



Full wwPDB X-ray Structure Validation Report

Oct 30, 2014 – 08:29 PM EDT

PDB ID : 2WL4
Title : BIOSYNTHETIC THIOLASE FROM Z. RAMIGERA. COMPLEX OF THE H348A 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

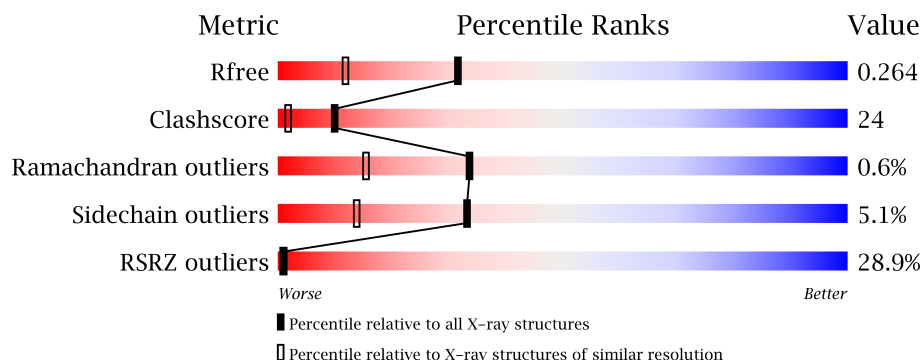
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

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}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	392	
2	B	392	
3	C	392	
4	D	392	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	SO4	A	1395	-	X
5	SO4	A	1397	-	X
5	SO4	A	1398	-	X
5	SO4	A	1399	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	SO4	A	1400	-	X
5	SO4	A	1401	-	X
5	SO4	B	1398	-	X
5	SO4	C	1393	-	X
5	SO4	D	1394	-	X
5	SO4	D	1397	-	X
7	CL	D	1399	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12721 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	5	0
			2837	1765	511	539	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	ALA	SEE REMARK 999	UNP P07097
A	348	ALA	HIS	ENGINEERED MUTATION	UNP P07097

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	389	Total	C	N	O	S	0	7	0
			2843	1770	509	543	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	129	ARG	ALA	SEE REMARK 999	UNP P07097
B	348	ALA	HIS	ENGINEERED MUTATION	UNP P07097

- Molecule 3 is a protein called ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	389	Total	C	N	O	S	0	1	0
			2816	1747	509	539	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	129	ARG	ALA	SEE REMARK 999	UNP P07097
C	348	ALA	HIS	ENGINEERED MUTATION	UNP P07097

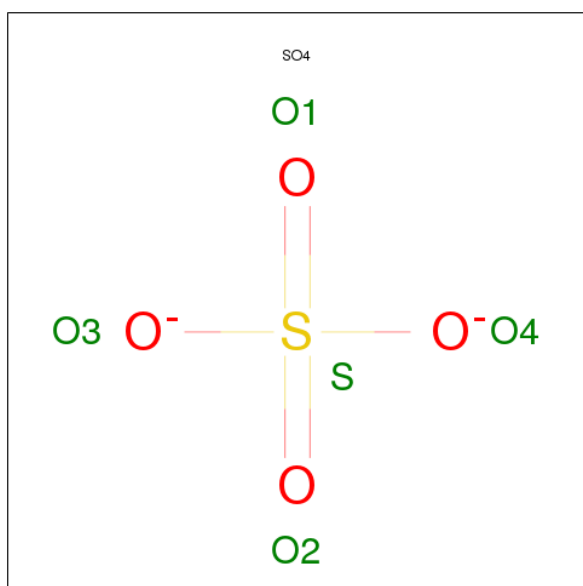
- Molecule 4 is a protein called ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	389	Total	C	N	O	S	0	3	0
			2828	1755	513	539	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	ALA	SEE REMARK 999	UNP P07097
D	348	ALA	HIS	ENGINEERED MUTATION	UNP P07097

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



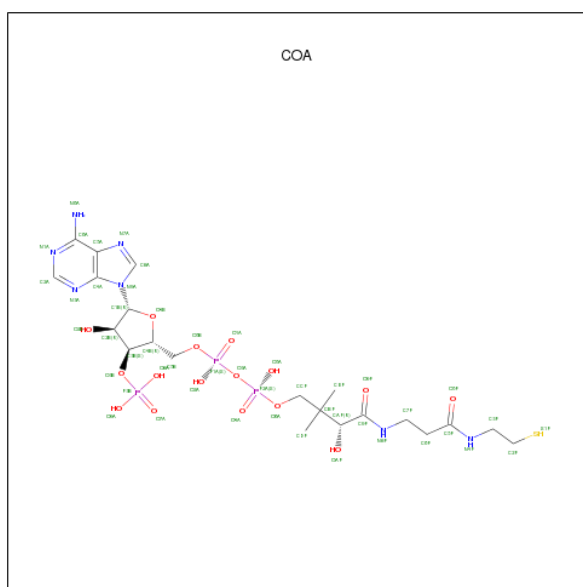
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 6 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
6	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Na	0	0
			1	1		
8	C	2	Total	Na	0	0
			2	2		

- Molecule 9 is water.

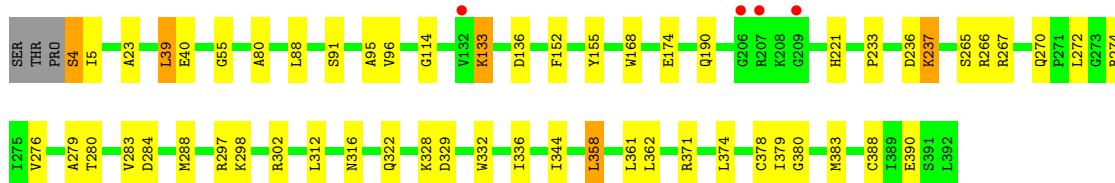
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	426	Total 426	O 426	0	0
9	B	407	Total 407	O 407	0	0
9	C	149	Total 149	O 149	0	0
9	D	188	Total 188	O 188	0	0

3 Residue-property plots

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

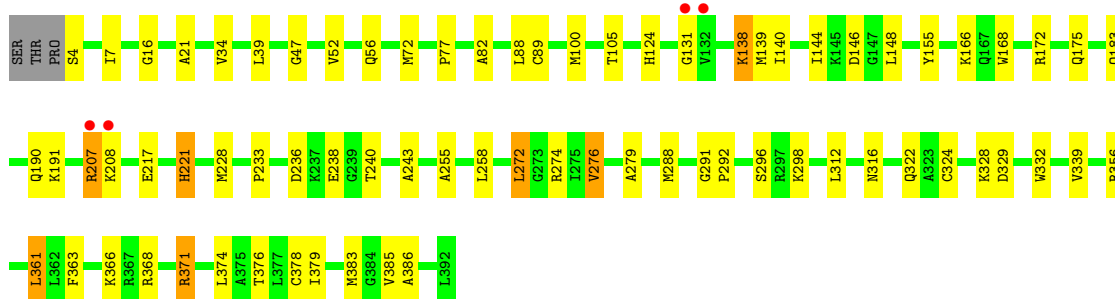
• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

Chain A: 



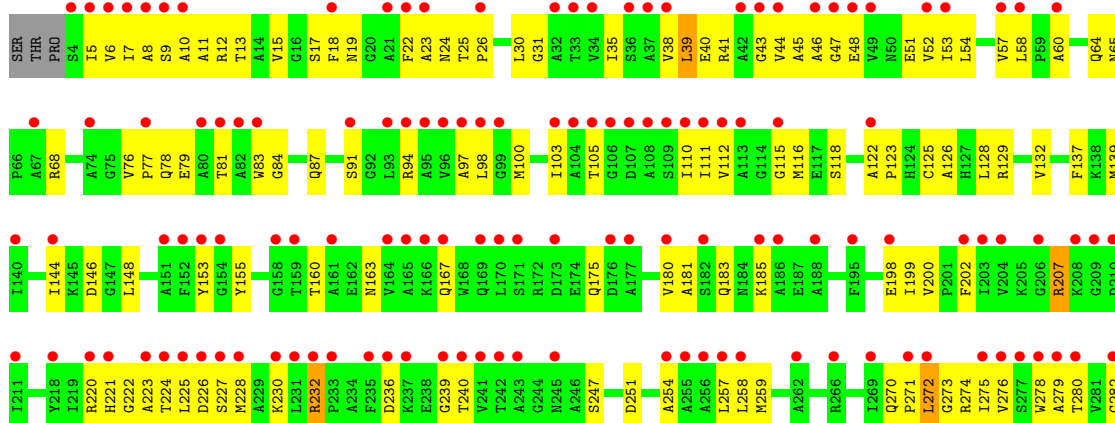
• Molecule 2: ACETYL-COA ACETYLTRANSFERASE

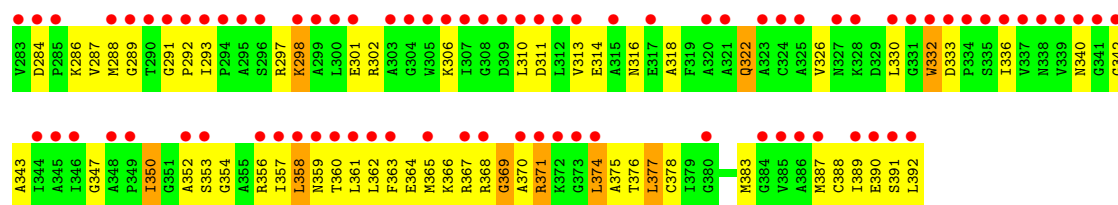
Chain B: 



• Molecule 3: ACETYL-COA ACETYLTRANSFERASE

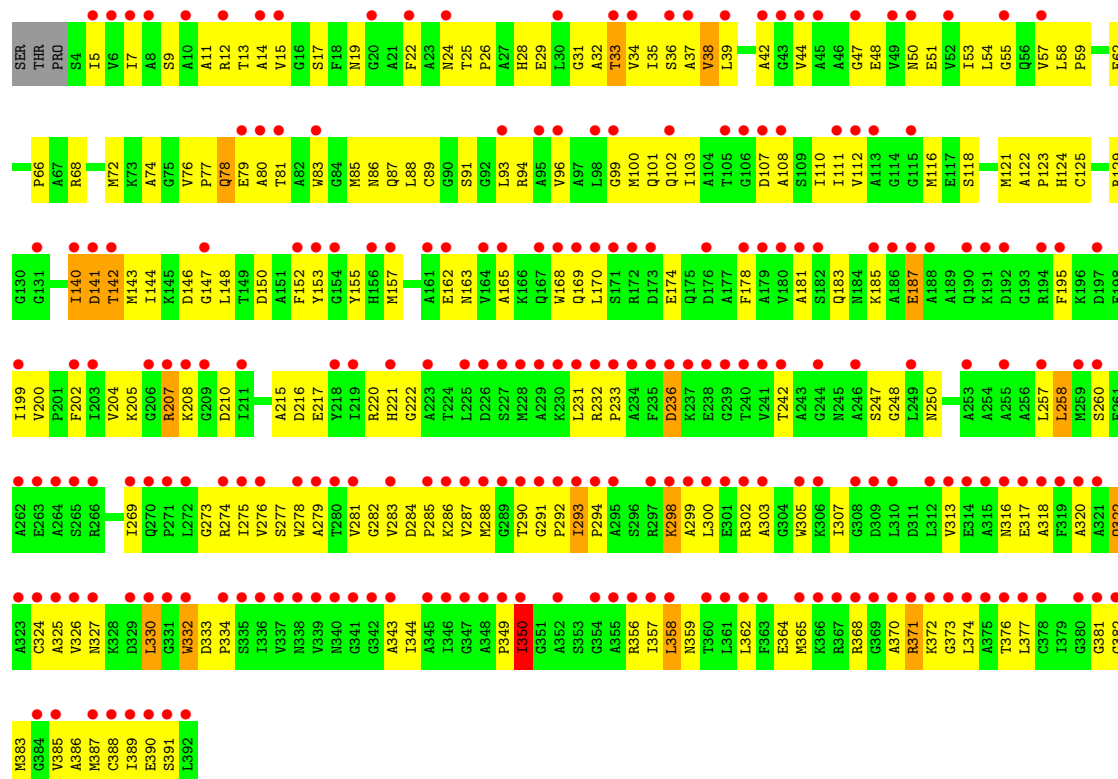
Chain C: 





