



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:35 PM UTC

PDB ID : 2WL5 / pdb_00002wl5
Title : BIOSYNTHETIC THIOLASE FROM Z. RAMIGERA. COMPLEX OF THE H348N MUTANT WITH COENZYME A.
Authors : Merilainen, G.; Poikela, V.; Kursula, P.; Wierenga, R.K.
Deposited on : 2009-06-22
Resolution : 1.80 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

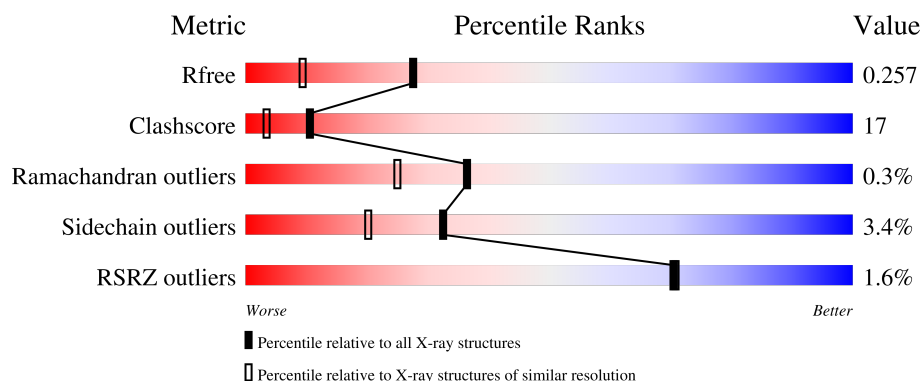
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	392	 83% 15% ..
1	B	392	 85% 13% ..
2	C	392	 2% 58% 39% ..
2	D	392	 5% 64% 33% ..

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
4	DNO	A	1398	X	-	-	-
4	DNO	C	1397	X	-	-	-
4	DNO	C	1398	X	-	-	-
4	DNO	C	1399	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12780 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 ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	8	0
			2856	1783	513	539	21			
1	B	389	Total	C	N	O	S	0	7	0
			2850	1775	511	541	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	ALA	SEE REMARK 999	UNP P07097
A	348	ASN	HIS	engineered mutation	UNP P07097
B	129	ARG	ALA	SEE REMARK 999	UNP P07097
B	348	ASN	HIS	engineered mutation	UNP P07097

- Molecule 2 is a protein called ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	389	Total	C	N	O	S	0	1	0
			2815	1748	508	538	21			
2	D	389	Total	C	N	O	S	0	0	0
			2811	1744	508	538	21			

There are 4 discrepancies between the modelled and reference sequences:

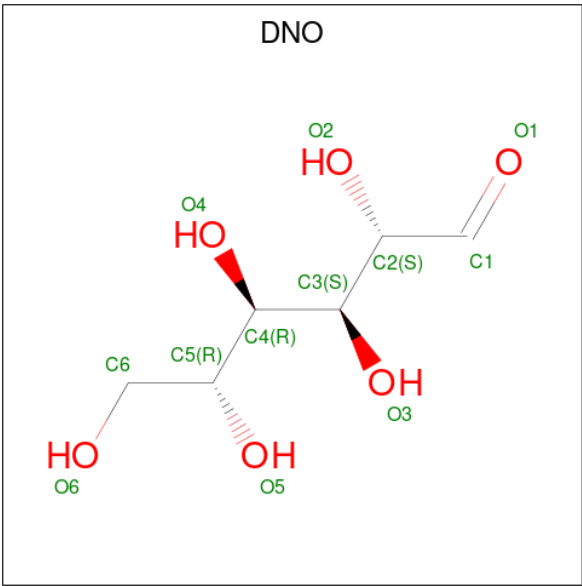
Chain	Residue	Modelled	Actual	Comment	Reference
C	129	ARG	ALA	SEE REMARK 999	UNP P07097
C	348	ASN	HIS	engineered mutation	UNP P07097
D	129	ARG	ALA	SEE REMARK 999	UNP P07097
D	348	ASN	HIS	engineered mutation	UNP P07097

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



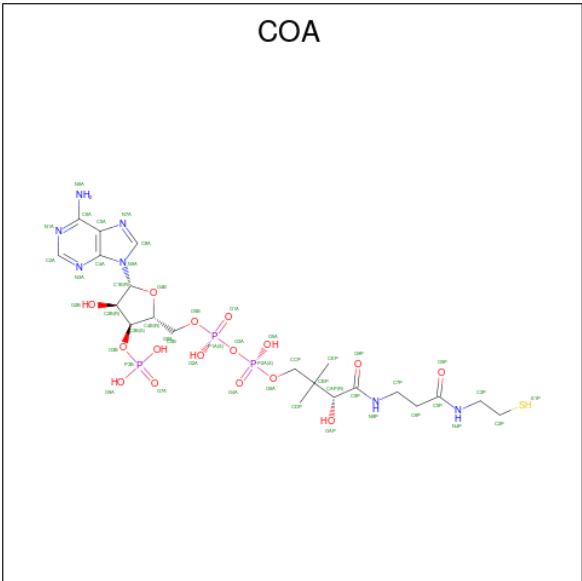
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total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

- Molecule 4 is D-mannose (CCD ID: DNO) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	
			48	21	7	16	3	1	
5	B	1	Total	C	N	O	P	S	
			48	21	7	16	3	1	

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na		
			1	1	0	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl		
			1	1	0	0

- Molecule 8 is water.

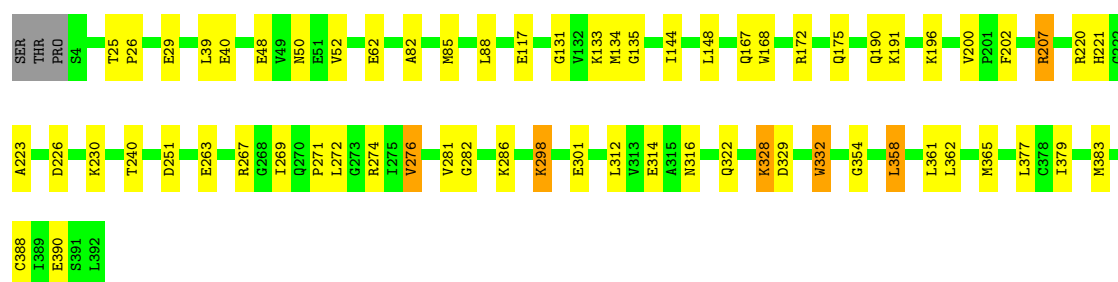
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	453	Total	O		
			453	453	0	0
8	B	479	Total	O		
			479	479	0	0
8	C	171	Total	O		
			171	171	0	0
8	D	129	Total	O		
			129	129	0	0

3 Residue-property plots

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

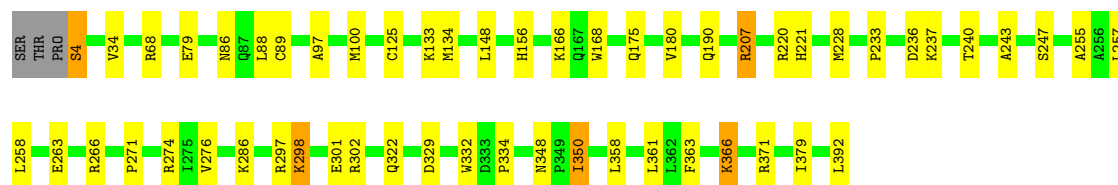
• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

Chain A: 



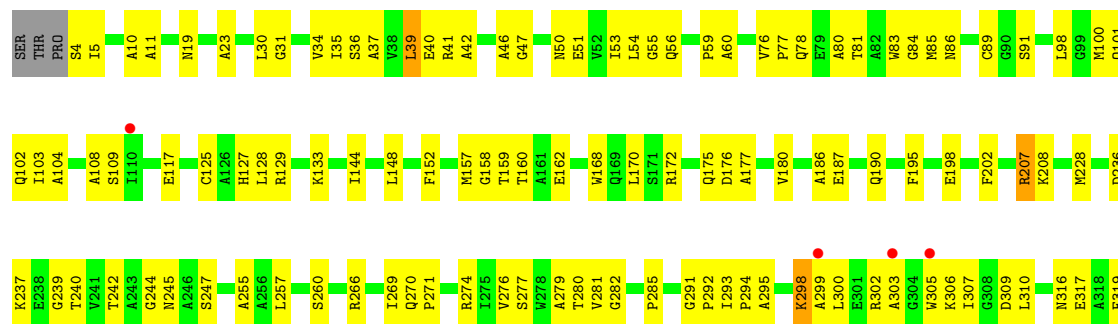
• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

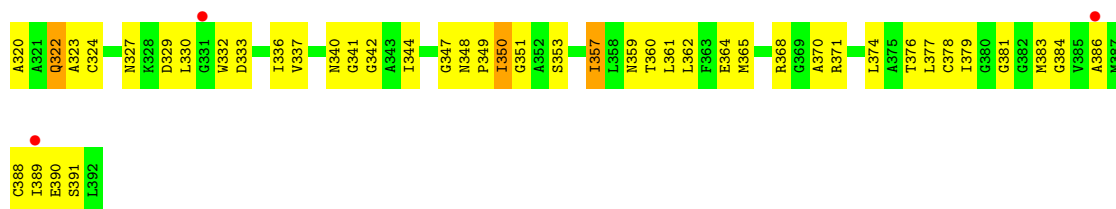
Chain B: 



