



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:53 PM GMT

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

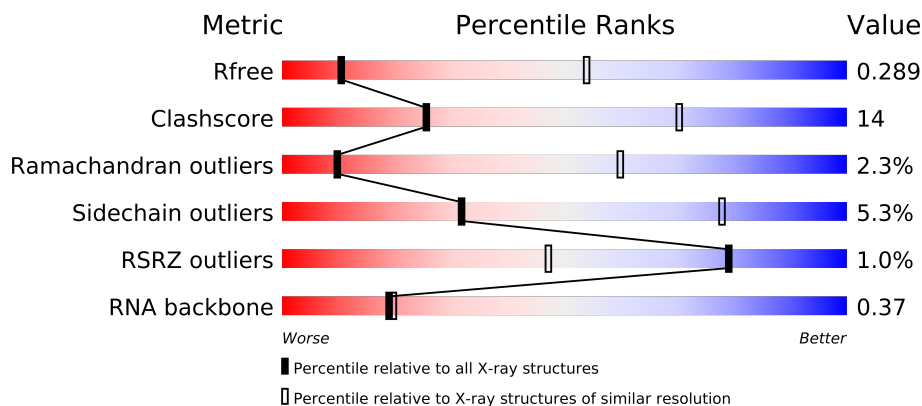
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 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}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	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 hydrogen and 0 are deuterium.

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

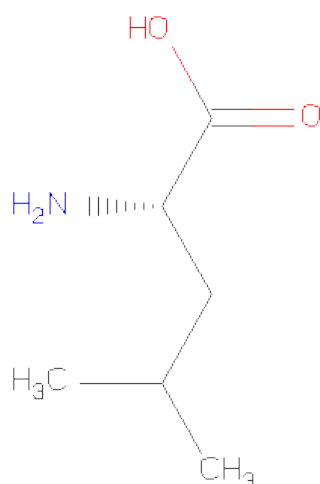
- Molecule 1 is a protein called AMINOACYL-TRNA SYNTHETASE.

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: C₆H₁₃NO₂).



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		

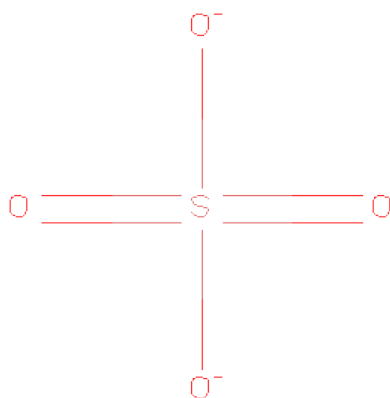
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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: O₄S).



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

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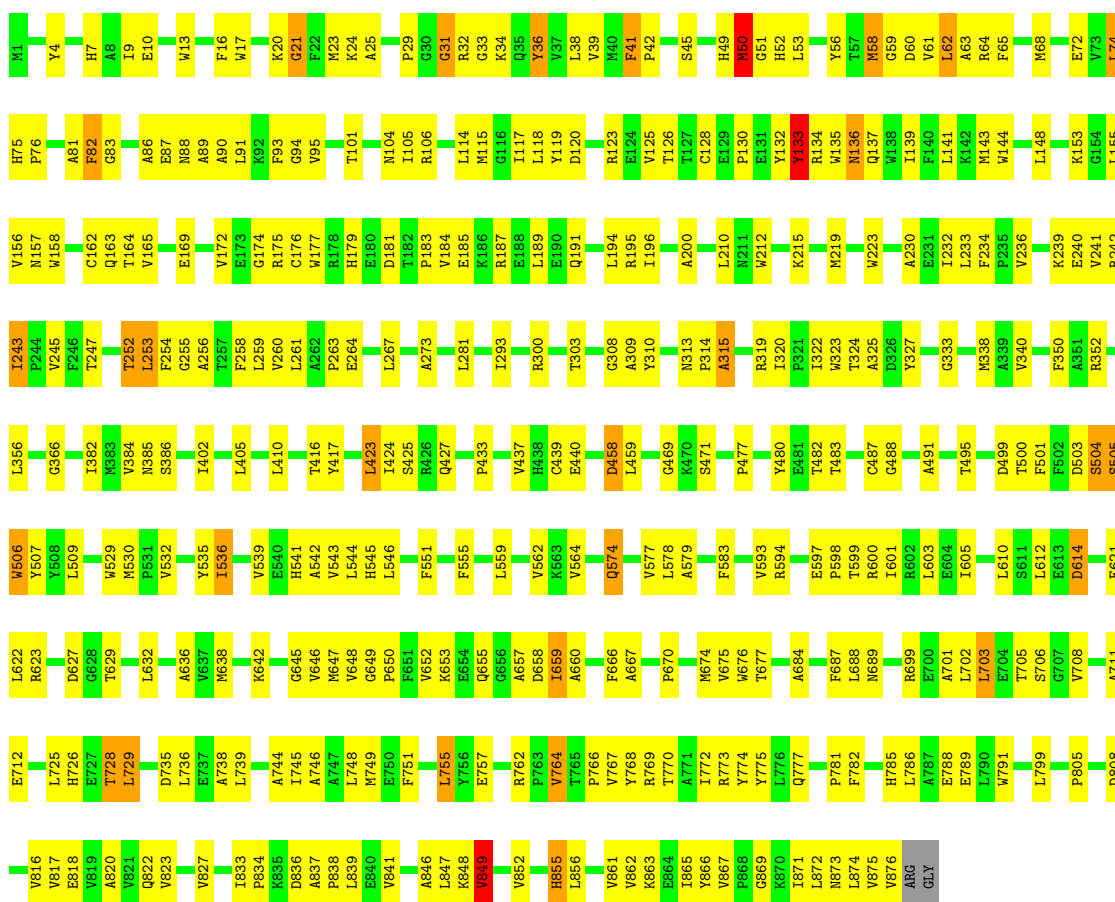
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

