



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:04 am BST

PDB ID : 3L0O  
Title : Structure of RNA-free Rho transcription termination factor from *Thermotoga maritima*  
Authors : Canals, A.; Uson, I.; Coll, M.  
Deposited on : 2009-12-10  
Resolution : 2.35 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  
buster-report : 1.1.7 (2018)  
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

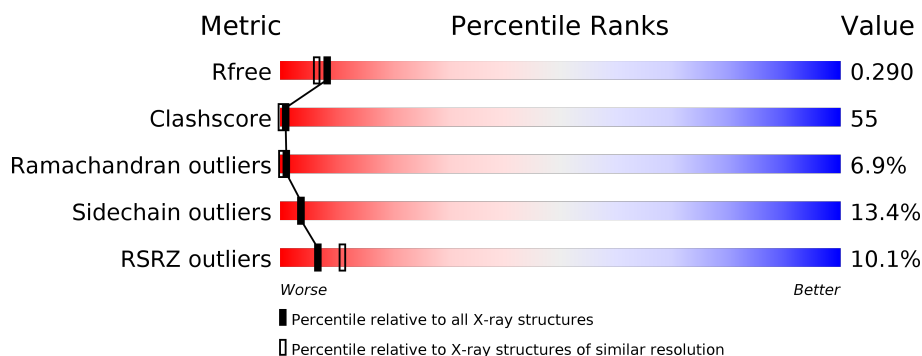
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	427	<div> <div>7%</div> <div>51%</div> <div>32%</div> <div>10%</div> <div>• •</div> </div>
1	B	427	<div> <div>11%</div> <div>37%</div> <div>33%</div> <div>8%</div> <div>•</div> <div>19%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IUM	A	429	-	-	-	X
3	SO4	B	432	-	-	X	-
3	SO4	B	434	-	-	X	-
3	SO4	B	435	-	-	X	-

## 2 Entry composition [i](#)

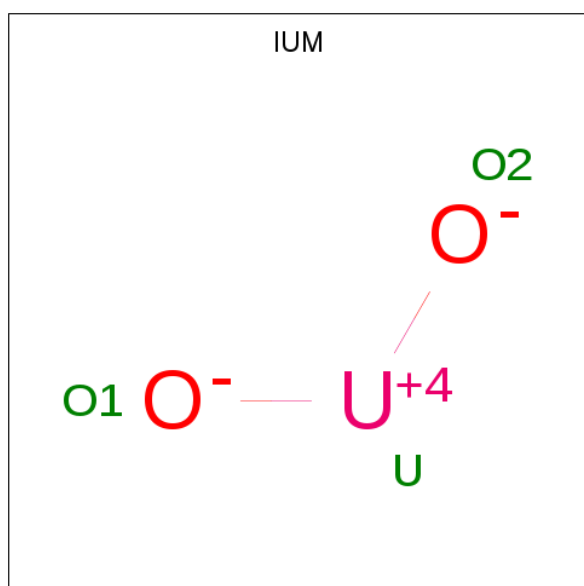
There are 5 unique types of molecules in this entry. The entry contains 6194 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transcription termination factor rho.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	1	0	0
			3283	2101	556	616	10			
1	B	347	Total	C	N	O	S	3	0	0
			2737	1749	466	514	8			

- Molecule 2 is URANYL (VI) ION (three-letter code: IUM) (formula: O<sub>2</sub>U).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	U	0	0
			3	2	1		
2	A	1	Total	O	U	0	0
			3	2	1		
2	A	1	Total	O	U	0	0
			3	2	1		
2	B	1	Total	O	U	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	U	0	0
			3	2	1		
2	B	1	Total	O	U	0	0
			3	2	1		
2	B	1	Total	O	U	0	0
			3	2	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

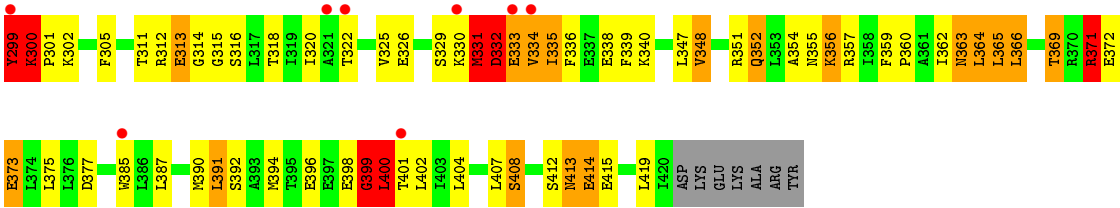
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Na	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	36	Total	O	0	0
			36	36		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.00Å 139.00Å 150.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.55 – 2.35 38.55 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.55-2.35) 98.5 (38.55-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.68 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.268 , 0.297 0.264 , 0.290	Depositor DCC
$R_{free}$ test set	4886 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, IUM, 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	0.69	0/3336	0.89	5/4504 (0.1%)
1	B	0.55	0/2779	0.87	7/3758 (0.2%)
All	All	0.63	0/6115	0.88	12/8262 (0.1%)

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	6
1	B	0	7
All	All	0	13

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	PRO	C-N-CD	-15.05	87.48	120.60
1	A	294	ASP	C-N-CD	-10.05	98.49	120.60
1	A	117	TYR	N-CA-C	9.73	137.28	111.00
1	B	300	LYS	N-CA-C	-8.08	89.19	111.00
1	A	234	ALA	C-N-CD	-7.81	103.41	120.60
1	B	408	SER	N-CA-C	-7.74	90.11	111.00
1	B	371	ARG	N-CA-C	-7.36	91.14	111.00
1	A	79	LEU	CA-CB-CG	6.95	131.27	115.30
1	A	116	LYS	C-N-CA	6.46	137.85	121.70
1	B	299	TYR	N-CA-C	-6.17	94.35	111.00
1	B	96	PHE	N-CA-C	5.71	126.42	111.00
1	B	356	LYS	N-CA-C	5.64	126.23	111.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Peptide
1	A	234	ALA	Peptide
1	A	294	ASP	Peptide
1	A	395	THR	Peptide
1	A	79	LEU	Peptide
1	A	82	SER	Peptide
1	B	283	PRO	Peptide
1	B	298	LEU	Peptide
1	B	331	MET	Peptide
1	B	333	GLU	Peptide
1	B	399	GLY	Peptide
1	B	400	LEU	Peptide
1	B	407	LEU	Peptide

## 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	3283	0	3400	377	0
1	B	2737	0	2835	307	0
2	A	9	0	0	0	0
2	B	12	0	0	3	0
3	A	25	0	0	3	0
3	B	20	0	0	7	0
4	B	2	0	0	0	0
5	A	70	0	0	6	0
5	B	36	0	0	0	0
All	All	6194	0	6235	678	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 55.