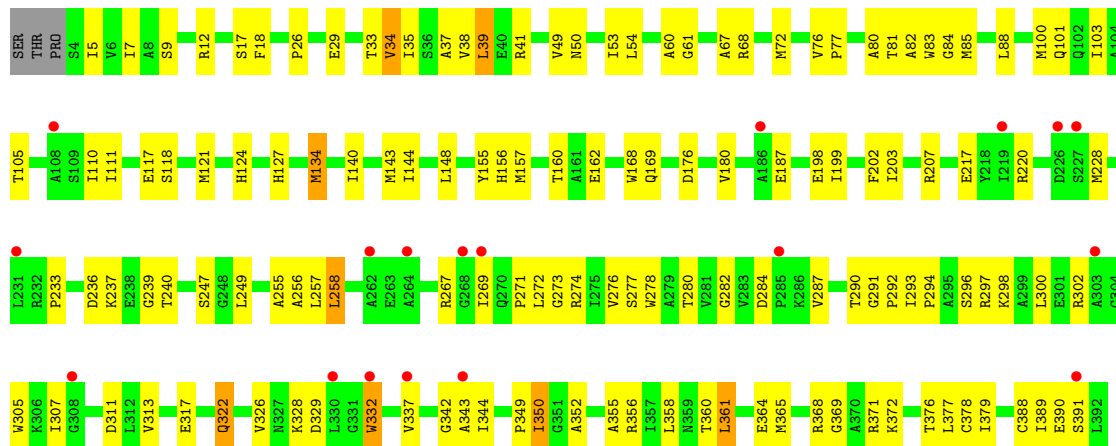
• Molecule 2: ACETYL-COA ACETYLTRANSFERASE

Chain C: 





● Molecule 2: ACETYL-COA ACETYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.70Å 79.20Å 153.00Å 90.00° 92.50° 90.00°	Depositor
Resolution (Å)	19.39 – 1.80 19.39 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.39-1.80) 86.6 (19.39-1.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.257 0.221 , 0.257	Depositor DCC
R_{free} test set	9226 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 67.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.176 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12780	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, NA, CL, DNO, SO4, COA

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	0/2912	0.91	2/3928 (0.1%)
1	B	0.70	0/2900	0.94	0/3910
2	C	0.35	0/2858	0.77	2/3859 (0.1%)
2	D	0.34	0/2851	0.80	0/3849
All	All	0.55	0/11521	0.86	4/15546 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	VAL	CA-C-N	-5.77	114.02	119.85
1	A	200	VAL	C-N-CA	-5.77	114.02	119.85
2	C	270	GLN	CA-C-N	5.05	124.98	119.78
2	C	270	GLN	C-N-CA	5.05	124.98	119.78

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2856	0	2910	74	0
1	B	2850	0	2888	55	0
2	C	2815	0	2827	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2811	0	2818	121	0
3	A	20	0	0	0	0
3	B	25	0	0	0	0
3	C	20	0	0	0	0
3	D	5	0	0	0	0
4	A	12	0	12	0	0
4	C	36	0	36	2	0
5	A	48	0	32	5	0
5	B	48	0	32	3	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0
8	A	453	0	0	28	0
8	B	479	0	0	18	0
8	C	171	0	0	48	0
8	D	129	0	0	25	0
All	All	12780	0	11555	388	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 17.