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

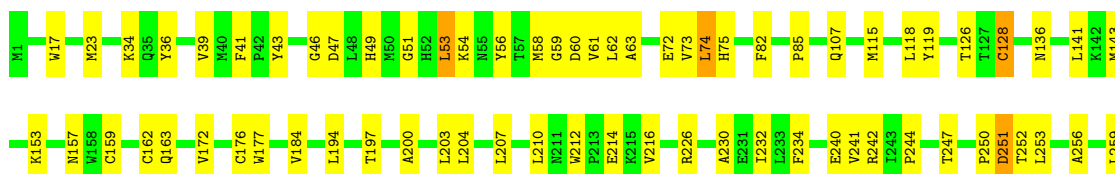
• Molecule 1: AMINOACYL-TRNA SYNTHETASE

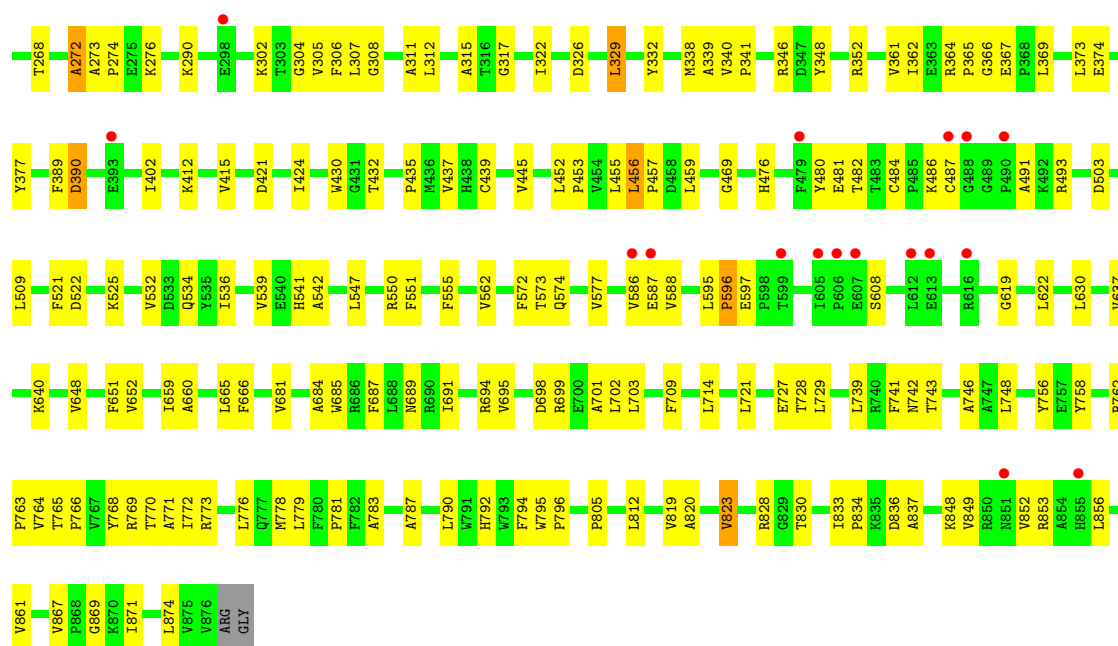
Chain A: 