Molecule 4: ACETYL-COA ACETYLTRANSFERASE

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.31Å 79.14Å 149.41Å 90.00° 92.68° 90.00°	Depositor
Resolution (Å)	19.61 – 1.80 19.61 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.61-1.80) 86.6 (19.61-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 1.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.231 , 0.270 0.223 , 0.264	Depositor DCC
R_{free} test set	9049 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 84.9	EDS
Estimated twinning fraction	0.159 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 181001 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12721	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.50	0/2884	0.64	1/3892 (0.0%)
2	B	0.50	0/2888	0.64	0/3896
3	C	0.25	0/2864	0.45	0/3867
4	D	0.28	0/2869	0.47	0/3870
All	All	0.40	0/11505	0.56	1/15525 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2837	0	2870	54	0
2	B	2843	0	2882	76	0
3	C	2816	0	2825	205	0
4	D	2828	0	2848	230	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	45	0	0	9	0
5	B	40	0	0	2	0
5	C	20	0	0	0	0
5	D	20	0	0	5	0
6	A	48	0	32	1	0
6	B	48	0	32	8	0
7	B	1	0	0	0	0
7	C	1	0	0	6	0
7	D	1	0	0	7	0
8	C	2	0	0	0	0
8	D	1	0	0	0	0
9	A	426	0	0	22	0
9	B	407	0	0	24	0
9	C	149	0	0	39	0
9	D	188	0	0	77	0
All	All	12721	0	11489	551	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (551) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:64:GLN:HG2	4:D:88:LEU:HD11	1.42	1.00
2:B:296:SER:OG	2:B:376[B]:THR:HG21	1.62	0.99
3:C:298:LYS:HE2	3:C:302:ARG:HE	1.24	0.99
4:D:140:ILE:CD1	4:D:141:ASP:H	1.76	0.98
3:C:356:ARG:HH21	3:C:357:ILE:HG22	1.25	0.97
2:B:374:LEU:HD21	2:B:376[B]:THR:HG23	1.46	0.95
4:D:357:ILE:HD11	4:D:377:LEU:HD11	1.51	0.93
3:C:374:LEU:HD22	3:C:375:ALA:H	1.37	0.90
3:C:38:VAL:HA	3:C:41:ARG:HD2	1.56	0.87
2:B:56:GLN:HB2	9:B:2073:HOH:O	1.75	0.86
3:C:146:ASP:HB2	9:C:2063:HOH:O	1.76	0.86
4:D:35:ILE:HG23	4:D:112:VAL:HG11	1.58	0.85
2:B:124:HIS:HD2	9:B:2164:HOH:O	1.60	0.85
4:D:125:CYS:SG	4:D:140:ILE:HD11	2.18	0.84
3:C:207:ARG:HD3	3:C:207:ARG:H	1.42	0.84
2:B:376[B]:THR:HG22	2:B:386:ALA:CB	2.06	0.84
1:A:279:ALA:HA	5:A:1401:SO4:O1	1.77	0.84
3:C:354:GLY:HA2	3:C:377:LEU:HD21	1.57	0.83
2:B:279:ALA:HB1	9:B:2310:HOH:O	1.78	0.82
3:C:207:ARG:HH11	3:C:207:ARG:HG2	1.40	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:376[B]:THR:HG22	2:B:386:ALA:HB2	1.62	0.81
2:B:374:LEU:HD21	2:B:376[B]:THR:CG2	2.10	0.81
1:A:95:ALA:HB3	9:A:2127:HOH:O	1.79	0.81
3:C:7:ILE:HD12	3:C:362:LEU:HD21	1.62	0.81
4:D:344:ILE:HB	9:D:2103:HOH:O	1.81	0.80
1:A:4:SER:HA	9:A:2295:HOH:O	1.81	0.80
2:B:207:ARG:H	2:B:207:ARG:HD3	1.47	0.80
4:D:231:LEU:HB3	9:D:2129:HOH:O	1.81	0.80
4:D:62:GLU:HB3	9:D:2043:HOH:O	1.81	0.80
1:A:23:ALA:HB1	9:A:2023:HOH:O	1.82	0.80
4:D:140:ILE:HD12	4:D:141:ASP:H	1.47	0.80
3:C:100:MET:HG3	3:C:275:ILE:HG21	1.62	0.79
4:D:125:CYS:HB3	7:D:1399:CL:CL	2.20	0.79
3:C:58:LEU:HD22	9:C:2063:HOH:O	1.80	0.79
4:D:140:ILE:HD13	4:D:141:ASP:H	1.47	0.78
4:D:207:ARG:H	4:D:207:ARG:HD3	1.47	0.78
1:A:267:ARG:NH1	9:A:2304:HOH:O	2.16	0.78
3:C:38:VAL:CG1	3:C:257:LEU:HB2	2.13	0.78
3:C:364:GLU:HA	3:C:367:ARG:HG2	1.64	0.78
3:C:298:LYS:HE2	3:C:302:ARG:NE	1.99	0.77
3:C:180:VAL:HG21	3:C:225:LEU:HA	1.65	0.77
3:C:374:LEU:HD22	3:C:375:ALA:N	2.00	0.76
3:C:356:ARG:NH2	3:C:357:ILE:HG22	1.98	0.76
4:D:276:VAL:HG11	4:D:305:TRP:CH2	2.19	0.76
1:A:280:THR:HG22	5:A:1401:SO4:O4	1.84	0.75
4:D:14:ALA:HB1	9:D:2121:HOH:O	1.86	0.75
4:D:316:ASN:OD1	4:D:357:ILE:HD13	1.85	0.75
4:D:273:GLY:HA2	4:D:391:SER:HB3	1.67	0.75
1:A:270:GLN:HG3	9:A:2306:HOH:O	1.86	0.75
3:C:54:LEU:HB3	9:C:2025:HOH:O	1.85	0.75
3:C:105:THR:HG21	4:D:101:GLN:HG2	1.68	0.75
4:D:140:ILE:HD13	4:D:142:THR:H	1.51	0.74
2:B:339:VAL:HG11	2:B:368:ARG:NH2	2.04	0.73
4:D:15:VAL:HG13	9:D:2142:HOH:O	1.88	0.73
3:C:47:GLY:HA2	3:C:77:PRO:HG3	1.69	0.72
4:D:216:ASP:HA	9:D:2121:HOH:O	1.88	0.72
2:B:374:LEU:CD2	2:B:376[B]:THR:HG23	2.18	0.72
3:C:374:LEU:CD2	3:C:375:ALA:H	2.01	0.72
3:C:64:GLN:HG2	4:D:88:LEU:CD1	2.18	0.72
4:D:140:ILE:HD12	4:D:141:ASP:N	2.05	0.72
4:D:282:GLY:HA2	4:D:383:MET:HA	1.72	0.72
2:B:207:ARG:HG2	2:B:208:LYS:H	1.55	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:174:GLU:HB2	9:D:2100:HOH:O	1.88	0.72
4:D:123:PRO:HB2	7:D:1399:CL:CL	2.27	0.72
3:C:125:CYS:HB2	7:D:1399:CL:CL	2.26	0.71
4:D:368:ARG:HG3	9:D:2182:HOH:O	1.89	0.71
3:C:128:LEU:HD21	3:C:137:PHE:CE2	2.25	0.71
2:B:371:ARG:HG3	9:B:2373:HOH:O	1.90	0.71
4:D:42:ALA:HB1	9:D:2031:HOH:O	1.89	0.71
4:D:47:GLY:HA2	4:D:77:PRO:HG2	1.71	0.71
2:B:139:MET:O	9:B:2164:HOH:O	2.08	0.71
2:B:124:HIS:CD2	9:B:2164:HOH:O	2.38	0.70
4:D:162:GLU:HG3	9:D:2132:HOH:O	1.91	0.70
4:D:207:ARG:HD3	4:D:207:ARG:N	2.06	0.70
3:C:279:ALA:HA	9:C:2112:HOH:O	1.92	0.70
3:C:280:THR:HG23	4:D:81:THR:HG21	1.73	0.70
1:A:133:LYS:HB2	9:D:2013:HOH:O	1.91	0.69
4:D:35:ILE:HD12	9:D:2023:HOH:O	1.92	0.69
2:B:339:VAL:HG11	2:B:368:ARG:HH22	1.56	0.69
3:C:310:LEU:HG	9:C:2113:HOH:O	1.93	0.68
3:C:18:PHE:CZ	4:D:129:ARG:HD3	2.29	0.68
3:C:8:ALA:HB3	9:C:2095:HOH:O	1.91	0.68
4:D:326:VAL:HG13	9:D:2150:HOH:O	1.93	0.68
4:D:222:GLY:N	9:D:2127:HOH:O	2.27	0.68
4:D:292:PRO:HB2	9:D:2150:HOH:O	1.94	0.68
4:D:76:VAL:HG23	5:D:1397:SO4:O1	1.94	0.67
9:A:2138:HOH:O	2:B:105:THR:HG22	1.93	0.67
4:D:371:ARG:O	4:D:390:GLU:HA	1.94	0.67
3:C:259:MET:HB2	9:C:2097:HOH:O	1.94	0.67
4:D:207:ARG:HG2	4:D:208:LYS:HG3	1.76	0.67
4:D:299:ALA:HB2	9:D:2152:HOH:O	1.94	0.66
3:C:65:ASN:OD1	9:C:2035:HOH:O	2.13	0.66
3:C:83:TRP:HH2	3:C:98:LEU:HD13	1.59	0.66
4:D:100:MET:HB2	9:D:2061:HOH:O	1.94	0.66
3:C:43:GLY:HA3	9:C:2021:HOH:O	1.95	0.66
1:A:378:CSD:SG	9:A:2343:HOH:O	2.53	0.66
4:D:35:ILE:HB	9:D:2023:HOH:O	1.96	0.65
3:C:68:ARG:CB	7:C:1396:CL:CL	2.81	0.65
1:A:283:VAL:HA	5:A:1400:SO4:O4	1.96	0.65
1:A:280:THR:N	5:A:1401:SO4:O3	2.30	0.65
3:C:302:ARG:NH1	4:D:107:ASP:HA	2.11	0.65
1:A:371:ARG:HG2	9:A:2387:HOH:O	1.95	0.65
3:C:274:ARG:HH21	3:C:392:LEU:HD21	1.62	0.65
3:C:6:VAL:HG13	9:C:2098:HOH:O	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:140:ILE:N	9:D:2083:HOH:O	2.29	0.65
3:C:228:MET:HG3	9:C:2093:HOH:O	1.96	0.64
1:A:302:ARG:NH1	5:A:1401:SO4:O1	2.30	0.64
6:B:1401:COA:H31	9:B:2172:HOH:O	1.95	0.64
3:C:31:GLY:O	3:C:35:ILE:HG13	1.98	0.64
3:C:65:ASN:HB3	7:C:1396:CL:CL	2.35	0.64
2:B:175:GLN:HE22	2:B:240:THR:CG2	2.10	0.64
3:C:60:ALA:HB1	9:C:2029:HOH:O	1.97	0.64
3:C:371:ARG:HA	9:C:2141:HOH:O	1.96	0.64
3:C:38:VAL:HG12	3:C:257:LEU:HB2	1.80	0.64