All (678) 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:B:93:ILE:HG22	1:B:94:ARG:CA	1.33	1.57
1:B:93:ILE:CG2	1:B:94:ARG:HA	1.30	1.52
1:B:228:ASN:CA	1:B:229:ALA:HB2	1.27	1.52
1:B:228:ASN:CA	1:B:229:ALA:CB	1.82	1.50
1:B:333:GLU:CA	1:B:334:VAL:HG23	1.41	1.48
1:A:297:ALA:CB	1:A:299:TYR:N	1.82	1.42
1:B:298:LEU:CA	1:B:299:TYR:O	1.69	1.41
1:A:296:ALA:H	1:A:297:ALA:CA	1.36	1.38
1:A:221:THR:C	1:A:225:GLU:HG3	1.45	1.36
1:A:297:ALA:CB	1:A:299:TYR:H	1.36	1.33
1:A:222:ASP:N	1:A:225:GLU:HG3	1.44	1.33
1:A:297:ALA:HB1	1:A:299:TYR:N	1.00	1.32
1:B:298:LEU:HA	1:B:299:TYR:O	1.17	1.31
1:B:90:PRO:CD	1:B:91:SER:HB2	1.61	1.30
1:B:90:PRO:N	1:B:91:SER:HB2	1.46	1.29
1:A:276:ARG:NH2	3:A:435:SO4:O1	1.66	1.27
1:A:185:LYS:N	1:A:186:ALA:HB2	1.48	1.27
1:B:330:LYS:O	1:B:334:VAL:CG2	1.81	1.27
1:A:382:LYS:O	1:A:386:LEU:CD1	1.80	1.27
1:B:228:ASN:HA	1:B:229:ALA:CB	0.87	1.27
1:A:225:GLU:CB	1:A:226:SER:HB2	1.64	1.26
1:A:5:GLN:CB	1:A:6:LYS:HB2	1.64	1.26
1:A:220:VAL:O	1:A:223:ILE:CG2	1.83	1.25
1:B:333:GLU:CB	1:B:334:VAL:HG23	1.65	1.25
1:A:5:GLN:N	1:A:6:LYS:HB3	1.51	1.25
1:B:90:PRO:CB	1:B:91:SER:HB2	1.65	1.24
1:A:116:LYS:CG	1:A:116:LYS:O	1.85	1.24
1:A:329:SER:CA	1:A:330:LYS:HB2	1.65	1.23
1:A:157:ASP:HB2	5:A:487:HOH:O	1.09	1.23
1:A:297:ALA:HB1	1:A:298:LEU:C	1.59	1.23
1:A:222:ASP:H	1:A:225:GLU:CB	1.53	1.21
1:A:386:LEU:CD1	1:A:386:LEU:H	1.52	1.21
1:B:291:GLY:CA	1:B:293:VAL:HG23	1.71	1.20
1:A:222:ASP:CB	1:A:223:ILE:HB	1.71	1.20
1:A:82:SER:HB2	1:A:83:ASN:C	1.61	1.19
1:A:382:LYS:O	1:A:386:LEU:HD11	1.36	1.19
1:B:333:GLU:N	1:B:334:VAL:HG23	1.59	1.18
1:A:221:THR:O	1:A:225:GLU:HG3	1.43	1.18
1:B:91:SER:H	1:B:94:ARG:HB2	1.03	1.17
1:B:399:GLY:HA3	1:B:400:LEU:HB2	1.26	1.17
1:A:223:ILE:N	1:A:226:SER:OG	1.76	1.17
1:A:222:ASP:HB3	1:A:223:ILE:CB	1.76	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:THR:O	1:A:224:ARG:HB2	1.46	1.15
1:A:295:PRO:O	1:A:298:LEU:HB2	1.47	1.15
1:B:90:PRO:CA	1:B:91:SER:HB2	1.73	1.15
1:B:235:PRO:HD2	1:B:238:MET:HE3	1.29	1.15
1:A:296:ALA:N	1:A:297:ALA:HA	1.37	1.13
1:B:298:LEU:C	1:B:299:TYR:O	1.75	1.12
1:B:228:ASN:HA	1:B:229:ALA:HB3	1.17	1.10
1:B:333:GLU:HB2	1:B:334:VAL:CG2	1.81	1.10
1:A:5:GLN:CB	1:A:6:LYS:CB	2.30	1.10
1:A:8:ILE:HA	1:A:11:SER:HB2	1.15	1.10
1:A:294:ASP:HB3	1:A:296:ALA:HB3	1.27	1.10
1:A:290:THR:HG22	1:A:292:GLY:HA2	1.29	1.10
1:B:225:GLU:O	1:B:226:SER:HB3	1.51	1.10
1:B:90:PRO:HB2	1:B:91:SER:OG	1.51	1.09
1:A:222:ASP:N	1:A:225:GLU:CG	2.16	1.09
1:B:89:SER:CB	1:B:92:GLN:HB3	1.81	1.09
1:A:54:GLY:HA2	1:A:110:LYS:HD2	1.27	1.09
1:B:89:SER:HB2	1:B:92:GLN:HB3	1.30	1.09
1:B:90:PRO:CB	1:B:91:SER:CB	2.30	1.09
1:A:291:GLY:HA2	1:A:293:VAL:HG12	1.24	1.08
1:B:90:PRO:HB2	1:B:91:SER:CB	1.84	1.08
1:B:90:PRO:CD	1:B:91:SER:CB	2.30	1.08
1:B:95:LYS:O	1:B:95:LYS:CG	2.00	1.08
1:A:289:LEU:HD23	1:A:295:PRO:HD2	1.33	1.08
1:A:8:ILE:HA	1:A:11:SER:CB	1.83	1.08
1:A:5:GLN:HB2	1:A:6:LYS:HB2	1.27	1.07
1:B:330:LYS:O	1:B:334:VAL:HG21	0.91	1.07
1:A:221:THR:O	1:A:225:GLU:CG	2.03	1.06
1:A:386:LEU:N	1:A:386:LEU:HD12	1.49	1.06
1:A:289:LEU:HD23	1:A:295:PRO:CD	1.84	1.06
1:A:8:ILE:O	1:A:10:ILE:N	1.88	1.06
1:A:220:VAL:O	1:A:223:ILE:HG21	1.52	1.06
1:B:333:GLU:CB	1:B:334:VAL:CG2	2.33	1.05
1:A:227:THR:HB	1:A:228:ASN:HA	1.11	1.05
1:A:329:SER:HA	1:A:330:LYS:CB	1.87	1.05
1:A:222:ASP:H	1:A:225:GLU:HB2	1.23	1.03
1:A:294:ASP:HB3	1:A:295:PRO:HB2	1.36	1.03
1:B:90:PRO:CG	1:B:91:SER:HB2	1.88	1.03
1:A:224:ARG:N	1:A:225:GLU:HB2	1.73	1.02
1:B:298:LEU:O	1:B:298:LEU:HG	1.21	1.02
1:A:185:LYS:N	1:A:186:ALA:CB	2.23	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:VAL:C	1:A:223:ILE:HG21	1.78	1.02
1:A:222:ASP:H	1:A:225:GLU:CG	1.72	1.02
1:A:386:LEU:HD12	1:A:386:LEU:H	0.88	1.02
1:B:333:GLU:CA	1:B:334:VAL:CG2	2.37	1.02
1:B:291:GLY:HA3	1:B:293:VAL:CG2	1.91	1.01
1:A:5:GLN:CA	1:A:6:LYS:HB3	1.91	1.01
1:B:390:MET:O	1:B:391:LEU:HB2	1.59	1.01
1:A:357:ARG:HH11	1:A:357:ARG:HG2	0.88	1.01
1:A:220:VAL:O	1:A:223:ILE:HG22	1.58	1.00
1:A:5:GLN:CA	1:A:6:LYS:CB	2.39	1.00
1:B:228:ASN:N	1:B:229:ALA:HB2	1.76	1.00
1:B:298:LEU:CA	1:B:299:TYR:C	2.29	1.00
1:A:86:ILE:HD13	1:A:108:ILE:HD13	1.44	0.99
1:B:144:THR:OG1	1:B:313:GLU:OE2	1.78	0.99
1:A:293:VAL:HG22	1:A:294:ASP:O	1.61	0.99
1:A:365:LEU:HD11	1:A:391:LEU:HB3	1.43	0.99
1:A:129:ARG:HH11	1:A:129:ARG:CG	1.75	0.98
1:A:82:SER:CB	1:A:83:ASN:C	2.32	0.98
1:A:116:LYS:HG2	1:A:116:LYS:O	1.20	0.98
1:B:291:GLY:HA3	1:B:293:VAL:HG23	1.00	0.98
1:B:89:SER:HB2	1:B:92:GLN:OE1	1.62	0.98
1:A:396:GLU:HB2	5:A:485:HOH:O	1.61	0.98
1:B:173:GLY:H	1:B:176:GLN:HE21	1.07	0.97
1:A:113:GLU:N	1:A:114:GLY:HA3	1.79	0.97
1:A:287:LYS:O	1:A:288:LEU:HB3	1.64	0.97
1:B:298:LEU:O	1:B:298:LEU:CG	2.09	0.97
1:A:225:GLU:CA	1:A:226:SER:HB2	1.93	0.97
1:A:227:THR:HB	1:A:228:ASN:CA	1.96	0.96
1:A:289:LEU:CD2	1:A:295:PRO:CD	2.42	0.96
1:B:73:ARG:HG2	1:B:79:LEU:O	1.65	0.96
1:B:287:LYS:HG3	1:B:287:LYS:O	1.61	0.96
1:A:227:THR:CB	1:A:228:ASN:HA	1.94	0.96
1:A:294:ASP:CB	1:A:295:PRO:HB2	1.95	0.95
1:A:77:ASP:O	1:A:80:LEU:HB2	1.66	0.95
1:A:357:ARG:NH1	1:A:357:ARG:HG2	1.67	0.94
1:A:5:GLN:N	1:A:6:LYS:CB	2.30	0.94
1:B:188:LYS:HB3	3:B:432:SO4:O1	1.68	0.94
1:A:294:ASP:CB	1:A:296:ALA:HB3	1.96	0.94
1:B:333:GLU:N	1:B:334:VAL:CG2	2.31	0.93
1:A:6:LYS:CB	1:A:7:THR:HA	1.99	0.93
1:B:95:LYS:N	1:B:97:ASN:H	1.64	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.30	0.93
1:A:185:LYS:H	1:A:186:ALA:HB2	1.12	0.93
1:A:222:ASP:HB3	1:A:223:ILE:HB	0.95	0.93
1:A:107:VAL:HG13	1:A:122:LYS:HB3	1.49	0.93
1:B:92:GLN:HG2	1:B:92:GLN:O	1.68	0.92
1:A:89:SER:H	1:A:92:GLN:HE21	1.14	0.92
1:B:333:GLU:O	1:B:336:PHE:HB3	1.68	0.92
1:A:289:LEU:CD2	1:A:295:PRO:HD3	1.99	0.92
1:A:8:ILE:CA	1:A:11:SER:HB2	1.99	0.92
1:B:90:PRO:N	1:B:91:SER:CB	2.30	0.92
1:B:332:ASP:H	1:B:335:ILE:HD12	1.31	0.92
1:B:283:PRO:HB2	1:B:284:PRO:HD3	1.51	0.92
1:A:5:GLN:HB3	1:A:6:LYS:CA	2.00	0.91
1:B:90:PRO:HD2	1:B:91:SER:HB3	1.53	0.91
1:A:82:SER:CB	1:A:83:ASN:O	2.19	0.90
1:B:283:PRO:CB	1:B:284:PRO:HD3	2.00	0.90
1:A:225:GLU:HB3	1:A:226:SER:HB2	1.49	0.90
1:A:291:GLY:HA2	1:A:293:VAL:CG1	2.02	0.90
1:B:311:THR:OG1	1:B:314:GLY:HA2	1.70	0.90
1:B:90:PRO:HD2	1:B:91:SER:CB	1.99	0.90
1:B:363:ASN:C	1:B:363:ASN:HD22	1.73	0.89
1:A:329:SER:HA	1:A:330:LYS:HB2	0.92	0.89
1:B:153:ILE:H	1:B:203:HIS:HE1	1.16	0.89
1:A:289:LEU:HD21	1:A:295:PRO:HD3	1.53	0.89
1:B:91:SER:N	1:B:94:ARG:HB2	1.87	0.89
1:A:82:SER:HB2	1:A:84:ASP:N	1.86	0.89
1:B:330:LYS:C	1:B:334:VAL:HG21	1.92	0.89
1:A:289:LEU:CD2	1:A:295:PRO:HD2	2.02	0.88
1:A:235:PRO:HD3	1:A:238:MET:HG3	1.54	0.88
1:A:185:LYS:HA	1:A:186:ALA:HB3	1.56	0.88
1:A:185:LYS:CA	1:A:186:ALA:CB	2.51	0.88
1:B:235:PRO:CD	1:B:238:MET:HE3	2.04	0.87
1:A:222:ASP:N	1:A:225:GLU:CB	2.37	0.87
1:B:128:TYR:O	1:B:129:ARG:HG2	1.74	0.87
1:A:297:ALA:HB2	1:A:299:TYR:HB3	1.57	0.87
1:A:215:GLU:HB2	1:A:216:ARG:HH21	1.37	0.87
1:A:67:GLU:N	1:A:67:GLU:OE2	2.08	0.86
1:A:293:VAL:CG2	1:A:294:ASP:O	2.22	0.86
1:A:216:ARG:HD2	1:A:216:ARG:N	1.91	0.86
1:A:5:GLN:HB3	1:A:6:LYS:HB2	1.58	0.86
1:A:297:ALA:HB2	1:A:299:TYR:H	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:GLU:O	1:B:226:SER:CB	2.22	0.86
1:A:185:LYS:H	1:A:186:ALA:CB	1.85	0.85
1:A:329:SER:CA	1:A:330:LYS:CB	2.46	0.85
1:B:298:LEU:HA	1:B:301:PRO:HD2	1.59	0.85
1:A:216:ARG:H	1:A:216:ARG:HD2	1.39	0.84