• Molecule 1: AMINOACYL-TRNA SYNTHETASE

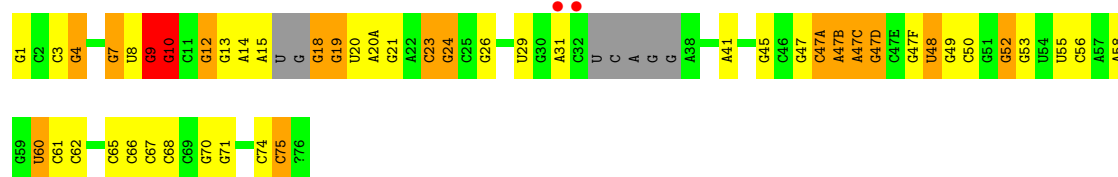
Chain D: 





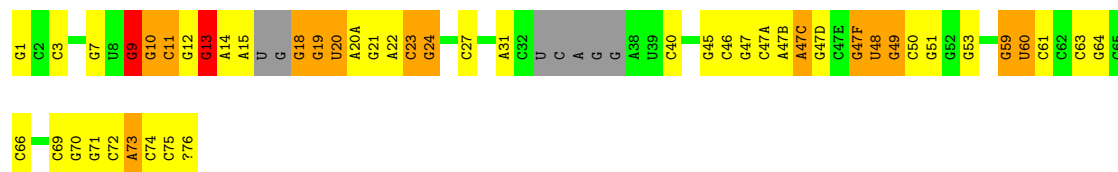
• Molecule 2: TRNALEU

Chain B:



• Molecule 2: TRNALEU

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.245 , 0.314 0.234 , 0.289	Depositor DCC
R_{free} test set	2324 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 24.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 45761 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17604	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7122	0	7036	250	0
1	D	7122	0	7037	158	0
2	B	1643	0	832	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1643	0	832	23	0
3	A	9	0	10	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (446) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:509:LEU:HG	1:A:530:MET:HE2	1.67	0.76
1:A:157:ASN:HB3	1:A:184:VAL:HG11	1.66	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	Distance(Å)	Clash(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:D:482:THR:HG21	1:D:493:ARG:HG3	1.76	0.68
1:A:169:GLU:HG3	1:A:223:TRP:CZ2	2.28	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:833:ILE:HD12	1:D:834:PRO:O	2.00	0.62
1:D:58:MET:CE	1:D:574:GLN:HE22	2.12	0.62
1:A:666:PHE:HE1	1:A:746:ALA:HB2	1.64	0.62
1:A:323:TRP:CZ2	1:A:356:LEU:HD21	2.35	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
1:A:649:GLY:O	1:A:653:LYS:HG2	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:659:ILE:HG22	1:A:684:ALA:CB	2.33	0.59
1:A:61:VAL:HG12	1:A:62:LEU:N	2.16	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:D:304:GLY:O	1:D:305:VAL:HG23	2.03	0.58
1:A:31:GLY:O	1:A:33:GLY:N	2.37	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: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:A:627:ASP:OD2	1:A:629:THR:OG1	2.22	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:D:232:ILE:O	1:D:244:PRO:HA	2.06	0.56
1:A:210:LEU:HD21	1:A:212:TRP:CE2	2.40	0.56
1:D:659:ILE:HG23	1:D:684:ALA:CB	2.36	0.56
2:B:4:G:H1'	2:B:70:G:N2	2.21	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:666:PHE:CG	1:A:666:PHE:O	2.58	0.56
1:A:482:THR:O	1:A:491:ALA:HB3	2.06	0.56
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:820:ALA:O	1:A:871:ILE:HD12	2.06	0.54
1:A:82:PHE:CD1	1:A:128:CYS:HB2	2.43	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:822:GLN:O	1:A:873:ASN:HA	2.07	0.54
1:A:241:VAL:HG22	1:A:242:ARG:N	2.22	0.54
2:B:14:A:C2	2:B:21:G:C4'	2.90	0.54
1:A:137:GLN:NE2	1:A:433:PRO:O	2.39	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: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:141:LEU:O	1:A:144:TRP:N	2.41	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:O	1:D:204:LEU:HD12	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:D:290:LYS:NZ	1:D:326:ASP:OD2	2.42	0.53
1:A:477:PRO:HA	1:A:480:TYR:CE2	2.44	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:838:PRO:HD2	1:A:841:VAL:HG23	1.92	0.52
1:A:254:PHE:CZ	1:A:315:ALA:HB1	2.44	0.51
1:D:58:MET:HE2	1:D:574:GLN:HE22	1.74	0.51
1:A:215:LYS:CE	1:A:539:VAL:HG11	2.40	0.51
1:A:817:VAL:HG12	1:A:818:GLU:N	2.25	0.51
1:A:253:LEU:HA	1:A:338:MET:CE	2.39	0.51
1:A:243:ILE:CD1	1:A:261:LEU:HD21	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
2:F:48:U:C2	2:F:59:G:O4'	2.63	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
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:51:GLY:HA2	1:A:577:VAL:CG2	2.41	0.50
1:A:41:PHE:CE2	1:A:507:TYR:CG	2.99	0.50
1:D:216:VAL:HG13	1:D:542:ALA:CB	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
2:B:66:C:C1'	2:F:47(C):A:H1'	2.41	0.50
1:A:60:ASP:OD2	1:A:117:ILE:HA	2.10	0.50
1:A:49:HIS:O	1:A:51:GLY:N	2.44	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: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:405:LEU:HD22	1:A:410:LEU:HB2	1.94	0.49
1:A:319:ARG:O	1:A:320:ILE:HG23	2.11	0.49
1:A:9:ILE:HG21	1:A:789:GLU:HG2	1.93	0.49
1:A:148:LEU:CD2	1:A:195:ARG:HB3	2.43	0.49
1:A:791:TRP:CE3	1:A:799:LEU:HD21	2.47	0.49