All (388) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:HG2	1:A:207:ARG:HH11	1.10	1.14
1:A:207:ARG:H	1:A:207:ARG:HD3	1.29	0.97
2:C:274:ARG:HE	2:C:390:GLU:HG2	1.33	0.93
2:D:207:ARG:H	2:D:207:ARG:HD3	1.36	0.90
2:C:125:CYS:SG	8:D:2021:HOH:O	2.30	0.89
1:A:226:ASP:HB3	8:A:2448:HOH:O	1.74	0.88
2:C:207:ARG:H	2:C:207:ARG:HD3	1.36	0.88
2:C:388:CYS:HB2	8:C:2120:HOH:O	1.74	0.88
2:C:160:THR:HG21	8:C:2125:HOH:O	1.74	0.87
2:D:389:ILE:HG23	8:D:2095:HOH:O	1.75	0.86
2:C:305:TRP:CZ3	2:C:388:CYS:HB3	2.14	0.82
1:A:207:ARG:HG2	1:A:207:ARG:NH1	1.90	0.82
1:A:202:PHE:HZ	8:A:2049:HOH:O	1.63	0.82
2:C:5:ILE:HD13	2:C:100:MET:HG2	1.61	0.81
2:D:61:GLY:HA3	8:D:2021:HOH:O	1.83	0.79
2:C:168:TRP:HA	8:C:2078:HOH:O	1.83	0.79
1:B:207:ARG:HG2	1:B:207:ARG:HH11	1.46	0.79
2:C:247:SER:OG	2:C:348:ASN:HB2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:293:ILE:HB	2:C:294:PRO:HD3	1.66	0.78
2:C:279:ALA:HB2	8:C:2121:HOH:O	1.83	0.77
2:C:302:ARG:HD2	8:C:2121:HOH:O	1.83	0.77
2:C:379:ILE:HG12	8:C:2152:HOH:O	1.84	0.77
2:D:49:VAL:HG13	8:D:2016:HOH:O	1.83	0.76
1:B:207:ARG:HH11	1:B:207:ARG:H	1.31	0.76
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.21	0.75
2:C:187:GLU:HA	8:C:2085:HOH:O	1.85	0.75
1:B:168:TRP:HH2	1:B:329:ASP:HB2	1.52	0.74
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.24	0.73
2:C:31:GLY:O	2:C:34[B]:VAL:HG12	1.88	0.73
1:A:196[A]:LYS:HD3	8:A:2121:HOH:O	1.89	0.73
2:C:180:VAL:HG22	8:C:2100:HOH:O	1.89	0.72
1:B:125:CYS:SG	8:B:2183:HOH:O	2.48	0.72
1:B:237:LYS:N	1:B:237:LYS:HD2	2.03	0.71
2:D:291:GLY:O	2:D:294:PRO:HD2	1.90	0.71
1:A:301:GLU:HG3	8:A:2366:HOH:O	1.91	0.71
2:C:47:GLY:HA2	2:C:77:PRO:HG3	1.73	0.70
2:C:317:GLU:CD	2:C:342:GLY:HA3	2.16	0.70
2:C:320:ALA:HA	8:C:2138:HOH:O	1.90	0.70
1:B:79:GLU:HB3	8:B:2139:HOH:O	1.91	0.69
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.58	0.69
1:A:26:PRO:HB3	8:A:2085:HOH:O	1.91	0.69
1:A:207:ARG:HH11	1:A:207:ARG:CG	1.95	0.68
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.57	0.68
2:C:379:ILE:HB	2:C:383:MET:HB2	1.77	0.67
1:A:220[B]:ARG:NH1	8:A:2300:HOH:O	2.27	0.67
2:D:236:ASP:HB3	2:D:239:GLY:HA3	1.75	0.67
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.08	0.67
1:B:243:ALA:HB1	8:B:2470:HOH:O	1.94	0.66
2:D:88:LEU:HB2	2:D:379:ILE:HG23	1.78	0.66
2:C:144:ILE:HD13	2:C:148:LEU:HD12	1.76	0.66
2:C:282:GLY:HA2	8:C:2155:HOH:O	1.96	0.65
1:B:134:MET:CE	2:C:144:ILE:HD11	2.26	0.65
1:A:148:LEU:HD23	8:A:2198:HOH:O	1.96	0.65
1:B:207:ARG:HG2	1:B:207:ARG:NH1	2.08	0.65
2:D:35:ILE:O	2:D:38:VAL:HG22	1.96	0.65
2:C:128:LEU:O	8:C:2065:HOH:O	2.14	0.65
1:A:362:LEU:HD22	8:A:2344:HOH:O	1.97	0.64
2:C:91:SER:HB2	8:C:2029:HOH:O	1.96	0.64
1:A:62:GLU:CD	8:A:2085:HOH:O	2.40	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:81:THR:HG21	2:D:280:THR:HG23	1.77	0.64
2:D:317:GLU:CD	2:D:342:GLY:HA3	2.22	0.64
2:C:330:LEU:HD12	2:C:332:TRP:CH2	2.33	0.64
2:C:236:ASP:HB3	2:C:239:GLY:HA3	1.79	0.64
2:D:207:ARG:HD3	2:D:207:ARG:N	2.12	0.63
5:A:1399:COA:H32	8:A:2198:HOH:O	1.96	0.63
1:A:358[B]:LEU:HD21	1:A:362:LEU:HD11	1.80	0.62
2:C:383:MET:HG2	8:C:2155:HOH:O	1.96	0.62
2:D:292:PRO:HD3	2:D:378:CYS:HB3	1.82	0.62
2:C:299:ALA:HA	8:C:2121:HOH:O	1.98	0.62
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.13	0.62
2:D:33:THR:HG1	2:D:202:PHE:HD1	1.48	0.62
2:D:293:ILE:HB	2:D:294:PRO:HD3	1.81	0.62
2:C:5:ILE:HD11	2:C:104:ALA:HB2	1.82	0.61
2:C:293:ILE:HG23	2:C:330:LEU:HD21	1.83	0.61
1:B:371:ARG:HD2	8:B:2437:HOH:O	2.00	0.61
2:D:313:VAL:HB	2:D:337:VAL:HG22	1.82	0.61
2:D:34:VAL:CG1	2:D:255:ALA:HB3	2.31	0.61
2:C:228:MET:HB2	8:C:2100:HOH:O	2.01	0.60
2:C:292:PRO:HD3	8:C:2156:HOH:O	2.00	0.60
1:A:25:THR:HG23	8:A:2049:HOH:O	2.00	0.60
1:A:251:ASP:HA	8:A:2158:HOH:O	2.00	0.60
1:A:196[A]:LYS:NZ	8:A:2268:HOH:O	2.33	0.60
2:C:274:ARG:NE	2:C:390:GLU:HG2	2.13	0.60
1:A:362:LEU:CD2	8:A:2344:HOH:O	2.50	0.60
1:B:156:HIS:HD2	4:C:1397:DNO:O2	1.84	0.60
2:D:290:THR:HB	8:D:2098:HOH:O	2.00	0.60
1:B:220:ARG:HD2	8:B:2310:HOH:O	2.00	0.60
1:B:263:GLU:OE1	1:B:266:ARG:NH2	2.35	0.60
1:B:297:ARG:NE	8:B:2379:HOH:O	2.34	0.59
1:A:117:GLU:HB3	8:A:2158:HOH:O	2.02	0.59
2:C:53:ILE:HD13	2:C:83:TRP:CZ2	2.38	0.59
1:A:281:VAL:HG13	8:B:2139:HOH:O	2.01	0.59
2:C:327:ASN:HD21	2:C:337:VAL:HG11	1.67	0.59
5:B:1399:COA:H8A	8:B:2470:HOH:O	2.03	0.58
2:C:277:SER:N	8:C:2120:HOH:O	2.35	0.58
2:C:364:GLU:O	2:C:368:ARG:HG2	2.03	0.58
2:C:152:PHE:CZ	2:D:72:MET:HG3	2.39	0.58
2:C:77:PRO:HA	4:C:1398:DNO:H5	1.86	0.58
2:D:198:GLU:OE1	2:D:360:THR:HA	2.03	0.57
2:D:276:VAL:CG1	2:D:388:CYS:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:ARG:NE	8:D:2115:HOH:O	2.36	0.57
2:C:35:ILE:O	2:C:39:LEU:HD13	2.04	0.57
1:B:175:GLN:HE22	1:B:240:THR:HG21	1.70	0.57
1:B:298:LYS:HE2	1:B:302:ARG:HG3	1.87	0.57
2:C:362:LEU:HD21	2:C:389:ILE:HG21	1.87	0.57
2:D:257:LEU:HD23	2:D:258:LEU:N	2.20	0.57
2:D:35:ILE:O	2:D:39:LEU:HD22	2.05	0.57
2:C:276:VAL:O	2:C:277:SER:HB3	2.05	0.56
2:D:269:ILE:O	2:D:271:PRO:HD3	2.04	0.56
1:A:134:MET:HG3	2:D:143:MET:HE1	1.87	0.56
2:C:281:VAL:N	8:C:2123:HOH:O	2.38	0.56
2:C:291:GLY:O	2:C:294:PRO:HD2	2.06	0.56
1:A:269:ILE:O	1:A:271:PRO:HD3	2.05	0.56
2:D:148:LEU:HD13	2:D:156:HIS:HE2	1.71	0.56
1:A:312:LEU:HD23	1:A:361[B]:LEU:HD12	1.88	0.55
2:C:198:GLU:OE1	2:C:360:THR:HA	2.05	0.55
2:D:12:ARG:O	2:D:199:ILE:HA	2.06	0.55
2:D:34:VAL:HG11	2:D:255:ALA:HB3	1.88	0.55
2:D:344:ILE:HG23	8:D:2078:HOH:O	2.05	0.55
2:D:292:PRO:HG3	2:D:377:LEU:C	2.32	0.55
1:A:191:LYS:HG3	8:A:2250:HOH:O	2.07	0.54
1:A:358[B]:LEU:CD2	1:A:362:LEU:HD11	2.37	0.54
2:C:98:LEU:O	2:C:102:GLN:HG2	2.07	0.54
2:C:378:CYS:HB2	8:C:2156:HOH:O	2.07	0.54
2:D:7:ILE:HG12	2:D:258:LEU:CD1	2.37	0.54
2:D:237:LYS:HB3	8:D:2075:HOH:O	2.08	0.54
1:A:207:ARG:H	1:A:207:ARG:CD	2.10	0.54
1:B:133:LYS:HD2	2:C:19:ASN:ND2	2.22	0.54
2:C:282:GLY:CA	8:C:2155:HOH:O	2.54	0.54
1:B:190:GLN:OE1	1:B:221:HIS:HE1	1.90	0.54
1:B:271:PRO:HG2	1:B:392:LEU:HD12	1.89	0.54
1:B:286:LYS:HD3	8:B:2216:HOH:O	2.07	0.54
2:D:9:SER:HA	2:D:272:LEU:HD23	1.90	0.54
5:A:1399:COA:O5P	5:A:1399:COA:H21	2.06	0.54
2:D:180:VAL:HG22	2:D:228:MET:HE3	1.89	0.53
1:A:220[A]:ARG:NH2	8:A:2298:HOH:O	2.41	0.53
1:A:298:LYS:HA	1:A:298:LYS:NZ	2.22	0.53
1:A:332:TRP:HZ2	8:A:2391:HOH:O	1.90	0.53
2:C:51:GLU:CD	2:C:83:TRP:HE1	2.16	0.53
2:C:127:HIS:HD2	8:D:2042:HOH:O	1.91	0.53
1:B:4:SER:HB3	8:B:2366:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:281:VAL:HG22	8:C:2122:HOH:O	2.08	0.53
1:B:334:PRO:HA	8:B:2403:HOH:O	2.08	0.53
2:D:276:VAL:HG13	2:D:388:CYS:HB2	1.89	0.53
2:D:305:TRP:CH2	2:D:372:LYS:HB3	2.44	0.53
1:A:276:VAL:HG22	1:A:388:CYS:HB2	1.91	0.53
2:C:109:SER:HB3	8:C:2111:HOH:O	2.09	0.53
2:C:374:LEU:C	2:C:374:LEU:HD23	2.33	0.53
2:C:365:MET:HA	2:C:370:ALA:HB3	1.91	0.53
2:C:19:ASN:C	2:C:23:ALA:HB2	2.34	0.52
1:A:274:ARG:NH2	1:A:390:GLU:OE1	2.42	0.52
2:C:300:LEU:HD13	2:C:307:ILE:HG12	1.91	0.52
2:C:376:THR:HB	8:C:2150:HOH:O	2.10	0.52
1:A:40:GLU:HG3	8:A:2059:HOH:O	2.09	0.52
1:A:361[A]:LEU:CD1	1:A:365:MET:SD	2.98	0.52
2:C:37:ALA:O	2:C:41:ARG:HG3	2.10	0.52
2:C:159:THR:O	2:C:162:GLU:HB2	2.09	0.52
2:C:274:ARG:HG2	2:C:390:GLU:O	2.09	0.52
2:D:7:ILE:HG23	2:D:256:ALA:HB1	1.92	0.52
2:D:26:PRO:HD2	2:D:29:GLU:OE1	2.09	0.52
2:D:111:ILE:HA	8:D:2016:HOH:O	2.10	0.52
2:D:292:PRO:HD3	2:D:378:CYS:CB	2.39	0.52
2:C:333:ASP:O	2:C:336:ILE:HG12	2.10	0.52
2:C:228:MET:HE2	8:C:2100:HOH:O	2.09	0.52
2:C:55:GLY:C	8:C:2029:HOH:O	2.52	0.51
1:A:133:LYS:O	2:C:129:ARG:HG2	2.10	0.51
2:C:300:LEU:HD21	2:C:310:LEU:HD11	1.92	0.51
1:A:379:ILE:HB	1:A:383:MET:HB2	1.93	0.51
2:C:170:LEU:HD13	2:C:324:CYS:HB2	1.93	0.51
1:B:237:LYS:HD2	1:B:237:LYS:H	1.76	0.51
2:C:280:THR:HG23	2:D:81:THR:HG21	1.91	0.51
2:C:281:VAL:HG12	2:C:282:GLY:N	2.26	0.51
2:D:53:ILE:HD12	2:D:111:ILE:HG21	1.91	0.51
2:C:190:GLN:HB3	8:C:2085:HOH:O	2.11	0.51
2:D:5:ILE:HG21	2:D:100:MET:CG	2.41	0.51
2:D:371:ARG:O	2:D:390:GLU:HA	2.10	0.51
1:B:34:VAL:HG12	1:B:255:ALA:HB3	1.93	0.50
2:D:124:HIS:HA	2:D:140:ILE:O	2.10	0.50
2:D:305:TRP:CZ3	2:D:372:LYS:HB3	2.46	0.50
2:C:5:ILE:HG21	2:C:100:MET:HG2	1.93	0.50
2:D:203:ILE:HB	8:D:2068:HOH:O	2.11	0.50
1:B:166:LYS:HG3	8:B:2222:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ARG:NH1	1:A:207:ARG:CG	2.63	0.49
1:A:301:GLU:CG	8:A:2366:HOH:O	2.55	0.49
1:B:68:ARG:NH2	8:B:2114:HOH:O	2.45	0.49
1:A:190:GLN:OE1	1:A:221:HIS:HE1	1.95	0.49
2:C:291:GLY:HA3	8:C:2156:HOH:O	2.12	0.49
2:C:371:ARG:HA	2:C:391:SER:OG	2.13	0.49
2:D:100:MET:HE2	2:D:101:GLN:HG3	1.94	0.49
1:B:134:MET:HE2	2:C:144:ILE:HD11	1.93	0.49
1:A:134:MET:HG2	2:D:144:ILE:HD11	1.94	0.49
2:C:269:ILE:O	2:C:271:PRO:HD3	2.13	0.49
2:D:247:SER:HB3	2:D:317:GLU:O	2.12	0.49