1:A:290:THR:HG22	1:A:292:GLY:CA	2.08	0.84
1:A:5:GLN:HB3	1:A:6:LYS:CB	2.07	0.84
1:A:223:ILE:HG22	1:A:224:ARG:N	1.92	0.84
1:A:153:ILE:H	1:A:203:HIS:HE1	1.23	0.84
1:B:95:LYS:HG2	1:B:95:LYS:O	1.11	0.84
1:A:225:GLU:HB2	1:A:226:SER:HB2	1.60	0.84
1:A:295:PRO:O	1:A:298:LEU:CB	2.25	0.84
1:B:62:LEU:HD11	1:B:64:ILE:HG13	1.59	0.83
1:A:289:LEU:HD13	1:A:289:LEU:O	1.78	0.83
1:A:220:VAL:C	1:A:223:ILE:CG2	2.41	0.83
1:A:294:ASP:HA	1:A:295:PRO:HG2	1.59	0.83
1:A:294:ASP:OD1	1:A:295:PRO:HG2	1.78	0.83
1:A:338:GLU:HA	1:A:338:GLU:OE1	1.79	0.82
1:B:334:VAL:H	1:B:336:PHE:N	1.77	0.82
1:B:90:PRO:O	1:B:93:ILE:HD12	1.78	0.82
1:A:222:ASP:C	1:A:226:SER:OG	2.17	0.82
1:B:171:PRO:O	1:B:369:THR:HG21	1.80	0.82
1:A:277:VAL:O	1:A:281:VAL:HG23	1.78	0.82
1:A:82:SER:HB3	1:A:83:ASN:O	1.78	0.82
1:A:357:ARG:HH11	1:A:357:ARG:CG	1.81	0.81
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.43	0.81
1:B:261:ASN:ND2	1:B:314:GLY:O	2.13	0.81
1:B:93:ILE:HG22	1:B:94:ARG:CB	2.10	0.81
1:A:171:PRO:O	1:A:369:THR:HG21	1.80	0.81
1:B:143:LEU:CD2	1:B:313:GLU:HG3	2.10	0.81
1:B:89:SER:HB3	1:B:91:SER:C	2.01	0.81
1:B:95:LYS:CA	1:B:97:ASN:H	1.94	0.80
1:B:298:LEU:HA	1:B:299:TYR:C	1.95	0.80
1:A:6:LYS:HB3	1:A:7:THR:HA	1.62	0.80
1:A:89:SER:H	1:A:92:GLN:NE2	1.79	0.80
1:A:357:ARG:O	1:A:357:ARG:HG3	1.81	0.80
1:A:112:LYS:C	1:A:114:GLY:HA3	2.02	0.80
1:A:288:LEU:HB2	1:A:289:LEU:HB2	1.62	0.80
1:B:256:ARG:NH1	1:B:259:GLU:OE2	2.15	0.80
1:B:173:GLY:H	1:B:176:GLN:NE2	1.81	0.79
1:A:235:PRO:CD	1:A:238:MET:CG	2.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:SER:HB2	1:A:330:LYS:HB3	1.65	0.79
1:A:365:LEU:CD1	1:A:391:LEU:HB3	2.12	0.79
1:B:287:LYS:O	1:B:288:LEU:HB3	1.81	0.79
1:B:372:GLU:N	1:B:372:GLU:OE2	2.15	0.79
1:A:222:ASP:N	1:A:224:ARG:H	1.80	0.78
1:A:215:GLU:HB2	1:A:216:ARG:NH2	1.96	0.78
1:B:398:GLU:O	1:B:399:GLY:C	2.21	0.78
1:A:112:LYS:HB3	1:A:115:GLU:H	1.47	0.78
1:A:80:LEU:HD23	1:A:80:LEU:H	1.48	0.78
1:B:62:LEU:CD1	1:B:64:ILE:HG13	2.13	0.78
1:A:86:ILE:CD1	1:A:108:ILE:HD13	2.14	0.77
1:B:90:PRO:CG	1:B:91:SER:CB	2.55	0.77
1:A:113:GLU:O	1:A:113:GLU:HG2	1.82	0.77
1:B:153:ILE:H	1:B:203:HIS:CE1	2.01	0.77
1:A:294:ASP:HA	1:A:295:PRO:CG	2.12	0.77
1:B:143:LEU:HD23	1:B:313:GLU:HG3	1.65	0.77
1:B:227:THR:C	1:B:229:ALA:HB2	2.05	0.77
1:B:78:ASN:ND2	1:B:233:ALA:O	2.18	0.77
1:B:235:PRO:HD2	1:B:238:MET:CE	2.13	0.77
1:B:92:GLN:O	1:B:92:GLN:CG	2.33	0.76
1:B:228:ASN:CB	1:B:229:ALA:HB3	2.16	0.76
1:B:93:ILE:CB	1:B:94:ARG:HA	2.15	0.76
1:A:129:ARG:NH1	1:A:129:ARG:CG	2.39	0.75
1:B:278:TYR:O	1:B:282:VAL:HG13	1.85	0.75
1:B:126:ILE:HG13	1:B:126:ILE:O	1.86	0.75
1:B:296:ALA:O	1:B:297:ALA:C	2.25	0.75
1:B:400:LEU:O	1:B:404:LEU:HG	1.87	0.75
1:B:108:ILE:HG23	1:B:119:ALA:O	1.87	0.75
1:A:86:ILE:HD13	1:A:108:ILE:CD1	2.15	0.75
1:A:223:ILE:CG2	1:A:224:ARG:N	2.49	0.75
1:B:91:SER:H	1:B:94:ARG:CB	1.93	0.75
1:A:356:LYS:O	1:A:357:ARG:HB3	1.86	0.74
1:B:302:LYS:NZ	1:B:338:GLU:HG3	2.02	0.74
1:A:222:ASP:C	1:A:226:SER:HG	1.90	0.74
1:B:67:GLU:OE2	1:B:69:PHE:HE2	1.70	0.74
1:A:6:LYS:O	1:A:9:SER:HB2	1.87	0.74
1:B:164:ARG:HE	1:B:413:ASN:ND2	1.86	0.74
1:B:291:GLY:H	1:B:293:VAL:H	1.35	0.74
1:B:228:ASN:CA	1:B:229:ALA:HB3	1.83	0.73
1:A:185:LYS:CA	1:A:186:ALA:HB3	2.16	0.73
1:B:302:LYS:HZ3	1:B:338:GLU:HG3	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:LEU:HD13	1:A:391:LEU:HD23	1.70	0.73
1:A:414:GLU:OE1	1:A:418:LYS:HE3	1.89	0.73
1:A:228:ASN:HD22	1:A:228:ASN:H	1.37	0.72
1:B:286:GLY:HA3	1:B:294:ASP:OD2	1.89	0.72
1:A:222:ASP:N	1:A:225:GLU:HB2	2.02	0.72
1:B:89:SER:HB3	1:B:92:GLN:HB3	1.67	0.72
1:B:371:ARG:HB3	2:B:430:IUM:O2	1.89	0.72
1:A:223:ILE:N	1:A:226:SER:CB	2.52	0.72
1:A:235:PRO:HD2	1:A:238:MET:HG2	1.70	0.72
1:A:6:LYS:CB	1:A:7:THR:CA	2.67	0.72
1:B:203:HIS:CD2	3:B:435:SO4:O3	2.42	0.72
1:A:83:ASN:HA	1:A:85:ASP:H	1.53	0.72
1:A:221:THR:O	1:A:225:GLU:HG2	1.89	0.71
1:A:5:GLN:HB3	1:A:6:LYS:HA	1.71	0.71
1:A:235:PRO:HD3	1:A:238:MET:CG	2.20	0.71
1:A:221:THR:N	1:A:222:ASP:HB2	2.05	0.71
1:A:235:PRO:HD2	1:A:238:MET:CG	2.20	0.71
1:A:329:SER:HB2	1:A:330:LYS:CB	2.20	0.71
1:A:8:ILE:HG22	1:A:9:SER:N	2.06	0.71
1:B:298:LEU:H	1:B:299:TYR:C	1.94	0.71
1:A:256:ARG:NH1	1:A:259:GLU:OE2	2.23	0.70
1:B:400:LEU:O	1:B:404:LEU:N	2.22	0.70
1:A:414:GLU:HG3	1:A:415:GLU:N	2.04	0.70
1:A:225:GLU:CB	1:A:226:SER:CB	2.59	0.70
1:A:83:ASN:HA	1:A:85:ASP:N	2.06	0.70
1:B:298:LEU:N	1:B:299:TYR:C	2.44	0.69
1:B:86:ILE:CG2	1:B:87:TYR:N	2.55	0.69
1:A:129:ARG:NH1	1:A:129:ARG:HG2	2.06	0.69
1:B:287:LYS:O	1:B:288:LEU:CB	2.39	0.69
1:B:390:MET:O	1:B:391:LEU:CB	2.39	0.69
1:B:89:SER:HB3	1:B:92:GLN:N	2.07	0.69
1:B:333:GLU:H	1:B:334:VAL:CG2	2.05	0.69
1:A:297:ALA:HB1	1:A:298:LEU:CA	2.22	0.69
1:B:299:TYR:HD1	1:B:300:LYS:HG3	1.56	0.69
1:B:331:MET:O	1:B:334:VAL:HB	1.92	0.69
1:A:223:ILE:HG22	1:A:224:ARG:H	1.56	0.69
1:B:203:HIS:HD2	3:B:435:SO4:O3	1.76	0.68
1:A:4:GLU:C	1:A:6:LYS:HB3	2.13	0.68
1:B:332:ASP:H	1:B:335:ILE:CD1	2.06	0.68
1:B:291:GLY:HA3	1:B:292:GLY:C	2.14	0.68
1:A:77:ASP:O	1:A:80:LEU:CB	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:GLY:HA3	1:B:293:VAL:N	2.09	0.68
1:B:95:LYS:HA	1:B:97:ASN:H	1.58	0.68
1:A:294:ASP:HB3	1:A:296:ALA:CB	2.15	0.68
1:A:329:SER:CB	1:A:330:LYS:HB2	2.25	0.67
1:A:223:ILE:C	1:A:226:SER:HB3	2.15	0.67
1:A:222:ASP:HB3	1:A:223:ILE:CG2	2.25	0.67
1:A:227:THR:HG22	1:A:228:ASN:C	2.15	0.67
1:B:311:THR:HG1	1:B:314:GLY:HA2	1.60	0.67
1:A:227:THR:CB	1:A:228:ASN:CA	2.62	0.66
1:A:235:PRO:CD	1:A:238:MET:HG2	2.25	0.66
1:B:89:SER:HB2	1:B:92:GLN:CB	2.17	0.66
1:B:172:ILE:HD13	1:B:320:ILE:HD12	1.76	0.66
1:B:331:MET:O	1:B:335:ILE:HG13	1.95	0.66
1:A:145:PRO:O	1:B:221:THR:HG21	1.94	0.66
1:A:329:SER:CB	1:A:330:LYS:CB	2.73	0.66
1:B:126:ILE:O	1:B:127:ASN:HB2	1.96	0.66
1:B:95:LYS:HA	1:B:97:ASN:N	2.10	0.66
1:B:172:ILE:HD13	1:B:320:ILE:CD1	2.25	0.66
1:A:109:ARG:HG2	1:A:109:ARG:NH1	2.08	0.65
1:A:294:ASP:CG	1:A:296:ALA:HB3	2.16	0.65
1:A:7:THR:N	1:A:8:ILE:C	2.49	0.65
1:B:67:GLU:OE2	1:B:69:PHE:CE2	2.49	0.65
1:A:131:VAL:HG12	1:A:131:VAL:O	1.96	0.65
1:A:287:LYS:HD2	1:B:284:PRO:HB3	1.78	0.65
1:A:287:LYS:O	1:A:288:LEU:CB	2.40	0.65
1:A:312:ARG:NH2	1:B:225:GLU:OE2	2.29	0.65
1:B:90:PRO:CB	1:B:91:SER:OG	2.33	0.65
1:A:244:VAL:O	1:A:248:GLU:HG3	1.97	0.65
1:B:363:ASN:C	1:B:363:ASN:ND2	2.46	0.64
1:B:387:LEU:O	1:B:390:MET:O	2.14	0.64
1:B:90:PRO:HB2	1:B:91:SER:HG	1.62	0.64
1:A:153:ILE:H	1:A:203:HIS:CE1	2.12	0.64
1:A:289:LEU:CB	1:A:293:VAL:O	2.46	0.64
1:B:102:ASP:OD1	1:B:256:ARG:HG3	1.98	0.64
1:A:225:GLU:HB3	1:A:226:SER:CB	2.25	0.64
1:A:290:THR:CG2	1:A:292:GLY:HA2	2.16	0.64
1:A:382:LYS:O	1:A:386:LEU:HD12	1.94	0.64
1:B:128:TYR:C	1:B:129:ARG:HG2	2.17	0.64
1:A:294:ASP:CA	1:A:295:PRO:CG	2.75	0.64
1:A:294:ASP:HB3	1:A:295:PRO:CB	2.20	0.63
1:A:294:ASP:CB	1:A:295:PRO:CB	2.75	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:THR:HA	1:A:224:ARG:HG3	1.78	0.63
1:A:296:ALA:H	1:A:297:ALA:HA	0.52	0.63
1:B:332:ASP:N	1:B:335:ILE:HD12	2.11	0.63
1:A:223:ILE:O	1:A:226:SER:HB3	1.99	0.63
1:A:289:LEU:HB2	1:A:293:VAL:O	1.99	0.63
1:B:224:ARG:HA	1:B:231:VAL:HG21	1.80	0.63
1:B:394:MET:CE	1:B:399:GLY:O	2.46	0.63
1:A:73:ARG:HH11	1:A:73:ARG:CG	2.11	0.62
1:A:111:PRO:HB3	1:A:116:LYS:HB2	1.82	0.62
1:A:220:VAL:O	1:A:224:ARG:HG3	2.00	0.62
1:A:171:PRO:HD2	1:A:369:THR:HG23	1.82	0.62
1:A:7:THR:N	1:A:8:ILE:O	2.33	0.62
