



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 11:07 AM BST

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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

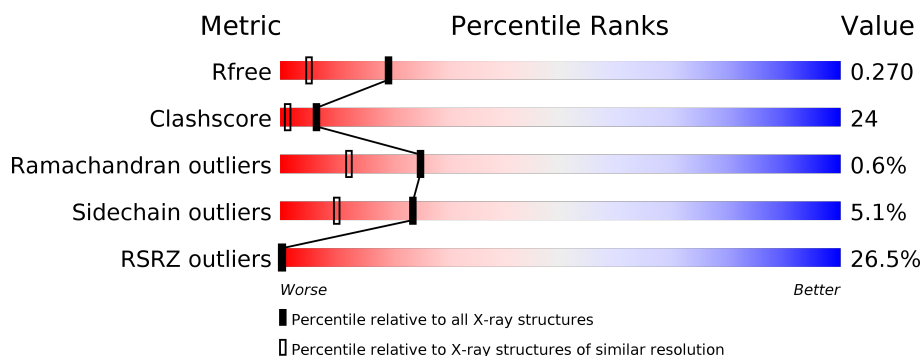
1 Overall quality at a glance

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	<div> <div style="width: 100%;"></div> <div> <div style="width: 85%;"></div> <div style="width: 13%;"></div> <div style="width: 2%;"></div> </div> </div>
2	B	392	<div> <div style="width: 100%;"></div> <div> <div style="width: 80%;"></div> <div style="width: 17%;"></div> <div style="width: 3%;"></div> </div> </div>
3	C	392	<div> <div style="width: 49%;"></div> <div style="width: 53%;"></div> <div style="width: 43%;"></div> <div style="width: 2%;"></div> </div>
4	D	392	<div> <div style="width: 54%;"></div> <div style="width: 49%;"></div> <div style="width: 46%;"></div> <div style="width: 2%;"></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	1401	-	-	X	-
5	SO4	B	1398	-	-	X	-
5	SO4	D	1394	-	-	X	-
5	SO4	D	1397	-	-	-	X
7	CL	C	1396	-	-	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 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

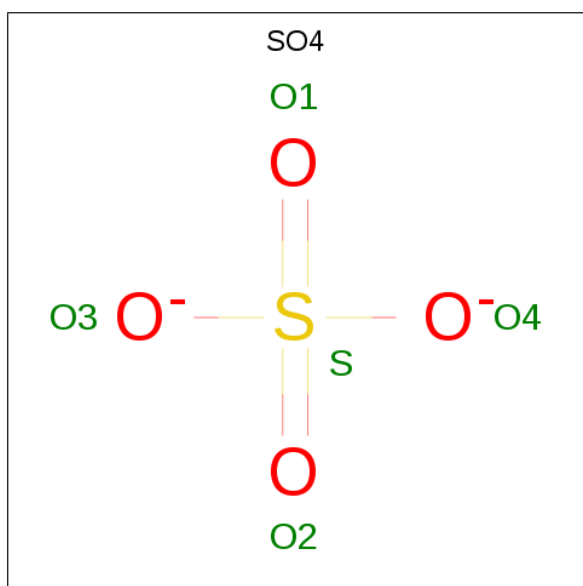
- Molecule 4 is a protein called ACETYL-COA ACETYLTRANSFERASE.

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).



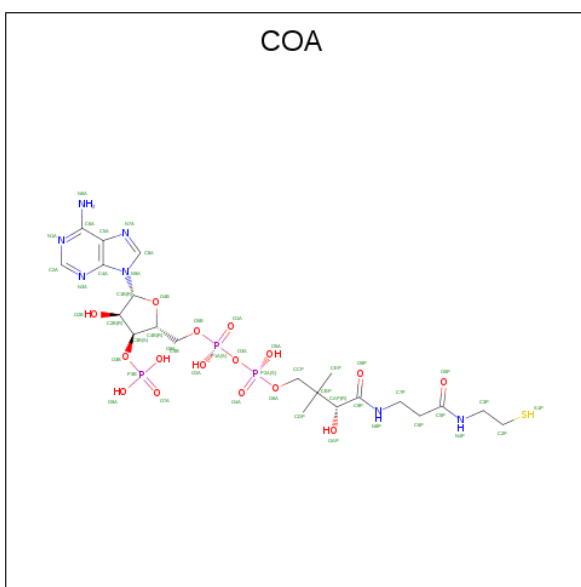
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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		

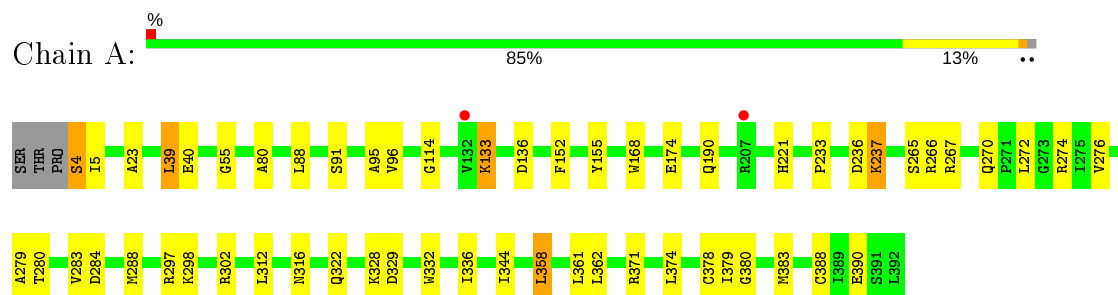
- Molecule 9 is water.