1:B:133:LYS:HD2	2:C:19:ASN:HD22	1.77	0.49
2:C:127:HIS:CD2	8:D:2042:HOH:O	2.64	0.49
2:C:242:THR:C	2:C:244:GLY:H	2.20	0.49
2:C:175:GLN:HE22	2:C:240:THR:HG21	1.78	0.48
2:C:281:VAL:HG22	8:C:2058:HOH:O	2.13	0.48
2:D:293:ILE:O	2:D:297:ARG:HG3	2.13	0.48
2:C:50:ASN:O	2:C:80:ALA:HB1	2.13	0.48
2:D:103:ILE:HD11	2:D:111:ILE:HG12	1.96	0.48
2:D:278:TRP:O	2:D:302:ARG:NH1	2.44	0.48
2:D:157:MET:HA	2:D:157:MET:HE2	1.95	0.48
2:C:298:LYS:O	2:C:298:LYS:HD3	2.14	0.48
2:D:369:GLY:HA2	8:D:2117:HOH:O	2.13	0.48
2:D:12:ARG:HE	2:D:198:GLU:CD	2.21	0.48
2:D:155:TYR:HE1	2:D:160:THR:HG22	1.78	0.48
2:D:168:TRP:CH2	2:D:329:ASP:HB2	2.49	0.48
2:D:317:GLU:OE2	2:D:342:GLY:HA3	2.13	0.48
1:A:50:ASN:HB3	8:A:2037:HOH:O	2.13	0.48
2:C:285:PRO:HG3	2:C:381:GLY:O	2.13	0.48
2:D:50:ASN:HB2	2:D:110:ILE:O	2.14	0.47
2:D:361:LEU:O	2:D:365:MET:HG3	2.14	0.47
1:B:263:GLU:CD	8:B:2348:HOH:O	2.58	0.47
2:C:347:GLY:HA2	8:C:2141:HOH:O	2.14	0.47
2:D:68:ARG:N	8:D:2027:HOH:O	2.46	0.47
5:A:1399:COA:O7A	2:C:208:LYS:NZ	2.47	0.47
1:B:86:ASN:HB2	8:B:2090:HOH:O	2.13	0.47
2:C:186:ALA:HB2	2:C:341:GLY:HA3	1.96	0.47
2:C:316:ASN:HB2	2:C:377:LEU:HG	1.96	0.47
1:B:190:GLN:OE1	1:B:221:HIS:CE1	2.67	0.47
1:B:247[A]:SER:OG	1:B:348:ASN:HB2	2.15	0.47
1:B:298:LYS:HE2	1:B:302:ARG:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:ALA:O	2:C:11:ALA:HB2	2.15	0.47
2:C:85:MET:HE3	2:C:98:LEU:HD11	1.97	0.47
2:C:306:LYS:HB2	2:C:309:ASP:OD1	2.14	0.47
1:A:202:PHE:CZ	8:A:2049:HOH:O	2.51	0.47
1:B:207:ARG:H	1:B:207:ARG:NH1	2.07	0.47
2:D:284:ASP:HB3	2:D:287:VAL:HG22	1.97	0.47
2:C:5:ILE:CD1	2:C:100:MET:HG2	2.40	0.47
2:C:362:LEU:CD2	2:C:389:ILE:HG21	2.45	0.47
2:C:34[A]:VAL:HG12	2:C:255:ALA:HB3	1.96	0.47
2:C:280:THR:OG1	2:D:81:THR:HG21	2.15	0.47
1:A:167:GLN:NE2	8:A:2218:HOH:O	2.47	0.46
2:C:269:ILE:HG12	8:C:2023:HOH:O	2.14	0.46
2:D:60:ALA:C	8:D:2021:HOH:O	2.58	0.46
1:B:97:ALA:O	1:B:100[B]:MET:HG3	2.15	0.46
2:D:34:VAL:O	2:D:38:VAL:HG13	2.15	0.46
2:D:127:HIS:CG	8:D:2043:HOH:O	2.68	0.46
2:C:177:ALA:HB1	8:C:2080:HOH:O	2.14	0.46
2:C:54:LEU:O	2:C:84:GLY:HA2	2.16	0.46
2:C:168:TRP:CH2	2:C:329:ASP:HB2	2.51	0.46
2:C:295:ALA:HA	8:C:2123:HOH:O	2.16	0.46
1:A:207:ARG:HD3	1:A:207:ARG:N	2.11	0.46
2:C:379:ILE:HG21	2:C:383:MET:HE3	1.96	0.46
2:C:101:GLN:HG2	2:D:105:THR:HG21	1.98	0.46
2:C:378:CYS:HA	8:C:2156:HOH:O	2.16	0.46
2:D:26:PRO:HD2	2:D:29:GLU:CD	2.40	0.46
2:D:233:PRO:HB2	2:D:236:ASP:O	2.15	0.46
1:B:89:CSO:SG	1:B:350:ILE:HG23	2.56	0.46
2:C:59:PRO:O	2:C:60:ALA:C	2.59	0.46
2:C:353:SER:O	2:C:357:ILE:HG23	2.16	0.46
2:D:257:LEU:O	2:D:258:LEU:HD13	2.15	0.46
2:C:47:GLY:HA2	2:C:77:PRO:CG	2.45	0.46
2:C:245:ASN:HB2	2:C:320:ALA:CB	2.46	0.46
2:D:118:SER:OG	2:D:121:MET:HB2	2.16	0.46
1:A:286:LYS:NZ	8:A:2353:HOH:O	2.50	0.45
2:D:307:ILE:HG23	2:D:332:TRP:HB3	1.99	0.45
2:C:129:ARG:HD3	2:D:18:PHE:CZ	2.51	0.45
2:D:176:ASP:O	2:D:180:VAL:HG23	2.17	0.45
2:C:317:GLU:OE2	2:C:342:GLY:HA3	2.16	0.45
2:D:355:ALA:O	2:D:356:ARG:C	2.58	0.45
1:A:281:VAL:HG12	1:A:282:GLY:N	2.29	0.45
1:A:358[B]:LEU:CD2	1:A:362:LEU:CD1	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:VAL:CG1	1:B:255:ALA:HB3	2.47	0.45
2:C:86:ASN:HA	8:C:2031:HOH:O	2.16	0.45
2:C:319:PHE:O	2:C:322:GLN:HG3	2.16	0.45
2:C:281:VAL:HG23	8:C:2123:HOH:O	2.16	0.45
2:D:276:VAL:O	2:D:277:SER:HB3	2.17	0.45
2:C:157:MET:HE2	2:C:157:MET:HA	1.98	0.45
2:D:162:GLU:OE1	2:D:240:THR:HG22	2.16	0.45
2:C:5:ILE:CD1	2:C:104:ALA:HB2	2.45	0.45
2:C:78:GLN:O	2:D:282:GLY:HA3	2.17	0.45
2:C:344:ILE:HD11	8:C:2139:HOH:O	2.17	0.45
2:C:379:ILE:HD12	8:C:2157:HOH:O	2.17	0.45
2:C:11:ALA:N	2:C:359:ASN:OD1	2.50	0.44
1:A:52:VAL:O	1:A:82:ALA:HA	2.17	0.44
1:B:228[B]:MET:HG2	8:B:2474:HOH:O	2.18	0.44
2:C:319:PHE:C	8:C:2139:HOH:O	2.59	0.44
2:D:292:PRO:HB3	2:D:376:THR:OG1	2.17	0.44
2:D:257:LEU:C	2:D:258:LEU:HD13	2.43	0.44
2:C:36:SER:HA	2:C:39:LEU:HD22	1.98	0.44
2:C:176:ASP:O	2:C:180:VAL:HG23	2.17	0.44
2:D:144:ILE:HA	2:D:148:LEU:HB2	1.98	0.44
1:A:88:LEU:HB2	1:A:379:ILE:HG23	2.00	0.44
1:A:314:GLU:HG3	1:A:361[A]:LEU:HB2	1.98	0.44
2:D:76:VAL:HA	2:D:77:PRO:HD2	1.80	0.44
1:B:228[B]:MET:HE2	5:B:1399:COA:H61A	1.82	0.44
2:C:349:PRO:O	2:C:350:ILE:C	2.61	0.44
1:A:354:GLY:HA2	1:A:377:LEU:HD11	2.00	0.43
1:B:301:GLU:CD	8:B:2380:HOH:O	2.61	0.43
1:B:363:PHE:CD1	1:B:366[A]:LYS:NZ	2.86	0.43
2:D:368:ARG:HA	8:D:2120:HOH:O	2.18	0.43
1:A:135:GLY:HA2	2:D:144:ILE:HD12	2.00	0.43
2:C:89:CYS:O	2:C:377:LEU:HD22	2.18	0.43
2:C:133:LYS:HG2	8:C:2066:HOH:O	2.18	0.43
2:D:7:ILE:HG12	2:D:258:LEU:HD12	2.00	0.43
2:D:53:ILE:HG12	2:D:83:TRP:CE2	2.53	0.43
1:A:220[A]:ARG:CZ	5:A:1399:COA:N6A	2.81	0.43
1:A:361[A]:LEU:HD11	1:A:365:MET:SD	2.57	0.43
1:B:274:ARG:NH2	1:B:392:LEU:HD21	2.33	0.43
2:C:237:LYS:HA	2:C:237:LYS:HD2	1.74	0.43
2:D:37:ALA:O	2:D:41:ARG:HG3	2.18	0.43
1:B:134:MET:HE3	2:C:144:ILE:HD11	2.00	0.43
1:A:316:ASN:HB3	8:A:2427:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:158:GLY:HA2	2:C:319:PHE:CE1	2.54	0.43
2:D:17:SER:OG	2:D:217:GLU:HG3	2.17	0.43
2:D:61:GLY:CA	8:D:2021:HOH:O	2.55	0.43
1:B:100[A]:MET:HE2	1:B:100[A]:MET:HB3	1.96	0.43
2:C:56:GLN:N	8:C:2029:HOH:O	2.52	0.43
2:C:274:ARG:HE	2:C:390:GLU:CG	2.18	0.43
2:C:386:ALA:HA	8:C:2150:HOH:O	2.18	0.43
2:D:38:VAL:HG23	2:D:39:LEU:N	2.33	0.43
2:C:4:SER:O	2:C:260:SER:HA	2.19	0.42
2:C:298:LYS:HE2	2:C:302:ARG:HG3	2.01	0.42
2:D:293:ILE:HB	8:D:2098:HOH:O	2.18	0.42
2:C:56:GLN:C	8:C:2031:HOH:O	2.62	0.42
1:A:220[A]:ARG:HH12	1:A:223:ALA:CB	2.32	0.42
2:C:30:LEU:HD23	2:C:202:PHE:CE1	2.55	0.42
2:D:361:LEU:HD22	2:D:365:MET:SD	2.59	0.42
1:A:134:MET:SD	2:D:249:LEU:HD11	2.59	0.42
1:A:328:LYS:HB2	1:A:328:LYS:HE2	1.38	0.42
1:B:180:VAL:CG2	1:B:228[B]:MET:HG3	2.49	0.42
2:C:103:ILE:HG12	2:C:108:ALA:O	2.19	0.42
2:D:364:GLU:O	2:D:368:ARG:HG2	2.18	0.42
2:C:195:PHE:HZ	2:C:340:ASN:O	2.02	0.42
2:D:349:PRO:O	2:D:350:ILE:C	2.62	0.42
2:C:379:ILE:HG13	2:C:384:GLY:HA2	2.01	0.42
2:D:33:THR:OG1	2:D:202:PHE:HD1	2.02	0.42
2:D:54:LEU:O	2:D:84:GLY:HA2	2.19	0.42
2:D:67:ALA:HB3	8:D:2027:HOH:O	2.20	0.42
2:D:82:ALA:C	8:D:2027:HOH:O	2.62	0.42
2:D:311:ASP:HA	8:D:2103:HOH:O	2.19	0.42
2:D:349:PRO:HB2	2:D:352:ALA:HB3	2.02	0.42
1:A:172:ARG:HA	1:A:240:THR:OG1	2.19	0.42
2:D:85:MET:HE2	2:D:85:MET:HB2	1.98	0.42
2:C:85:MET:HA	2:D:85:MET:HA	2.01	0.42
2:D:274:ARG:N	8:D:2095:HOH:O	2.53	0.42
2:D:328:LYS:HB2	2:D:328:LYS:HE3	1.84	0.42
1:A:220[A]:ARG:NH2	8:A:2299:HOH:O	2.46	0.41
1:B:207:ARG:HH11	1:B:207:ARG:CG	2.23	0.41
1:B:233:PRO:HB2	1:B:236:ASP:O	2.18	0.41
2:C:266:ARG:HA	8:C:2165:HOH:O	2.20	0.41
2:C:276:VAL:HG23	2:C:303:ALA:HB2	2.02	0.41
2:D:143:MET:HE2	2:D:143:MET:HB3	1.95	0.41
2:D:322:GLN:O	2:D:326:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:172:ARG:HA	2:C:240:THR:OG1	2.20	0.41
2:D:273:GLY:HA2	2:D:391:SER:HA	2.01	0.41
2:C:323:ALA:CB	8:C:2138:HOH:O	2.67	0.41
2:D:307:ILE:HD12	2:D:307:ILE:H	1.85	0.41
1:A:29:GLU:OE1	8:A:2049:HOH:O	2.22	0.41
1:A:131:GLY:CA	8:C:2065:HOH:O	2.68	0.41
2:C:4:SER:C	2:C:5:ILE:HG13	2.44	0.41
2:C:46:ALA:HB1	2:C:76:VAL:HA	2.03	0.41
2:C:292:PRO:HA	2:C:295:ALA:HB3	2.01	0.41
2:D:88:LEU:HB2	2:D:379:ILE:CG2	2.48	0.41
1:B:207:ARG:HH11	1:B:207:ARG:N	2.08	0.41
2:C:42:ALA:HB3	2:C:257:LEU:HD13	2.03	0.41
2:D:267:ARG:NH2	8:D:2088:HOH:O	2.52	0.41
2:D:292:PRO:CD	2:D:378:CYS:HB3	2.51	0.41
2:D:317:GLU:O	2:D:343:ALA:HB3	2.20	0.41
2:D:53:ILE:HD12	2:D:111:ILE:CG2	2.51	0.41
5:A:1399:COA:O5A	2:D:134:MET:HE1	2.20	0.41
1:B:148:LEU:HD22	5:B:1399:COA:C5P	2.50	0.41
2:D:296:SER:O	2:D:300:LEU:HG	2.20	0.41
1:A:85:MET:HE2	1:A:85:MET:HB2	1.89	0.41
1:B:257[A]:LEU:HD23	1:B:258:LEU:N	2.35	0.41
2:C:242:THR:C	2:C:244:GLY:N	2.78	0.41
2:D:117:GLU:HA	2:D:117:GLU:OE1	2.21	0.41
1:A:144:ILE:HD13	1:A:148:LEU:HD12	2.03	0.41
2:C:117:GLU:OE1	2:C:351:GLY:HA3	2.21	0.41
2:C:302:ARG:CZ	8:C:2132:HOH:O	2.69	0.41
2:D:68:ARG:NH1	2:D:80:ALA:O	2.51	0.41
1:A:131:GLY:HA2	8:C:2065:HOH:O	2.22	0.41
1:B:88:LEU:HB2	1:B:379:ILE:HG23	2.02	0.41
1:B:298:LYS:CE	8:B:2380:HOH:O	2.69	0.41
2:C:86:ASN:CB	8:C:2031:HOH:O	2.69	0.41
2:D:100:MET:HE2	2:D:101:GLN:N	2.36	0.40
1:A:220[A]:ARG:NH1	1:A:223:ALA:HB2	2.36	0.40
2:C:42:ALA:CB	2:C:257:LEU:HD13	2.52	0.40
2:D:293:ILE:HD12	8:D:2098:HOH:O	2.21	0.40
1:A:48:GLU:OE1	1:A:267:ARG:NH2	2.52	0.40
1:A:190:GLN:OE1	1:A:221:HIS:CE1	2.74	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	394/392 (100%)	378 (96%)	16 (4%)	0	100	100
1	B	393/392 (100%)	380 (97%)	12 (3%)	1 (0%)	36	25
2	C	388/392 (99%)	365 (94%)	22 (6%)	1 (0%)	36	25
2	D	387/392 (99%)	359 (93%)	26 (7%)	2 (0%)	24	14
All	All	1562/1568 (100%)	1482 (95%)	76 (5%)	4 (0%)	36	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	350	ILE
2	D	350	ILE
2	D	169	GLN
1	B	350	ILE

