



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:17 AM GMT

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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

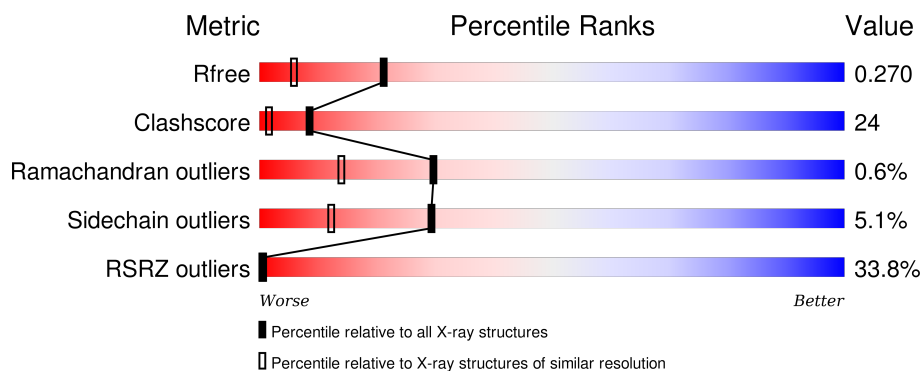
1 Overall quality at a glance

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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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. 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	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
2	B	392	<div> <div>3%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
3	C	392	<div> <div>61%</div> <div>53%</div> <div>43%</div> <div>..</div> </div>
4	D	392	<div> <div>67%</div> <div>49%</div> <div>46%</div> <div>..</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CSO	B	89	-	-	X	-
5	SO4	A	1396	-	-	-	X
5	SO4	A	1397	-	-	-	X
5	SO4	A	1400	-	-	-	X
5	SO4	A	1401	-	-	X	X
5	SO4	B	1398	-	-	X	-
5	SO4	D	1394	-	-	X	-
5	SO4	D	1397	-	-	-	X
6	COA	A	1402	-	-	-	X
6	COA	B	1401	-	-	-	X
7	CL	C	1396	-	-	X	-
7	CL	D	1399	-	-	X	X
8	NA	C	1395	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12721 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	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

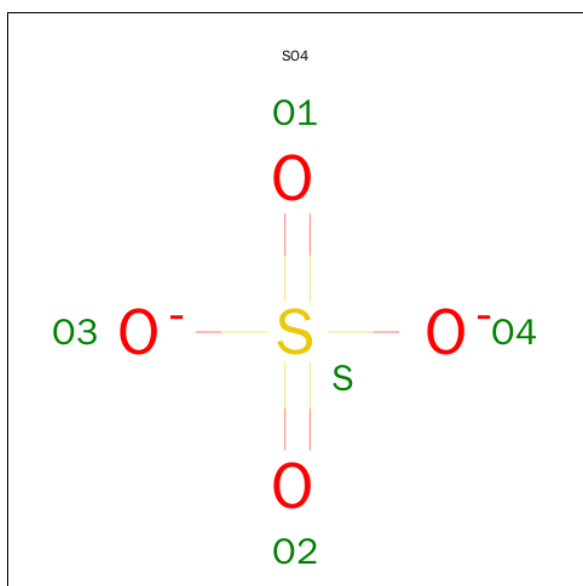
- Molecule 4 is a protein called ACETYL-COA ACETYLTRANSFERASE.

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).



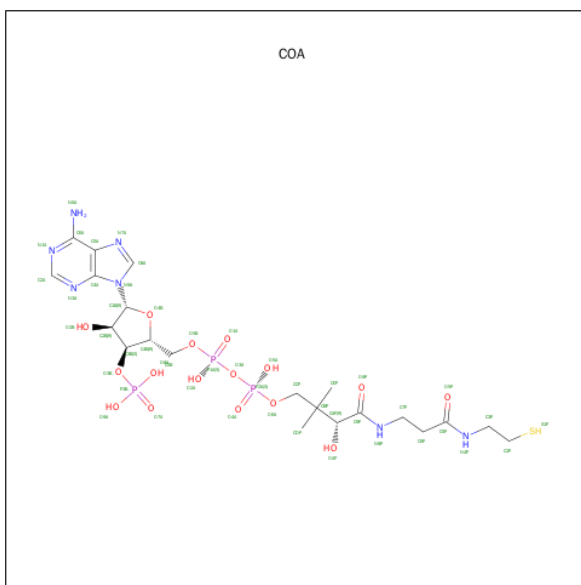
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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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		

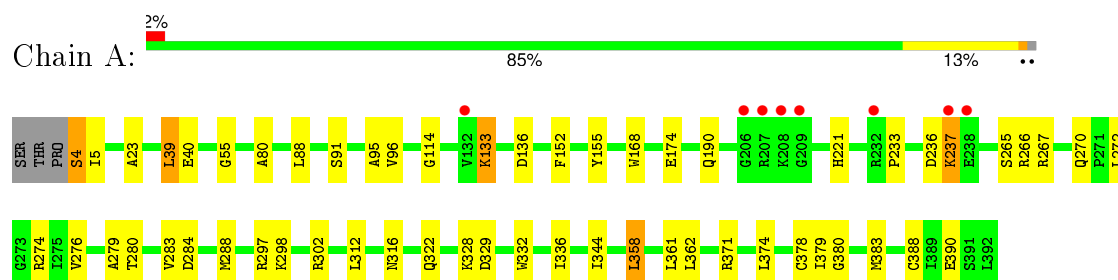
- Molecule 9 is water.

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

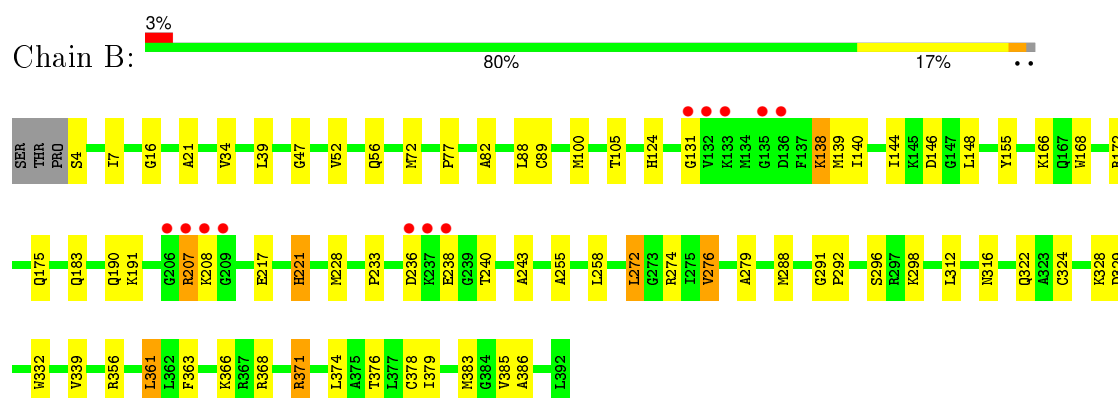
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

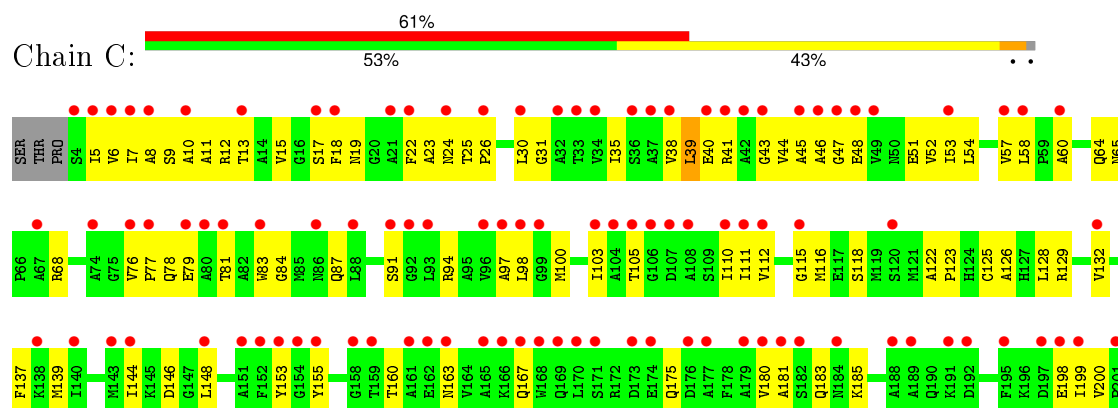
• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