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

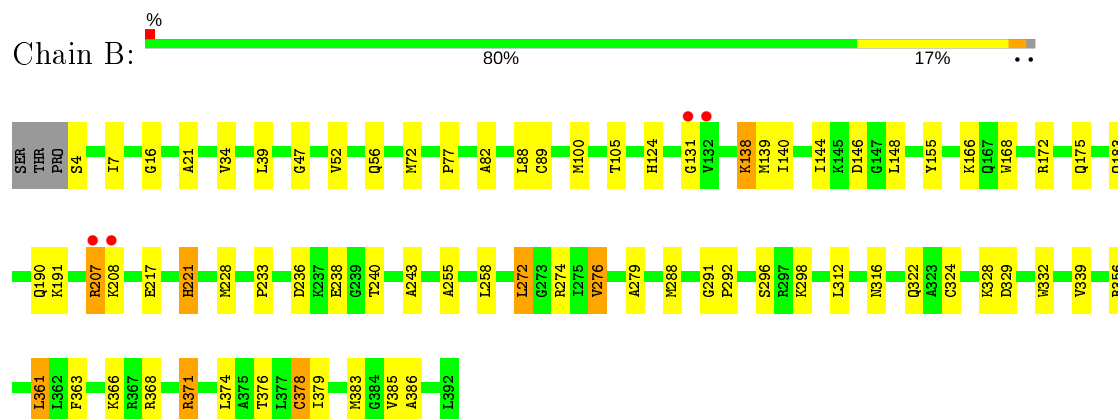
3 Residue-property plots [i](#)

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

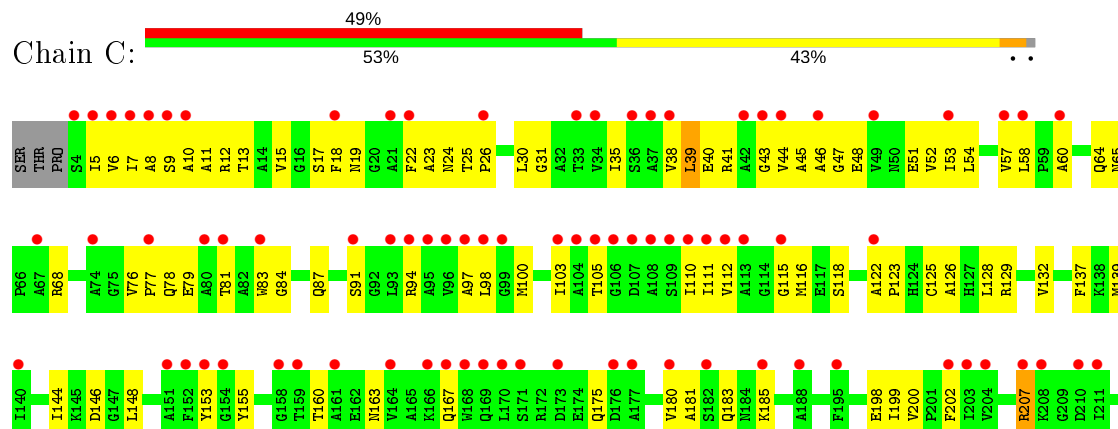
• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