4:D:298:LYS:HE3	9:D:2153:HOH:O	1.97	0.64
3:C:183:GLN:OE1	3:C:220:ARG:HG2	1.96	0.64
1:A:265:SER:HA	9:A:2298:HOH:O	1.98	0.63
4:D:150:ASP:HB2	9:D:2086:HOH:O	1.98	0.63
4:D:178:PHE:HB2	5:D:1396:SO4:O1	1.98	0.63
4:D:247:SER:HB3	4:D:318:ALA:HA	1.79	0.63
2:B:228:MET:HE1	9:B:2404:HOH:O	1.99	0.63
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.33	0.63
3:C:53:ILE:HG12	3:C:83:TRP:CE2	2.34	0.62
4:D:183:GLN:NE2	4:D:220:ARG:HD3	2.15	0.62
2:B:339:VAL:HG13	9:B:2357:HOH:O	1.99	0.62
3:C:65:ASN:ND2	7:C:1396:CL:CL	2.70	0.62
1:A:316:ASN:HB3	9:A:2343:HOH:O	2.00	0.61
4:D:199:ILE:HD12	9:D:2120:HOH:O	1.99	0.61
3:C:374:LEU:HD21	3:C:387:MET:O	1.99	0.61
3:C:362:LEU:HD12	9:C:2132:HOH:O	2.00	0.61
1:A:279:ALA:HB1	1:A:298:LYS:HD3	1.83	0.61
3:C:333:ASP:O	3:C:336:ILE:HG12	2.01	0.61
4:D:51:GLU:HB3	4:D:111:ILE:CD1	2.30	0.61
2:B:207:ARG:HG2	2:B:208:LYS:N	2.14	0.61
3:C:51:GLU:HA	3:C:81:THR:O	2.01	0.61
4:D:142:THR:O	4:D:146:ASP:HB2	2.00	0.61
4:D:232:ARG:HH11	4:D:232:ARG:HB2	1.66	0.61
4:D:305:TRP:CZ3	4:D:388:CYS:HB3	2.36	0.61
2:B:139:MET:HG3	3:C:139:MET:HE2	1.81	0.61
2:B:166:LYS:HG3	9:B:2187:HOH:O	2.00	0.61
4:D:232:ARG:NH1	4:D:232:ARG:HB2	2.15	0.60
4:D:110:ILE:HG23	4:D:257:LEU:HD21	1.84	0.60
3:C:232:ARG:H	3:C:232:ARG:NE	1.99	0.60
3:C:5:ILE:HG13	3:C:100:MET:HG2	1.83	0.60
3:C:52:VAL:HG13	3:C:112:VAL:HG12	1.82	0.60
4:D:269:ILE:HD13	9:D:2031:HOH:O	2.02	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:279:ALA:HB3	9:D:2152:HOH:O	2.01	0.60
2:B:89:CSO:HD	6:B:1401:COA:H22	1.67	0.60
3:C:293:ILE:HA	3:C:330:LEU:HD21	1.83	0.60
2:B:376[A]:THR:HG23	2:B:385:VAL:O	2.01	0.59
3:C:358:LEU:HD22	3:C:362:LEU:HG	1.83	0.59
3:C:144:ILE:HD13	3:C:148:LEU:HD12	1.81	0.59
4:D:57:VAL:C	4:D:59:PRO:HD3	2.23	0.59
4:D:168:TRP:HB3	9:D:2099:HOH:O	2.01	0.59
3:C:200:VAL:HG13	9:C:2080:HOH:O	2.00	0.59
4:D:250:ASN:HB3	9:D:2142:HOH:O	2.02	0.59
1:A:312:LEU:HD23	1:A:361:LEU:HD12	1.84	0.59
2:B:207:ARG:HD3	2:B:207:ARG:N	2.15	0.59
4:D:12:ARG:HH22	4:D:199:ILE:HD11	1.68	0.59
3:C:316:ASN:ND2	3:C:377:LEU:HD23	2.18	0.59
4:D:140:ILE:CD1	4:D:141:ASP:N	2.54	0.58
1:A:284:ASP:OD2	9:A:2312:HOH:O	2.17	0.58
3:C:57:VAL:HG12	3:C:58:LEU:HD23	1.86	0.58
4:D:140:ILE:HD12	9:D:2083:HOH:O	2.02	0.58
1:A:371:ARG:HD2	9:A:2381:HOH:O	2.03	0.58
4:D:275:ILE:CD1	9:D:2061:HOH:O	2.52	0.58
4:D:277:SER:HB3	4:D:303:ALA:HB2	1.85	0.58
4:D:94:ARG:NH2	9:D:2059:HOH:O	2.36	0.58
3:C:153:TYR:HB3	3:C:155:TYR:CE2	2.38	0.58
2:B:221:HIS:HD2	9:B:2220:HOH:O	1.86	0.58
2:B:374:LEU:HD21	2:B:376[A]:THR:OG1	2.04	0.58
4:D:274:ARG:HB3	4:D:390:GLU:O	2.02	0.58
2:B:16:GLY:HA2	9:B:2261:HOH:O	2.04	0.58
4:D:258:LEU:HD12	9:D:2007:HOH:O	2.04	0.57
3:C:274:ARG:NH2	3:C:392:LEU:HD21	2.19	0.57
3:C:87:GLN:N	3:C:91:SER:OG	2.37	0.57
4:D:50:ASN:HB2	4:D:110:ILE:O	2.04	0.57
4:D:242:THR:HB	9:D:2129:HOH:O	2.04	0.57
3:C:83:TRP:CH2	3:C:98:LEU:HD13	2.40	0.57
4:D:96:VAL:HG12	9:D:2061:HOH:O	2.04	0.57
3:C:68:ARG:HG3	4:D:152:PHE:HZ	1.70	0.57
2:B:363:PHE:CD1	2:B:366[A]:LYS:NZ	2.72	0.57
3:C:116:MET:HG2	9:C:2025:HOH:O	2.04	0.57
3:C:272:LEU:HD12	3:C:366:LYS:HD2	1.87	0.57
3:C:125:CYS:CB	7:D:1399:CL:CL	2.90	0.57
9:C:2029:HOH:O	4:D:125:CYS:SG	2.54	0.57
4:D:96:VAL:O	9:D:2061:HOH:O	2.18	0.57
2:B:243:ALA:HB1	6:B:1401:COA:O2A	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:9:SER:OG	4:D:42:ALA:HB2	2.05	0.56
4:D:141:ASP:O	4:D:143:MET:N	2.31	0.56
4:D:287:VAL:HB	4:D:290:THR:HG23	1.87	0.56
4:D:80:ALA:HB2	9:D:2033:HOH:O	2.05	0.56
3:C:342:GLY:HA3	9:C:2116:HOH:O	2.03	0.56
3:C:180:VAL:HG13	3:C:223:ALA:O	2.06	0.56
3:C:353:SER:O	3:C:357:ILE:HG23	2.06	0.56
2:B:183:GLN:HG3	9:B:2404:HOH:O	2.06	0.56
3:C:316:ASN:HB2	3:C:377:LEU:HA	1.88	0.56
4:D:349:PRO:HG3	9:D:2142:HOH:O	2.06	0.56
2:B:100:MET:SD	5:B:1398:SO4:O4	2.64	0.56
4:D:51:GLU:HB3	4:D:111:ILE:HD12	1.88	0.56
4:D:44:VAL:HG13	4:D:48:GLU:OE1	2.06	0.56
2:B:175:GLN:HE22	2:B:240:THR:HG21	1.71	0.56
3:C:276:VAL:HG22	3:C:388:CYS:HB3	1.88	0.56
4:D:165:ALA:HA	4:D:170:LEU:HD12	1.88	0.56
4:D:305:TRP:CE2	4:D:372:LYS:HD3	2.40	0.56
1:A:114:GLY:HA2	9:A:2127:HOH:O	2.05	0.55
3:C:110:ILE:HG23	3:C:257:LEU:HD21	1.89	0.55
3:C:330:LEU:HD13	3:C:332:TRP:CZ2	2.42	0.55
4:D:35:ILE:HG23	4:D:112:VAL:HG21	1.89	0.55
4:D:298:LYS:HB3	9:D:2153:HOH:O	2.06	0.55
2:B:316:ASN:HB3	9:B:2381:HOH:O	2.05	0.55
3:C:146:ASP:HB3	5:D:1394:SO4:O1	2.07	0.55
4:D:327:ASN:HB3	9:D:2165:HOH:O	2.05	0.55
3:C:272:LEU:CD1	3:C:366:LYS:HD2	2.37	0.55
3:C:314:GLU:O	3:C:375:ALA:HA	2.07	0.54
2:B:34:VAL:HG12	2:B:255:ALA:HB3	1.90	0.54
4:D:85:MET:HG3	9:D:2039:HOH:O	2.06	0.54
4:D:283:VAL:HG11	4:D:290:THR:O	2.06	0.54
3:C:306:LYS:HB3	9:C:2114:HOH:O	2.07	0.54
3:C:340[C]:ASN:HD21	3:C:360:THR:HG23	1.73	0.54
3:C:100:MET:HG3	3:C:275:ILE:CG2	2.36	0.54
1:A:174:GLU:HG3	9:A:2210:HOH:O	2.07	0.54
4:D:34:VAL:O	4:D:38:VAL:HG13	2.07	0.54
2:B:21:ALA:HB3	9:B:2261:HOH:O	2.08	0.54
4:D:357:ILE:HD11	4:D:377:LEU:CD1	2.31	0.54
1:A:298:LYS:HE2	1:A:302:ARG:NH2	2.23	0.53
3:C:230:LYS:HA	9:C:2094:HOH:O	2.07	0.53
4:D:187:GLU:HG3	9:D:2127:HOH:O	2.07	0.53
4:D:204:VAL:HB	9:D:2119:HOH:O	2.07	0.53
4:D:236:ASP:HB2	9:D:2132:HOH:O	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:7:ILE:HD13	4:D:362:LEU:HD11	1.89	0.53
1:A:266:ARG:NH2	5:A:1394:SO4:O1	2.39	0.53
6:A:1402:COA:H141	6:A:1402:COA:O9P	2.07	0.53
3:C:11:ALA:HB3	3:C:38:VAL:HG23	1.89	0.53
4:D:215:ALA:HA	9:D:2120:HOH:O	2.08	0.53
4:D:316:ASN:OD1	4:D:357:ILE:HG21	2.07	0.53
6:B:1401:COA:H122	6:B:1401:COA:O2A	2.09	0.53
2:B:207:ARG:HH11	2:B:207:ARG:N	2.06	0.53
3:C:68:ARG:HB3	7:C:1396:CL:CL	2.46	0.53
4:D:178:PHE:HE1	4:D:317:GLU:CD	2.12	0.53
4:D:300:LEU:HD13	4:D:307:ILE:HG13	1.90	0.53
4:D:93:LEU:HD23	4:D:385:VAL:HG13	1.91	0.53
4:D:169:GLN:HG3	9:D:2095:HOH:O	2.09	0.52
3:C:207:ARG:HH11	3:C:207:ARG:CG	2.15	0.52
4:D:103:ILE:HG23	4:D:108:ALA:O	2.09	0.52
4:D:35:ILE:HG12	4:D:112:VAL:HG11	1.91	0.52
2:B:324:CYS:O	2:B:328:LYS:HG3	2.09	0.52
4:D:35:ILE:O	4:D:39:LEU:HD23	2.09	0.52
1:A:297:ARG:NE	9:A:2319:HOH:O	2.43	0.52
2:B:316:ASN:ND2	9:B:2335:HOH:O	2.42	0.52
3:C:25:THR:HG21	3:C:30:LEU:HD21	1.91	0.52
3:C:302:ARG:NH1	9:C:2112:HOH:O	2.42	0.52
4:D:281:VAL:HG13	9:D:2151:HOH:O	2.09	0.52
4:D:300:LEU:HD13	4:D:307:ILE:CD1	2.40	0.52
4:D:274:ARG:H	4:D:389:ILE:HG23	1.74	0.52
2:B:146:ASP:HB3	9:B:2076:HOH:O	2.09	0.52
3:C:284:ASP:HA	9:D:2055:HOH:O	2.10	0.52
3:C:322:GLN:O	3:C:326:VAL:HG23	2.10	0.52
4:D:163:ASN:HD22	4:D:286:LYS:HB3	1.75	0.52
2:B:274:ARG:NH2	9:B:2307:HOH:O	2.43	0.52
3:C:247:SER:HB2	3:C:318:ALA:O	2.10	0.52