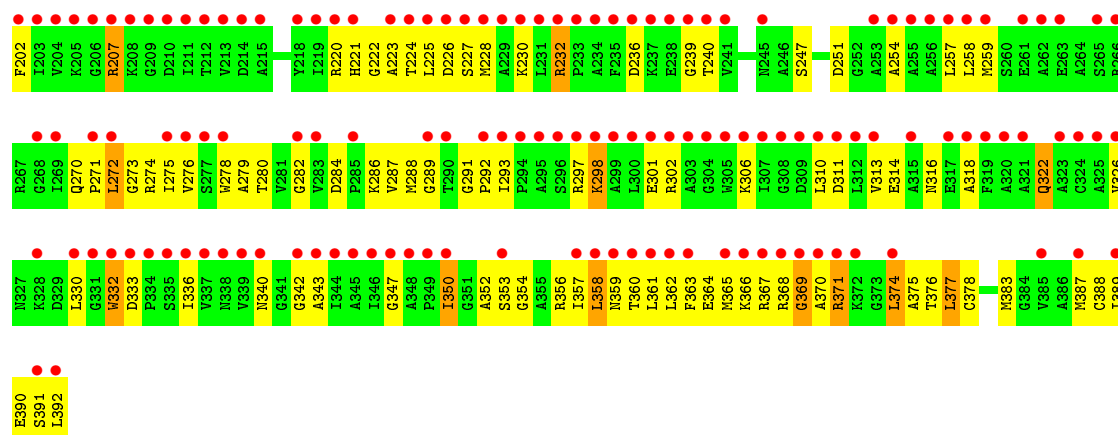


• Molecule 2: ACETYL-COA ACETYLTRANSFERASE

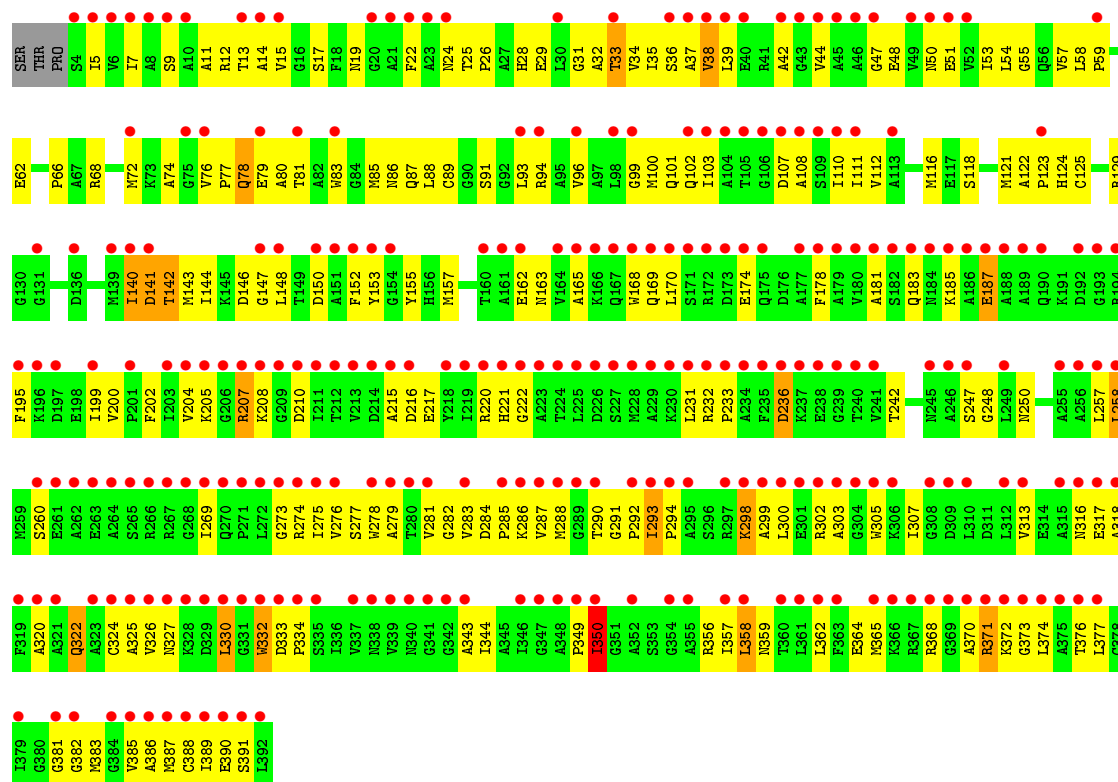


• Molecule 3: ACETYL-COA ACETYLTRANSFERASE





● Molecule 4: 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	84.31Å 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) 99.6 (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 0.232 , 0.270	Depositor DCC
R_{free} test set	9051 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 102.6	EDS
Estimated twinning fraction	0.159 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 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 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	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
5	A	45	0	0	9	0
5	B	40	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 24.