1:A:414:GLU:OE1	1:A:418:LYS:CE	2.47	0.62
1:A:297:ALA:CB	1:A:299:TYR:CA	2.77	0.61
1:B:291:GLY:HA2	1:B:293:VAL:HG23	1.76	0.61
1:A:117:TYR:CE2	1:A:119:ALA:HB2	2.35	0.61
1:A:227:THR:CG2	1:A:228:ASN:C	2.68	0.61
1:A:382:LYS:O	1:A:386:LEU:HD13	1.93	0.61
1:B:311:THR:OG1	1:B:314:GLY:CA	2.44	0.61
1:A:297:ALA:HB2	1:A:299:TYR:N	2.01	0.61
1:B:330:LYS:O	1:B:334:VAL:CB	2.45	0.61
1:A:221:THR:H	1:A:222:ASP:HB2	1.64	0.60
1:A:338:GLU:OE1	1:A:338:GLU:CA	2.49	0.60
1:B:287:LYS:CG	1:B:287:LYS:O	2.40	0.60
1:B:299:TYR:CD1	1:B:300:LYS:HG3	2.35	0.60
1:A:221:THR:O	1:A:224:ARG:CB	2.37	0.60
1:B:325:VAL:HG12	1:B:326:GLU:HG3	1.82	0.60
1:A:242:LYS:HE3	3:A:432:SO4:O3	2.00	0.60
1:B:362:ILE:HG22	1:B:364:LEU:HD13	1.83	0.60
1:B:291:GLY:H	1:B:293:VAL:N	1.98	0.60
1:B:74:ARG:HB2	1:B:77:ASP:HB2	1.84	0.60
1:B:331:MET:HB3	1:B:332:ASP:HB2	1.83	0.59
1:B:82:SER:OG	2:B:431:IUM:O2	2.11	0.59
1:A:216:ARG:HD3	1:A:219:GLU:HB2	1.84	0.59
1:B:289:LEU:O	1:B:290:THR:HG23	2.03	0.59
1:A:330:LYS:O	1:A:334:VAL:HG23	2.03	0.59
1:A:8:ILE:HA	1:A:11:SER:HB3	1.83	0.59
1:A:330:LYS:H	1:A:333:GLU:H	1.50	0.59
1:A:31:PRO:O	1:A:32:ARG:HB2	2.03	0.59
1:A:89:SER:N	1:A:92:GLN:HE21	1.95	0.59
1:B:73:ARG:HH12	1:B:81:PRO:HG3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ASN:HB2	1:B:229:ALA:HB3	1.85	0.58
1:A:296:ALA:N	1:A:297:ALA:CA	2.18	0.58
1:B:288:LEU:HD23	1:B:289:LEU:O	2.03	0.58
1:A:6:LYS:HB3	1:A:7:THR:CA	2.31	0.58
1:A:80:LEU:HD23	1:A:80:LEU:N	2.10	0.58
1:B:291:GLY:CA	1:B:292:GLY:C	2.72	0.58
1:A:78:ASN:O	1:A:79:LEU:HB2	2.02	0.58
1:A:113:GLU:CG	1:A:113:GLU:O	2.49	0.58
1:B:108:ILE:HG13	1:B:119:ALA:O	2.04	0.58
1:B:95:LYS:CA	1:B:97:ASN:N	2.64	0.58
1:A:221:THR:N	1:A:222:ASP:CB	2.68	0.57
1:B:329:SER:HB2	1:B:332:ASP:CB	2.34	0.57
1:B:87:TYR:O	1:B:88:ILE:HD13	2.04	0.57
1:B:394:MET:HE2	1:B:399:GLY:O	2.03	0.57
1:A:161:TYR:OH	1:A:408:SER:HB3	2.04	0.57
1:A:197:ASN:ND2	5:A:505:HOH:O	2.38	0.57
1:A:216:ARG:CD	1:A:216:ARG:N	2.62	0.57
1:B:333:GLU:HB2	1:B:334:VAL:HG22	1.79	0.57
1:B:348:VAL:HG11	1:B:366:LEU:HB3	1.85	0.57
1:A:224:ARG:H	1:A:225:GLU:HB2	1.68	0.57
1:B:188:LYS:CB	3:B:432:SO4:O1	2.49	0.57
1:A:116:LYS:HG3	1:A:116:LYS:O	1.97	0.57
1:B:400:LEU:H	1:B:402:LEU:N	2.03	0.57
1:A:54:GLY:CA	1:A:110:LYS:HD2	2.19	0.57
1:B:144:THR:CB	1:B:313:GLU:OE2	2.53	0.56
1:A:220:VAL:CA	1:A:223:ILE:HG21	2.35	0.56
1:B:173:GLY:N	1:B:176:GLN:HE21	1.90	0.56
1:A:112:LYS:O	1:A:116:LYS:HB3	2.06	0.56
1:B:356:LYS:H	1:B:357:ARG:HA	1.69	0.56
1:A:157:ASP:HB3	1:A:160:ILE:HD12	1.88	0.56
1:A:288:LEU:HD22	1:A:288:LEU:O	2.05	0.56
1:B:208:ARG:NE	1:B:228:ASN:O	2.24	0.56
1:B:399:GLY:CA	1:B:400:LEU:HB2	2.18	0.56
1:A:23:GLU:HG3	1:A:24:ILE:N	2.21	0.56
1:A:151:ARG:NH1	1:A:376:LEU:CD2	2.68	0.56
1:B:228:ASN:HA	1:B:229:ALA:HB2	0.56	0.56
1:B:87:TYR:CD1	1:B:88:ILE:N	2.74	0.56
1:B:235:PRO:CD	1:B:238:MET:CE	2.79	0.56
1:B:334:VAL:H	1:B:336:PHE:H	1.53	0.56
1:B:63:GLU:HG3	1:B:73:ARG:HD3	1.87	0.56
1:A:291:GLY:CA	1:A:293:VAL:HG12	2.17	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LYS:HE2	3:B:434:SO4:O2	2.05	0.55
1:A:222:ASP:OD2	1:A:222:ASP:C	2.43	0.55
1:A:8:ILE:HG22	1:A:9:SER:H	1.70	0.55
1:A:183:PRO:HA	1:A:325:VAL:O	2.06	0.55
1:B:143:LEU:HD22	1:B:313:GLU:HG3	1.86	0.55
1:B:365:LEU:HD21	1:B:392:SER:HA	1.88	0.55
1:A:289:LEU:N	1:A:290:THR:HG23	2.21	0.55
1:B:334:VAL:N	1:B:336:PHE:N	2.51	0.55
1:A:294:ASP:CG	1:A:295:PRO:HB2	2.26	0.55
1:B:291:GLY:CA	1:B:293:VAL:N	2.70	0.55
1:A:294:ASP:OD1	1:A:295:PRO:CG	2.53	0.55
1:A:363:ASN:HD22	1:A:363:ASN:C	2.09	0.55
1:B:59:GLU:HB3	1:B:105:SER:HB3	1.89	0.55
1:A:73:ARG:HH11	1:A:73:ARG:HG3	1.72	0.55
1:B:96:PHE:O	1:B:97:ASN:C	2.43	0.55
1:A:188:LYS:HE2	1:A:269:ASP:OD1	2.06	0.54
1:A:212:LEU:HB2	1:A:233:ALA:HB2	1.88	0.54
1:A:73:ARG:HG3	1:A:73:ARG:NH1	2.21	0.54
1:A:289:LEU:HG	1:A:293:VAL:O	2.07	0.54
1:B:228:ASN:CB	1:B:229:ALA:CB	2.71	0.54
1:A:256:ARG:NH1	1:A:259:GLU:CD	2.60	0.54
1:A:288:LEU:CB	1:A:289:LEU:HB2	2.34	0.54
1:A:33:TYR:HA	1:A:36:MET:HE3	1.88	0.54
1:B:399:GLY:HA3	1:B:400:LEU:CB	2.11	0.54
1:A:386:LEU:CD1	1:A:386:LEU:N	2.25	0.54
1:B:334:VAL:N	1:B:336:PHE:H	2.05	0.54
1:A:371:ARG:HA	1:A:373:GLU:OE2	2.08	0.54
1:B:362:ILE:HG22	1:B:364:LEU:CD1	2.37	0.54
1:B:93:ILE:CG2	1:B:94:ARG:CA	2.23	0.54
1:B:356:LYS:N	1:B:357:ARG:HA	2.23	0.54
1:A:122:LYS:CG	1:A:124:GLU:OE1	2.56	0.53
1:A:287:LYS:HE2	1:B:282:VAL:O	2.09	0.53
1:A:129:ARG:HG2	1:A:129:ARG:HH11	1.64	0.53
1:A:288:LEU:HD22	1:A:288:LEU:C	2.28	0.53
1:B:88:ILE:CG2	1:B:92:GLN:O	2.57	0.53
1:B:333:GLU:CB	1:B:334:VAL:HG22	2.33	0.53
1:A:102:ASP:OD2	1:A:137:ARG:NH2	2.42	0.53
1:B:362:ILE:CG2	1:B:364:LEU:CD1	2.86	0.53
1:A:223:ILE:C	1:A:226:SER:CB	2.77	0.53
1:A:265:VAL:HG12	1:A:267:LEU:CD1	2.38	0.53
1:B:93:ILE:CB	1:B:94:ARG:CA	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:O	1:B:98:LEU:HD12	2.09	0.53
1:A:76:GLU:CD	5:A:500:HOH:O	2.47	0.52
1:B:86:ILE:HG22	1:B:87:TYR:N	2.23	0.52
1:A:225:GLU:CA	1:A:226:SER:CB	2.77	0.52
1:B:354:ALA:C	1:B:356:LYS:H	2.12	0.52
1:A:219:GLU:O	1:A:222:ASP:OD1	2.26	0.52
1:A:357:ARG:O	1:A:357:ARG:CG	2.57	0.52
1:B:80:LEU:HD13	1:B:246:VAL:CG2	2.39	0.52
1:A:289:LEU:HD13	1:A:289:LEU:C	2.29	0.52
1:B:184:PRO:HD3	1:B:325:VAL:O	2.10	0.52
1:B:144:THR:HB	1:B:312:ARG:CG	2.39	0.52
1:B:396:GLU:O	1:B:399:GLY:HA3	2.09	0.52
1:A:216:ARG:H	1:A:216:ARG:CD	2.08	0.52
1:A:289:LEU:H	1:A:290:THR:HG23	1.74	0.52
1:B:65:HIS:HB3	1:B:66:PRO:HD2	1.91	0.52
1:B:59:GLU:CB	1:B:105:SER:HB3	2.40	0.52
1:B:279:ASN:HD21	1:B:294:ASP:H	1.56	0.52
1:A:363:ASN:OD1	1:A:366:LEU:HD22	2.09	0.52
1:B:92:GLN:H	1:B:93:ILE:HB	1.75	0.52
1:A:171:PRO:CD	1:A:369:THR:HG23	2.40	0.52
1:B:234:ALA:HB1	1:B:243:GLN:HG2	1.91	0.52
1:B:91:SER:O	1:B:92:GLN:CB	2.57	0.52
1:B:144:THR:HB	1:B:312:ARG:HG2	1.92	0.51
1:B:287:LYS:HB2	1:B:287:LYS:NZ	2.24	0.51
1:A:293:VAL:HG23	1:A:294:ASP:O	2.09	0.51
1:A:370:ARG:CZ	1:B:216:ARG:NH2	2.73	0.51
1:A:4:GLU:HG2	1:A:4:GLU:O	2.11	0.51
1:A:107:VAL:CG1	1:A:122:LYS:HB3	2.32	0.51
1:A:227:THR:HG22	1:A:228:ASN:O	2.10	0.51
1:A:212:LEU:HB2	1:A:233:ALA:CB	2.40	0.51
1:B:412:SER:OG	1:B:414:GLU:HB3	2.11	0.51
1:A:265:VAL:HG12	1:A:267:LEU:HD13	1.93	0.51
1:A:265:VAL:HG22	1:A:318:THR:HB	1.91	0.51
1:A:279:ASN:HD21	1:A:293:VAL:HA	1.76	0.51
1:B:329:SER:O	1:B:332:ASP:HB3	2.11	0.51
1:B:400:LEU:C	1:B:400:LEU:HD22	2.31	0.51
1:A:280:ILE:HG22	1:A:280:ILE:O	2.10	0.51
1:A:145:PRO:O	1:B:221:THR:CG2	2.58	0.50
1:B:285:SER:O	1:B:286:GLY:O	2.29	0.50
1:A:37:ARG:O	1:A:40:ASP:HB2	2.11	0.50
1:B:64:ILE:HD11	1:B:99:ASN:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:MET:O	1:B:334:VAL:CB	2.59	0.50
1:B:86:ILE:HG23	1:B:87:TYR:H	1.77	0.50
1:B:291:GLY:N	1:B:293:VAL:N	2.59	0.50
1:B:93:ILE:O	1:B:96:PHE:HB2	2.11	0.50
1:A:170:ALA:HA	1:A:369:THR:HG22	1.93	0.50
1:A:131:VAL:CG1	1:A:131:VAL:O	2.59	0.50
1:B:138:VAL:O	1:B:259:GLU:HG2	2.12	0.50
1:B:171:PRO:HD2	1:B:369:THR:HG23	1.94	0.50
1:A:383:LYS:HA	1:A:386:LEU:HD13	1.94	0.50
1:B:352:GLN:O	1:B:356:LYS:HB2	2.12	0.50
1:B:95:LYS:N	1:B:97:ASN:N	2.46	0.50
1:A:17:ASN:ND2	1:A:20:GLN:H	2.10	0.50
1:B:185:LYS:CE	3:B:434:SO4:O2	2.60	0.50
1:B:252:GLU:OE1	1:B:256:ARG:NH2	2.35	0.49
1:A:33:TYR:HA	1:A:36:MET:CE	2.41	0.49
1:A:111:PRO:HA	1:A:116:LYS:HA	1.95	0.49
1:A:356:LYS:NZ	1:A:397:GLU:OE2	2.23	0.49
1:B:72:LEU:HD11	1:B:104:ILE:HB	1.93	0.49