3:C:44:VAL:HG13	3:C:48:GLU:HB2	1.92	0.52
4:D:349:PRO:O	4:D:350:ILE:C	2.48	0.52
3:C:232:ARG:H	3:C:232:ARG:HE	1.57	0.51
4:D:216:ASP:CA	9:D:2121:HOH:O	2.53	0.51
4:D:44:VAL:HG23	9:D:2031:HOH:O	2.10	0.51
2:B:356:ARG:HD2	2:B:356:ARG:C	2.31	0.51
2:B:312:LEU:HD23	2:B:361:LEU:HD22	1.91	0.51
3:C:377:LEU:HD22	9:C:2044:HOH:O	2.09	0.51
3:C:97:ALA:HA	3:C:387:MET:CE	2.41	0.51
4:D:293:ILE:HB	4:D:294:PRO:HD3	1.91	0.51
3:C:39:LEU:HD21	3:C:46:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:381:GLY:N	9:D:2088:HOH:O	2.43	0.51
1:A:96:VAL:HG23	9:A:2127:HOH:O	2.10	0.51
4:D:200:VAL:HG22	9:D:2114:HOH:O	2.10	0.51
3:C:97:ALA:HA	3:C:387:MET:HE1	1.91	0.51
4:D:247:SER:HA	4:D:344:ILE:HA	1.92	0.51
4:D:144:ILE:HA	4:D:148:LEU:HB2	1.93	0.51
4:D:93:LEU:HD11	4:D:387:MET:HB3	1.93	0.51
4:D:33:THR:HG21	4:D:202:PHE:HD1	1.76	0.51
3:C:163:ASN:O	3:C:167:GLN:HB2	2.10	0.50
3:C:330:LEU:HD13	3:C:332:TRP:CH2	2.46	0.50
4:D:275:ILE:HD12	9:D:2004:HOH:O	2.11	0.50
4:D:364:GLU:OE2	4:D:368:ARG:HG2	2.11	0.50
4:D:47:GLY:HA2	4:D:77:PRO:CG	2.38	0.50
4:D:99:GLY:O	4:D:103:ILE:HD12	2.11	0.50
2:B:190:GLN:OE1	2:B:221:HIS:HE1	1.94	0.50
3:C:51:GLU:OE2	3:C:83:TRP:CD1	2.65	0.50
4:D:55:GLY:HA3	4:D:91[B]:SER:OG	2.11	0.50
1:A:133:LYS:HD3	1:A:133:LYS:H	1.77	0.50
4:D:153:TYR:HB3	4:D:155:TYR:CE2	2.47	0.50
3:C:12:ARG:HB2	3:C:254:ALA:HB2	1.94	0.50
3:C:81:THR:HG23	4:D:383:MET:SD	2.51	0.50
4:D:66:PRO:HB2	4:D:116:MET:HE3	1.94	0.50
4:D:87:GLN:OE1	4:D:94:ARG:HG2	2.12	0.50
3:C:128:LEU:HD12	4:D:124:HIS:HB2	1.94	0.49
4:D:32:ALA:HA	9:D:2023:HOH:O	2.12	0.49
4:D:371:ARG:HD3	4:D:371:ARG:N	2.27	0.49
4:D:386:ALA:HB3	9:D:2152:HOH:O	2.11	0.49
3:C:374:LEU:CD2	3:C:375:ALA:N	2.69	0.49
3:C:365:MET:HE2	3:C:391:SER:H	1.77	0.49
4:D:140:ILE:O	4:D:141:ASP:HB2	2.12	0.49
1:A:274:ARG:NH2	1:A:390:GLU:OE1	2.45	0.49
2:B:47:GLY:HA2	2:B:77:PRO:CG	2.42	0.49
3:C:227:SER:HA	3:C:230:LYS:HE3	1.94	0.49
4:D:317:GLU:O	4:D:344:ILE:HG13	2.12	0.49
4:D:305:TRP:HZ3	4:D:388:CYS:HB3	1.75	0.49
1:A:80:ALA:HB2	9:A:2064:HOH:O	2.13	0.49
3:C:207:ARG:NH1	3:C:207:ARG:HG2	2.18	0.49
3:C:153:TYR:CE1	3:C:286:LYS:HG3	2.48	0.49
3:C:6:VAL:HB	3:C:271:PRO:HB3	1.94	0.49
2:B:148:LEU:HD23	9:B:2172:HOH:O	2.12	0.49
3:C:84:GLY:N	9:C:2035:HOH:O	2.41	0.49
4:D:387:MET:HG2	4:D:389:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:9:SER:OG	3:C:38:VAL:HG13	2.12	0.49
4:D:248:GLY:HA2	9:D:2138:HOH:O	2.12	0.49
4:D:26:PRO:HD2	4:D:29:GLU:OE1	2.13	0.49
3:C:183:GLN:CD	3:C:220:ARG:HG2	2.33	0.49
3:C:7:ILE:HD13	3:C:362:LEU:HD11	1.93	0.49
1:A:298:LYS:NZ	5:A:1401:SO4:O2	2.46	0.48
1:A:40:GLU:HG3	9:A:2045:HOH:O	2.13	0.48
3:C:22:PHE:HB3	3:C:25:THR:HB	1.95	0.48
3:C:387:MET:CG	3:C:388:CYS:N	2.76	0.48
1:A:4:SER:C	1:A:5:ILE:HD12	2.33	0.48
2:B:379:ILE:HB	2:B:383:MET:HB2	1.95	0.48
4:D:183:GLN:OE1	4:D:220:ARG:HG2	2.13	0.48
1:A:276:VAL:HG22	1:A:388:CYS:HB2	1.96	0.48
3:C:316:ASN:CG	3:C:377:LEU:HD23	2.34	0.48
3:C:358:LEU:CD2	3:C:362:LEU:HG	2.44	0.48
3:C:387:MET:CG	3:C:388:CYS:H	2.25	0.48
3:C:78:GLN:HG3	3:C:79:GLU:OE2	2.14	0.48
2:B:191[A]:LYS:NZ	2:B:191[A]:LYS:HB3	2.29	0.48
3:C:17:SER:HB3	9:C:2008:HOH:O	2.13	0.48
3:C:313:VAL:HA	3:C:374:LEU:O	2.14	0.48
4:D:283:VAL:CG1	4:D:294:PRO:HG2	2.43	0.48
2:B:376[B]:THR:HG22	2:B:386:ALA:HB1	1.91	0.48
3:C:369:GLY:HA3	9:C:2138:HOH:O	2.13	0.48
3:C:78:GLN:NE2	4:D:285:PRO:HD3	2.28	0.48
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.77	0.47
3:C:278:TRP:HA	3:C:387:MET:HA	1.94	0.47
3:C:7:ILE:HG12	3:C:258:LEU:HD11	1.96	0.47
4:D:12:ARG:NH1	4:D:13:THR:O	2.47	0.47
4:D:207:ARG:NH1	4:D:208:LYS:H	2.11	0.47
3:C:284:ASP:HB3	3:C:287:VAL:HG22	1.96	0.47
4:D:284:ASP:OD1	4:D:286:LYS:HB2	2.14	0.47
3:C:291:GLY:HA3	3:C:383:MET:O	2.14	0.47
3:C:354:GLY:HA3	9:C:2044:HOH:O	2.15	0.47
3:C:68:ARG:HB2	7:C:1396:CL:CL	2.52	0.47
4:D:35:ILE:CG2	4:D:112:VAL:HG11	2.38	0.47
4:D:326:VAL:O	4:D:330:LEU:HB2	2.14	0.47
4:D:53:ILE:HD13	4:D:83:TRP:CZ2	2.50	0.47
3:C:123:PRO:HD2	9:C:2026:HOH:O	2.15	0.47
4:D:19:ASN:N	4:D:19:ASN:HD22	2.13	0.47
3:C:132:VAL:HG21	3:C:137:PHE:CD1	2.50	0.47
3:C:236:ASP:HB3	3:C:239:GLY:HA3	1.97	0.47
3:C:257:LEU:HD22	9:C:2095:HOH:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:328:LYS:HB2	1:A:328:LYS:HE3	1.58	0.46
3:C:19:ASN:C	3:C:23:ALA:HB2	2.36	0.46
3:C:289:GLY:O	3:C:292:PRO:HD2	2.16	0.46
3:C:115:GLY:HA3	3:C:352:ALA:HA	1.96	0.46
2:B:190:GLN:OE1	2:B:221:HIS:CE1	2.68	0.46
3:C:357:ILE:CD1	3:C:375:ALA:HB1	2.45	0.46
4:D:170:LEU:HD21	9:D:2099:HOH:O	2.15	0.46
4:D:388:CYS:C	4:D:389:ILE:HD12	2.35	0.46
1:A:237:LYS:HE2	9:A:2282:HOH:O	2.14	0.46
2:B:172:ARG:HA	2:B:240:THR:OG1	2.15	0.46
4:D:385:VAL:HB	9:D:2056:HOH:O	2.16	0.46
4:D:358:LEU:HD22	4:D:362:LEU:HG	1.98	0.46
4:D:74:ALA:HB2	9:D:2023:HOH:O	2.15	0.46
1:A:298:LYS:HE2	1:A:302:ARG:CZ	2.46	0.46
3:C:129:ARG:CZ	9:C:2056:HOH:O	2.62	0.46
3:C:371:ARG:O	3:C:390:GLU:HA	2.15	0.46
4:D:283:VAL:N	4:D:382:GLY:O	2.46	0.46
1:A:133:LYS:H	1:A:133:LYS:CD	2.28	0.46
2:B:168:TRP:CH2	2:B:329:ASP:HB2	2.51	0.46
2:B:89:CSO:HD	6:B:1401:COA:C2P	2.27	0.46
3:C:198:GLU:HG3	3:C:199:ILE:N	2.31	0.46
4:D:302:ARG:HG3	9:D:2153:HOH:O	2.15	0.46
4:D:141:ASP:OD1	4:D:143:MET:HB3	2.16	0.46
4:D:181:ALA:O	4:D:185:LYS:HG3	2.16	0.46
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.70	0.45
2:B:276:VAL:O	5:B:1398:SO4:O2	2.33	0.45
2:B:298:LYS:HG2	9:B:2310:HOH:O	2.16	0.45
4:D:123:PRO:C	7:D:1399:CL:CL	2.91	0.45
3:C:13:THR:HA	9:C:2080:HOH:O	2.16	0.45
3:C:103:ILE:HD13	3:C:259:MET:HA	1.98	0.45
4:D:368:ARG:HB3	9:D:2179:HOH:O	2.16	0.45
3:C:94:ARG:HH22	4:D:51:GLU:CD	2.20	0.45
3:C:202:PHE:HD1	9:C:2014:HOH:O	2.00	0.45
3:C:45:ALA:HB3	3:C:48:GLU:OE1	2.16	0.45
3:C:129:ARG:HD2	9:D:2068:HOH:O	2.17	0.45
4:D:140:ILE:HD13	4:D:142:THR:N	2.28	0.45
4:D:66:PRO:CG	9:D:2043:HOH:O	2.64	0.45
3:C:316:ASN:OD1	3:C:357:ILE:HG21	2.17	0.45
2:B:236:ASP:OD1	2:B:238:GLU:HG2	2.17	0.45
3:C:316:ASN:OD1	3:C:377:LEU:HD23	2.17	0.45
4:D:292:PRO:HB3	4:D:376:THR:OG1	2.16	0.45
4:D:59:PRO:HB2	5:D:1394:SO4:O3	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:122:ALA:HA	9:C:2026:HOH:O	2.15	0.45
3:C:356:ARG:NH1	9:C:2133:HOH:O	2.49	0.45
3:C:87:GLN:HG3	9:D:2046:HOH:O	2.17	0.45
3:C:146:ASP:HB3	5:D:1394:SO4:S	2.57	0.45
3:C:38:VAL:HG11	3:C:257:LEU:N	2.30	0.45
3:C:83:TRP:HA	9:C:2035:HOH:O	2.17	0.45
4:D:233:PRO:HB2	4:D:236:ASP:O	2.16	0.45
4:D:58:LEU:N	4:D:59:PRO:HD3	2.31	0.45
2:B:378:CSD:OD1	6:B:1401:COA:S1P	2.71	0.45
2:B:4:SER:HB3	9:B:2394:HOH:O	2.17	0.45
3:C:298:LYS:HE3	3:C:301:GLU:OE1	2.17	0.45