All (551) 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)
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	Interatomic distance (Å)	Clash overlap (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
4:D:231:LEU:HB3	9:D:2129:HOH:O	1.81	0.80
2:B:207:ARG:H	2:B:207:ARG:HD3	1.47	0.80
4:D:62:GLU:HB3	9:D:2043:HOH:O	1.81	0.80
4:D:140:ILE:HD12	4:D:141:ASP:H	1.47	0.80
1:A:23:ALA:HB1	9:A:2023:HOH:O	1.82	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
4:D:216:ASP:HA	9:D:2121:HOH:O	1.88	0.72
3:C:47:GLY:HA2	3:C:77:PRO:HG3	1.69	0.72
2:B:374:LEU:CD2	2:B:376[B]:THR:HG23	2.18	0.72
3:C:64:GLN:HG2	4:D:88:LEU:CD1	2.18	0.72
3:C:374:LEU:CD2	3:C:375:ALA:H	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:ARG:HG2	2:B:208:LYS:H	1.55	0.72
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:207:ARG:HD3	4:D:207:ARG:N	2.06	0.70
4:D:162:GLU:HG3	9:D:2132:HOH:O	1.91	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:8:ALA:HB3	9:C:2095:HOH:O	1.91	0.68
3:C:18:PHE:CZ	4:D:129:ARG:HD3	2.29	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
3:C:302:ARG:NH1	4:D:107:ASP:HA	2.11	0.65
1:A:280:THR:N	5:A:1401:SO4:O3	2.30	0.65
1:A:371:ARG:HG2	9:A:2387:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:C:65:ASN:HB3	7:C:1396:CL:CL	2.35	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:60:ALA:HB1	9:C:2029:HOH:O	1.97	0.64
2:B:175:GLN:HE22	2:B:240:THR:CG2	2.10	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:371:ARG:HA	9:C:2141:HOH:O	1.96	0.64
3:C:183:GLN:OE1	3:C:220:ARG:HG2	1.96	0.64
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
4:D:150:ASP:HB2	9:D:2086:HOH:O	1.98	0.63
1:A:265:SER:HA	9:A:2298:HOH:O	1.98	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:HB2	4:D:232:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:269:ILE:HD13	9:D:2031:HOH:O	2.02	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: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
4:D:57:VAL:C	4:D:59:PRO:HD3	2.23	0.59
3:C:144:ILE:HD13	3:C:148:LEU:HD12	1.81	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
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
1:A:312:LEU:HD23	1:A:361:LEU:HD12	1.84	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
4:D:140:ILE:HD12	9:D:2083:HOH:O	2.02	0.58
3:C:57:VAL:HG12	3:C:58:LEU:HD23	1.86	0.58
1:A:284:ASP:OD2	9:A:2312:HOH:O	2.17	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:94:ARG:NH2	9:D:2059:HOH:O	2.36	0.58
4:D:277:SER:HB3	4:D:303:ALA:HB2	1.85	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
4:D:242:THR:HB	9:D:2129:HOH:O	2.04	0.57
4:D:50:ASN:HB2	4:D:110:ILE:O	2.04	0.57
3:C:87:GLN:N	3:C:91:SER:OG	2.37	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
3:C:125:CYS:CB	7:D:1399:CL:CL	2.90	0.57
3:C:116:MET:HG2	9:C:2025:HOH:O	2.04	0.57
2:B:363:PHE:CD1	2:B:366[A]:LYS:NZ	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:272:LEU:HD12	3:C:366:LYS:HD2	1.87	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
4:D:9:SER:OG	4:D:42:ALA:HB2	2.05	0.56
2:B:243:ALA:HB1	6:B:1401:COA:O2A	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
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:183:GLN:HG3	9:B:2404:HOH:O	2.06	0.56
4:D:44:VAL:HG13	4:D:48:GLU:OE1	2.06	0.56
4:D:51:GLU:HB3	4:D:111:ILE:HD12	1.88	0.56
2:B:100:MET:SD	5:B:1398:SO4:O4	2.64	0.56
3:C:276:VAL:HG22	3:C:388:CYS:HB3	1.88	0.56
4:D:305:TRP:CE2	4:D:372:LYS:HD3	2.40	0.56
2:B:175:GLN:HE22	2:B:240:THR:HG21	1.71	0.56
4:D:165:ALA:HA	4:D:170:LEU:HD12	1.88	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
4:D:35:ILE:HG23	4:D:112:VAL:HG21	1.89	0.55
3:C:330:LEU:HD13	3:C:332:TRP:CZ2	2.42	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:340[C]:ASN:HD21	3:C:360:THR:HG23	1.73	0.54
3:C:306:LYS:HB3	9:C:2114:HOH:O	2.07	0.54
3:C:100:MET:HG3	3:C:275:ILE:CG2	2.36	0.54
4:D:34:VAL:O	4:D:38:VAL:HG13	2.07	0.54
1:A:174:GLU:HG3	9:A:2210:HOH:O	2.07	0.54
4:D:357:ILE:HD11	4:D:377:LEU:CD1	2.31	0.54
2:B:21:ALA:HB3	9:B:2261:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LYS:HE2	1:A:302:ARG:NH2	2.23	0.53
4:D:187:GLU:HG3	9:D:2127:HOH:O	2.07	0.53
3:C:230:LYS:HA	9:C:2094: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
4:D:7:ILE:HD13	4:D:362:LEU:HD11	1.89	0.53
3:C:11:ALA:HB3	3:C:38:VAL:HG23	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
4:D:316:ASN:OD1	4:D:357:ILE:HG21	2.07	0.53
4:D:215:ALA:HA	9:D:2120:HOH:O	2.08	0.53
6:B:1401:COA:H122	6:B:1401:COA:O2A	2.09	0.53
4:D:178:PHE:HE1	4:D:317:GLU:CD	2.12	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:93:LEU:HD23	4:D:385:VAL:HG13	1.91	0.53
4:D:300:LEU:HD13	4:D:307:ILE:HG13	1.90	0.53
4:D:169:GLN:HG3	9:D:2095:HOH:O	2.09	0.52
4:D:35:ILE:HG12	4:D:112:VAL:HG11	1.91	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:O	4:D:39:LEU:HD23	2.09	0.52
2:B:324:CYS:O	2:B:328:LYS:HG3	2.09	0.52
3:C:302:ARG:NH1	9:C:2112:HOH:O	2.42	0.52
2:B:316:ASN:ND2	9:B:2335:HOH:O	2.42	0.52
1:A:297:ARG:NE	9:A:2319:HOH:O	2.43	0.52
3:C:25:THR:HG21	3:C:30:LEU:HD21	1.91	0.52
4:D:281:VAL:HG13	9:D:2151:HOH:O	2.09	0.52
4:D:274:ARG:H	4:D:389:ILE:HG23	1.74	0.52
4:D:300:LEU:HD13	4:D:307:ILE:CD1	2.40	0.52
2:B:146:ASP:HB3	9:B:2076:HOH:O	2.09	0.52
3:C:322:GLN:O	3:C:326:VAL:HG23	2.10	0.52
3:C:284:ASP:HA	9:D:2055:HOH:O	2.10	0.52
4:D:163:ASN:HD22	4:D:286:LYS:HB3	1.75	0.52