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	283/278 (102%)	269 (95%)	14 (5%)	22	10
1	B	282/278 (101%)	271 (96%)	11 (4%)	28	16
2	C	277/279 (99%)	270 (98%)	7 (2%)	42	30
2	D	276/279 (99%)	265 (96%)	11 (4%)	28	15
All	All	1118/1114 (100%)	1075 (96%)	43 (4%)	32	17

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	207	ARG
1	A	230[A]	LYS
1	A	230[B]	LYS
1	A	263	GLU
1	A	272[A]	LEU
1	A	272[B]	LEU
1	A	276	VAL
1	A	298	LYS
1	A	322	GLN
1	A	328	LYS
1	A	332	TRP
1	A	358[A]	LEU
1	A	358[B]	LEU
1	B	4	SER
1	B	207	ARG
1	B	276	VAL
1	B	298	LYS
1	B	322	GLN
1	B	332	TRP
1	B	358[A]	LEU
1	B	358[B]	LEU
1	B	361	LEU
1	B	366[A]	LYS
1	B	366[B]	LYS
2	C	39	LEU
2	C	40	GLU
2	C	207	ARG
2	C	298	LYS
2	C	322	GLN
2	C	357	ILE
2	C	361	LEU
2	D	34	VAL
2	D	39	LEU
2	D	134	MET
2	D	187	GLU
2	D	220	ARG
2	D	258	LEU
2	D	298	LYS
2	D	322	GLN
2	D	332	TRP
2	D	358	LEU

