
2	F	47(F)	G
2	F	48	U
2	F	49	G
2	F	53	G
2	F	60	U
2	F	61	C
2	F	63	C
2	F	66	C
2	F	73	A
2	F	74	C

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	18	G
2	B	20	U
2	B	31	A
2	B	48	U
2	B	60	U
2	B	74	C
2	F	7	G
2	F	9	G
2	F	10	G
2	F	18	G
2	F	20	U
2	F	47	G
2	F	60	U

## 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 [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	$\# Z  > 2$
6	SO4	D	1878	-	4,4,4	0.13	0	6,6,6	0.10	0
6	SO4	A	1883	-	4,4,4	0.15	0	6,6,6	0.16	0
6	SO4	A	1882	-	4,4,4	0.15	0	6,6,6	0.17	0
6	SO4	A	1885	-	4,4,4	0.17	0	6,6,6	0.21	0
6	SO4	A	1880	-	4,4,4	0.18	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	SO4	A	1881	-	4,4,4	0.13	0	6,6,6	0.32	0
6	SO4	A	1886	-	4,4,4	0.14	0	6,6,6	0.12	0
6	SO4	D	1879	-	4,4,4	0.13	0	6,6,6	0.10	0
6	SO4	A	1884	-	4,4,4	0.16	0	6,6,6	0.11	0
6	SO4	D	1877	-	4,4,4	0.11	0	6,6,6	0.25	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.35	1 (0%) 95 95	24, 57, 95, 114	0
1	D	876/878 (99%)	-0.11	10 (1%) 80 75	55, 87, 130, 150	0
2	B	75/83 (90%)	-0.01	2 (2%) 54 48	27, 74, 124, 160	0
2	F	75/83 (90%)	0.07	3 (4%) 38 33	51, 84, 139, 177	0
All	All	1902/1922 (98%)	-0.21	16 (0%) 86 81	24, 72, 124, 177	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	32	C	3.7
1	D	586	VAL	3.6
1	D	587	GLU	3.2
1	D	488	GLY	3.1
2	B	31	A	3.1
1	D	393	GLU	2.8
1	D	487	CYS	2.8
1	D	605	ILE	2.6
2	F	30	G	2.3
1	D	606	PRO	2.3
2	F	31	A	2.2
1	D	298	GLU	2.1
1	D	851	ASN	2.1
1	D	599	THR	2.0
2	F	32	C	2.0
1	A	292	GLU	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 [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( $\text{\AA}^2$ )	Q<0.9
6	SO4	A	1883	5/5	0.77	0.22	149,149,149,149	0
4	ZN	D	1880	1/1	0.84	0.19	178,178,178,178	0
6	SO4	D	1878	5/5	0.85	0.26	139,139,139,139	0
6	SO4	A	1882	5/5	0.87	0.37	102,102,102,102	0
6	SO4	A	1885	5/5	0.87	0.24	110,110,111,111	0
4	ZN	A	1877	1/1	0.90	0.17	164,164,164,164	0
6	SO4	D	1879	5/5	0.90	0.22	128,128,129,129	0
6	SO4	A	1886	5/5	0.90	0.16	130,130,130,130	0
3	LEU	D	1883	9/9	0.92	0.47	80,81,81,81	0
3	LEU	A	1887	9/9	0.93	0.30	60,60,61,61	0
6	SO4	A	1880	5/5	0.94	0.24	89,89,89,89	0
6	SO4	D	1877	5/5	0.95	0.11	95,95,95,96	0
6	SO4	A	1881	5/5	0.96	0.14	75,76,76,76	0
6	SO4	A	1884	5/5	0.97	0.14	102,102,102,103	0
4	ZN	D	1881	1/1	0.98	0.15	70,70,70,70	0
4	ZN	A	1878	1/1	0.99	0.16	25,25,25,25	0
5	HG	D	1882	1/1	0.99	0.11	140,140,140,140	0
5	HG	A	1879	1/1	0.99	0.12	79,79,79,79	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.