4:D:349:PRO:O	4:D:350:ILE:C	2.48	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
2:B:274:ARG:NH2	9:B:2307:HOH:O	2.43	0.52
4:D:44:VAL:HG23	9:D:2031:HOH:O	2.10	0.51
4:D:216:ASP:CA	9:D:2121:HOH:O	2.53	0.51
3:C:232:ARG:H	3:C:232:ARG:HE	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:312:LEU:HD23	2:B:361:LEU:HD22	1.91	0.51
2:B:356:ARG:HD2	2:B:356:ARG:C	2.31	0.51
3:C:39:LEU:HD21	3:C:46:ALA:HA	1.92	0.51
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:93:LEU:HD11	4:D:387:MET:HB3	1.93	0.51
4:D:144:ILE:HA	4:D:148:LEU:HB2	1.93	0.51
4:D:33:THR:HG21	4:D:202:PHE:HD1	1.76	0.51
3:C:330:LEU:HD13	3:C:332:TRP:CH2	2.46	0.50
3:C:163:ASN:O	3:C:167:GLN:HB2	2.10	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:275:ILE:HD12	9:D:2004:HOH:O	2.11	0.50
4:D:99:GLY:O	4:D:103:ILE:HD12	2.11	0.50
3:C:51:GLU:OE2	3:C:83:TRP:CD1	2.65	0.50
2:B:190:GLN:OE1	2:B:221:HIS:HE1	1.94	0.50
4:D:55:GLY:HA3	4:D:91[B]:SER:OG	2.11	0.50
1:A:133:LYS:H	1:A:133:LYS:HD3	1.77	0.50
4:D:153:TYR:HB3	4:D:155:TYR:CE2	2.47	0.50
3:C:81:THR:HG23	4:D:383:MET:SD	2.51	0.50
3:C:12:ARG:HB2	3:C:254:ALA:HB2	1.94	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
4:D:140:ILE:O	4:D:141:ASP:HB2	2.12	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:317:GLU:O	4:D:344:ILE:HG13	2.12	0.49
3:C:227:SER:HA	3:C:230:LYS:HE3	1.94	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
4:D:305:TRP:HZ3	4:D:388:CYS:HB3	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:207:ARG:NH1	3:C:207:ARG:HG2	2.18	0.49
3:C:6:VAL:HB	3:C:271:PRO:HB3	1.94	0.49
3:C:153:TYR:CE1	3:C:286:LYS:HG3	2.48	0.49
1:A:80:ALA:HB2	9:A:2064:HOH:O	2.13	0.49
4:D:387:MET:HG2	4:D:389:ILE:HD11	1.94	0.49
3:C:84:GLY:N	9:C:2035:HOH:O	2.41	0.49
2:B:148:LEU:HD23	9:B:2172:HOH:O	2.12	0.49
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:7:ILE:HD13	3:C:362:LEU:HD11	1.93	0.49
3:C:183:GLN:CD	3:C:220:ARG:HG2	2.33	0.49
3:C:387:MET:CG	3:C:388:CYS:N	2.76	0.48
1:A:298:LYS:NZ	5:A:1401:SO4:O2	2.46	0.48
3:C:22:PHE:HB3	3:C:25:THR:HB	1.95	0.48
1:A:40:GLU:HG3	9:A:2045:HOH:O	2.13	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
3:C:316:ASN:CG	3:C:377:LEU:HD23	2.34	0.48
1:A:276:VAL:HG22	1:A:388:CYS:HB2	1.96	0.48
3:C:387:MET:CG	3:C:388:CYS:H	2.25	0.48
3:C:358:LEU:CD2	3:C:362:LEU:HG	2.44	0.48
3:C:78:GLN:HG3	3:C:79:GLU:OE2	2.14	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
3:C:17:SER:HB3	9:C:2008:HOH:O	2.13	0.48
2:B:191[A]:LYS:NZ	2:B:191[A]:LYS:HB3	2.29	0.48
2:B:376[B]:THR:HG22	2:B:386:ALA:HB1	1.91	0.48
3:C:78:GLN:NE2	4:D:285:PRO:HD3	2.28	0.48
3:C:369:GLY:HA3	9:C:2138:HOH:O	2.13	0.48
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
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.77	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:354:GLY:HA3	9:C:2044:HOH:O	2.15	0.47
4:D:35:ILE:CG2	4:D:112:VAL:HG11	2.38	0.47
3:C:68:ARG:HB2	7:C:1396:CL:CL	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:326:VAL:O	4:D:330:LEU:HB2	2.14	0.47
3:C:291:GLY:HA3	3:C:383:MET:O	2.14	0.47
4:D:53:ILE:HD13	4:D:83:TRP:CZ2	2.50	0.47
4:D:19:ASN:N	4:D:19:ASN:HD22	2.13	0.47
3:C:123:PRO:HD2	9:C:2026:HOH:O	2.15	0.47
3:C:132:VAL:HG21	3:C:137:PHE:CD1	2.50	0.47
3:C:257:LEU:HD22	9:C:2095:HOH:O	2.14	0.47
3:C:236:ASP:HB3	3:C:239:GLY:HA3	1.97	0.47
3:C:19:ASN:C	3:C:23:ALA:HB2	2.36	0.46
3:C:115:GLY:HA3	3:C:352:ALA:HA	1.96	0.46
1:A:328:LYS:HB2	1:A:328:LYS:HE3	1.58	0.46
3:C:289:GLY:O	3:C:292:PRO:HD2	2.16	0.46
3:C:357:ILE:CD1	3:C:375:ALA:HB1	2.45	0.46
4:D:388:CYS:C	4:D:389:ILE:HD12	2.35	0.46
4:D:170:LEU:HD21	9:D:2099:HOH:O	2.15	0.46
2:B:190:GLN:OE1	2:B:221:HIS:CE1	2.68	0.46
4:D:385:VAL:HB	9:D:2056:HOH:O	2.16	0.46
2:B:172:ARG:HA	2:B:240:THR:OG1	2.15	0.46
1:A:237:LYS:HE2	9:A:2282:HOH:O	2.14	0.46
4:D:74:ALA:HB2	9:D:2023:HOH:O	2.15	0.46
4:D:358:LEU:HD22	4:D:362:LEU:HG	1.98	0.46
1:A:298:LYS:HE2	1:A:302:ARG:CZ	2.46	0.46
4:D:283:VAL:N	4:D:382:GLY:O	2.46	0.46
3:C:371:ARG:O	3:C:390:GLU:HA	2.15	0.46
3:C:129:ARG:CZ	9:C:2056:HOH:O	2.62	0.46
1:A:133:LYS:H	1:A:133:LYS:CD	2.28	0.46
2:B:89:CSO:HD	6:B:1401:COA:C2P	2.27	0.46
2:B:168:TRP:CH2	2:B:329:ASP:HB2	2.51	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
4:D:123:PRO:C	7:D:1399:CL:CL	2.91	0.45
2:B:298:LYS:HG2	9:B:2310:HOH:O	2.16	0.45
2:B:276:VAL:O	5:B:1398:SO4:O2	2.33	0.45
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.70	0.45
4:D:368:ARG:HB3	9:D:2179:HOH:O	2.16	0.45
3:C:103:ILE:HD13	3:C:259:MET:HA	1.98	0.45
3:C:94:ARG:HH22	4:D:51:GLU:CD	2.20	0.45
3:C:13:THR:HA	9:C:2080:HOH:O	2.16	0.45
3:C:45:ALA:HB3	3:C:48:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:PHE:HD1	9:C:2014:HOH:O	2.00	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:129:ARG:HD2	9:D:2068:HOH:O	2.17	0.45
3:C:316:ASN:OD1	3:C:357:ILE:HG21	2.17	0.45
3:C:316:ASN:OD1	3:C:377:LEU:HD23	2.17	0.45
4:D:59:PRO:HB2	5:D:1394:SO4:O3	2.17	0.45
4:D:292:PRO:HB3	4:D:376:THR:OG1	2.16	0.45
2:B:236:ASP:OD1	2:B:238:GLU:HG2	2.17	0.45
3:C:356:ARG:NH1	9:C:2133:HOH:O	2.49	0.45
3:C:146:ASP:HB3	5:D:1394:SO4:S	2.57	0.45
3:C:87:GLN:HG3	9:D:2046:HOH:O	2.17	0.45
3:C:122:ALA:HA	9:C:2026:HOH:O	2.15	0.45
3:C:38:VAL:HG11	3:C:257:LEU:N	2.30	0.45
4:D:58:LEU:N	4:D:59:PRO:HD3	2.31	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
3:C:298:LYS:HE3	3:C:301:GLU:OE1	2.17	0.45