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Mol	Chain	Res	Type
2	D	361	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	167	GLN
1	A	169	GLN
1	A	175	GLN
1	A	184	ASN
1	A	221	HIS
1	B	78	GLN
1	B	175	GLN
1	B	184	ASN
1	B	221	HIS
2	C	19	ASN
2	C	78	GLN
2	C	127	HIS
2	C	184	ASN
2	C	327	ASN
2	D	175	GLN
2	D	184	ASN
2	D	190	GLN
2	D	322	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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
1	CSO	A	89	1	3,6,7	0.66	0	1,6,8	1.37	0
1	CSO	B	89	1	3,6,7	0.57	0	1,6,8	1.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	A	89	1	-	0/1/5/7	-
1	CSO	B	89	1	-	0/1/5/7	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	89	CSO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	1396	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	B	1394	-	4,4,4	0.26	0	6,6,6	0.11	0
3	SO4	B	1401	-	4,4,4	0.24	0	6,6,6	0.12	0
4	DNO	C	1399	-	10,11,11	2.34	3 (30%)	13,14,14	1.96	5 (38%)
4	DNO	C	1397	-	10,11,11	2.20	2 (20%)	13,14,14	1.64	3 (23%)
3	SO4	B	1395	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	C	1396	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	A	1395	-	4,4,4	0.28	0	6,6,6	0.13	0
3	SO4	C	1394	-	4,4,4	0.25	0	6,6,6	0.06	0
5	COA	A	1399	-	47,50,50	2.83	17 (36%)	69,75,75	2.05	17 (24%)
3	SO4	D	1393	-	4,4,4	0.23	0	6,6,6	0.14	0
4	DNO	A	1398	-	10,11,11	2.35	3 (30%)	13,14,14	1.91	5 (38%)
3	SO4	C	1395	-	4,4,4	0.24	0	6,6,6	0.12	0
5	COA	B	1399	-	47,50,50	2.77	17 (36%)	69,75,75	1.96	15 (21%)
4	DNO	C	1398	-	10,11,11	2.28	3 (30%)	13,14,14	1.82	4 (30%)
3	SO4	A	1397	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	A	1394	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	B	1397	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	C	1393	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	1396	-	4,4,4	0.23	0	6,6,6	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DNO	A	1398	-	2/2/4/5	3/15/16/16	-
4	DNO	C	1399	-	2/2/4/5	5/15/16/16	-
5	COA	B	1399	-	-	7/48/64/64	0/3/3/3
4	DNO	C	1397	-	2/2/4/5	5/15/16/16	-
4	DNO	C	1398	-	2/2/4/5	4/15/16/16	-
5	COA	A	1399	-	-	9/48/64/64	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1399	COA	P1A-O3A	7.52	1.67	1.59
5	A	1399	COA	P2A-O3A	7.28	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1399	COA	P1A-O3A	7.11	1.67	1.59
5	B	1399	COA	P2A-O3A	6.25	1.66	1.59
5	B	1399	COA	C9P-N8P	6.14	1.48	1.33
5	A	1399	COA	C9P-N8P	6.02	1.47	1.33
5	B	1399	COA	C5P-N4P	5.72	1.46	1.33
5	A	1399	COA	C5P-N4P	5.69	1.46	1.33
5	B	1399	COA	C8A-N7A	5.50	1.42	1.31
5	A	1399	COA	C8A-N7A	5.33	1.41	1.31
4	A	1398	DNO	C4-C3	5.11	1.63	1.53
4	C	1399	DNO	C4-C3	5.03	1.62	1.53
5	B	1399	COA	P3B-O7A	4.96	1.65	1.50
4	C	1397	DNO	O1-C1	4.86	1.38	1.20
5	A	1399	COA	P3B-O7A	4.84	1.65	1.50
4	C	1398	DNO	C4-C3	4.83	1.62	1.53
4	C	1398	DNO	O1-C1	4.78	1.38	1.20
4	C	1399	DNO	O1-C1	4.74	1.38	1.20
4	A	1398	DNO	O1-C1	4.73	1.37	1.20
4	C	1397	DNO	C4-C3	4.42	1.61	1.53
5	A	1399	COA	C6A-N6A	4.32	1.45	1.34
5	B	1399	COA	P1A-O1A	4.32	1.65	1.50
5	A	1399	COA	P2A-O4A	4.29	1.65	1.50
5	A	1399	COA	P1A-O1A	4.29	1.65	1.50
5	B	1399	COA	C6A-N6A	4.29	1.45	1.34
5	B	1399	COA	P2A-O4A	4.22	1.65	1.50
5	B	1399	COA	C4A-N9A	3.44	1.44	1.37
5	A	1399	COA	C2A-N3A	3.40	1.40	1.33
5	B	1399	COA	C2A-N3A	3.27	1.39	1.33
5	A	1399	COA	C4A-N9A	3.20	1.44	1.37
5	B	1399	COA	P3B-O8A	2.82	1.65	1.54
5	B	1399	COA	P3B-O3B	2.78	1.64	1.59
5	A	1399	COA	P3B-O8A	2.78	1.65	1.54
5	A	1399	COA	P3B-O3B	2.66	1.64	1.59
5	A	1399	COA	C8A-N9A	-2.56	1.33	1.37
5	A	1399	COA	C5A-C4A	-2.50	1.34	1.39
5	B	1399	COA	C5A-C4A	-2.33	1.34	1.39
4	A	1398	DNO	C3-C2	2.29	1.56	1.53
4	C	1399	DNO	C3-C2	2.26	1.56	1.53
5	A	1399	COA	P2A-O6A	2.23	1.68	1.59
5	A	1399	COA	P1A-O5B	2.11	1.67	1.59
5	B	1399	COA	P2A-O6A	2.08	1.67	1.59
4	C	1398	DNO	C3-C2	2.06	1.56	1.53
5	B	1399	COA	C8A-N9A	-2.06	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1399	COA	O5P-C5P	-2.03	1.19	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1399	COA	C2B-C1B-N9A	6.52	129.51	113.30
5	B	1399	COA	N3A-C2A-N1A	-6.28	119.08	128.58
5	A	1399	COA	N3A-C2A-N1A	-5.76	119.86	128.58
5	B	1399	COA	C2B-C1B-N9A	4.93	125.56	113.30
5	A	1399	COA	N9A-C8A-N7A	-4.89	107.00	113.94
5	B	1399	COA	N9A-C8A-N7A	-4.87	107.03	113.94
5	A	1399	COA	C5A-C4A-N3A	-4.45	120.58	126.72
5	B	1399	COA	C5A-C4A-N3A	-4.27	120.84	126.72
5	A	1399	COA	C3P-N4P-C5P	-4.00	115.38	122.82
5	A	1399	COA	O2B-C2B-C3B	3.99	122.34	111.19
5	B	1399	COA	O4B-C1B-N9A	3.85	115.48	108.09
5	A	1399	COA	O6A-CCP-CBP	3.83	116.70	110.55
5	B	1399	COA	O3B-C3B-C4B	3.70	123.09	110.03
5	B	1399	COA	C4A-N9A-C8A	3.64	109.56	105.74
4	A	1398	DNO	O6-C6-C5	3.52	118.55	111.16
5	A	1399	COA	O2B-C2B-C1B	3.46	122.00	110.10
5	B	1399	COA	C2A-N3A-C4A	3.36	120.03	111.83
4	C	1399	DNO	O6-C6-C5	3.29	118.07	111.16
5	B	1399	COA	O2B-C2B-C3B	3.23	120.22	111.19
5	A	1399	COA	C4A-N9A-C8A	3.21	109.11	105.74
5	A	1399	COA	C2A-N3A-C4A	3.20	119.65	111.83
5	B	1399	COA	N3A-C4A-N9A	3.16	132.54	127.17
5	A	1399	COA	C5A-N7A-C8A	3.12	108.35	103.45
5	B	1399	COA	O2B-C2B-C1B	2.99	120.40	110.10
5	A	1399	COA	O3B-C3B-C4B	2.95	120.42	110.03
4	C	1399	DNO	O4-C4-C3	2.94	116.33	109.46
5	A	1399	COA	N3A-C4A-N9A	2.89	132.08	127.17
4	C	1397	DNO	O5-C5-C4	2.86	115.94	109.25
4	C	1398	DNO	O6-C6-C5	2.78	116.99	111.16
5	B	1399	COA	C5A-N7A-C8A	2.75	107.77	103.45
5	B	1399	COA	CDP-CBP-CCP	2.61	112.53	108.22
4	C	1398	DNO	O5-C5-C4	2.60	115.33	109.25
4	A	1398	DNO	O5-C5-C4	2.59	115.30	109.25
5	B	1399	COA	C7P-C6P-C5P	2.57	116.67	112.39
4	A	1398	DNO	O4-C4-C3	2.51	115.32	109.46
5	A	1399	COA	C7P-C6P-C5P	2.49	116.54	112.39
5	A	1399	COA	O3B-C3B-C2B	2.39	120.24	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1399	DNO	O5-C5-C4	2.37	114.80	109.25
4	C	1399	DNO	O5-C5-C6	2.33	114.32	109.03
4	C	1397	DNO	O6-C6-C5	2.29	115.97	111.16
4	C	1397	DNO	O5-C5-C6	2.29	114.22	109.03
4	C	1398	DNO	O4-C4-C3	2.21	114.61	109.46
4	A	1398	DNO	O5-C5-C6	2.12	113.84	109.03
5	A	1399	COA	O4B-C1B-N9A	2.10	112.13	108.09
5	A	1399	COA	C4A-C5A-N7A	-2.08	108.20	110.58
4	C	1399	DNO	O4-C4-C5	2.05	113.60	108.93
4	C	1398	DNO	O4-C4-C5	2.05	113.58	108.93
4	A	1398	DNO	O2-C2-C3	2.03	114.21	109.46
5	B	1399	COA	OAP-CAP-CBP	2.03	114.87	110.18