1:A:214:ASP:O	1:A:214:ASP:CG	2.47	0.49
1:B:331:MET:O	1:B:334:VAL:CG1	2.61	0.49
1:A:221:THR:C	1:A:224:ARG:H	2.15	0.49
1:B:153:ILE:N	1:B:203:HIS:HE1	1.98	0.49
1:B:227:THR:O	1:B:229:ALA:HB2	2.13	0.48
1:B:256:ARG:HH11	1:B:259:GLU:CD	2.15	0.48
1:B:108:ILE:HD12	1:B:108:ILE:N	2.28	0.48
1:B:173:GLY:O	1:B:176:GLN:HB2	2.12	0.48
1:A:222:ASP:O	1:A:226:SER:OG	2.21	0.48
1:B:128:TYR:C	1:B:129:ARG:CG	2.82	0.48
1:B:188:LYS:N	3:B:432:SO4:O1	2.46	0.48
1:B:86:ILE:HG23	1:B:87:TYR:N	2.27	0.48
1:A:122:LYS:HG3	1:A:124:GLU:OE1	2.14	0.48
1:A:289:LEU:CG	1:A:293:VAL:O	2.61	0.48
1:A:356:LYS:O	1:A:357:ARG:CB	2.57	0.48
1:A:63:GLU:HG3	1:A:73:ARG:NH1	2.28	0.48
1:A:49:GLN:HG3	1:A:56:PHE:CD1	2.49	0.48
1:A:83:ASN:CA	1:A:85:ASP:H	2.26	0.48
1:B:89:SER:CB	1:B:92:GLN:OE1	2.49	0.48
1:A:288:LEU:CA	1:A:289:LEU:HB2	2.44	0.48
1:A:63:GLU:HG3	1:A:73:ARG:HH11	1.79	0.48
1:B:62:LEU:HD11	1:B:64:ILE:CG1	2.38	0.48
1:B:143:LEU:O	1:B:145:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLY:HA3	1:A:108:ILE:HD12	1.95	0.48
1:A:75:ILE:HD13	1:A:79:LEU:HD21	1.95	0.48
1:B:298:LEU:H	1:B:300:LYS:N	2.11	0.48
1:B:88:ILE:O	1:B:89:SER:O	2.32	0.48
1:A:129:ARG:HD2	1:A:262:TYR:OH	2.14	0.47
1:A:235:PRO:O	1:A:236:PHE:C	2.53	0.47
1:A:297:ALA:HB2	1:A:299:TYR:CB	2.34	0.47
1:B:270:SER:HB3	1:B:322:THR:OG1	2.15	0.47
1:A:289:LEU:HB3	1:A:290:THR:HA	1.97	0.47
1:B:162:SER:O	1:B:166:ILE:HG13	2.14	0.47
1:B:294:ASP:O	1:B:295:PRO:C	2.49	0.47
1:B:298:LEU:HA	1:B:301:PRO:CD	2.39	0.47
1:A:220:VAL:O	1:A:224:ARG:CG	2.62	0.47
1:B:377:ASP:C	1:B:377:ASP:OD2	2.52	0.47
1:B:294:ASP:O	1:B:296:ALA:N	2.48	0.47
1:A:224:ARG:CA	1:A:225:GLU:HB2	2.42	0.47
1:A:373:GLU:HA	1:A:381:LEU:HD11	1.95	0.47
1:A:400:LEU:O	1:A:404:LEU:HG	2.14	0.47
1:B:106:GLY:O	1:B:108:ILE:HD12	2.15	0.47
1:A:397:GLU:O	1:A:401:THR:OG1	2.15	0.47
1:A:365:LEU:CD1	1:A:391:LEU:HD23	2.44	0.47
1:A:363:ASN:ND2	1:A:363:ASN:C	2.68	0.46
1:A:30:ILE:HG21	1:A:36:MET:HE1	1.97	0.46
1:B:359:PHE:HA	1:B:360:PRO:C	2.36	0.46
1:A:157:ASP:HB3	1:A:160:ILE:CD1	2.46	0.46
1:A:79:LEU:N	1:A:80:LEU:HB2	2.31	0.46
1:B:121:ILE:O	1:B:122:LYS:HB2	2.16	0.46
1:B:313:GLU:N	1:B:314:GLY:CA	2.79	0.46
1:B:151:ARG:HD3	1:B:153:ILE:CG1	2.46	0.46
1:B:73:ARG:NH1	1:B:81:PRO:HG3	2.30	0.46
1:A:222:ASP:CG	1:A:223:ILE:HB	2.30	0.46
1:A:290:THR:HA	1:A:291:GLY:HA3	1.81	0.46
1:A:171:PRO:CD	1:A:369:THR:CG2	2.94	0.46
1:B:108:ILE:HG23	1:B:119:ALA:HB3	1.97	0.46
1:A:273:ARG:HD2	5:A:461:HOH:O	2.15	0.46
1:B:151:ARG:HD3	1:B:153:ILE:HG12	1.98	0.46
1:A:411:SER:OG	1:A:415:GLU:HG3	2.16	0.45
1:A:223:ILE:C	1:A:225:GLU:HB2	2.35	0.45
1:B:354:ALA:C	1:B:356:LYS:N	2.68	0.45
1:A:113:GLU:N	1:A:114:GLY:CA	2.63	0.45
1:B:415:GLU:O	1:B:419:LEU:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.80	0.45
1:A:151:ARG:NH1	1:A:376:LEU:HD23	2.31	0.45
1:A:298:LEU:HA	1:A:298:LEU:HD12	1.67	0.45
1:A:288:LEU:HA	1:A:289:LEU:CB	2.47	0.45
1:B:311:THR:OG1	1:B:315:GLY:N	2.50	0.45
1:B:373:GLU:CD	1:B:373:GLU:H	2.19	0.45
1:A:270:SER:HA	1:A:322:THR:OG1	2.17	0.45
1:A:288:LEU:HA	1:A:289:LEU:CD2	2.46	0.45
1:B:177:ARG:HG2	1:B:305:PHE:CZ	2.52	0.45
1:B:326:GLU:HB3	1:B:351:ARG:NH1	2.32	0.45
1:B:387:LEU:O	1:B:391:LEU:HB2	2.16	0.45
1:A:8:ILE:C	1:A:10:ILE:N	2.66	0.45
1:A:225:GLU:N	1:A:226:SER:HB2	2.32	0.44
1:A:138:VAL:O	1:A:259:GLU:HG2	2.16	0.44
1:B:183:PRO:HB3	1:B:326:GLU:OE1	2.17	0.44
1:B:394:MET:HE3	1:B:399:GLY:O	2.16	0.44
1:A:297:ALA:HB1	1:A:299:TYR:H	0.92	0.44
1:A:171:PRO:HG2	1:A:369:THR:CG2	2.48	0.44
1:A:220:VAL:C	1:A:223:ILE:HG22	2.26	0.44
1:B:147:TYR:CD1	1:B:371:ARG:CZ	3.00	0.44
1:B:96:PHE:O	1:B:97:ASN:O	2.35	0.44
1:A:293:VAL:C	1:A:294:ASP:O	2.54	0.44
1:A:203:HIS:HD2	3:A:433:SO4:O1	2.00	0.44
1:A:235:PRO:CD	1:A:238:MET:HG3	2.24	0.44
1:A:278:TYR:CE2	1:A:300:LYS:HB3	2.53	0.44
1:A:90:PRO:O	1:A:94:ARG:HG3	2.17	0.44
1:A:227:THR:CG2	1:A:228:ASN:CA	2.96	0.44
1:B:365:LEU:HD12	1:B:365:LEU:HA	1.73	0.44
1:B:398:GLU:O	1:B:399:GLY:O	2.34	0.44
1:B:74:ARG:HB3	1:B:76:GLU:HG2	2.00	0.44
1:A:86:ILE:CD1	1:A:108:ILE:CD1	2.87	0.44
1:A:289:LEU:C	1:A:289:LEU:CD1	2.86	0.44
1:A:223:ILE:HA	1:A:223:ILE:HD13	1.76	0.43
1:A:280:ILE:CG2	1:A:280:ILE:O	2.67	0.43
1:A:80:LEU:HD22	1:A:80:LEU:HA	1.85	0.43
1:B:256:ARG:HD3	1:B:256:ARG:HA	1.37	0.43
1:A:366:LEU:HA	1:A:366:LEU:HD12	1.88	0.43
1:A:144:THR:O	1:A:311:THR:HA	2.19	0.43
1:B:58:GLY:N	1:B:108:ILE:HD13	2.33	0.43
1:B:210:ILE:HG22	1:B:212:LEU:HD21	1.99	0.43
1:B:236:PHE:C	1:B:236:PHE:CD1	2.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:MET:HB2	1:B:238:MET:HE3	1.83	0.43
1:A:222:ASP:N	1:A:224:ARG:N	2.57	0.43
1:A:73:ARG:CZ	5:A:452:HOH:O	2.66	0.43
1:B:172:ILE:HD13	1:B:320:ILE:HD11	1.98	0.43
1:A:222:ASP:CB	1:A:223:ILE:CB	2.60	0.43
1:B:176:GLN:HB3	1:B:318:THR:HG23	2.00	0.43
1:A:6:LYS:C	1:A:9:SER:HB2	2.39	0.43
1:B:278:TYR:O	1:B:282:VAL:HG22	2.19	0.43
1:A:256:ARG:HH11	1:A:259:GLU:CD	2.21	0.42
1:B:298:LEU:CA	1:B:301:PRO:HD2	2.37	0.42
1:A:402:LEU:HA	1:A:402:LEU:HD23	1.92	0.42
1:B:126:ILE:O	1:B:127:ASN:CB	2.65	0.42
1:A:297:ALA:CB	1:A:300:LYS:H	2.32	0.42
1:A:330:LYS:HB3	1:A:331:MET:H	1.72	0.42
1:B:271:LEU:HD13	1:B:339:PHE:CD2	2.54	0.42
1:A:62:LEU:HD13	1:A:64:ILE:HG13	2.01	0.42
1:A:8:ILE:N	1:A:11:SER:HB2	2.32	0.42
1:A:161:TYR:OH	1:A:408:SER:CB	2.67	0.42
1:B:362:ILE:CG2	1:B:364:LEU:HD13	2.49	0.42
1:B:396:GLU:O	1:B:399:GLY:CA	2.67	0.42
1:B:76:GLU:OE1	1:B:76:GLU:N	2.51	0.42
1:B:152:PHE:CZ	1:B:174:LYS:HG2	2.54	0.42
1:B:65:HIS:HB3	1:B:66:PRO:CD	2.49	0.42
1:A:117:TYR:HE2	1:A:119:ALA:HB2	1.82	0.42
1:A:372:GLU:HG3	1:A:381:LEU:HD21	2.02	0.41
1:B:354:ALA:O	1:B:356:LYS:N	2.50	0.41
1:A:147:TYR:OH	2:B:429:IUM:O2	2.26	0.41
1:A:227:THR:HG21	1:A:229:ALA:HB3	2.02	0.41
1:A:20:GLN:O	1:A:24:ILE:HD12	2.19	0.41
1:A:294:ASP:CA	1:A:295:PRO:CB	2.98	0.41
1:A:36:MET:HE3	1:A:41:LEU:HD13	2.01	0.41
1:A:334:VAL:O	1:A:337:GLU:HB2	2.21	0.41
1:B:138:VAL:HG12	1:B:139:ASN:N	2.35	0.41
1:B:170:ALA:HA	1:B:369:THR:HG22	2.03	0.41
1:B:400:LEU:C	1:B:400:LEU:CD2	2.87	0.41
1:A:56:PHE:O	1:A:107:VAL:HA	2.21	0.41
1:A:352:GLN:CG	1:A:353:LEU:N	2.83	0.41
1:A:357:ARG:NH1	1:A:357:ARG:CG	2.52	0.41
1:A:23:GLU:OE2	1:A:124:GLU:OE1	2.38	0.41
1:A:177:ARG:HG2	1:A:305:PHE:CZ	2.56	0.41
1:B:144:THR:O	1:B:311:THR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LYS:HG2	1:A:124:GLU:OE1	2.21	0.41
1:B:126:ILE:O	1:B:126:ILE:CG1	2.57	0.41
1:A:47:LYS:HD3	1:A:51:GLU:OE1	2.21	0.41
1:B:77:ASP:O	1:B:78:ASN:HB2	2.21	0.41
1:B:89:SER:HB3	1:B:92:GLN:CB	2.45	0.41
1:B:89:SER:N	1:B:92:GLN:OE1	2.42	0.41
1:A:188:LYS:HE3	1:A:324:LEU:HD21	2.03	0.41
1:A:48:ALA:O	1:A:49:GLN:C	2.58	0.41
1:B:107:VAL:C	1:B:108:ILE:HD12	2.42	0.41
1:B:157:ASP:HA	1:B:158:PRO:HD3	1.92	0.41
1:B:339:PHE:O	1:B:340:LYS:C	2.60	0.40
1:B:286:GLY:CA	1:B:294:ASP:OD2	2.63	0.40
1:B:93:ILE:CG2	1:B:94:ARG:CB	2.85	0.40
1:A:228:ASN:H	1:A:228:ASN:ND2	2.13	0.40
1:B:329:SER:HB2	1:B:332:ASP:CG	2.42	0.40
1:B:79:LEU:HB3	1:B:249:LEU:HD23	2.02	0.40
1:A:216:ARG:NH2	1:A:219:GLU:HG3	2.36	0.40
1:A:157:ASP:HA	1:A:158:PRO:HD2	1.82	0.40
1:B:279:ASN:HA	1:B:279:ASN:HD22	1.68	0.40
1:B:332:ASP:H	1:B:335:ILE:CG1	2.33	0.40
1:B:394:MET:HE3	1:B:402:LEU:HD12	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	409/427 (96%)	363 (89%)	23 (6%)	23 (6%)	2	0
1	B	341/427 (80%)	284 (83%)	28 (8%)	29 (8%)	1	0
All	All	750/854 (88%)	647 (86%)	51 (7%)	52 (7%)	1	0