4:D:124:HIS:C	7:D:1399:CL:CL	2.92	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
2:B:378:CSD:OD1	6:B:1401:COA:S1P	2.71	0.45
4:D:278:TRP:HH2	9:D:2059:HOH:O	1.99	0.45
2:B:4:SER:HB3	9:B:2394:HOH:O	2.17	0.45
3:C:207:ARG:HG2	9:C:2086:HOH:O	2.17	0.45
4:D:365:MET:HE2	4:D:370:ALA:O	2.17	0.44
4:D:293:ILE:CB	4:D:294:PRO:HD3	2.47	0.44
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
3:C:76:VAL:HG13	3:C:77:PRO:HD2	1.98	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
4:D:275:ILE:HD13	9:D:2061:HOH:O	2.15	0.44
2:B:144:ILE:HD13	2:B:148:LEU:HD12	1.98	0.44
4:D:88:LEU:HA	4:D:88:LEU:HD23	1.86	0.44
4:D:140:ILE:C	9:D:2083:HOH:O	2.55	0.44
3:C:316:ASN:HD21	3:C:377:LEU:HD23	1.82	0.44
3:C:207:ARG:NH1	3:C:207:ARG:CG	2.77	0.44
1:A:280:THR:O	5:A:1401:SO4:O3	2.34	0.44
4:D:96:VAL:HG21	4:D:358:LEU:HD12	2.00	0.44
2:B:89:CSO:OD	6:B:1401:COA:H22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:334:PRO:HD3	9:D:2165:HOH:O	2.16	0.44
3:C:48:GLU:N	3:C:48:GLU:OE1	2.51	0.44
4:D:147:GLY:O	4:D:148:LEU:HD23	2.17	0.44
3:C:273:GLY:HA2	3:C:391:SER:HA	2.00	0.44
4:D:140:ILE:CA	9:D:2083:HOH:O	2.66	0.44
3:C:274:ARG:O	3:C:389:ILE:HA	2.18	0.44
1:A:379:ILE:HB	1:A:383:MET:HB2	2.00	0.44
4:D:343:ALA:O	4:D:344:ILE:C	2.55	0.44
4:D:298:LYS:HD2	9:D:2154:HOH:O	2.17	0.44
3:C:374:LEU:CD2	3:C:387:MET:O	2.66	0.44
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
4:D:123:PRO:CB	7:D:1399:CL:CL	3.00	0.44
3:C:207:ARG:HD3	3:C:207:ARG:N	2.21	0.44
4:D:370:ALA:N	9:D:2182:HOH:O	2.50	0.44
3:C:118:SER:HB2	9:C:2050:HOH:O	2.17	0.44
3:C:343:ALA:N	9:C:2116:HOH:O	2.50	0.43
1:A:233:PRO:HB2	1:A:236:ASP:O	2.17	0.43
1:A:136:ASP:OD1	4:D:140:ILE:HA	2.18	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:47:GLY:HA2	3:C:77:PRO:CG	2.45	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
4:D:293:ILE:O	4:D:330:LEU:HD21	2.18	0.43
3:C:220:ARG:O	3:C:222:GLY:N	2.52	0.43
4:D:22:PHE:HB3	4:D:25:THR:HB	2.01	0.43
3:C:282:GLY:HA2	3:C:383:MET:HA	2.00	0.43
2:B:291:GLY:N	2:B:292:PRO:CD	2.81	0.43
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
1:A:374:LEU:HD23	1:A:374:LEU:C	2.39	0.42
1:A:336:ILE:HA	9:A:2376:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:195:PHE:HB2	9:D:2110:HOH:O	2.19	0.42
3:C:357:ILE:HD11	3:C:375:ALA:HB1	2.00	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
4:D:25:THR:HA	4:D:26:PRO:HD3	1.87	0.42
3:C:24:ASN:O	3:C:26:PRO:HD3	2.18	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
4:D:89:CSO:O	4:D:377:LEU:HD22	2.20	0.42
4:D:93:LEU:HD11	4:D:387:MET:CB	2.50	0.42
4:D:365:MET:HA	9:D:2182:HOH:O	2.19	0.42
4:D:78:GLN:NE2	9:D:2055:HOH:O	2.53	0.42
1:A:88:LEU:HD12	1:A:380:GLY:O	2.19	0.42
4:D:207:ARG:HH11	4:D:208:LYS:H	1.66	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
3:C:274:ARG:HH21	3:C:392:LEU:HD11	1.84	0.42
3:C:112:VAL:HG12	3:C:112:VAL:O	2.19	0.42
2:B:233:PRO:HB2	2:B:236:ASP:O	2.20	0.42
1:A:344:ILE:HG22	9:A:2215:HOH:O	2.20	0.42
3:C:155:TYR:HE1	3:C:160:THR:HG22	1.85	0.42
1:A:190:GLN:OE1	1:A:221:HIS:HE1	2.02	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
4:D:333:ASP:HA	4:D:334:PRO:HD2	1.88	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
3:C:293:ILE:O	3:C:297:ARG:HG3	2.20	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
4:D:313:VAL:HA	4:D:374:LEU:O	2.20	0.41
4:D:389:ILE:N	4:D:389:ILE:HD12	2.35	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
2:B:272:LEU:HD12	2:B:366[A]:LYS:HD3	2.02	0.41
4:D:5:ILE:HD12	4:D:103:ILE:HB	2.02	0.41
3:C:15:VAL:HG11	3:C:347:GLY:HA3	2.02	0.41
2:B:7:ILE:HA	2:B:258[A]:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:LEU:HD23	2:B:374:LEU:C	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
4:D:300:LEU:HD13	4:D:307:ILE:CG1	2.50	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
3:C:51:GLU:HG3	3:C:81:THR:O	2.20	0.41
4:D:187:GLU:HG3	4:D:221:HIS:HA	2.02	0.41
3:C:25:THR:HG21	3:C:30:LEU:CD2	2.50	0.41
4:D:33:THR:HG21	4:D:202:PHE:CD1	2.54	0.41
4:D:320:ALA:O	4:D:324:CYS:SG	2.75	0.41
4:D:102:GLN:NE2	9:D:2063:HOH:O	2.54	0.41
4:D:205:LYS:HA	4:D:210:ASP:OD1	2.20	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
3:C:374:LEU:HA	3:C:374:LEU:HD23	1.74	0.40
4:D:35:ILE:HD11	4:D:54:LEU:HD11	2.04	0.40
4:D:38:VAL:CG2	4:D:257:LEU:HB2	2.50	0.40
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
4:D:356:ARG:NH1	9:D:2173:HOH:O	2.31	0.40
3:C:64:GLN:HE22	4:D:157:MET:CE	2.35	0.40
3:C:57:VAL:C	3:C:58:LEU:HD23	2.42	0.40
4:D:31:GLY:O	4:D:35:ILE:HD12	2.21	0.40
1:A:298:LYS:HD3	5:A:1401:SO4:O3	2.20	0.40
3:C:7:ILE:HG21	3:C:362:LEU:HD13	2.02	0.40
1:A:274:ARG:HD3	9:A:2310:HOH:O	2.21	0.40
2:B:217:GLU:HG2	9:B:2261:HOH:O	2.21	0.40
1:A:276:VAL:HG22	1:A:388:CYS:CB	2.52	0.40
4:D:11:ALA:HB3	4:D:38:VAL:HG12	2.02	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
3:C:387:MET:HG2	3:C:388:CYS:N	2.37	0.40
4:D:39:LEU:HD12	4:D:44:VAL:O	2.21	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
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
4:D:68:ARG:O	4:D:72:MET:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/392 (100%)	376 (96%)	15 (4%)	0	100	100
2	B	392/392 (100%)	378 (96%)	13 (3%)	1 (0%)	46	29
3	C	389/392 (99%)	350 (90%)	36 (9%)	3 (1%)	24	8
4	D	389/392 (99%)	352 (90%)	31 (8%)	6 (2%)	13	3
All	All	1561/1568 (100%)	1456 (93%)	95 (6%)	10 (1%)	30	14