1:D:268:THR:HG23	1:D:307:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:F:51:G:C6	2:F:64:G:N1	2.81	0.49
1:D:699:ARG:O	1:D:703:LEU:HD12	2.12	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:364:ARG:HD3	1:D:377:TYR:CE1	2.48	0.49
1:D:341:PRO:O	1:D:348:TYR:HB2	2.13	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
2:B:14:A:H2	2:B:21:G:H4'	1.77	0.48
2:B:66:C:O4'	2:F:47(C):A:H1'	2.13	0.48
2:F:45:G:H2'	2:F:46:C:H6	1.77	0.48
1:A:667:ALA:HB3	1:A:674:MET:HE3	1.95	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:D:833:ILE:CD1	1:D:837:ALA:HB3	2.41	0.48
1:D:23:MET:HE1	1:D:73:VAL:HG11	1.94	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:A:219:MET:CE	1:A:542:ALA:HB3	2.44	0.48
1:D:259:LEU:HD23	1:D:338:MET:HA	1.95	0.48
1:A:41:PHE:HD1	1:A:41:PHE:O	1.96	0.48
1:D:509:LEU:HD13	1:D:521:PHE:CZ	2.49	0.48
1:D:172:VAL:HG13	2:F:72:C:OP1	2.14	0.48
1:A:638:MET:CG	1:A:645:GLY:HA2	2.42	0.48
1:A:38:LEU:HD23	1:A:535:TYR:CD1	2.49	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:D:54:LYS:O	1:D:58:MET:HG2	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:24:LYS:HA	1:A:120:ASP:OD1	2.14	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
1:D:61:VAL:HG13	1:D:781:PRO:CB	2.45	0.47
2:B:8:U:H2'	2:B:8:U:O2	2.14	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:D:23:MET:CE	1:D:63:ALA:HB1	2.45	0.46
1:A:833:ILE:HD13	1:A:837:ALA:HB3	1.96	0.46
1:D:729:LEU:HD21	1:D:805:PRO:HB2	1.98	0.46
1:D:306:PHE:CE2	1:D:308:GLY:HA2	2.50	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
2:B:20(A):A:H2'	2:B:21:G:O4'	2.15	0.46
1:A:219:MET:HE2	1:A:542:ALA:HB3	1.98	0.46
1:D:823:VAL:HG13	1:D:874:LEU:HB2	1.97	0.46
1:A:61:VAL:HG22	1:A:781:PRO:O	2.16	0.46
1:A:245:VAL:HG23	1:A:245:VAL:O	2.15	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:745:ILE:HG22	1:A:749:MET:HE3	1.98	0.46
1:A:725:LEU:HD13	1:A:751:PHE:CE2	2.50	0.46
1:D:276:LYS:HG3	1:D:308:GLY:HA3	1.97	0.46
1:D:823:VAL:HG23	1:D:828:ARG:CG	2.46	0.46
1:A:487:CYS:SG	1:A:488:GLY:N	2.89	0.46
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:A:735:ASP:HB3	1:A:744:ALA:HB2	1.98	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:39:VAL:HG11	1:D:56:TYR:HA	1.98	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
2:F:12:G:C6	2:F:13:G:H1'	2.51	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:D:273:ALA:HB1	1:D:274:PRO:HD2	1.98	0.45
1:A:49:HIS:O	1:A:52:HIS:N	2.45	0.45
1:A:702:LEU:O	1:A:705:THR:N	2.49	0.45
1:D:17:TRP:HB3	1:D:118:LEU:HD21	1.99	0.45
1:D:143:MET:HG2	1:D:555:PHE:CE2	2.52	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:822:GLN:CG	1:A:871:ILE:HD11	2.44	0.45
1:A:260:VAL:HG13	1:A:325:ALA:H	1.82	0.45
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:236:VAL:HB	1:A:241:VAL:HG13	1.99	0.44
1:D:256:ALA:HA	1:D:339:ALA:O	2.17	0.44
1:A:158:TRP:N	1:A:185:GLU:O	2.43	0.44
1:A:621:GLU:OE2	1:A:623:ARG:NE	2.50	0.44
1:A:501:PHE:CZ	1:A:544:LEU:HD13	2.53	0.44
1:A:163:GLN:NE2	1:A:469:GLY:HA2	2.32	0.44
1:A:729:LEU:HD21	1:A:805:PRO:HB2	1.99	0.44
1:D:332:TYR:OH	2:F:76:ANZ:O1P	2.31	0.44
1:D:74:LEU:C	1:D:74:LEU:HD12	2.37	0.44
1:D:480:TYR:O	1:D:482:THR:HG22	2.17	0.44
1:D:509:LEU:HD11	1:D:562:VAL:HG21	1.99	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: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:155:LEU:HD11	1:A:264:GLU:HG2	1.99	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
1:A:555:PHE:O	1:A:559:LEU:HG	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:711:ALA:HB3	1:A:712:GLU:OE1	2.18	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:74:LEU:HD11	1:A:76:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:203:LEU:O	1:D:207:LEU:HB2	2.18	0.43
1:A:636:ALA:HB1	1:A:642:LYS:HE2	2.00	0.43
1:D:46:GLY:HA3	1:D:640:LYS:NZ	2.32	0.43
1:D:128:CYS:HB2	1:D:430:TRP:CZ2	2.52	0.43