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	6	LYS
1	A	9	SER
1	A	117	TYR
1	A	186	ALA
1	A	222	ASP
1	A	226	SER
1	A	235	PRO
1	A	288	LEU
1	A	295	PRO
1	A	296	ALA
1	A	330	LYS
1	B	89	SER
1	B	92	GLN
1	B	93	ILE
1	B	95	LYS
1	B	96	PHE
1	B	229	ALA
1	B	284	PRO
1	B	286	GLY
1	B	297	ALA
1	B	298	LEU
1	B	299	TYR
1	B	334	VAL
1	B	408	SER
1	A	8	ILE
1	A	227	THR
1	B	97	ASN
1	B	331	MET
1	B	335	ILE
1	B	355	ASN
1	B	391	LEU
1	B	399	GLY
1	B	400	LEU
1	A	7	THR
1	A	225	GLU
1	A	229	ALA
1	B	283	PRO
1	B	287	LYS
1	B	288	LEU
1	B	401	THR
1	A	32	ARG

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Mol	Chain	Res	Type
1	A	223	ILE
1	B	68	GLY
1	B	90	PRO
1	B	91	SER
1	B	332	ASP
1	A	80	LEU
1	A	289	LEU
1	A	83	ASN
1	B	300	LYS
1	A	284	PRO