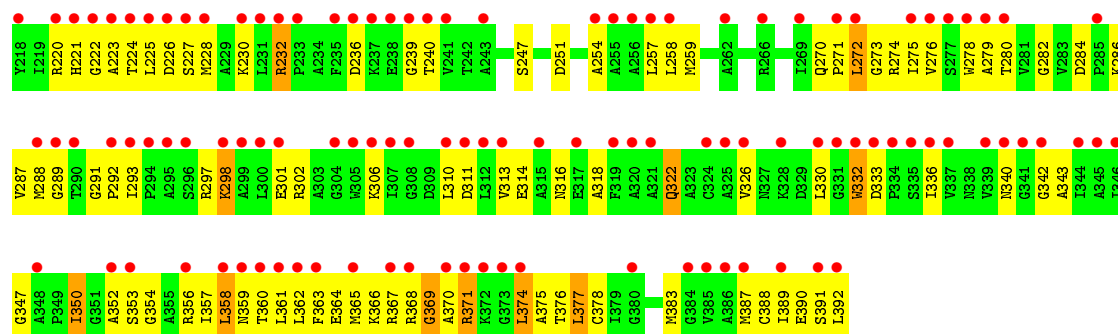


• Molecule 2: ACETYL-COA ACETYLTRANSFERASE

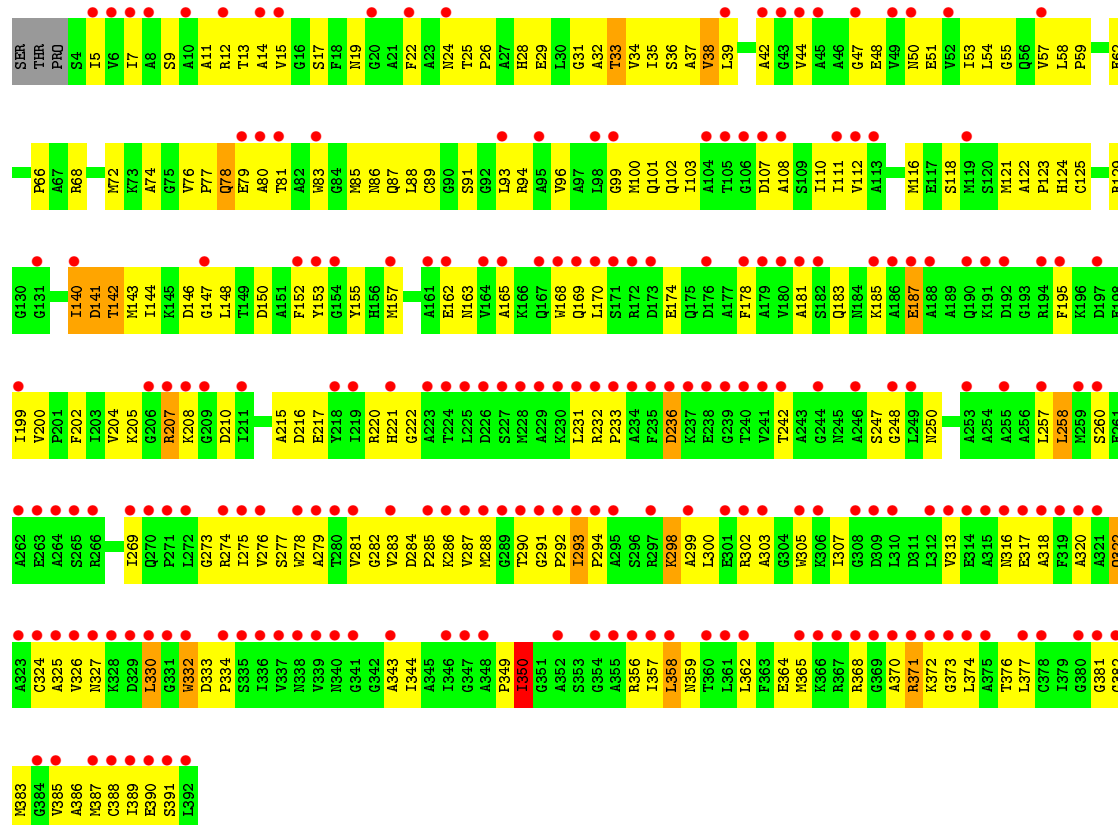


• Molecule 3: ACETYL-COA ACETYLTRANSFERASE





● 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) 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 0.232 , 0.270	Depositor DCC
R_{free} test set	9051 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.159 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
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

Continued on next page...

Continued from previous page...

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: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

Continued on next page...

Continued from previous page...

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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:302:ARG:NH1	9:C:2112:HOH:O	2.42	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ALA:HB2	9:A:2064:HOH:O	2.13	0.49
3:C:153:TYR:CE1	3:C:286:LYS:HG3	2.48	0.49
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
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
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:7:ILE:HG12	3:C:258:LEU:HD11	1.96	0.47
3:C:278:TRP:HA	3:C:387:MET:HA	1.94	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:122:ALA:HA	9:C:2026:HOH:O	2.15	0.45
3:C:146:ASP:HB3	5:D:1394:SO4:S	2.57	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:57:VAL:HG21	3:C:350:ILE:CG2	2.47	0.43
3:C:47:GLY:HA2	3:C:77:PRO:CG	2.45	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
3:C:15:VAL:HG11	3:C:347:GLY:HA3	2.02	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:282:GLY:O	4:D:79:GLU:HA	2.21	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
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 [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%)	41	27
3	C	389/392 (99%)	350 (90%)	36 (9%)	3 (1%)	19	7
4	D	389/392 (99%)	352 (90%)	31 (8%)	6 (2%)	10	2
All	All	1561/1568 (100%)	1456 (93%)	95 (6%)	10 (1%)	25	12

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%)	35	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	280/276 (101%)	268 (96%)	12 (4%)	29	14
3	C	277/278 (100%)	260 (94%)	17 (6%)	18	7
4	D	277/277 (100%)	260 (94%)	17 (6%)	18	7
All	All	1113/1108 (100%)	1057 (95%)	56 (5%)	24	10

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
2	CSD	B	378	2	3,7,8	0.66	0	1,8,10	2.40	1 (100%)
1	CSD	A	378	1	3,7,8	0.75	0	1,8,10	1.94	0
4	CSO	D	89	4	3,6,7	0.60	0	0,6,8	0.00	-
2	CSO	B	89	2	3,6,7	0.60	0	0,6,8	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSD	B	378	2	-	0/2/6/8	-
1	CSD	A	378	1	-	0/2/6/8	-
4	CSO	D	89	4	-	1/1/5/7	-
2	CSO	B	89	2	-	0/1/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	378	CSD	OD1-SG-CB	2.40	110.10	105.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	89	CSO	N-CA-CB-SG

There are no ring outliers.