1:A:241:VAL:CG2	1:A:242:ARG:N	2.82	0.43
1:A:176:CYS:SG	1:A:179:HIS:ND1	2.87	0.43
1:A:674:MET:HB2	1:A:674:MET:HE3	1.82	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: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:645:GLY:O	1:A:647:MET:HE2	2.18	0.43
2:F:12:G:C5	2:F:13:G:H1'	2.54	0.43
1:D:765:THR:HB	1:D:766:PRO:CD	2.49	0.43
1:A:273:ALA:HB2	1:A:308:GLY:O	2.18	0.43
2:F:69:C:H2'	2:F:70:G:H8	1.83	0.43
1:A:230:ALA:HB2	1:A:402:ILE:CD1	2.41	0.43
1:D:194:LEU:HD12	1:D:424:ILE:CG2	2.44	0.43
1:A:748:LEU:HD22	1:A:775:TYR:CE2	2.54	0.43
1:D:729:LEU:CD2	1:D:805:PRO:HB2	2.48	0.43
1:A:105:ILE:O	1:A:106:ARG:C	2.57	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
1:D:143:MET:HE1	1:D:551:PHE:CZ	2.54	0.43
2:B:26:G:H8	2:B:26:G:O5'	2.01	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:D:234:PHE:CG	1:D:259:LEU:HD11	2.54	0.42
1:D:687:PHE:CZ	1:D:691:ILE:HD11	2.53	0.42
1:A:688:LEU:HD22	1:A:786:LEU:HD23	2.00	0.42
1:A:10:GLU:OE1	1:A:657:ALA:HB3	2.20	0.42
1:A:867:VAL:O	1:A:867:VAL:HG12	2.17	0.42
1:D:698:ASP:O	1:D:702:LEU:HD13	2.19	0.42
1:A:215:LYS:HZ3	1:A:539:VAL:HG11	1.84	0.42
1:D:230:ALA:HB2	1:D:402:ILE:CD1	2.49	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:595:LEU:HD23	1:D:596:PRO:N	2.34	0.42
1:D:389:PHE:O	1:D:390:ASP:C	2.57	0.42
1:A:256:ALA:HB2	1:A:338:MET:HE3	2.01	0.42
1:A:183:PRO:HB3	1:A:293:ILE:HD12	2.02	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:223:TRP:CD1	1:A:223:TRP:C	2.92	0.42
1:A:135:TRP:C	1:A:137:GLN:N	2.73	0.42
1:D:794:PHE:HB2	1:D:795:TRP:CE3	2.55	0.42
1:A:599:THR:HG22	1:A:599:THR:O	2.19	0.42
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:333:GLY:HA2	1:A:416:THR:HG21	2.02	0.41
1:A:309:ALA:O	1:A:310:TYR:CD1	2.73	0.41
1:A:36:TYR:CE2	1:A:532:VAL:HG22	2.55	0.41
2:B:66:C:H1'	2:F:47(C):A:H1'	2.03	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
1:A:4:TYR:HB3	1:A:689:ASN:OD1	2.20	0.41
1:A:667:ALA:HB3	1:A:674:MET:CE	2.51	0.41
1:A:382:ILE:HD13	1:A:382:ILE:N	2.36	0.41
1:A:194:LEU:HD21	1:A:424:ILE:HD11	2.02	0.41
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:D:23:MET:HE1	1:D:73:VAL:CG1	2.51	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:164:THR:OG1	1:A:165:VAL:N	2.53	0.41
1:A:509:LEU:CD2	1:A:562:VAL:HG21	2.50	0.41
1:A:139:ILE:HG23	1:A:143:MET:HE2	2.02	0.41
1:A:866:TYR:HD1	1:A:872:LEU:HD13	1.85	0.41
1:A:725:LEU:HD13	1:A:751:PHE:CZ	2.55	0.41
1:A:162:CYS:SG	1:A:179:HIS:CE1	3.14	0.41
1:D:445:VAL:HG11	1:D:484:CYS:SG	2.60	0.41
1:A:593:VAL:CG2	1:A:612:LEU:HD23	2.50	0.41
1:A:200:ALA:HB3	1:A:417:TYR:CD2	2.56	0.41
1:D:234:PHE:CE1	1:D:259:LEU:HD21	2.56	0.41
1:A:36:TYR:CD1	1:A:74:LEU:HG	2.56	0.41
1:A:725:LEU:HD21	1:A:774:TYR:CD2	2.56	0.41
1:D:701:ALA:HB1	1:D:764:VAL:HB	2.02	0.41
1:D:53:LEU:HD12	1:D:115:MET:HG3	2.02	0.41
1:D:666:PHE:HE1	1:D:746:ALA:HB2	1.86	0.41
1:D:247:THR:HG23	1:D:250:PRO:HB3	2.03	0.41
1:A:256:ALA:N	1:A:340:VAL:HG22	2.36	0.41
1:A:745:ILE:HG22	1:A:749:MET:HE2	2.01	0.41
1:A:738:ALA:O	1:A:739:LEU:HB2	2.21	0.41
1:A:156:VAL:HG12	1:A:423:LEU:HD11	2.03	0.40
1:A:117:ILE:CG2	1:A:119:TYR:CE2	3.04	0.40
1:A:817:VAL:HG12	1:A:818:GLU:H	1.86	0.40
1:A:622:LEU:HD23	1:A:632:LEU:HA	2.03	0.40
1:D:694:ARG:HB2	1:D:756:TYR:CE1	2.56	0.40
2:B:47:G:N2	2:B:47(D):G:C4	2.89	0.40
1:D:59:GLY:O	1:D:60:ASP:C	2.60	0.40
1:D:47:ASP:OD2	1:D:107:GLN:HB3	2.21	0.40
1:A:259:LEU:CD2	1:A:338:MET:HA	2.51	0.40
1:D:665:LEU:HD22	1:D:741:PHE:CB	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
1:A:13:TRP:O	1:A:16:PHE:HB3	2.21	0.40
1:D:141:LEU:CD1	1:D:452:LEU:HD11	2.45	0.40
1:A:130:PRO:HA	1:A:133:TYR:CZ	2.56	0.40
1:D:702:LEU:HD12	1:D:764:VAL:HG11	2.04	0.40
1:D:459:LEU:HD21	1:D:476:HIS:CD2	2.56	0.40
1:A:846:ALA:O	1:A:848:LYS:N	2.54	0.40
1:A:68:MET:HE1	1:A:777:GLN:HB3	2.03	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