3:C:364:GLU:OE1	3:C:367:ARG:HD2	2.17	0.45
3:C:54:LEU:N	9:C:2024:HOH:O	2.49	0.45
4:D:124:HIS:C	7:D:1399:CL:CL	2.92	0.45
4:D:278:TRP:HH2	9:D:2059:HOH:O	1.99	0.45
3:C:207:ARG:HG2	9:C:2086:HOH:O	2.17	0.45
2:B:89:CSO:SG	9:B:2376:HOH:O	2.62	0.44
3:C:79:GLU:O	4:D:281:VAL:HG23	2.17	0.44
4:D:293:ILE:CB	4:D:294:PRO:HD3	2.47	0.44
4:D:365:MET:HE2	4:D:370:ALA:O	2.17	0.44
3:C:10:ALA:HB3	3:C:363:PHE:CE2	2.52	0.44
3:C:311:ASP:HB2	3:C:370:ALA:HB1	1.99	0.44
3:C:76:VAL:HG13	3:C:77:PRO:HD2	1.98	0.44
2:B:144:ILE:HD13	2:B:148:LEU:HD12	1.98	0.44
4:D:275:ILE:HD13	9:D:2061:HOH:O	2.15	0.44
1:A:280:THR:O	5:A:1401:SO4:O3	2.34	0.44
2:B:89:CSO:OD	6:B:1401:COA:H22	2.17	0.44
3:C:207:ARG:NH1	3:C:207:ARG:CG	2.77	0.44
3:C:316:ASN:HD21	3:C:377:LEU:HD23	1.82	0.44
3:C:273:GLY:HA2	3:C:391:SER:HA	2.00	0.44
3:C:48:GLU:N	3:C:48:GLU:OE1	2.51	0.44
4:D:140:ILE:C	9:D:2083:HOH:O	2.55	0.44
4:D:147:GLY:O	4:D:148:LEU:HD23	2.17	0.44
4:D:334:PRO:HD3	9:D:2165:HOH:O	2.16	0.44
4:D:96:VAL:HG21	4:D:358:LEU:HD12	2.00	0.44
4:D:88:LEU:HD23	4:D:88:LEU:HA	1.86	0.44
1:A:379:ILE:HB	1:A:383:MET:HB2	2.00	0.44
3:C:274:ARG:O	3:C:389:ILE:HA	2.18	0.44
4:D:140:ILE:CA	9:D:2083:HOH:O	2.66	0.44
4:D:298:LYS:HD2	9:D:2154:HOH:O	2.17	0.44
4:D:343:ALA:O	4:D:344:ILE:C	2.55	0.44
3:C:374:LEU:CD2	3:C:387:MET:O	2.66	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:287:VAL:HB	4:D:290:THR:CG2	2.48	0.44
4:D:291:GLY:N	4:D:292:PRO:CD	2.81	0.44
3:C:118:SER:HB2	9:C:2050:HOH:O	2.17	0.44
3:C:207:ARG:HD3	3:C:207:ARG:N	2.21	0.44
4:D:123:PRO:CB	7:D:1399:CL:CL	3.00	0.44
4:D:370:ALA:N	9:D:2182:HOH:O	2.50	0.44
1:A:233:PRO:HB2	1:A:236:ASP:O	2.17	0.43
3:C:343:ALA:N	9:C:2116:HOH:O	2.50	0.43
1:A:136:ASP:OD1	4:D:140:ILE:HA	2.18	0.43
3:C:47:GLY:HA2	3:C:77:PRO:CG	2.45	0.43
3:C:57:VAL:HG21	3:C:350:ILE:CG2	2.47	0.43
4:D:66:PRO:HD2	9:D:2048:HOH:O	2.18	0.43
3:C:126:ALA:O	3:C:128:LEU:HG	2.18	0.43
4:D:291:GLY:O	4:D:294:PRO:HD2	2.18	0.43
4:D:300:LEU:CD1	4:D:307:ILE:HG13	2.48	0.43
3:C:129:ARG:NH2	4:D:122:ALA:O	2.40	0.43
2:B:378:CSD:SG	9:B:2381:HOH:O	2.62	0.43
2:B:207:ARG:HG2	2:B:208:LYS:HG2	2.00	0.43
3:C:364:GLU:O	3:C:368:ARG:HG2	2.19	0.43
4:D:326:VAL:CG1	4:D:332:TRP:HZ2	2.32	0.43
4:D:33:THR:O	4:D:37:ALA:HB2	2.19	0.43
3:C:270:GLN:HA	3:C:271:PRO:HD3	1.86	0.43
3:C:220:ARG:O	3:C:222:GLY:N	2.52	0.43
4:D:293:ILE:O	4:D:330:LEU:HD21	2.18	0.43
2:B:291:GLY:N	2:B:292:PRO:CD	2.81	0.43
3:C:282:GLY:HA2	3:C:383:MET:HA	2.00	0.43
4:D:22:PHE:HB3	4:D:25:THR:HB	2.01	0.43
1:A:336:ILE:HA	9:A:2376:HOH:O	2.18	0.42
1:A:374:LEU:HD23	1:A:374:LEU:C	2.39	0.42
3:C:7:ILE:HG21	3:C:362:LEU:CD1	2.49	0.42
4:D:38:VAL:HG23	4:D:257:LEU:HB2	2.01	0.42
4:D:195:PHE:HB2	9:D:2110:HOH:O	2.19	0.42
2:B:138:LYS:HD3	2:B:140:ILE:HD11	2.01	0.42
1:A:152:PHE:CZ	2:B:72:MET:HG3	2.54	0.42
3:C:357:ILE:HD11	3:C:375:ALA:HB1	2.00	0.42
3:C:24:ASN:O	3:C:26:PRO:HD3	2.18	0.42
4:D:25:THR:HA	4:D:26:PRO:HD3	1.87	0.42
3:C:68:ARG:HG2	7:C:1396:CL:CL	2.57	0.42
4:D:383:MET:N	9:D:2184:HOH:O	2.52	0.42
1:A:88:LEU:HD12	1:A:380:GLY:O	2.19	0.42
4:D:365:MET:HA	9:D:2182:HOH:O	2.19	0.42
4:D:89:CSO:O	4:D:377:LEU:HD22	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:93:LEU:HD11	4:D:387:MET:CB	2.50	0.42
4:D:78:GLN:NE2	9:D:2055:HOH:O	2.53	0.42
4:D:207:ARG:HH11	4:D:208:LYS:H	1.66	0.42
1:A:344:ILE:HG22	9:A:2215:HOH:O	2.20	0.42
2:B:233:PRO:HB2	2:B:236:ASP:O	2.20	0.42
3:C:112:VAL:HG12	3:C:112:VAL:O	2.19	0.42
3:C:274:ARG:HH21	3:C:392:LEU:HD11	1.84	0.42
4:D:28:HIS:HA	4:D:116:MET:SD	2.60	0.42
9:C:2035:HOH:O	4:D:86:ASN:O	2.21	0.42
1:A:190:GLN:OE1	1:A:221:HIS:HE1	2.02	0.42
3:C:155:TYR:HE1	3:C:160:THR:HG22	1.85	0.42
2:B:124:HIS:HA	2:B:140:ILE:O	2.20	0.41
3:C:6:VAL:HG12	3:C:274:ARG:HD3	2.01	0.41
4:D:5:ILE:HD13	4:D:260:SER:HA	2.00	0.41
3:C:292:PRO:HB3	3:C:376:THR:OG1	2.20	0.41
4:D:325:ALA:HB2	9:D:2163:HOH:O	2.21	0.41
3:C:175:GLN:HE22	3:C:240:THR:CG2	2.33	0.41
4:D:118:SER:OG	4:D:121:MET:HB2	2.21	0.41
4:D:333:ASP:HA	4:D:334:PRO:HD2	1.88	0.41
2:B:168:TRP:N	2:B:168:TRP:CD1	2.88	0.41
3:C:181:ALA:O	3:C:185:LYS:HG3	2.20	0.41
3:C:293:ILE:O	3:C:297:ARG:HG3	2.20	0.41
4:D:313:VAL:HA	4:D:374:LEU:O	2.20	0.41
2:B:272:LEU:HD12	2:B:366[A]:LYS:HD3	2.02	0.41
2:B:7:ILE:HA	2:B:258[A]:LEU:HD13	2.02	0.41
3:C:15:VAL:HG11	3:C:347:GLY:HA3	2.02	0.41
3:C:53:ILE:HD12	3:C:111:ILE:HG21	2.03	0.41
3:C:6:VAL:CG1	3:C:274:ARG:HD3	2.50	0.41
4:D:389:ILE:N	4:D:389:ILE:HD12	2.35	0.41
4:D:5:ILE:HD12	4:D:103:ILE:HB	2.02	0.41
2:B:374:LEU:C	2:B:374:LEU:HD23	2.40	0.41
2:B:52:VAL:O	2:B:82:ALA:HA	2.21	0.41
3:C:224:THR:C	3:C:226:ASP:N	2.74	0.41
3:C:282:GLY:O	4:D:79:GLU:HA	2.21	0.41
4:D:17:SER:OG	4:D:217:GLU:HG3	2.21	0.41
4:D:300:LEU:HD13	4:D:307:ILE:CG1	2.50	0.41
3:C:25:THR:HG21	3:C:30:LEU:CD2	2.50	0.41
3:C:51:GLU:HG3	3:C:81:THR:O	2.20	0.41
4:D:102:GLN:NE2	9:D:2063:HOH:O	2.54	0.41
4:D:187:GLU:HG3	4:D:221:HIS:HA	2.02	0.41
4:D:205:LYS:HA	4:D:210:ASP:OD1	2.20	0.41
4:D:320:ALA:O	4:D:324:CYS:SG	2.75	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:33:THR:HG21	4:D:202:PHE:CD1	2.54	0.41
4:D:220:ARG:HG2	4:D:220:ARG:H	1.74	0.41
4:D:322:GLN:HE21	4:D:322:GLN:HB2	1.68	0.41
1:A:358:LEU:HD22	1:A:362:LEU:HG	2.03	0.40
1:A:55:GLY:HA3	1:A:91:SER:HB3	2.03	0.40
3:C:374:LEU:HA	3:C:374:LEU:HD23	1.74	0.40
4:D:356:ARG:NH1	9:D:2173:HOH:O	2.31	0.40
4:D:38:VAL:CG2	4:D:257:LEU:HB2	2.50	0.40
4:D:35:ILE:HD11	4:D:54:LEU:HD11	2.04	0.40
1:A:298:LYS:HD3	5:A:1401:SO4:O3	2.20	0.40
1:A:274:ARG:HD3	9:A:2310:HOH:O	2.21	0.40
3:C:57:VAL:C	3:C:58:LEU:HD23	2.42	0.40
3:C:64:GLN:HE22	4:D:157:MET:CE	2.35	0.40
3:C:7:ILE:HG21	3:C:362:LEU:HD13	2.02	0.40
4:D:31:GLY:O	4:D:35:ILE:HD12	2.21	0.40
1:A:276:VAL:HG22	1:A:388:CYS:CB	2.52	0.40
2:B:217:GLU:HG2	9:B:2261:HOH:O	2.21	0.40
3:C:340[C]:ASN:HD21	3:C:360:THR:CG2	2.35	0.40
4:D:285:PRO:HB2	9:D:2087:HOH:O	2.21	0.40
4:D:11:ALA:HB3	4:D:38:VAL:HG12	2.02	0.40
6:B:1401:COA:O9P	6:B:1401:COA:H141	2.22	0.40
2:B:88:LEU:HB2	2:B:379:ILE:HG23	2.02	0.40
3:C:387:MET:HG2	3:C:388:CYS:N	2.37	0.40
3:C:7:ILE:HG12	3:C:258:LEU:CD1	2.51	0.40
4:D:365:MET:HE1	4:D:373:GLY:N	2.36	0.40
4:D:39:LEU:HD12	4:D:44:VAL:O	2.21	0.40
4:D:68:ARG:O	4:D:72:MET:HG2	2.21	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	391/392 (100%)	376 (96%)	15 (4%)	0	100	100
2	B	392/392 (100%)	378 (96%)	13 (3%)	1 (0%)	50	31
3	C	389/392 (99%)	350 (90%)	36 (9%)	3 (1%)	27	9
4	D	389/392 (99%)	352 (90%)	31 (8%)	6 (2%)	15	3
All	All	1561/1568 (100%)	1456 (93%)	95 (6%)	10 (1%)	33	15