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 [i](#)

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%)	42	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	280/276 (101%)	268 (96%)	12 (4%)	35	17
3	C	277/278 (100%)	260 (94%)	17 (6%)	23	8
4	D	277/277 (100%)	260 (94%)	17 (6%)	23	8
All	All	1113/1108 (100%)	1057 (95%)	56 (5%)	29	13

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

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
4	D	163	ASN
4	D	184	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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	3,7,8	0.68	0	3,8,10	1.53	1 (33%)
2	CSD	B	378	2	3,7,8	0.62	0	3,8,10	1.91	1 (33%)
2	CSO	B	89	2	3,6,7	0.53	0	1,6,8	1.75	0
4	CSO	D	89	4	3,6,7	0.52	0	1,6,8	1.69	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	-	0/2/6/8	0/0/0/0
2	CSD	B	378	2	-	0/2/6/8	0/0/0/0
2	CSO	B	89	2	-	0/1/5/7	0/0/0/0
4	CSO	D	89	4	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	CSD	OD1-SG-CB	2.29	109.22	105.40
2	B	378	CSD	OD1-SG-CB	2.82	110.10	105.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	378	CSD	1	0
2	B	378	CSD	2	0
2	B	89	CSO	4	0
4	D	89	CSO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.29	0	6,6,6	0.15	0
5	SO4	A	1395	-	4,4,4	0.22	0	6,6,6	0.09	0
5	SO4	A	1396	-	4,4,4	0.18	0	6,6,6	0.10	0
5	SO4	A	1397	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	A	1398	-	4,4,4	0.22	0	6,6,6	0.09	0
5	SO4	A	1399	-	4,4,4	0.21	0	6,6,6	0.08	0
5	SO4	A	1400	-	4,4,4	0.23	0	6,6,6	0.12	0
5	SO4	A	1401	-	4,4,4	0.34	0	6,6,6	0.20	0
6	COA	A	1402	-	40,50,50	1.55	5 (12%)	50,75,75	1.57	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	1403	-	4,4,4	0.21	0	6,6,6	0.09	0
5	SO4	B	1395	-	4,4,4	0.29	0	6,6,6	0.11	0
5	SO4	B	1396	-	4,4,4	0.20	0	6,6,6	0.11	0
5	SO4	B	1397	-	4,4,4	0.24	0	6,6,6	0.13	0
5	SO4	B	1398	-	4,4,4	0.28	0	6,6,6	0.18	0
5	SO4	B	1399	-	4,4,4	0.22	0	6,6,6	0.07	0
6	COA	B	1401	-	40,50,50	1.59	5 (12%)	50,75,75	1.71	8 (16%)
5	SO4	B	1402	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	B	1403	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	B	1404	-	4,4,4	0.21	0	6,6,6	0.09	0
5	SO4	C	1393	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	C	1397	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	C	1398	-	4,4,4	0.21	0	6,6,6	0.09	0
5	SO4	C	1399	-	4,4,4	0.21	0	6,6,6	0.07	0
5	SO4	D	1394	-	4,4,4	0.20	0	6,6,6	0.08	0
5	SO4	D	1395	-	4,4,4	0.22	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	0.27	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	-	-	0/44/64/64	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	-	-	0/44/64/64	0/3/3/3
5	SO4	B	1402	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1402	COA	C5A-C4A	2.13	1.45	1.40
6	B	1401	COA	C5A-C4A	2.47	1.46	1.40
6	A	1402	COA	P1A-O2A	3.39	1.69	1.54
6	B	1401	COA	P1A-O2A	3.54	1.70	1.54
6	A	1402	COA	P2A-O5A	3.55	1.70	1.54
6	B	1401	COA	P2A-O5A	3.58	1.70	1.54
6	A	1402	COA	P3B-O8A	4.29	1.70	1.54
6	B	1401	COA	P3B-O8A	4.38	1.70	1.54
6	A	1402	COA	P3B-O7A	5.86	1.70	1.51
6	B	1401	COA	P3B-O7A	5.86	1.70	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1402	COA	N3A-C2A-N1A	-6.77	123.71	128.89
6	B	1401	COA	N3A-C2A-N1A	-5.24	124.89	128.89
6	B	1401	COA	P2A-O3A-P1A	-5.08	118.46	132.73
6	B	1401	COA	C7P-C6P-C5P	-4.66	104.63	112.31
6	A	1402	COA	P2A-O3A-P1A	-3.60	122.61	132.73
6	B	1401	COA	C7P-N8P-C9P	-2.86	116.86	122.53
6	B	1401	COA	C3P-N4P-C5P	-2.72	117.45	122.79
6	A	1402	COA	C7P-N8P-C9P	-2.69	117.20	122.53
6	A	1402	COA	C1B-N9A-C4A	-2.67	122.92	126.94
6	A	1402	COA	C7P-C6P-C5P	-2.61	108.02	112.31
6	B	1401	COA	C2B-C1B-N9A	-2.22	110.91	114.29
6	A	1402	COA	C4B-O4B-C1B	-2.20	107.30	109.72
6	A	1402	COA	C2A-N1A-C6A	2.09	122.51	118.77
6	B	1401	COA	C6P-C5P-N4P	2.22	120.31	116.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1402	COA	C6P-C7P-N8P	2.42	117.19	111.88
6	B	1401	COA	C6P-C7P-N8P	2.94	118.34	111.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1394	SO4	1	0
5	A	1400	SO4	1	0
5	A	1401	SO4	7	0
6	A	1402	COA	1	0
5	B	1398	SO4	2	0
6	B	1401	COA	8	0
5	D	1394	SO4	3	0
5	D	1396	SO4	1	0
5	D	1397	SO4	1	0