4 monomers are involved in 8 short contacts:

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

5.5 Carbohydrates

There are no monosaccharides 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	1399	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	D	1395	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	A	1395	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	A	1394	-	4,4,4	0.17	0	6,6,6	0.20	0
5	SO4	B	1402	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	C	1397	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	1403	-	4,4,4	0.13	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	C	1399	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	C	1398	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	D	1394	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	D	1396	-	4,4,4	0.13	0	6,6,6	0.10	0
5	SO4	B	1399	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	1396	-	4,4,4	0.14	0	6,6,6	0.09	0
6	COA	B	1401	-	41,50,50	1.56	5 (12%)	52,75,75	1.51	7 (13%)
5	SO4	A	1398	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	1398	-	4,4,4	0.17	0	6,6,6	0.15	0
5	SO4	C	1393	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	A	1397	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	A	1400	-	4,4,4	0.16	0	6,6,6	0.14	0
5	SO4	A	1396	-	4,4,4	0.19	0	6,6,6	0.09	0
5	SO4	B	1397	-	4,4,4	0.13	0	6,6,6	0.08	0
5	SO4	B	1403	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	A	1401	-	4,4,4	0.16	0	6,6,6	0.22	0
5	SO4	B	1404	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	D	1397	-	4,4,4	0.14	0	6,6,6	0.09	0
6	COA	A	1402	-	41,50,50	1.53	4 (9%)	52,75,75	1.23	8 (15%)
5	SO4	B	1395	-	4,4,4	0.17	0	6,6,6	0.09	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
6	COA	B	1401	-	-	10/44/64/64	0/3/3/3
6	COA	A	1402	-	-	3/44/64/64	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1401	COA	P3B-O7A	6.17	1.70	1.50
6	A	1402	COA	P3B-O7A	6.17	1.70	1.50
6	B	1401	COA	P3B-O8A	4.05	1.70	1.54
6	A	1402	COA	P3B-O8A	3.96	1.70	1.54
6	B	1401	COA	P2A-O5A	3.18	1.70	1.55
6	A	1402	COA	P2A-O5A	3.15	1.70	1.55
6	B	1401	COA	P1A-O2A	3.14	1.70	1.55
6	A	1402	COA	P1A-O2A	3.00	1.69	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1401	COA	C2A-N3A	2.03	1.35	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1401	COA	C7P-C6P-C5P	-4.64	104.63	112.36
6	B	1401	COA	P2A-O3A-P1A	-4.19	118.46	132.83
6	B	1401	COA	C7P-N8P-C9P	-3.21	116.86	122.59
6	B	1401	COA	C6P-C7P-N8P	3.19	118.34	111.90
6	A	1402	COA	N3A-C2A-N1A	-3.18	123.71	128.68
6	A	1402	COA	C7P-N8P-C9P	-3.02	117.20	122.59
6	A	1402	COA	P2A-O3A-P1A	-2.98	122.61	132.83
6	B	1401	COA	C3P-N4P-C5P	-2.90	117.45	122.84
6	A	1402	COA	C6P-C7P-N8P	2.62	117.19	111.90
6	A	1402	COA	C7P-C6P-C5P	-2.61	108.02	112.36
6	B	1401	COA	N3A-C2A-N1A	-2.43	124.89	128.68
6	B	1401	COA	C6P-C5P-N4P	2.31	120.31	116.42
6	A	1402	COA	C2A-N1A-C6A	2.19	122.51	118.75
6	A	1402	COA	C1B-N9A-C4A	-2.12	122.92	126.64
6	A	1402	COA	C5A-C6A-N1A	-2.02	115.78	120.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

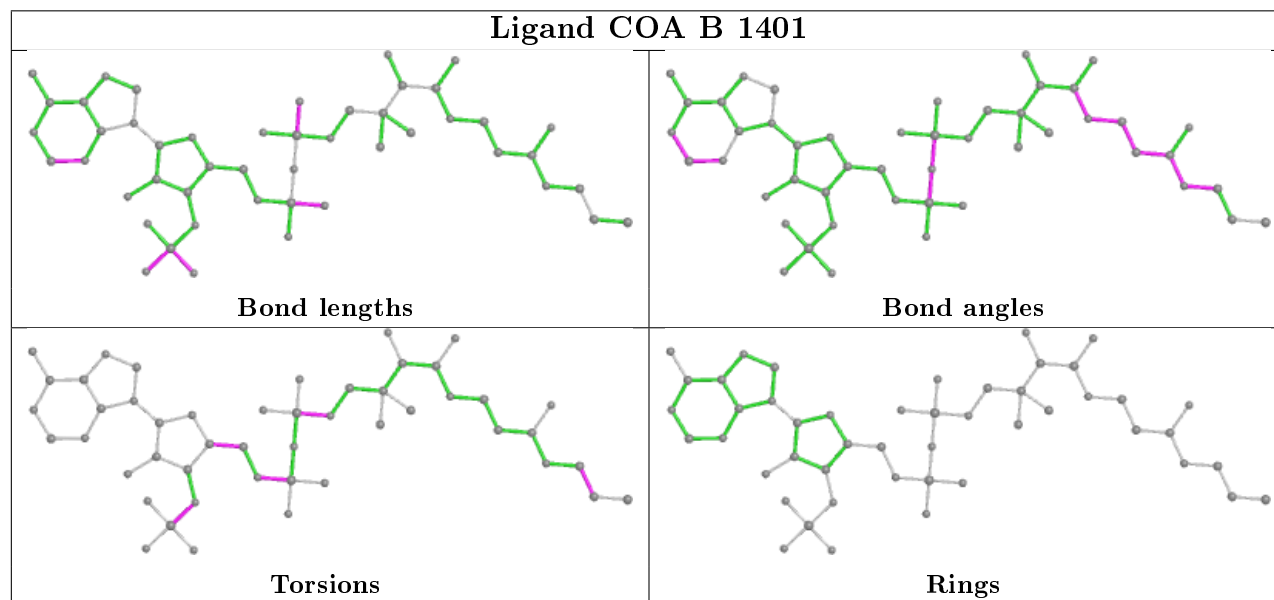
Mol	Chain	Res	Type	Atoms
6	B	1401	COA	C3B-O3B-P3B-O7A
6	B	1401	COA	C5B-O5B-P1A-O1A
6	B	1401	COA	C5B-O5B-P1A-O2A
6	A	1402	COA	C2P-C3P-N4P-C5P
6	B	1401	COA	O4B-C4B-C5B-O5B
6	B	1401	COA	S1P-C2P-C3P-N4P
6	B	1401	COA	C3B-O3B-P3B-O9A
6	B	1401	COA	C3B-C4B-C5B-O5B
6	A	1402	COA	P1A-O3A-P2A-O4A
6	B	1401	COA	C5B-O5B-P1A-O3A
6	B	1401	COA	CCP-O6A-P2A-O3A
6	B	1401	COA	CCP-O6A-P2A-O5A
6	A	1402	COA	CCP-O6A-P2A-O4A