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	140	ILE
4	D	141	ASP
4	D	330	LEU
4	D	350	ILE
2	B	131	GLY
3	C	221	HIS
3	C	350	ILE
4	D	142	THR
4	D	236	ASP
3	C	369	GLY

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	279/277 (101%)	269 (96%)	10 (4%)	47	27
2	B	280/276 (101%)	268 (96%)	12 (4%)	40	19
3	C	277/278 (100%)	260 (94%)	17 (6%)	26	9
4	D	277/277 (100%)	260 (94%)	17 (6%)	26	9
All	All	1113/1108 (100%)	1057 (95%)	56 (5%)	33	14

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	39	LEU

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Mol	Chain	Res	Type
1	A	133	LYS
1	A	155	TYR
1	A	237	LYS
1	A	272	LEU
1	A	288	MET
1	A	322	GLN
1	A	332	TRP
1	A	358	LEU
2	B	39	LEU
2	B	138	LYS
2	B	155	TYR
2	B	207	ARG
2	B	221	HIS
2	B	272	LEU
2	B	276	VAL
2	B	288	MET
2	B	322	GLN
2	B	332	TRP
2	B	361	LEU
2	B	371	ARG
3	C	39	LEU
3	C	40	GLU
3	C	207	ARG
3	C	232	ARG
3	C	251	ASP
3	C	272	LEU
3	C	288	MET
3	C	298	LYS
3	C	322	GLN
3	C	332	TRP
3	C	358	LEU
3	C	359	ASN
3	C	361	LEU
3	C	371	ARG
3	C	374	LEU
3	C	377	LEU
3	C	378	CYS
4	D	24	ASN
4	D	33	THR
4	D	36	SER
4	D	38	VAL
4	D	78	GLN

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Mol	Chain	Res	Type
4	D	187	GLU
4	D	207	ARG
4	D	258	LEU
4	D	288	MET
4	D	293	ILE
4	D	298	LYS
4	D	322	GLN
4	D	332	TRP
4	D	350	ILE
4	D	358	LEU
4	D	359	ASN
4	D	371	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	169	GLN
1	A	184	ASN
1	A	221	HIS
2	B	78	GLN
2	B	175	GLN
2	B	184	ASN
2	B	221	HIS
2	B	316	ASN
3	C	64	GLN
3	C	78	GLN
3	C	175	GLN
3	C	184	ASN
3	C	322	GLN
4	D	19	ASN
4	D	163	ASN
4	D	184	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 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	CSD	A	378	1	7,7,8	8.04	2 (28%)	6,8,10	2.12	3 (50%)
2	CSD	B	378	2	7,7,8	7.62	3 (42%)	6,8,10	2.79	4 (66%)
2	CSO	B	89	2	6,6,7	7.25	2 (33%)	3,6,8	0.96	0
4	CSO	D	89	4	6,6,7	7.27	2 (33%)	3,6,8	1.06	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	CSD	A	378	1	-	0/3/6/8	0/0/0/0
2	CSD	B	378	2	-	0/3/6/8	0/0/0/0
2	CSO	B	89	2	-	0/2/5/7	0/0/0/0
4	CSO	D	89	4	-	0/2/5/7	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	89	CSO	O-C	17.32	1.23	1.11
2	B	89	CSO	O-C	17.20	1.23	1.11
1	A	378	CSD	OD1-SG	16.64	1.65	1.47
2	B	378	CSD	OD1-SG	16.18	1.65	1.47
1	A	378	CSD	O-C	12.98	1.20	1.11
2	B	378	CSD	O-C	11.75	1.19	1.11
2	B	89	CSO	OD-SG	3.77	1.78	1.62
4	D	89	CSO	OD-SG	3.61	1.77	1.62
2	B	378	CSD	CA-C	2.06	1.53	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	378	CSD	CA-CB-SG	4.98	117.92	110.82
1	A	378	CSD	OD2-SG-CB	3.83	112.44	98.82
2	B	378	CSD	C-CA-N	-2.99	110.85	113.83
2	B	378	CSD	OD1-SG-CB	2.78	110.10	105.29
1	A	378	CSD	C-CA-N	-2.32	111.51	113.83
1	A	378	CSD	OD1-SG-CB	2.27	109.22	105.29
2	B	378	CSD	OD2-SG-CB	2.20	106.63	98.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 6 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	A	1394	-	4,4,4	0.28	0	6,6,6	0.15	0
5	SO4	A	1395	-	4,4,4	0.21	0	6,6,6	0.09	0
5	SO4	A	1396	-	4,4,4	0.18	0	6,6,6	0.09	0
5	SO4	A	1397	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	A	1398	-	4,4,4	0.21	0	6,6,6	0.09	0
5	SO4	A	1399	-	4,4,4	0.20	0	6,6,6	0.08	0
5	SO4	A	1400	-	4,4,4	0.22	0	6,6,6	0.12	0
5	SO4	A	1401	-	4,4,4	0.33	0	6,6,6	0.19	0
6	COA	A	1402	-	50,50,50	1.54	7 (14%)	75,75,75	1.83	13 (17%)
5	SO4	A	1403	-	4,4,4	0.21	0	6,6,6	0.09	0
5	SO4	B	1395	-	4,4,4	0.28	0	6,6,6	0.10	0
5	SO4	B	1396	-	4,4,4	0.19	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	1397	-	4,4,4	0.23	0	6,6,6	0.13	0
5	SO4	B	1398	-	4,4,4	0.27	0	6,6,6	0.17	0
5	SO4	B	1399	-	4,4,4	0.21	0	6,6,6	0.07	0
6	COA	B	1401	-	50,50,50	1.52	6 (12%)	75,75,75	1.90	13 (17%)
5	SO4	B	1402	-	4,4,4	0.22	0	6,6,6	0.10	0
5	SO4	B	1403	-	4,4,4	0.22	0	6,6,6	0.10	0
5	SO4	B	1404	-	4,4,4	0.21	0	6,6,6	0.09	0
5	SO4	C	1393	-	4,4,4	0.23	0	6,6,6	0.06	0
5	SO4	C	1397	-	4,4,4	0.22	0	6,6,6	0.07	0
5	SO4	C	1398	-	4,4,4	0.20	0	6,6,6	0.08	0
5	SO4	C	1399	-	4,4,4	0.20	0	6,6,6	0.06	0
5	SO4	D	1394	-	4,4,4	0.20	0	6,6,6	0.08	0
5	SO4	D	1395	-	4,4,4	0.21	0	6,6,6	0.06	0
5	SO4	D	1396	-	4,4,4	0.22	0	6,6,6	0.11	0
5	SO4	D	1397	-	4,4,4	0.26	0	6,6,6	0.10	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
5	SO4	A	1394	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1395	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1396	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1397	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1398	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1399	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1400	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1401	-	-	0/0/0/0	0/0/0/0
6	COA	A	1402	-	-	0/48/64/64	0/3/3/3
5	SO4	A	1403	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1395	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1396	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1397	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1398	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1399	-	-	0/0/0/0	0/0/0/0
6	COA	B	1401	-	-	0/48/64/64	0/3/3/3
5	SO4	B	1402	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1403	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1404	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1393	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	C	1397	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1398	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1399	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1394	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1395	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1396	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1397	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1401	COA	P3B-O7A	5.81	1.70	1.51
6	A	1402	COA	P3B-O7A	5.81	1.70	1.51
6	B	1401	COA	P3B-O8A	4.35	1.70	1.54
6	A	1402	COA	P3B-O8A	4.26	1.70	1.54
6	A	1402	COA	CBP-CAP	-3.50	1.53	1.55
6	B	1401	COA	P2A-O5A	3.48	1.70	1.55
6	A	1402	COA	P2A-O5A	3.46	1.70	1.55
6	B	1401	COA	P1A-O2A	3.44	1.70	1.55
6	A	1402	COA	P1A-O2A	3.30	1.69	1.55
6	B	1401	COA	C4A-N9A	-3.07	1.33	1.37
6	A	1402	COA	C4A-N9A	-2.80	1.33	1.37
6	B	1401	COA	C5A-C4A	2.47	1.46	1.40
6	A	1402	COA	C5A-C4A	2.13	1.45	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1401	COA	C5A-C4A-N3A	-7.90	118.28	125.98
6	A	1402	COA	C5A-C4A-N3A	-7.32	118.84	125.98
6	B	1401	COA	N3A-C4A-N9A	6.78	137.03	125.39
6	A	1402	COA	N3A-C4A-N9A	6.61	136.73	125.39
6	A	1402	COA	N3A-C2A-N1A	-5.89	123.71	128.89
6	B	1401	COA	P2A-O3A-P1A	-4.86	118.46	131.93
6	B	1401	COA	C7P-C6P-C5P	-4.61	104.63	112.28
6	B	1401	COA	N3A-C2A-N1A	-4.55	124.89	128.89
6	A	1402	COA	CBP-CAP-C9P	-4.39	106.76	113.66
6	A	1402	COA	P2A-O3A-P1A	-3.37	122.61	131.93
6	A	1402	COA	C8A-N9A-C4A	3.07	109.45	106.96
6	B	1401	COA	CBP-CAP-C9P	-2.96	109.01	113.66
6	B	1401	COA	C6P-C7P-N8P	2.91	118.34	111.94
6	B	1401	COA	C7P-N8P-C9P	-2.90	116.86	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1402	COA	C7P-N8P-C9P	-2.72	117.20	122.58
6	B	1401	COA	C3P-N4P-C5P	-2.64	117.45	122.81
6	A	1402	COA	C7P-C6P-C5P	-2.57	108.02	112.28
6	A	1402	COA	C6P-C7P-N8P	2.39	117.19	111.94
6	A	1402	COA	C2A-N3A-C4A	2.29	119.85	113.27
6	B	1401	COA	C8A-N9A-C4A	2.28	108.81	106.96
6	A	1402	COA	C4B-O4B-C1B	-2.20	107.30	109.72
6	B	1401	COA	C2A-N3A-C4A	2.19	119.58	113.27
6	A	1402	COA	C1B-N9A-C4A	-2.15	122.92	126.64
6	B	1401	COA	C6P-C5P-N4P	2.11	120.31	116.48
6	A	1402	COA	C2A-N1A-C6A	2.10	122.51	118.76
6	B	1401	COA	C6A-C5A-C4A	2.01	119.81	117.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	389/392 (99%)	-0.05	4 (1%) 79 76	5, 13, 33, 69	0
2	B	389/392 (99%)	-0.04	4 (1%) 79 76	6, 13, 31, 79	0
3	C	389/392 (99%)	2.56	212 (54%) 0 1	23, 66, 100, 125	0
4	D	389/392 (99%)	2.84	230 (59%) 0 0	20, 60, 118, 148	0
All	All	1556/1568 (99%)	1.33	450 (28%) 1 1	5, 37, 97, 148	0