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%)	0.08	8 (2%) 67 62	5, 13, 33, 69	0
2	B	387/392 (98%)	0.11	12 (3%) 52 47	6, 13, 31, 79	0
3	C	389/392 (99%)	2.86	240 (61%) 0 0	23, 66, 100, 125	0
4	D	388/392 (98%)	3.19	264 (68%) 0 0	20, 60, 118, 148	0
All	All	1552/1568 (98%)	1.56	524 (33%) 0 0	5, 37, 97, 148	0

All (524) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	392	LEU	14.7
4	D	227	SER	12.9
4	D	330	LEU	12.2
4	D	331	GLY	12.1
4	D	47	GLY	11.4
3	C	223	ALA	10.9
3	C	106	GLY	10.8
4	D	310	LEU	10.7
3	C	334	PRO	10.6
4	D	206	GLY	10.2
3	C	307	ILE	10.0
4	D	340	ASN	9.8
4	D	367	ARG	9.0
4	D	207	ARG	9.0
3	C	299	ALA	9.0
4	D	339	VAL	8.9
4	D	236	ASP	8.8
4	D	389	ILE	8.6
4	D	269	ILE	8.5
3	C	325	ALA	8.2
4	D	229	ALA	8.1

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Mol	Chain	Res	Type	RSRZ
4	D	334	PRO	7.9
3	C	362	LEU	7.8
3	C	331	GLY	7.8
4	D	170	LEU	7.7
4	D	168	TRP	7.5
4	D	358	LEU	7.4
3	C	361	LEU	7.3
4	D	165	ALA	7.3
4	D	164	VAL	7.2
4	D	208	LYS	7.0
4	D	180	VAL	7.0
3	C	333	ASP	6.9
3	C	262	ALA	6.9
4	D	264	ALA	6.7
4	D	161	ALA	6.7
4	D	228	MET	6.6
4	D	219	ILE	6.6
3	C	42	ALA	6.6
3	C	371	ARG	6.6
4	D	262	ALA	6.6
4	D	388	CYS	6.5
4	D	329	ASP	6.5
3	C	153	TYR	6.5
3	C	105	THR	6.4
4	D	209	GLY	6.4
4	D	188	ALA	6.3
4	D	303	ALA	6.3
4	D	281	VAL	6.2
2	B	207	ARG	6.2
3	C	36	SER	6.2
3	C	232	ARG	6.2
3	C	348	ALA	6.2
1	A	132	VAL	6.2
3	C	177	ALA	6.1
4	D	192	ASP	6.1
3	C	171	SER	6.0
4	D	182	SER	6.0
3	C	208	LYS	6.0
3	C	305	TRP	5.9
4	D	352	ALA	5.9
4	D	362	LEU	5.9
3	C	276	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
3	C	308	GLY	5.9
3	C	392	LEU	5.8
4	D	186	ALA	5.8
3	C	206	GLY	5.8
3	C	218	TYR	5.8
4	D	347	GLY	5.7
4	D	232	ARG	5.7
3	C	239	GLY	5.7
4	D	81	THR	5.6
4	D	105	THR	5.6
3	C	161	ALA	5.6
3	C	5	ILE	5.6
3	C	151	ALA	5.5
4	D	305	TRP	5.5
4	D	185	LYS	5.5
3	C	108	ALA	5.5
3	C	97	ALA	5.4
4	D	289	GLY	5.4
3	C	180	VAL	5.4
4	D	231	LEU	5.4
4	D	45	ALA	5.3
3	C	342	GLY	5.3
3	C	107	ASP	5.3
3	C	207	ARG	5.2
4	D	265	SER	5.2
3	C	315	ALA	5.2
4	D	327	ASN	5.2
4	D	325	ALA	5.2
3	C	204	VAL	5.2
4	D	312	LEU	5.2
3	C	320	ALA	5.1
4	D	4	SER	5.1
3	C	158	GLY	5.1
3	C	304	GLY	5.1
3	C	233	PRO	5.1
3	C	330	LEU	5.1
2	B	208	LYS	5.0
4	D	241	VAL	5.0
4	D	299	ALA	5.0
4	D	308	GLY	5.0
4	D	221	HIS	5.0
3	C	47	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
4	D	172[A]	ARG	5.0
4	D	285	PRO	5.0
3	C	6	VAL	5.0
4	D	306	LYS	5.0
4	D	42	ALA	5.0
4	D	108	ALA	5.0
4	D	240	THR	5.0
4	D	197	ASP	5.0
3	C	103	ILE	5.0
4	D	349	PRO	5.0
3	C	45	ALA	5.0
4	D	246	ALA	4.9
4	D	24	ASN	4.9
3	C	209	GLY	4.9
3	C	152	PHE	4.9
3	C	370	ALA	4.9
3	C	275	ILE	4.9
3	C	335	SER	4.9
4	D	270	GLN	4.9
4	D	173	ASP	4.8
3	C	363	PHE	4.8
4	D	107	ASP	4.8
4	D	382	GLY	4.8
3	C	337	VAL	4.8
4	D	5	ILE	4.8
4	D	369	GLY	4.8
4	D	43	GLY	4.8
4	D	211	ILE	4.8
3	C	293	ILE	4.8
4	D	346	ILE	4.8
3	C	234	ALA	4.7
3	C	221	HIS	4.7
3	C	211	ILE	4.7
4	D	233	PRO	4.7
4	D	332	TRP	4.7
4	D	106	GLY	4.7
3	C	169	GLN	4.7
3	C	360	THR	4.6
4	D	52	VAL	4.6
4	D	391	SER	4.6
3	C	306	LYS	4.5
4	D	99	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
4	D	154	GLY	4.5
3	C	312	LEU	4.5
3	C	74	ALA	4.5
4	D	179	ALA	4.4
4	D	260	SER	4.4
4	D	317	GLU	4.4
4	D	288	MET	4.4
3	C	227	SER	4.4
3	C	340[A]	ASN	4.4
3	C	170	LEU	4.4
4	D	218	TYR	4.4
3	C	60	ALA	4.3
3	C	220	ARG	4.3
3	C	98	LEU	4.3
3	C	387	MET	4.3
1	A	207	ARG	4.3
4	D	295	ALA	4.3
3	C	67	ALA	4.3
4	D	385	VAL	4.3
3	C	353	SER	4.3
3	C	49	VAL	4.3
3	C	236	ASP	4.3
3	C	80	ALA	4.3
4	D	263	GLU	4.2
4	D	283	VAL	4.2
4	D	318	ALA	4.2
4	D	292	PRO	4.2
3	C	272	LEU	4.2
4	D	343	ALA	4.2
4	D	276	VAL	4.2
3	C	237	LYS	4.2
3	C	339	VAL	4.2
4	D	49	VAL	4.2
3	C	228	MET	4.2
3	C	214	ASP	4.2
4	D	360	THR	4.1
4	D	237	LYS	4.1
3	C	188	ALA	4.1
3	C	212	THR	4.1
3	C	202	PHE	4.1
3	C	154	GLY	4.1
3	C	346	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
3	C	18	PHE	4.1
3	C	277	SER	4.1
4	D	104	ALA	4.1
2	B	132	VAL	4.1
4	D	313	VAL	4.1
3	C	115	GLY	4.0
3	C	310	LEU	4.0
4	D	375	ALA	4.0
4	D	230	LYS	4.0
4	D	293	ILE	4.0
4	D	363	PHE	4.0
4	D	153	TYR	4.0
4	D	30	LEU	4.0
4	D	225	LEU	4.0
4	D	377	LEU	4.0
4	D	357	ILE	4.0
4	D	96	VAL	4.0
4	D	275	ILE	3.9
4	D	40	GLU	3.9
3	C	155	TYR	3.9
3	C	391	SER	3.9
3	C	311	ASP	3.9
4	D	175	GLN	3.9
4	D	370	ALA	3.9
4	D	371	ARG	3.9
3	C	96	VAL	3.9
3	C	321	ALA	3.9
4	D	348	ALA	3.9
3	C	258	LEU	3.9
4	D	272	LEU	3.9
4	D	390	GLU	3.9
3	C	301	GLU	3.8
3	C	210	ASP	3.8
3	C	230	LYS	3.8
3	C	292	PRO	3.8
4	D	290	THR	3.8
3	C	173	ASP	3.8
3	C	46	ALA	3.8
4	D	181	ALA	3.8
3	C	182	SER	3.8
4	D	167	GLN	3.8
3	C	92	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
3	C	229	ALA	3.8
4	D	326	VAL	3.8
3	C	367	ARG	3.8
3	C	323	ALA	3.7
3	C	389	ILE	3.7
3	C	30	LEU	3.7
4	D	39	LEU	3.7
4	D	194[A]	ARG	3.7
3	C	328	LYS	3.7
3	C	302	ARG	3.7
4	D	76	VAL	3.7
3	C	225	LEU	3.7
3	C	257	LEU	3.7
3	C	278	TRP	3.7
4	D	171	SER	3.6
4	D	280	THR	3.6
3	C	238	GLU	3.6
4	D	271	PRO	3.6
4	D	223	ALA	3.6
4	D	301	GLU	3.6
4	D	196	LYS	3.6
3	C	256	ALA	3.6
4	D	235	PHE	3.6
3	C	344	ILE	3.6
4	D	287	VAL	3.6
4	D	361	LEU	3.5
3	C	226	ASP	3.5
3	C	313	VAL	3.5
3	C	58	LEU	3.5
3	C	37	ALA	3.5
3	C	4	SER	3.5
3	C	261	GLU	3.5
4	D	373	GLY	3.5
3	C	43	GLY	3.5
3	C	374	LEU	3.5
1	A	206	GLY	3.4
4	D	203	ILE	3.4
4	D	15	VAL	3.4
3	C	357	ILE	3.4
4	D	22	PHE	3.4
4	D	152	PHE	3.4
2	B	133	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
4	D	278	TRP	3.4
4	D	368	ARG	3.4
4	D	98	LEU	3.4
3	C	255	ALA	3.3
4	D	309	ASP	3.3
3	C	21	ALA	3.3
3	C	104	ALA	3.3
1	A	208	LYS	3.3
4	D	294	PRO	3.3
3	C	195	PHE	3.3
4	D	212	THR	3.3
4	D	224	THR	3.3
3	C	201	PRO	3.3
3	C	231	LEU	3.3
4	D	7	ILE	3.3
3	C	254	ALA	3.3
4	D	234	ALA	3.3
4	D	162	GLU	3.3
4	D	199	ILE	3.3
2	B	206	GLY	3.2
3	C	345	ALA	3.2
1	A	238	GLU	3.2
3	C	224	THR	3.2
3	C	57	VAL	3.2
3	C	241	VAL	3.2
4	D	298	LYS	3.2
3	C	77	PRO	3.2
4	D	46	ALA	3.2
3	C	317	GLU	3.2
4	D	341	GLY	3.2