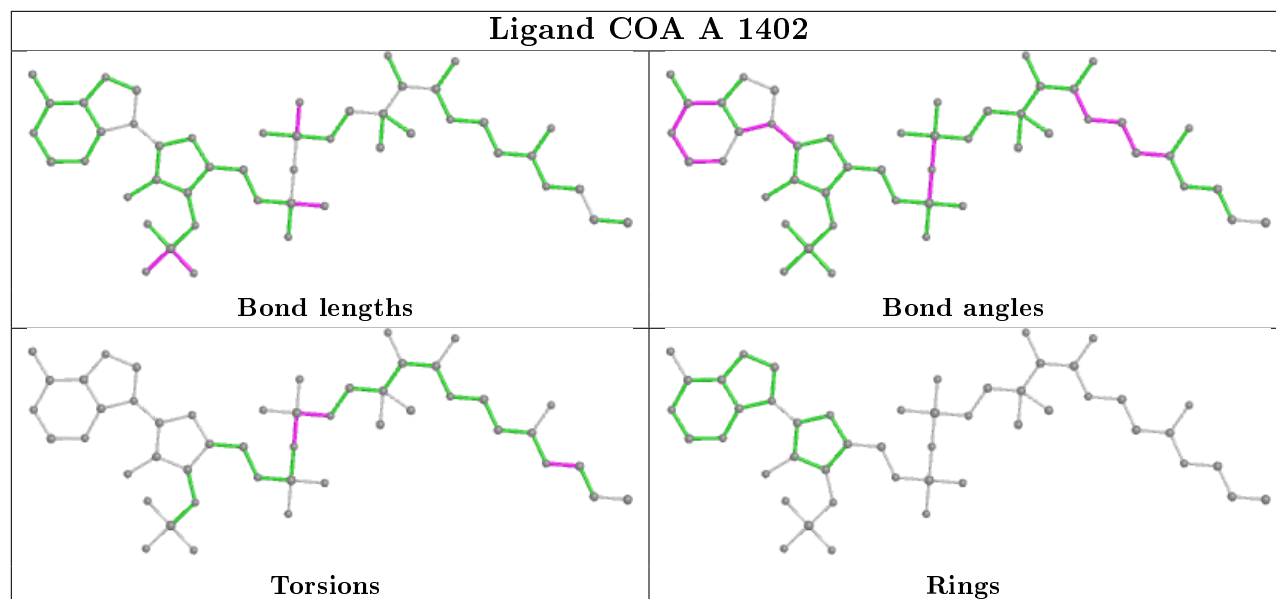
There are no ring outliers.

9 monomers are involved in 25 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/392 (98%)	-0.37	2 (0%) 91 89	5, 13, 33, 69	0
2	B	387/392 (98%)	-0.36	4 (1%) 82 80	6, 13, 31, 79	0
3	C	389/392 (99%)	2.34	192 (49%) 0 0	23, 66, 100, 125	0
4	D	388/392 (98%)	2.69	213 (54%) 0 0	20, 60, 118, 148	0
All	All	1552/1568 (98%)	1.08	411 (26%) 0 0	5, 37, 97, 148	0