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%)	119 (14%)	27 (3%)	7	53
1	D	874/878 (100%)	750 (86%)	110 (13%)	14 (2%)	14	68
All	All	1748/1756 (100%)	1478 (85%)	229 (13%)	41 (2%)	10	60

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
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

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Mol	Chain	Res	Type
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%)	22	69
1	D	741/742 (100%)	713 (96%)	28 (4%)	44	85
All	All	1482/1484 (100%)	1403 (95%)	79 (5%)	32	78

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

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
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

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Mol	Chain	Res	Type
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 ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANZ	B	76	2	37,37,38	1.69	4 (10%)	56,57,60	2.13	17 (30%)
2	ANZ	F	76	2	37,37,38	1.71	5 (13%)	56,57,60	2.21	15 (26%)

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
2	ANZ	B	76	2	-	1/9/47/48	0/0/6/6
2	ANZ	F	76	2	-	1/9/47/48	0/0/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	76	ANZ	B-CD2	-7.46	1.48	1.61
2	B	76	ANZ	B-CD2	-7.27	1.48	1.61
2	B	76	ANZ	CG-CD2	-4.11	1.37	1.40
2	F	76	ANZ	CG-CD2	-3.76	1.37	1.40
2	B	76	ANZ	C4-N9	-3.46	1.32	1.37
2	F	76	ANZ	C4-N9	-2.95	1.33	1.37
2	F	76	ANZ	CZ-CE1	2.32	1.41	1.36
2	B	76	ANZ	CZ-CE1	2.24	1.41	1.36
2	F	76	ANZ	B-O1	2.10	1.54	1.47

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	76	ANZ	N3-C2-N1	-8.46	121.64	128.71
2	F	76	ANZ	N3-C2-N1	-8.17	121.88	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	76	ANZ	CZ-CE2-CD2	-6.83	118.52	122.98
2	B	76	ANZ	CZ-CE2-CD2	-6.74	118.57	122.98
2	F	76	ANZ	C4-C5-N7	-4.20	105.92	109.52
2	F	76	ANZ	O2'-B-CD2	3.96	123.93	117.86
2	F	76	ANZ	N3-C4-N9	3.86	132.39	125.43
2	F	76	ANZ	CE2-CD2-CG	3.73	120.22	117.39
2	B	76	ANZ	CE2-CD2-CG	3.71	120.21	117.39
2	B	76	ANZ	N3-C4-N9	3.60	131.94	125.43
2	F	76	ANZ	C5-C4-N3	-3.28	118.57	125.70
2	F	76	ANZ	CZ-CE1-CD1	-3.25	118.85	123.32
2	B	76	ANZ	O2'-B-CD2	2.90	122.30	117.86
2	B	76	ANZ	CZ-CE1-CD1	-2.84	119.41	123.32
2	B	76	ANZ	C4-C5-N7	-2.71	107.20	109.52
2	B	76	ANZ	C5-C4-N3	-2.62	120.00	125.70
2	F	76	ANZ	CE2-CZ-CE1	2.60	121.08	118.33
2	B	76	ANZ	C1'-N9-C4	-2.56	122.21	126.64
2	F	76	ANZ	C2-N3-C4	2.51	121.16	114.01
2	F	76	ANZ	O1-CB-CG	-2.50	101.08	107.85
2	B	76	ANZ	O1P-P-O5'	-2.50	105.52	113.42
2	B	76	ANZ	B-O3'-C3'	-2.41	107.57	110.63
2	B	76	ANZ	CE2-CZ-CE1	2.38	120.84	118.33
2	F	76	ANZ	CB-CG-CD1	-2.21	124.47	129.41
2	B	76	ANZ	C2-N3-C4	2.20	120.27	114.01
2	B	76	ANZ	O1-CB-CG	-2.18	101.96	107.85
2	B	76	ANZ	C8-N9-C4	2.15	108.54	106.90
2	F	76	ANZ	C4'-O4'-C1'	2.14	112.08	109.75
2	F	76	ANZ	O1P-P-O5'	-2.14	106.67	113.42
2	F	76	ANZ	F-CE1-CZ	2.10	122.35	118.52
2	B	76	ANZ	B-O2'-C2'	-2.09	107.98	110.63
2	B	76	ANZ	O2'-B-O1	-2.08	100.57	107.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	76	ANZ	O1P-P-O5'-C5'
2	F	76	ANZ	O2P-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	1880	-	4,4,4	0.21	0	6,6,6	0.17	0
6	SO4	A	1881	-	4,4,4	0.17	0	6,6,6	0.23	0
6	SO4	A	1882	-	4,4,4	0.20	0	6,6,6	0.20	0
6	SO4	A	1883	-	4,4,4	0.19	0	6,6,6	0.17	0
6	SO4	A	1884	-	4,4,4	0.06	0	6,6,6	0.08	0
6	SO4	A	1885	-	4,4,4	0.22	0	6,6,6	0.20	0
6	SO4	A	1886	-	4,4,4	0.20	0	6,6,6	0.10	0
3	LEU	A	1887	-	8,8,8	0.72	0	10,10,10	0.74	0
6	SO4	D	1877	-	4,4,4	0.18	0	6,6,6	0.25	0
6	SO4	D	1878	-	4,4,4	0.18	0	6,6,6	0.12	0
6	SO4	D	1879	-	4,4,4	0.18	0	6,6,6	0.12	0
3	LEU	D	1883	-	8,8,8	0.68	0	10,10,10	1.23	2 (20%)