4	D	315	ALA	3.2
4	D	350	ILE	3.2
3	C	99	GLY	3.2
3	C	176	ASP	3.1
3	C	110	ILE	3.1
3	C	219	ILE	3.1
3	C	303	ALA	3.1
3	C	179	ALA	3.1
4	D	10	ALA	3.1
4	D	36	SER	3.1
2	B	131	GLY	3.1
3	C	181	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	332	TRP	3.1
3	C	289	GLY	3.1
4	D	300	LEU	3.1
4	D	365	MET	3.1
4	D	178	PHE	3.1
4	D	195	PHE	3.1
4	D	190	GLN	3.1
4	D	226	ASP	3.1
4	D	14	ALA	3.0
4	D	151	ALA	3.0
4	D	381	GLY	3.0
4	D	220	ARG	3.0
3	C	240	THR	3.0
3	C	298	LYS	3.0
3	C	253	ALA	3.0
4	D	103	ILE	3.0
4	D	304	GLY	3.0
4	D	302	ARG	3.0
4	D	316	ASN	3.0
4	D	324	CYS	3.0
4	D	239	GLY	3.0
3	C	215	ALA	3.0
3	C	22	PHE	2.9
4	D	21	ALA	2.9
3	C	338	ASN	2.9
4	D	93	LEU	2.9
4	D	238	GLU	2.9
4	D	273	GLY	2.9
4	D	222	GLY	2.9
4	D	268	GLY	2.9
4	D	111	ILE	2.9
4	D	379	ILE	2.9
3	C	326	VAL	2.9
3	C	235	PHE	2.9
4	D	160	THR	2.9
4	D	37	ALA	2.9
4	D	72	MET	2.9
4	D	374	LEU	2.9
3	C	263	GLU	2.9
3	C	32	ALA	2.9
4	D	337	VAL	2.9
4	D	338	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	210	ASP	2.8
3	C	88	LEU	2.8
4	D	213	VAL	2.8
4	D	83	TRP	2.8
3	C	48	GLU	2.8
3	C	336	ILE	2.8
3	C	138	LYS	2.8
3	C	13	THR	2.8
3	C	83	TRP	2.8
4	D	113	ALA	2.8
4	D	372	LYS	2.8
4	D	169	GLN	2.8
4	D	384	GLY	2.8
4	D	274	ARG	2.8
4	D	279	ALA	2.7
3	C	81	THR	2.7
3	C	309	ASP	2.7
1	A	209	GLY	2.7
2	B	209	GLY	2.7
3	C	8	ALA	2.7
4	D	33	THR	2.7
3	C	41	ARG	2.7
2	B	135	GLY	2.7
4	D	286	LYS	2.7
3	C	168	TRP	2.7
4	D	59	PRO	2.7
4	D	44	VAL	2.7
4	D	328	LYS	2.7
3	C	266	ARG	2.7
4	D	333	ASP	2.7
1	A	237	LYS	2.7
3	C	53	ILE	2.7
3	C	111	ILE	2.7
3	C	132	VAL	2.7
3	C	163	ASN	2.7
4	D	50	ASN	2.7
3	C	191	LYS	2.7
3	C	93	LEU	2.7
4	D	297	ARG	2.7
3	C	144	ILE	2.6
4	D	245	ASN	2.6
4	D	79	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
4	D	193	GLY	2.6
3	C	33	THR	2.6
3	C	17	SER	2.6
3	C	349	PRO	2.6
3	C	205	LYS	2.6
3	C	165	ALA	2.6
3	C	366	LYS	2.6
3	C	199	ILE	2.6
4	D	6	VAL	2.6
3	C	297	ARG	2.6
3	C	192	ASP	2.6
3	C	318	ALA	2.6
3	C	347	GLY	2.6
3	C	140	ILE	2.6
3	C	197	ASP	2.6
4	D	335	SER	2.6
3	C	343	ALA	2.5
3	C	271	PRO	2.5
3	C	369	GLY	2.5
4	D	255	ALA	2.5
4	D	266	ARG	2.5
3	C	166	LYS	2.5
4	D	174	GLU	2.5
4	D	215	ALA	2.5
4	D	249	LEU	2.5
4	D	319	PHE	2.5
4	D	140	ILE	2.5
4	D	355	ALA	2.5
3	C	174	GLU	2.5
4	D	13	THR	2.5
4	D	23	ALA	2.5
4	D	131	GLY	2.5
3	C	26	PRO	2.5
3	C	24	ASN	2.4
4	D	323	ALA	2.4
4	D	366	LYS	2.4
4	D	183	GLN	2.4
3	C	38	VAL	2.4
3	C	213	VAL	2.4
4	D	38	VAL	2.4
4	D	75	GLY	2.4
4	D	354	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	386	ALA	2.4
3	C	358	LEU	2.4
4	D	216	ASP	2.4
3	C	34	VAL	2.4
2	B	136	ASP	2.4
3	C	265	SER	2.4
4	D	205	LYS	2.4
4	D	257	LEU	2.4
3	C	10	ALA	2.4
4	D	139	MET	2.4
3	C	91	SER	2.4
4	D	177	ALA	2.3
3	C	283	VAL	2.3
4	D	342	GLY	2.3
3	C	148	LEU	2.3
4	D	321	ALA	2.3
3	C	76	VAL	2.3
3	C	350	ILE	2.3
4	D	110	ILE	2.3
4	D	376	THR	2.3
3	C	79	GLU	2.3
3	C	368	ARG	2.3
2	B	238	GLU	2.3
3	C	143	MET	2.3
3	C	300	LEU	2.3
3	C	365	MET	2.3
4	D	387	MET	2.3
3	C	245	ASN	2.3
4	D	187	GLU	2.3
4	D	256	ALA	2.3
3	C	324	CYS	2.2
4	D	204	VAL	2.2
3	C	319	PHE	2.2
3	C	290	THR	2.2
3	C	198	GLU	2.2
3	C	294	PRO	2.2
3	C	167	GLN	2.2
3	C	184	ASN	2.2
2	B	237	LYS	2.2
4	D	136	ASP	2.2
4	D	150	ASP	2.2
3	C	269	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	40	GLU	2.2
4	D	109	SER	2.2
4	D	320	ALA	2.2
3	C	285	PRO	2.2
3	C	282	GLY	2.2
4	D	267	ARG	2.2
3	C	385	VAL	2.2
3	C	86	ASN	2.1
4	D	214	ASP	2.1
3	C	372	LYS	2.1
4	D	258	LEU	2.1
3	C	120	SER	2.1
1	A	232	ARG	2.1
4	D	51	GLU	2.1
4	D	201	PRO	2.1
3	C	189	ALA	2.1
3	C	7	ILE	2.1
3	C	295	ALA	2.1
4	D	184	ASN	2.1
3	C	162	GLU	2.1
4	D	94	ARG	2.1
4	D	247	SER	2.1
3	C	259	MET	2.1
2	B	236	ASP	2.1
3	C	203	ILE	2.0
4	D	8	ALA	2.0
4	D	189	ALA	2.0
3	C	296	SER	2.0
4	D	9	SER	2.0
4	D	148	LEU	2.0
3	C	268	GLY	2.0
4	D	102	GLN	2.0
4	D	123	PRO	2.0
4	D	166	LYS	2.0
4	D	261	GLU	2.0
3	C	159	THR	2.0
3	C	112	VAL	2.0
3	C	359	ASN	2.0
4	D	20	GLY	2.0
4	D	141	ASP	2.0
4	D	147	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CSD	B	378	8/9	0.99	0.08	-	4,9,24,109	0
1	CSD	A	378	8/9	0.99	0.09	-	7,13,23,32	0
4	CSO	D	89	7/8	0.76	0.17	-	36,42,63,77	0
2	CSO	B	89	7/8	0.95	0.10	-	4,10,34,73	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	A	1400	5/5	0.82	0.36	30.23	60,60,69,75	0
5	SO4	A	1401	5/5	0.98	0.45	29.45	28,44,49,50	0
5	SO4	A	1397	5/5	0.95	0.29	7.39	47,48,56,56	0
7	CL	D	1399	1/1	0.07	0.38	6.25	80,80,80,80	0
5	SO4	D	1397	5/5	0.69	0.44	4.27	120,121,122,123	0
8	NA	C	1395	1/1	0.83	0.39	4.05	60,60,60,60	0
6	COA	B	1401	48/48	0.83	0.19	3.90	20,36,80,112	0
6	COA	A	1402	48/48	0.83	0.18	2.70	21,32,63,131	0
5	SO4	A	1396	5/5	0.86	0.18	2.50	31,39,50,57	0
5	SO4	C	1393	5/5	0.75	0.23	1.91	108,108,109,109	0
5	SO4	D	1394	5/5	0.88	0.18	-0.19	63,70,71,75	0
8	NA	C	1394	1/1	0.90	0.18	-0.38	34,34,34,34	0
8	NA	D	1398	1/1	0.91	0.20	-1.41	38,38,38,38	0
7	CL	C	1396	1/1	0.77	0.14	-1.91	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	CL	B	1400	1/1	0.98	0.05	-3.22	28,28,28,28	0
5	SO4	A	1394	5/5	0.98	0.17	-	41,43,48,48	0
5	SO4	B	1402	5/5	0.93	0.38	-	75,75,76,76	0
5	SO4	A	1398	5/5	0.89	0.26	-	71,78,79,81	0
5	SO4	B	1398	5/5	0.92	0.19	-	45,51,56,57	0
5	SO4	C	1397	5/5	0.93	0.40	-	84,84,85,86	0
5	SO4	A	1403	5/5	0.80	0.52	-	94,94,95,98	0
5	SO4	C	1399	5/5	0.68	0.28	-	90,91,94,94	0
5	SO4	C	1398	5/5	0.78	0.39	-	96,97,97,98	0
5	SO4	A	1399	5/5	0.63	0.35	-	95,99,101,101	0
5	SO4	D	1396	5/5	0.92	0.27	-	52,59,70,71	0
5	SO4	B	1397	5/5	0.91	0.30	-	66,66,71,73	0
5	SO4	B	1403	5/5	0.90	0.49	-	86,87,88,89	0
5	SO4	D	1395	5/5	0.78	0.31	-	89,89,90,91	0
5	SO4	B	1404	5/5	0.93	0.45	-	77,77,79,82	0
5	SO4	B	1399	5/5	0.92	0.44	-	78,78,80,81	0
5	SO4	B	1396	5/5	0.90	0.21	-	45,49,57,63	0
5	SO4	A	1395	5/5	0.94	0.18	-	46,54,58,59	0
5	SO4	B	1395	5/5	0.97	0.16	-	47,50,52,55	0

6.5 Other polymers

There are no such residues in this entry.