All (411) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	307	ILE	14.0
4	D	392	LEU	13.3
4	D	331	GLY	12.5
4	D	330	LEU	12.3
4	D	170	LEU	11.4
4	D	206	GLY	11.0
4	D	358	LEU	9.9
3	C	325	ALA	9.7
4	D	310	LEU	9.5
3	C	223	ALA	9.3
4	D	367	ARG	9.2
3	C	334	PRO	9.2
3	C	299	ALA	9.1
4	D	339	VAL	7.8
4	D	208	LYS	7.5
3	C	312	LEU	7.4
4	D	389	ILE	7.4
3	C	106	GLY	7.3
3	C	258	LEU	7.3
1	A	132	VAL	7.2
4	D	229	ALA	7.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	275	ILE	7.0
3	C	320	ALA	7.0
3	C	361	LEU	6.8
4	D	388	CYS	6.8
3	C	42	ALA	6.7
4	D	260	SER	6.5
4	D	340	ASN	6.5
4	D	325	ALA	6.4
4	D	185	LYS	6.4
4	D	334	PRO	6.4
4	D	269	ILE	6.4
4	D	262	ALA	6.3
4	D	326	VAL	6.2
4	D	108	ALA	6.2
3	C	177	ALA	6.2
3	C	5	ILE	6.2
4	D	5	ILE	6.2
4	D	369	GLY	6.2
4	D	192	ASP	6.1
3	C	276	VAL	6.1
4	D	186	ALA	6.0
4	D	329	ASP	6.0
4	D	289	GLY	5.9
4	D	227	SER	5.9
4	D	228	MET	5.8
3	C	371	ARG	5.8
3	C	340[A]	ASN	5.8
4	D	207	ARG	5.8
3	C	107	ASP	5.8
3	C	315	ALA	5.7
3	C	293	ILE	5.7
4	D	81	THR	5.7
4	D	168	TRP	5.7
4	D	165	ALA	5.7
3	C	6	VAL	5.6
4	D	362	LEU	5.6
4	D	197	ASP	5.5
4	D	232	ARG	5.5
4	D	246	ALA	5.4
3	C	180	VAL	5.4
4	D	265	SER	5.4
3	C	161	ALA	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	211	ILE	5.4
4	D	303	ALA	5.3
4	D	164	VAL	5.3
4	D	281	VAL	5.3
3	C	305	TRP	5.3
4	D	279	ALA	5.3
4	D	375	ALA	5.3
4	D	312	LEU	5.3
4	D	387	MET	5.2
4	D	332	TRP	5.2
4	D	180	VAL	5.2
4	D	316	ASN	5.2
4	D	179	ALA	5.2
4	D	347	GLY	5.2
4	D	47	GLY	5.1
4	D	219	ILE	5.1
3	C	272	LEU	5.1
3	C	43	GLY	5.1
3	C	337	VAL	5.0
3	C	97	ALA	5.0
4	D	181	ALA	5.0
4	D	315	ALA	5.0
3	C	372	LYS	5.0
3	C	353	SER	4.9
4	D	6	VAL	4.9
4	D	385	VAL	4.9
3	C	105	THR	4.8
3	C	36	SER	4.8
3	C	333	ASP	4.8
4	D	377	LEU	4.8
3	C	153	TYR	4.8
4	D	236	ASP	4.8
4	D	341	GLY	4.8
4	D	240	THR	4.8
4	D	225	LEU	4.7
4	D	231	LEU	4.7
4	D	188	ALA	4.7
3	C	239	GLY	4.6
4	D	209	GLY	4.6
4	D	305	TRP	4.6
3	C	321	ALA	4.6
2	B	132	VAL	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	169	GLN	4.6
3	C	4	SER	4.6
4	D	313	VAL	4.6
3	C	301	GLU	4.5
3	C	362	LEU	4.5
3	C	60	ALA	4.4
3	C	204	VAL	4.4
3	C	311	ASP	4.4
4	D	278	TRP	4.4
3	C	220	ARG	4.4
3	C	278	TRP	4.3
3	C	392	LEU	4.3
2	B	207	ARG	4.3
4	D	272	LEU	4.3
3	C	277	SER	4.3
4	D	15	VAL	4.3
4	D	360	THR	4.2
4	D	287	VAL	4.2
4	D	161	ALA	4.2
4	D	107	ASP	4.2
3	C	348	ALA	4.2
4	D	391	SER	4.2
3	C	342	GLY	4.2
4	D	7	ILE	4.2
4	D	382	GLY	4.1
3	C	391	SER	4.1
3	C	367	ARG	4.1
4	D	352	ALA	4.1
3	C	331	GLY	4.0
3	C	262	ALA	4.0
3	C	341	GLY	4.0
3	C	374	LEU	4.0
4	D	39	LEU	4.0
4	D	42	ALA	3.9
3	C	360	THR	3.9
4	D	182	SER	3.9
4	D	317	GLU	3.9
4	D	370	ALA	3.9
3	C	389	ILE	3.9
3	C	218	TYR	3.9
4	D	233	PRO	3.9
3	C	46	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	308	GLY	3.8
3	C	227	SER	3.8
4	D	171	SER	3.8
4	D	324	CYS	3.8
3	C	115	GLY	3.8
4	D	292	PRO	3.8
3	C	108	ALA	3.8
4	D	239	GLY	3.7
3	C	339	VAL	3.7
3	C	67	ALA	3.7
4	D	270	GLN	3.7
4	D	285	PRO	3.7
3	C	269	ILE	3.7
4	D	83	TRP	3.7
4	D	255	ALA	3.7
4	D	162	GLU	3.6
3	C	152	PHE	3.6
3	C	363	PHE	3.6
4	D	264	ALA	3.6
3	C	310	LEU	3.6
3	C	255	ALA	3.5
3	C	103	ILE	3.5
3	C	226	ASP	3.5
3	C	57	VAL	3.5
4	D	280	THR	3.5
2	B	208	LYS	3.5
3	C	241	VAL	3.5
3	C	370	ALA	3.5
4	D	8	ALA	3.5
4	D	226	ASP	3.5
4	D	290	THR	3.5
4	D	24	ASN	3.5
4	D	172[A]	ARG	3.5
4	D	390	GLU	3.5
4	D	361	LEU	3.4
3	C	151	ALA	3.4
4	D	343	ALA	3.4
3	C	225	LEU	3.4
4	D	44	VAL	3.4
3	C	256	ALA	3.4
3	C	170	LEU	3.4
4	D	321	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	233	PRO	3.3
4	D	357	ILE	3.3
3	C	49	VAL	3.3
3	C	80	ALA	3.3
3	C	330	LEU	3.3
3	C	8	ALA	3.3
4	D	275	ILE	3.3
4	D	147	GLY	3.2
4	D	241	VAL	3.2
3	C	298	LYS	3.2
4	D	320	ALA	3.2
3	C	292	PRO	3.2
4	D	14	ALA	3.2
4	D	113	ALA	3.2
4	D	293	ILE	3.2
3	C	257	LEU	3.2
4	D	105	THR	3.2
4	D	99	GLY	3.2
4	D	234	ALA	3.2
3	C	346	ILE	3.2
4	D	346	ILE	3.2
4	D	283	VAL	3.2
4	D	295	ALA	3.1
4	D	319	PHE	3.1