All (450) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	307	ILE	13.9
4	D	392	LEU	12.0
4	D	206	GLY	11.8
4	D	331	GLY	11.5
4	D	330	LEU	10.9
3	C	325	ALA	10.5
4	D	170	LEU	10.3
4	D	358	LEU	10.1
4	D	367	ARG	9.7
3	C	223	ALA	9.7
3	C	334	PRO	9.5
3	C	299	ALA	9.5
4	D	310	LEU	9.1
4	D	339	VAL	8.1
3	C	361	LEU	8.1
3	C	275	ILE	8.1
4	D	208	LYS	7.9
3	C	320	ALA	7.5
4	D	260	SER	7.4
4	D	389	ILE	7.3
4	D	325	ALA	7.2

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Mol	Chain	Res	Type	RSRZ
3	C	293	ILE	7.2
4	D	186	ALA	7.0
1	A	132	VAL	7.0
4	D	262	ALA	7.0
4	D	388	CYS	6.9
4	D	229	ALA	6.8
3	C	106	GLY	6.8
3	C	312	LEU	6.8
3	C	258	LEU	6.7
3	C	315	ALA	6.7
3	C	5	ILE	6.7
3	C	177	ALA	6.6
4	D	329	ASP	6.6
4	D	185	LYS	6.5
4	D	269	ILE	6.4
3	C	42	ALA	6.4
4	D	5	ILE	6.4
4	D	246	ALA	6.3
4	D	265	SER	6.3
4	D	334	PRO	6.3
4	D	81	THR	6.3
3	C	276	VAL	6.2
4	D	108	ALA	6.2
4	D	375	ALA	6.2
4	D	340	ASN	6.2
3	C	372	LYS	6.0
4	D	362	LEU	6.0
3	C	6	VAL	6.0
4	D	197	ASP	5.9
4	D	326	VAL	5.8
3	C	340[A]	ASN	5.8
4	D	240	THR	5.8
4	D	179	ALA	5.8
4	D	207	ARG	5.8
3	C	337	VAL	5.8
4	D	387	MET	5.8
4	D	369	GLY	5.7
3	C	97	ALA	5.7
4	D	168	TRP	5.7
3	C	43	GLY	5.7
4	D	232	ARG	5.6
4	D	188	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
3	C	107	ASP	5.6
3	C	353	SER	5.6
4	D	192	ASP	5.6
4	D	332	TRP	5.6
4	D	347	GLY	5.6
4	D	165	ALA	5.6
4	D	303	ALA	5.6
3	C	161	ALA	5.5
4	D	47	GLY	5.5
4	D	228	MET	5.5
3	C	305	TRP	5.5
4	D	289	GLY	5.5
4	D	315	ALA	5.5
4	D	6	VAL	5.4
4	D	341	GLY	5.4
3	C	180	VAL	5.4
3	C	333	ASP	5.4
4	D	219	ILE	5.3
4	D	227	SER	5.3
4	D	180	VAL	5.3
4	D	360	THR	5.3
4	D	377	LEU	5.3
3	C	321	ALA	5.2
3	C	211	ILE	5.2
4	D	231	LEU	5.2
3	C	153	TYR	5.1
4	D	236	ASP	5.1
4	D	292	PRO	5.1
3	C	311	ASP	5.0
3	C	60	ALA	5.0
4	D	164	VAL	5.0
3	C	371	ARG	5.0
3	C	239	GLY	5.0
4	D	316	ASN	5.0
4	D	312	LEU	5.0
4	D	279	ALA	4.9
3	C	272	LEU	4.9
4	D	209	GLY	4.9
4	D	305	TRP	4.8
3	C	277	SER	4.8
3	C	105	THR	4.7
3	C	389	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
4	D	281	VAL	4.7
4	D	161	ALA	4.7
3	C	158	GLY	4.7
4	D	7	ILE	4.7
3	C	278	TRP	4.6
3	C	342	GLY	4.6
3	C	4	SER	4.6
3	C	36	SER	4.6
3	C	169	GLN	4.6
4	D	107	ASP	4.6
4	D	308	GLY	4.5
4	D	264	ALA	4.5
4	D	385	VAL	4.5
3	C	362	LEU	4.5
3	C	301	GLU	4.5
4	D	15	VAL	4.5
3	C	204	VAL	4.5
4	D	352	ALA	4.4
4	D	275	ILE	4.4
2	B	132	VAL	4.4
3	C	115	GLY	4.4
3	C	256	ALA	4.4
4	D	382	GLY	4.4
4	D	233	PRO	4.3
4	D	99	GLY	4.3
3	C	348	ALA	4.3
4	D	42	ALA	4.3
4	D	278	TRP	4.3
3	C	360	THR	4.3
4	D	313	VAL	4.2
4	D	324	CYS	4.2
4	D	272	LEU	4.2
3	C	226	ASP	4.2
3	C	331	GLY	4.2
3	C	262	ALA	4.2
2	B	207	ARG	4.2
3	C	391	SER	4.2
3	C	341	GLY	4.2
3	C	269	ILE	4.1
3	C	310	LEU	4.1
3	C	227	SER	4.1
4	D	357	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
4	D	293	ILE	4.1
4	D	283	VAL	4.1
3	C	67	ALA	4.0
3	C	218	TYR	4.0
4	D	270	GLN	4.0
3	C	7	ILE	4.0
3	C	103	ILE	4.0
3	C	255	ALA	4.0
4	D	162	GLU	4.0
3	C	108	ALA	3.9
3	C	339	VAL	3.9
3	C	46	ALA	3.9
4	D	171	SER	3.9
4	D	285	PRO	3.9
3	C	367	ARG	3.9
4	D	255	ALA	3.9
4	D	317	GLU	3.9
3	C	220	ARG	3.9
4	D	320	ALA	3.8
4	D	83	TRP	3.8
4	D	113	ALA	3.8
4	D	391	SER	3.8
4	D	241	VAL	3.8
4	D	280	THR	3.8
4	D	14	ALA	3.7
3	C	8	ALA	3.7
4	D	8	ALA	3.7
3	C	292	PRO	3.7
3	C	392	LEU	3.7
3	C	80	ALA	3.7
3	C	386	ALA	3.7
3	C	49	VAL	3.7
4	D	343	ALA	3.7
2	B	208	LYS	3.7
3	C	113	ALA	3.7
4	D	181	ALA	3.7
3	C	257	LEU	3.6
3	C	374	LEU	3.6
3	C	151	ALA	3.6
4	D	370	ALA	3.6
4	D	361	LEU	3.6
4	D	39	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
4	D	295	ALA	3.6
4	D	24	ASN	3.6
4	D	338	ASN	3.6
3	C	96	VAL	3.5
3	C	313	VAL	3.5
3	C	370	ALA	3.5
3	C	152	PHE	3.5
4	D	290	THR	3.5
4	D	172[A]	ARG	3.5
4	D	287	VAL	3.4
3	C	365	MET	3.4
4	D	230	LYS	3.4
4	D	182	SER	3.4
3	C	95	ALA	3.4
4	D	390	GLU	3.4
3	C	57	VAL	3.4
3	C	93	LEU	3.4
4	D	319	PHE	3.4
4	D	173	ASP	3.4
4	D	253	ALA	3.3
3	C	240	THR	3.3
3	C	279	ALA	3.3
3	C	99	GLY	3.3
3	C	241	VAL	3.3
3	C	243	ALA	3.3
3	C	284	ASP	3.3
4	D	225	LEU	3.3
3	C	10	ALA	3.3
4	D	318	ALA	3.3
4	D	321	ALA	3.3
4	D	291	GLY	3.3
4	D	314	GLU	3.2
3	C	363	PHE	3.2
3	C	330	LEU	3.2
3	C	328	LYS	3.2
4	D	234	ALA	3.2
3	C	332	TRP	3.2
3	C	91	SER	3.2
3	C	387	MET	3.2
3	C	298	LYS	3.2
4	D	237	LYS	3.2
4	D	44	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	170	LEU	3.2
3	C	373	GLY	3.2
4	D	147	GLY	3.2
3	C	233	PRO	3.2
4	D	105	THR	3.2
4	D	276	VAL	3.2
4	D	274	ARG	3.2
4	D	257	LEU	3.2
3	C	83	TRP	3.2
3	C	37	ALA	3.1
4	D	223	ALA	3.1
4	D	195	PHE	3.1
4	D	95	ALA	3.1
4	D	239	GLY	3.1
3	C	77	PRO	3.1
4	D	271	PRO	3.0
4	D	384	GLY	3.0
3	C	176	ASP	3.0
4	D	309	ASP	3.0
3	C	235	PHE	3.0
3	C	188	ALA	3.0
3	C	98	LEU	3.0
3	C	280	THR	3.0
4	D	374	LEU	3.0
4	D	218	TYR	3.0
3	C	195	PHE	3.0
3	C	359	ASN	3.0
3	C	203	ILE	3.0
4	D	301	GLU	3.0
3	C	173	ASP	3.0
3	C	104	ALA	3.0
4	D	355	ALA	3.0
3	C	38	VAL	3.0
4	D	365	MET	3.0
3	C	58	LEU	3.0
4	D	226	ASP	3.0
3	C	308	GLY	3.0
3	C	122	ALA	3.0
4	D	199	ILE	2.9
3	C	202	PHE	2.9
3	C	230	LYS	2.9