### 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	363/375 (97%)	310 (85%)	53 (15%)	3	3
1	B	303/375 (81%)	267 (88%)	36 (12%)	5	4
All	All	666/750 (89%)	577 (87%)	89 (13%)	4	4

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	7	THR
1	A	11	SER
1	A	17	ASN
1	A	23	GLU
1	A	34	THR
1	A	53	THR
1	A	61	VAL
1	A	62	LEU
1	A	73	ARG
1	A	74	ARG
1	A	82	SER
1	A	107	VAL

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Mol	Chain	Res	Type
1	A	116	LYS
1	A	122	LYS
1	A	129	ARG
1	A	197	ASN
1	A	216	ARG
1	A	219	GLU
1	A	223	ILE
1	A	224	ARG
1	A	225	GLU
1	A	226	SER
1	A	228	ASN
1	A	256	ARG
1	A	261	ASN
1	A	271	LEU
1	A	288	LEU
1	A	289	LEU
1	A	290	THR
1	A	293	VAL
1	A	295	PRO
1	A	312	ARG
1	A	325	VAL
1	A	338	GLU
1	A	346	GLU
1	A	347	LEU
1	A	352	GLN
1	A	357	ARG
1	A	363	ASN
1	A	365	LEU
1	A	366	LEU
1	A	369	THR
1	A	373	GLU
1	A	375	LEU
1	A	379	GLU
1	A	382	LYS
1	A	386	LEU
1	A	392	SER
1	A	394	MET
1	A	405	ASN
1	A	410	THR
1	A	414	GLU
1	B	63	GLU
1	B	73	ARG

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Mol	Chain	Res	Type
1	B	80	LEU
1	B	89	SER
1	B	92	GLN
1	B	95	LYS
1	B	98	LEU
1	B	137	ARG
1	B	201	GLU
1	B	221	THR
1	B	226	SER
1	B	228	ASN
1	B	241	ASP
1	B	256	ARG
1	B	287	LYS
1	B	298	LEU
1	B	299	TYR
1	B	313	GLU
1	B	316	SER
1	B	331	MET
1	B	332	ASP
1	B	347	LEU
1	B	348	VAL
1	B	352	GLN
1	B	363	ASN
1	B	364	LEU
1	B	365	LEU
1	B	366	LEU
1	B	369	THR
1	B	371	ARG
1	B	373	GLU
1	B	375	LEU
1	B	385	TRP
1	B	400	LEU
1	B	413	ASN
1	B	414	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	49	GLN
1	A	92	GLN
1	A	97	ASN

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Mol	Chain	Res	Type
1	A	203	HIS
1	A	228	ASN
1	B	65	HIS
1	B	176	GLN
1	B	203	HIS
1	B	261	ASN
1	B	279	ASN
1	B	363	ASN
1	B	405	ASN
1	B	413	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	B	434	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	A	435	-	4,4,4	0.15	0	6,6,6	0.12	0
2	IUM	B	428	1	0,2,2	0.00	-	-		
2	IUM	A	428	1	0,2,2	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	431	-	4,4,4	0.17	0	6,6,6	0.24	0
2	IUM	B	431	1	0,2,2	0.00	-	-		
2	IUM	B	429	1,5	0,2,2	0.00	-	-		
3	SO4	A	434	-	4,4,4	0.13	0	6,6,6	0.26	0
3	SO4	B	432	4	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	B	435	-	4,4,4	0.18	0	6,6,6	0.09	0
3	SO4	A	433	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	B	433	-	4,4,4	0.18	0	6,6,6	0.10	0
2	IUM	A	429	1	0,2,2	0.00	-	-		
2	IUM	A	430	1,5	0,2,2	0.00	-	-		
2	IUM	B	430	1	0,2,2	0.00	-	-		
3	SO4	A	432	-	4,4,4	0.11	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