3	C	328	LYS	3.1
4	D	372	LYS	3.1
4	D	384	GLY	3.1
3	C	158	GLY	3.1
4	D	230	LYS	3.1
4	D	253	ALA	3.1
3	C	83	TRP	3.1
3	C	44	VAL	3.1
3	C	313	VAL	3.1
4	D	237	LYS	3.1
3	C	93	LEU	3.1
3	C	10	ALA	3.1
3	C	113	ALA	3.1
3	C	228	MET	3.1
4	D	218	TYR	3.1
4	D	299	ALA	3.1
4	D	302	ARG	3.1
3	C	7	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	211	ILE	3.1
3	C	243	ALA	3.1
3	C	254	ALA	3.1
3	C	232	ARG	3.0
4	D	195	PHE	3.0
4	D	276	VAL	3.0
3	C	22	PHE	3.0
3	C	235	PHE	3.0
4	D	318	ALA	3.0
4	D	327	ASN	3.0
4	D	191	LYS	3.0
3	C	365	MET	3.0
3	C	58	LEU	3.0
4	D	10	ALA	3.0
4	D	274	ARG	3.0
3	C	332	TRP	3.0
4	D	169	GLN	3.0
3	C	74	ALA	3.0
4	D	257	LEU	3.0
4	D	271	PRO	3.0
3	C	202	PHE	3.0
3	C	387	MET	2.9
3	C	324	CYS	2.9
3	C	110	ILE	2.9
3	C	203	ILE	2.9
3	C	195	PHE	2.9
3	C	240	THR	2.8
3	C	38	VAL	2.8
4	D	368	ARG	2.8
3	C	99	GLY	2.8
4	D	338	ASN	2.8
4	D	223	ALA	2.8
4	D	365	MET	2.8
4	D	187	GLU	2.8
4	D	235	PHE	2.8
1	A	207	ARG	2.8
3	C	210	ASP	2.8
3	C	306	LYS	2.8
3	C	386	ALA	2.8
4	D	306	LYS	2.8
3	C	94	ARG	2.8
3	C	96	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	57	VAL	2.8
4	D	314	GLU	2.8
3	C	356	ARG	2.8
4	D	112	VAL	2.8
3	C	230	LYS	2.7
3	C	280	THR	2.7
4	D	95	ALA	2.7
4	D	355	ALA	2.7
3	C	104	ALA	2.7
4	D	374	LEU	2.7
3	C	173	ASP	2.7
3	C	21	ALA	2.7
3	C	279	ALA	2.7
3	C	221	HIS	2.7
4	D	373	GLY	2.7
3	C	122	ALA	2.7
4	D	153	TYR	2.7
3	C	358	LEU	2.7
4	D	238	GLU	2.7
4	D	80	ALA	2.7
4	D	356	ARG	2.7
4	D	371	ARG	2.7
3	C	98	LEU	2.7
4	D	221	HIS	2.7
4	D	335	SER	2.7
3	C	295	ALA	2.6
3	C	112	VAL	2.6
3	C	164	VAL	2.6
4	D	366	LYS	2.6
4	D	173	ASP	2.6
3	C	300	LEU	2.6
4	D	336	ILE	2.6
3	C	77	PRO	2.6
3	C	182	SER	2.6
3	C	385	VAL	2.6
4	D	263	GLU	2.6
4	D	301	GLU	2.6
3	C	237	LYS	2.6
4	D	190	GLN	2.6
3	C	231	LEU	2.6
3	C	208	LYS	2.6
4	D	49	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	188	ALA	2.5
3	C	344	ILE	2.5
3	C	380	GLY	2.5
4	D	224	THR	2.5
4	D	286	LYS	2.5
4	D	22	PHE	2.5
3	C	352	ALA	2.5
3	C	37	ALA	2.5
3	C	236	ASP	2.5
3	C	224	THR	2.5
4	D	52	VAL	2.5
3	C	81	THR	2.5
3	C	359	ASN	2.5
3	C	168	TRP	2.4
4	D	294	PRO	2.4
4	D	348	ALA	2.4
3	C	266	ARG	2.4
3	C	91	SER	2.4
4	D	337	VAL	2.4
4	D	249	LEU	2.4
4	D	291	GLY	2.4
4	D	309	ASP	2.4
3	C	171	SER	2.4
4	D	111	ILE	2.4
4	D	140	ILE	2.4
4	D	199	ILE	2.4
3	C	271	PRO	2.4
4	D	98	LEU	2.4
3	C	308	GLY	2.4
4	D	43	GLY	2.4
4	D	152	PHE	2.4
3	C	290	THR	2.4
3	C	176	ASP	2.3
3	C	289	GLY	2.3
4	D	154	GLY	2.3
3	C	336	ILE	2.3
4	D	194[A]	ARG	2.3
3	C	288	MET	2.3
3	C	373	GLY	2.3
3	C	384	GLY	2.3
3	C	33	THR	2.3
4	D	178	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	140	ILE	2.3
4	D	242	THR	2.3
3	C	317	GLU	2.3
4	D	288	MET	2.3
3	C	111	ILE	2.3
4	D	378	CYS	2.3
3	C	154	GLY	2.2
3	C	285	PRO	2.2
3	C	294	PRO	2.2
3	C	95	ALA	2.2
3	C	109	SER	2.2
4	D	20	GLY	2.2
4	D	381	GLY	2.2
4	D	93	LEU	2.2
4	D	328	LYS	2.2
4	D	266	ARG	2.2
3	C	18	PHE	2.2
4	D	176	ASP	2.2
4	D	104	ALA	2.2
4	D	106	GLY	2.2
3	C	345	ALA	2.2
3	C	53	ILE	2.2
3	C	9	SER	2.2
3	C	26	PRO	2.1
4	D	354	GLY	2.1
4	D	323	ALA	2.1
3	C	296	SER	2.1
4	D	12	ARG	2.1
4	D	50	ASN	2.1
4	D	157	MET	2.1
2	B	131	GLY	2.1
4	D	297	ARG	2.1
3	C	319	PHE	2.1
3	C	167	GLN	2.1
4	D	119	MET	2.1
3	C	166	LYS	2.1
3	C	304	GLY	2.1
4	D	131	GLY	2.1
4	D	244	GLY	2.1
4	D	248	GLY	2.1
3	C	326	VAL	2.1
4	D	259	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	380	GLY	2.1
3	C	185	LYS	2.1
3	C	207	ARG	2.1
3	C	159	THR	2.0
3	C	238	GLU	2.0
3	C	335	SER	2.0
3	C	222	GLY	2.0
3	C	368	ARG	2.0
3	C	34	VAL	2.0
4	D	45	ALA	2.0
4	D	167	GLN	2.0
4	D	79	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CSO	D	89	7/8	0.85	0.13	36,42,63,77	0
2	CSO	B	89	7/8	0.96	0.08	4,10,34,73	0
2	CSD	B	378	8/9	0.98	0.07	4,9,24,109	0
1	CSD	A	378	8/9	0.98	0.08	7,13,23,32	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CL	D	1399	1/1	-0.13	0.34	80,80,80,80	0
5	SO4	A	1399	5/5	0.54	0.28	95,99,101,101	0