4	D	372	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	302	ARG	2.9
3	C	358	LEU	2.9
3	C	254	ALA	2.9
3	C	295	ALA	2.9
4	D	235	PHE	2.9
4	D	299	ALA	2.9
4	D	49	VAL	2.9
3	C	94	ARG	2.9
3	C	110	ILE	2.9
3	C	346	ILE	2.9
4	D	346	ILE	2.9
3	C	33	THR	2.9
3	C	324	CYS	2.9
3	C	345	ALA	2.9
4	D	356	ARG	2.9
3	C	300	LEU	2.9
3	C	21	ALA	2.9
3	C	210	ASP	2.9
4	D	242	THR	2.9
3	C	232	ARG	2.9
3	C	356	ARG	2.9
4	D	348	ALA	2.9
4	D	187	GLU	2.9
3	C	289	GLY	2.8
4	D	10	ALA	2.8
4	D	80	ALA	2.8
3	C	225	LEU	2.8
3	C	380	GLY	2.8
3	C	171	SER	2.8
3	C	236	ASP	2.8
3	C	323	ALA	2.8
4	D	190	GLN	2.8
4	D	263	GLU	2.8
4	D	98	LEU	2.8
3	C	385	VAL	2.8
4	D	327	ASN	2.8
4	D	153	TYR	2.8
4	D	140	ILE	2.8
3	C	22	PHE	2.8
3	C	44	VAL	2.8
3	C	182	SER	2.8
4	D	57	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	368	ARG	2.7
3	C	159	THR	2.7
3	C	294	PRO	2.7
3	C	144	ILE	2.7
3	C	338	ASN	2.7
4	D	238	GLU	2.7
3	C	335	SER	2.7
3	C	306	LYS	2.7
4	D	111	ILE	2.7
4	D	288	MET	2.7
4	D	221	HIS	2.7
4	D	336	ILE	2.7
4	D	178	PHE	2.7
4	D	380	GLY	2.7
4	D	349	PRO	2.7
4	D	306	LYS	2.7
3	C	154	GLY	2.7
3	C	228	MET	2.7
4	D	50	ASN	2.7
3	C	221	HIS	2.7
3	C	296	SER	2.7
4	D	45	ALA	2.7
3	C	224	THR	2.7
4	D	112	VAL	2.7
4	D	211	ILE	2.7
3	C	352	ALA	2.6
4	D	43	GLY	2.6
4	D	371	ARG	2.6
3	C	186	ALA	2.6
3	C	290	THR	2.6
3	C	34	VAL	2.6
3	C	53	ILE	2.6
3	C	208	LYS	2.6
3	C	344	ILE	2.6
3	C	317	GLU	2.6
3	C	47	GLY	2.6
4	D	34	VAL	2.6
3	C	384	GLY	2.6
3	C	74	ALA	2.5
4	D	152	PHE	2.5
4	D	191	LYS	2.5
3	C	140	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	336	ILE	2.5
4	D	79	GLU	2.5
4	D	169	GLN	2.5
4	D	266	ARG	2.5
1	A	207	ARG	2.5
3	C	283	VAL	2.5
4	D	335	SER	2.5
3	C	285	PRO	2.5
4	D	373	GLY	2.5
3	C	288	MET	2.5
4	D	294	PRO	2.5
3	C	164	VAL	2.5
3	C	242	THR	2.5
4	D	22	PHE	2.5
3	C	357	ILE	2.5
3	C	266	ARG	2.5
3	C	291	GLY	2.5
4	D	33	THR	2.5
4	D	323	ALA	2.5
3	C	112	VAL	2.5
3	C	167	GLN	2.5
3	C	81	THR	2.4
4	D	20	GLY	2.4
4	D	286	LYS	2.4
4	D	176	ASP	2.4
3	C	18	PHE	2.4
4	D	106	GLY	2.4
3	C	26	PRO	2.4
4	D	93	LEU	2.4
4	D	345	ALA	2.4
3	C	111	ILE	2.4
4	D	12	ARG	2.4
4	D	354	GLY	2.4
3	C	327	ASN	2.4
4	D	363	PHE	2.4
4	D	154	GLY	2.4
4	D	337	VAL	2.4
4	D	259	MET	2.4
3	C	304	GLY	2.3
3	C	109	SER	2.3
4	D	37	ALA	2.3
4	D	350	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	206	GLY	2.3
4	D	55	GLY	2.3
3	C	245	ASN	2.3
4	D	52	VAL	2.3
3	C	271	PRO	2.3
4	D	381	GLY	2.2
4	D	36	SER	2.2
4	D	244	GLY	2.2
3	C	23	ALA	2.2
4	D	378	CYS	2.2
4	D	203	ILE	2.2
3	C	309	ASP	2.2
4	D	96	VAL	2.2
4	D	298	LYS	2.2
4	D	142	THR	2.2
3	C	32	ALA	2.2
4	D	167	GLN	2.2
3	C	198	GLU	2.2
3	C	282	GLY	2.2
3	C	185	LYS	2.2
2	B	131	GLY	2.2
4	D	131	GLY	2.2
3	C	237	LYS	2.1
1	A	209	GLY	2.1
4	D	30	LEU	2.1
4	D	300	LEU	2.1
4	D	194[A]	ARG	2.1
3	C	165	ALA	2.1
4	D	156	HIS	2.1
3	C	82	ALA	2.1
3	C	303	ALA	2.1
3	C	52	VAL	2.1
3	C	231	LEU	2.1
4	D	202	PHE	2.1
4	D	366	LYS	2.1
3	C	206	GLY	2.1
4	D	342	GLY	2.1
3	C	166	LYS	2.1
4	D	376	THR	2.0
3	C	390	GLU	2.0
4	D	102	GLN	2.0
4	D	115	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	141	ASP	2.0
4	D	249	LEU	2.0
3	C	9	SER	2.0
3	C	48	GLU	2.0
3	C	368	ARG	2.0
4	D	297	ARG	2.0
4	D	157	MET	2.0
3	C	349	PRO	2.0
3	C	209	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CSD	A	378	8/9	0.10	0.92	7,13,23,32	0
2	CSD	B	378	8/9	0.09	-0.37	4,9,24,109	0
2	CSO	B	89	7/8	0.09	-0.99	4,10,34,73	0
4	CSO	D	89	7/8	0.14	-1.12	36,42,63,77	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	A	1401	5/5	0.41	20.85	28,44,49,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	A	1400	5/5	0.23	18.39	60,60,69,75	0
5	SO4	A	1399	5/5	0.27	10.24	95,99,101,101	0
5	SO4	D	1397	5/5	0.62	8.65	120,121,122,123	0
5	SO4	B	1398	5/5	0.17	5.53	45,51,56,57	0
5	SO4	A	1397	5/5	0.18	5.13	47,48,56,56	0
7	CL	D	1399	1/1	0.33	3.49	80,80,80,80	0
5	SO4	C	1393	5/5	0.26	2.91	108,108,109,109	0
5	SO4	D	1394	5/5	0.28	2.62	63,70,71,75	0
5	SO4	A	1395	5/5	0.15	2.06	46,54,58,59	0
5	SO4	A	1398	5/5	0.20	2.03	71,78,79,81	0
5	SO4	A	1396	5/5	0.14	1.97	31,39,50,57	0
5	SO4	B	1396	5/5	0.14	1.53	45,49,57,63	0
6	COA	B	1401	48/48	0.14	1.53	20,36,80,112	0
5	SO4	B	1397	5/5	0.14	1.29	66,66,71,73	0
6	COA	A	1402	48/48	0.13	1.18	21,32,63,131	0
5	SO4	B	1395	5/5	0.13	1.04	47,50,52,55	0
5	SO4	A	1394	5/5	0.13	0.40	41,43,48,48	0
5	SO4	D	1396	5/5	0.17	-0.97	52,59,70,71	0
8	NA	C	1394	1/1	0.12	-1.54	34,34,34,34	0
7	CL	C	1396	1/1	0.15	-1.65	58,58,58,58	0
8	NA	C	1395	1/1	0.12	-2.44	60,60,60,60	0
8	NA	D	1398	1/1	0.12	-2.54	38,38,38,38	0
7	CL	B	1400	1/1	0.05	-3.71	28,28,28,28	0
5	SO4	D	1395	5/5	0.17	-4.83	89,89,90,91	0
5	SO4	C	1399	5/5	0.17	-5.07	90,91,94,94	0
5	SO4	B	1403	5/5	0.24	-	86,87,88,89	0
5	SO4	B	1402	5/5	0.12	-	75,75,76,76	0
5	SO4	B	1404	5/5	0.26	-	77,77,79,82	0
5	SO4	B	1399	5/5	0.18	-	78,78,80,81	0
5	SO4	C	1398	5/5	0.21	-	96,97,97,98	0
5	SO4	C	1397	5/5	0.16	-	84,84,85,86	0
5	SO4	A	1403	5/5	0.35	-	94,94,95,98	0

6.5 Other polymers ⓘ

There are no such residues in this entry.