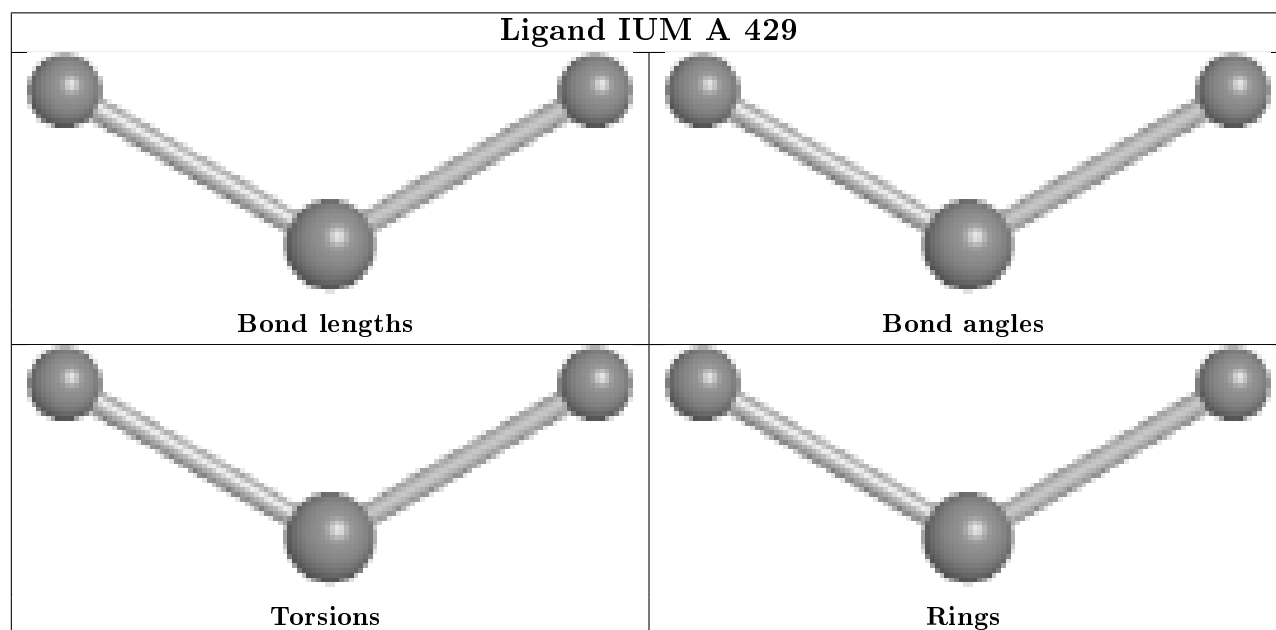
There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	434	SO4	2	0
3	A	435	SO4	1	0
2	B	431	IUM	1	0
2	B	429	IUM	1	0
3	B	432	SO4	3	0
3	B	435	SO4	2	0
3	A	433	SO4	1	0
2	B	430	IUM	1	0
3	A	432	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	413/427 (96%)	0.43	28 (6%) 17 25	23, 44, 77, 92	6 (1%)
1	B	347/427 (81%)	0.82	49 (14%) 2 4	30, 54, 100, 108	4 (1%)
All	All	760/854 (88%)	0.61	77 (10%) 7 11	23, 48, 94, 108	10 (1%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	ILE	11.6
1	B	108	ILE	10.2
1	A	236	PHE	6.6
1	B	71	PHE	6.6
1	B	90	PRO	6.2
1	B	107	VAL	5.4
1	B	91	SER	5.4
1	B	119	ALA	5.4
1	B	84	ASP	5.3
1	B	88	ILE	5.0
1	B	87	TYR	4.8
1	A	48	ALA	4.7
1	B	66	PRO	4.7
1	A	289	LEU	4.6
1	B	106	GLY	4.5
1	A	114	GLY	4.2
1	A	222	ASP	4.1
1	A	216	ARG	3.9
1	B	69	PHE	3.8
1	B	288	LEU	3.8
1	B	85	ASP	3.7
1	A	288	LEU	3.6
1	A	113	GLU	3.5
1	A	7	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	65	HIS	3.4
1	A	234	ALA	3.4
1	B	120	MET	3.4
1	A	291	GLY	3.3
1	B	287	LYS	3.3
1	B	94	ARG	3.3
1	B	286	GLY	3.2
1	B	289	LEU	3.2
1	A	290	THR	3.2
1	B	86	ILE	3.1
1	B	93	ILE	3.1
1	A	5	GLN	3.1
1	A	292	GLY	3.1
1	B	62	LEU	3.0
1	B	284	PRO	3.0
1	B	92	GLN	2.9
1	A	50	THR	2.9
1	A	285	SER	2.9
1	B	58	GLY	2.9
1	B	130	PRO	2.8
1	B	67	GLU	2.8
1	A	137	ARG	2.8
1	B	122	LYS	2.7
1	A	83	ASN	2.7
1	A	419	LEU	2.6
1	B	321	ALA	2.6
1	B	322	THR	2.6
1	A	8	ILE	2.6
1	B	123	ILE	2.6
1	B	299	TYR	2.5
1	B	97	ASN	2.5
1	A	232	ILE	2.5
1	A	225	GLU	2.5
1	B	95	LYS	2.4
1	B	72	LEU	2.4
1	B	330	LYS	2.4
1	B	293	VAL	2.3
1	A	230	ILE	2.3
1	B	70	GLY	2.3
1	B	209	ILE	2.3
1	B	230	ILE	2.3
1	B	333	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	334	VAL	2.2
1	B	401	THR	2.1
1	A	95	LYS	2.1
1	B	64	ILE	2.1
1	A	185	LYS	2.1
1	B	96	PHE	2.1
1	B	385	TRP	2.1
1	B	283	PRO	2.1
1	A	49	GLN	2.0
1	A	84	ASP	2.0
1	A	136	ASP	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.

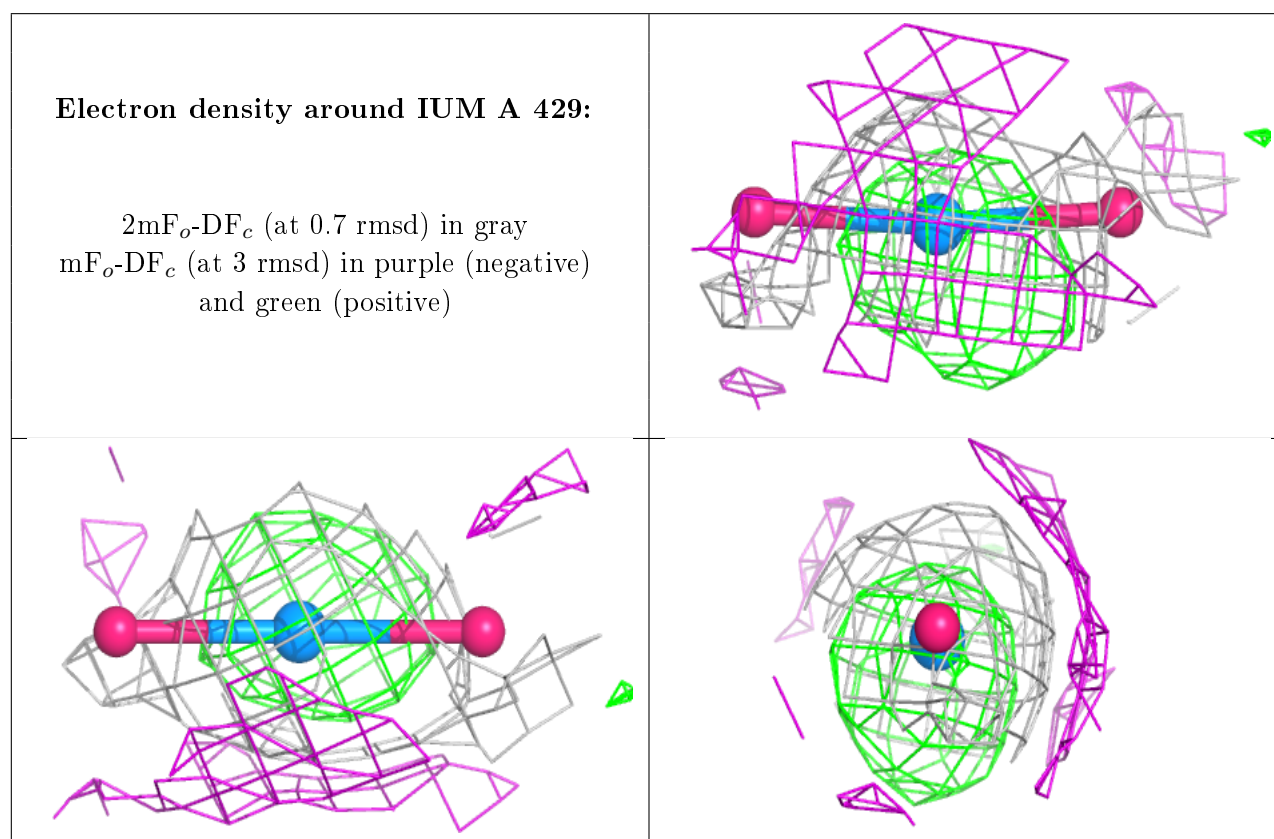
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	IUM	A	429	3/3	0.78	0.41	432,432,500,500	0
3	SO4	A	435	5/5	0.80	0.18	73,129,189,459	0
3	SO4	B	432	5/5	0.82	0.39	84,115,192,461	0
3	SO4	B	434	5/5	0.88	0.49	42,122,458,458	0
2	IUM	B	428	3/3	0.88	0.14	56,56,176,328	3
4	NA	B	437	1/1	0.88	0.10	66,66,66,66	0
2	IUM	B	430	3/3	0.89	0.33	211,211,480,480	3
4	NA	B	436	1/1	0.90	0.34	49,49,49,49	0
3	SO4	A	434	5/5	0.94	0.10	59,62,442,444	0
2	IUM	B	431	3/3	0.94	0.09	53,53,120,139	3
3	SO4	A	431	5/5	0.95	0.14	54,66,113,145	0
3	SO4	A	433	5/5	0.97	0.11	39,40,58,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	435	5/5	0.98	0.06	52,57,98,106	0
2	IUM	A	430	3/3	0.99	0.12	25,25,36,39	0
3	SO4	B	433	5/5	0.99	0.16	36,40,137,413	0
3	SO4	A	432	5/5	0.99	0.20	63,64,239,448	0
2	IUM	B	429	3/3	1.00	0.08	63,63,74,145	0
2	IUM	A	428	3/3	1.00	0.04	58,58,79,91	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.