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
6	SO4	A	1880	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1881	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1882	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1883	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1884	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1885	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1886	-	-	0/0/0/0	0/0/0/0
3	LEU	A	1887	-	-	0/8/8/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	D	1877	-	-	0/0/0/0	0/0/0/0
6	SO4	D	1878	-	-	0/0/0/0	0/0/0/0
6	SO4	D	1879	-	-	0/0/0/0	0/0/0/0
3	LEU	D	1883	-	-	0/8/8/8	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1883	LEU	OXT-C-O	-2.94	117.42	124.07
3	D	1883	LEU	OXT-C-CA	2.11	121.62	116.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	876/878 (99%)	-0.05	0 100 100	24, 57, 95, 114	0
1	D	876/878 (99%)	0.17	17 (1%) 64 32	55, 87, 130, 150	0
2	B	76/83 (91%)	-0.13	2 (2%) 53 24	27, 74, 124, 160	0
2	F	76/83 (91%)	-0.01	0 100 100	51, 84, 139, 177	0
All	All	1904/1922 (99%)	0.05	19 (0%) 79 47	24, 72, 124, 177	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	32	C	3.4
1	D	487	CYS	3.3
1	D	587	GLU	3.1
1	D	586	VAL	3.1
1	D	605	ILE	2.9
1	D	612	LEU	2.9
1	D	488	GLY	2.6
1	D	393	GLU	2.6
1	D	606	PRO	2.5
1	D	298	GLU	2.3
1	D	613	GLU	2.3
1	D	851	ASN	2.3
1	D	490	PRO	2.2
2	B	31	A	2.2
1	D	607	GLU	2.2
1	D	599	THR	2.1
1	D	616	ARG	2.1
1	D	855	HIS	2.0
1	D	479	PHE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ANZ	B	76	32/33	0.21	-	40,42,43,43	0
2	ANZ	F	76	32/33	0.25	-	50,55,58,58	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	LEU	A	1887	9/9	0.25	-	60,60,61,61	0
5	HG	D	1882	1/1	0.08	-	140,140,140,140	0
6	SO4	A	1883	5/5	0.27	-	149,149,149,149	0
4	ZN	D	1880	1/1	0.23	-	178,178,178,178	0
6	SO4	A	1882	5/5	0.38	-	102,102,102,102	0
6	SO4	D	1878	5/5	0.32	-	139,139,139,139	0
6	SO4	A	1885	5/5	0.20	-	110,110,111,111	0
4	ZN	A	1877	1/1	0.17	-	164,164,164,164	0
6	SO4	D	1879	5/5	0.23	-	128,128,129,129	0
6	SO4	A	1881	5/5	0.14	-	75,76,76,76	0
6	SO4	A	1886	5/5	0.16	-	130,130,130,130	0
6	SO4	D	1877	5/5	0.12	-	95,95,95,96	0
6	SO4	A	1884	5/5	0.17	-	102,102,102,103	0
4	ZN	A	1878	1/1	0.16	-	25,25,25,25	0
4	ZN	D	1881	1/1	0.16	-	70,70,70,70	0
3	LEU	D	1883	9/9	0.35	-	80,81,81,81	0
6	SO4	A	1880	5/5	0.24	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	HG	A	1879	1/1	0.12	-	79,79,79,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.