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1398	DNO	C2
4	A	1398	DNO	C3
4	C	1397	DNO	C2
4	C	1397	DNO	C3
4	C	1398	DNO	C2
4	C	1398	DNO	C3
4	C	1399	DNO	C2
4	C	1399	DNO	C3

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1398	DNO	O1-C1-C2-C3
4	C	1397	DNO	C3-C4-C5-C6
4	C	1397	DNO	O4-C4-C5-C6
4	C	1397	DNO	O4-C4-C5-O5
4	C	1398	DNO	O1-C1-C2-C3
4	C	1399	DNO	C2-C3-C4-C5
4	C	1399	DNO	C2-C3-C4-O4
4	C	1399	DNO	O3-C3-C4-C5
4	C	1399	DNO	O3-C3-C4-O4
5	A	1399	COA	CDP-CBP-CCP-O6A
5	A	1399	COA	CEP-CBP-CCP-O6A
5	A	1399	COA	CAP-CBP-CCP-O6A
5	A	1399	COA	C2P-C3P-N4P-C5P
5	B	1399	COA	S1P-C2P-C3P-N4P

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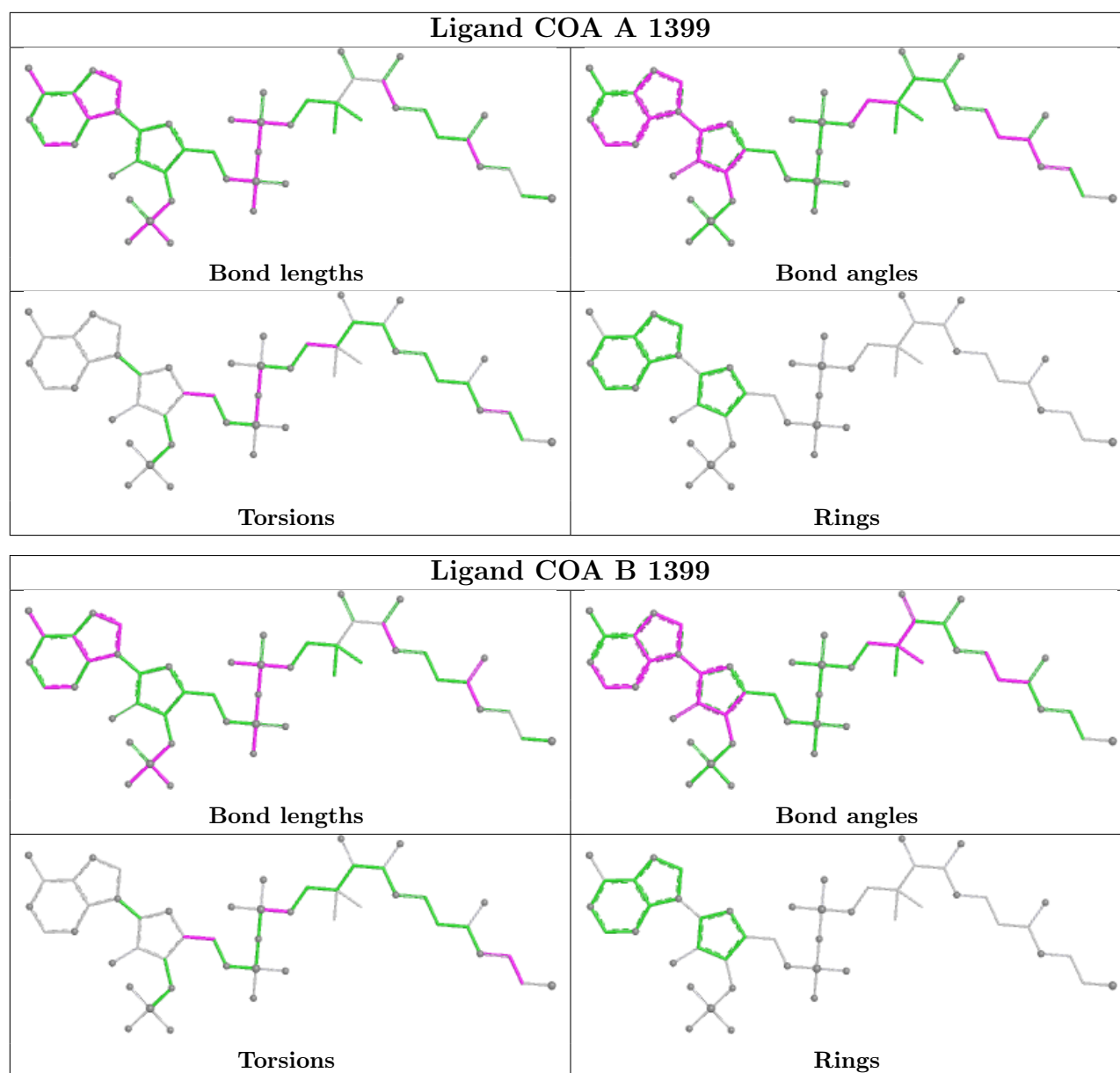
Mol	Chain	Res	Type	Atoms
4	C	1398	DNO	C3-C4-C5-O5
4	C	1397	DNO	C3-C4-C5-O5
4	C	1399	DNO	O4-C4-C5-C6
5	B	1399	COA	C2P-C3P-N4P-C5P
4	A	1398	DNO	C3-C4-C5-O5
5	A	1399	COA	C3B-C4B-C5B-O5B
5	A	1399	COA	P1A-O3A-P2A-O6A
4	C	1397	DNO	O2-C2-C3-C4
4	C	1398	DNO	C1-C2-C3-O3
5	B	1399	COA	CCP-O6A-P2A-O3A
5	B	1399	COA	CCP-O6A-P2A-O4A
5	B	1399	COA	CCP-O6A-P2A-O5A
4	A	1398	DNO	O5-C5-C6-O6
5	A	1399	COA	P2A-O3A-P1A-O2A
5	A	1399	COA	O4B-C4B-C5B-O5B
5	B	1399	COA	O4B-C4B-C5B-O5B
4	C	1398	DNO	O3-C3-C4-C5
5	B	1399	COA	C3B-C4B-C5B-O5B
5	A	1399	COA	P2A-O3A-P1A-O1A

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1397	DNO	1	0
5	A	1399	COA	5	0
5	B	1399	COA	3	0
4	C	1398	DNO	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, 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	388/392 (98%)	-1.32	0	100	100	4, 13, 34, 96	8 (2%)
1	B	388/392 (98%)	-1.34	0	100	100	4, 13, 32, 88	7 (1%)
2	C	389/392 (99%)	0.11	7 (1%)	67	68	18, 50, 79, 108	1 (0%)
2	D	389/392 (99%)	0.35	18 (4%)	37	36	20, 57, 102, 131	0
All	All	1554/1568 (99%)	-0.55	25 (1%)	70	71	4, 34, 81, 131	16 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	303	ALA	3.0
2	C	386	ALA	3.0
2	D	264	ALA	3.0
2	D	391	SER	2.9
2	D	285	PRO	2.9
2	D	332	TRP	2.7
2	D	308	GLY	2.6
2	D	262	ALA	2.6
2	C	110	ILE	2.6
2	C	299	ALA	2.6
2	D	269	ILE	2.5
2	D	108	ALA	2.5
2	C	389	ILE	2.3
2	D	227	SER	2.2
2	C	331	GLY	2.2
2	D	268	GLY	2.2
2	D	303	ALA	2.2
2	D	343	ALA	2.2
2	D	219	ILE	2.1
2	C	305	TRP	2.1
2	D	337	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	231	LEU	2.1
2	D	330	LEU	2.1
2	D	186	ALA	2.1
2	D	226	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSO	A	89	7/8	1.00	0.02	7,9,23,28	0
1	CSO	B	89	7/8	1.00	0.03	2,6,26,28	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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.

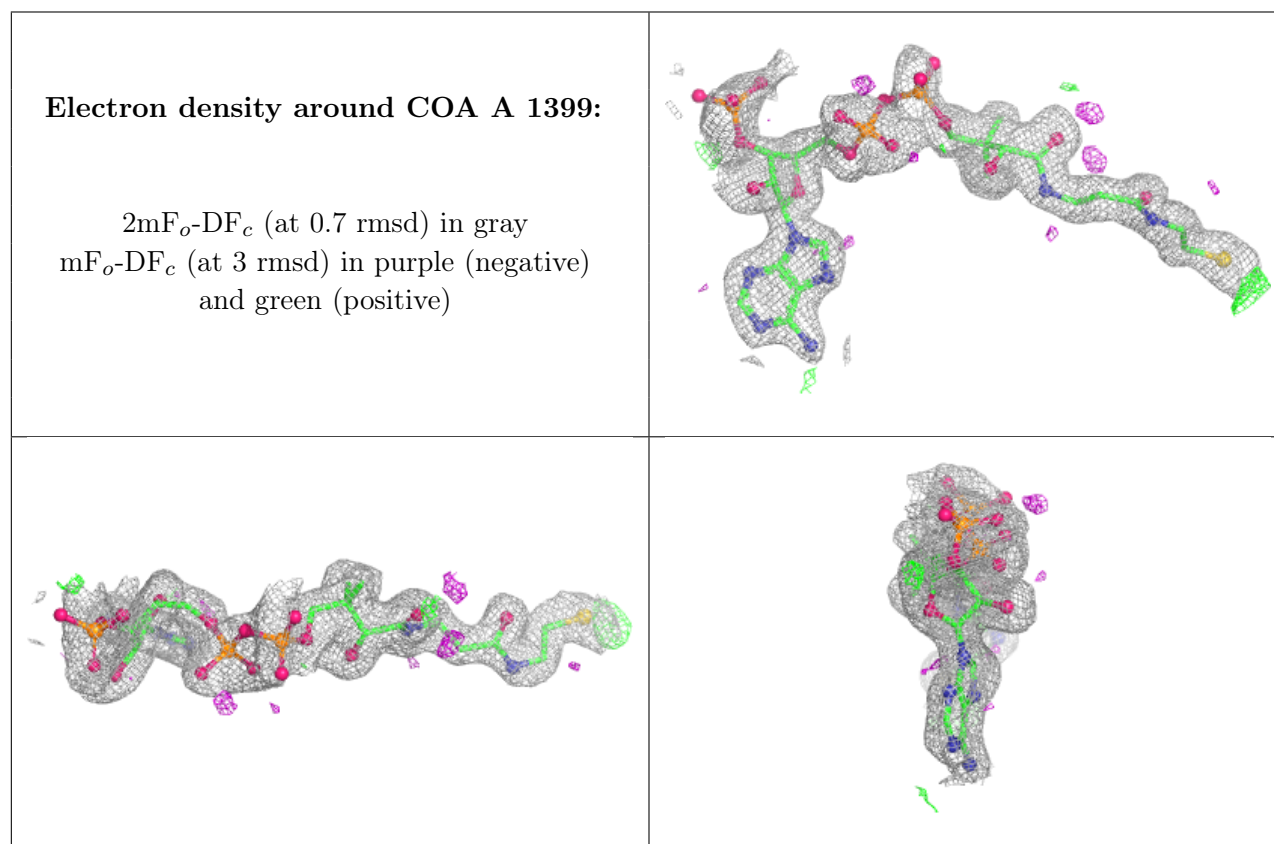
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	1396	5/5	0.94	0.07	64,64,66,66	0
3	SO4	C	1394	5/5	0.95	0.14	129,131,131,131	0
3	SO4	C	1393	5/5	0.96	0.08	75,77,78,79	0
3	SO4	B	1401	5/5	0.96	0.06	89,90,91,92	0
3	SO4	C	1395	5/5	0.96	0.09	81,83,86,87	0
4	DNO	C	1398	12/12	0.96	0.08	57,65,78,79	0
3	SO4	B	1396	5/5	0.97	0.10	77,80,81,82	0
4	DNO	A	1398	12/12	0.97	0.09	42,52,75,76	0
3	SO4	A	1397	5/5	0.97	0.07	72,73,76,77	0
4	DNO	C	1399	12/12	0.97	0.07	42,55,72,72	0
6	NA	B	1398	1/1	0.97	0.16	123,123,123,123	0
4	DNO	C	1397	12/12	0.98	0.06	44,55,91,93	0

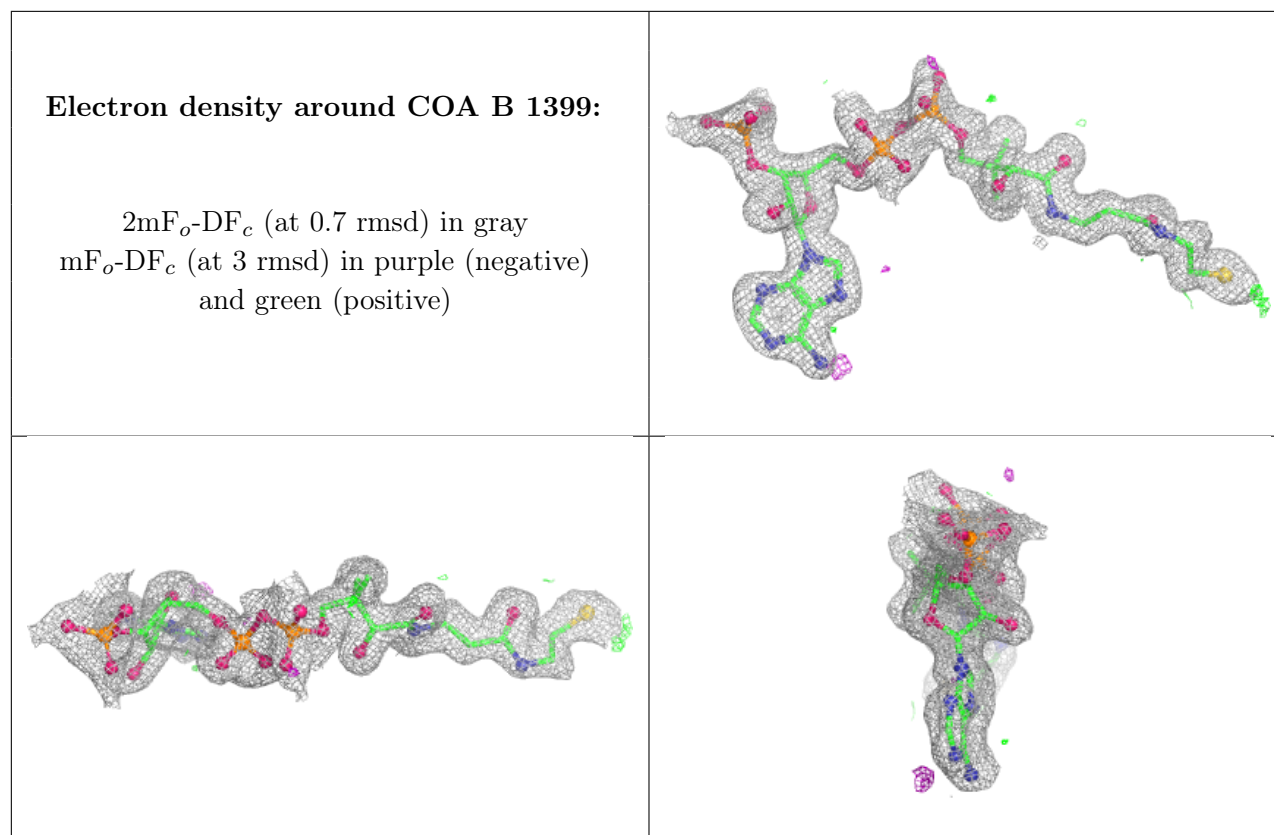
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	1396	5/5	0.98	0.05	64,66,67,71	0
3	SO4	D	1393	5/5	0.98	0.06	61,62,65,67	0
3	SO4	B	1395	5/5	0.98	0.04	41,44,47,48	0
3	SO4	B	1397	5/5	0.99	0.05	71,71,73,77	0
3	SO4	B	1394	5/5	0.99	0.04	30,39,41,43	0
3	SO4	A	1394	5/5	0.99	0.04	40,44,50,56	0
5	COA	A	1399	48/48	0.99	0.04	15,28,76,107	0
5	COA	B	1399	48/48	0.99	0.04	12,27,61,75	0
3	SO4	A	1395	5/5	0.99	0.04	43,50,53,57	0
7	CL	B	1400	1/1	0.99	0.03	68,68,68,68	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 [i](#)

There are no such residues in this entry.