Continued on next page...

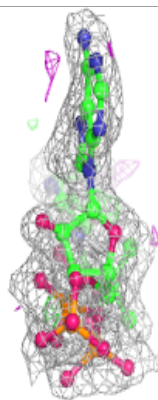
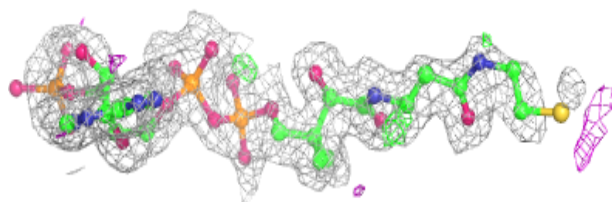
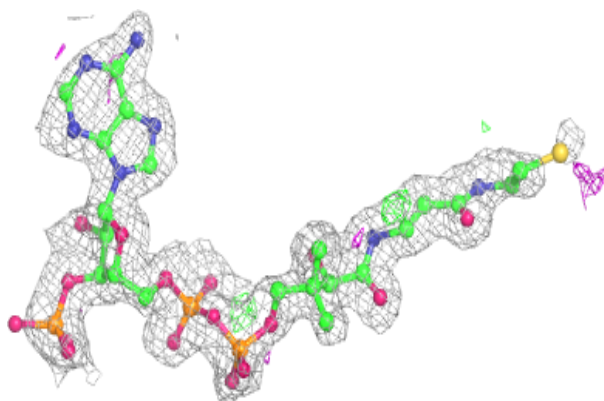
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	D	1397	5/5	0.69	0.56	120,121,122,123	0
5	SO4	A	1403	5/5	0.74	0.35	94,94,95,98	0
8	NA	C	1395	1/1	0.76	0.12	60,60,60,60	0
5	SO4	C	1393	5/5	0.76	0.24	108,108,109,109	0
5	SO4	C	1399	5/5	0.76	0.15	90,91,94,94	0
5	SO4	D	1394	5/5	0.82	0.27	63,70,71,75	0
5	SO4	C	1398	5/5	0.83	0.22	96,97,97,98	0
5	SO4	B	1397	5/5	0.84	0.14	66,66,71,73	0
5	SO4	B	1403	5/5	0.84	0.24	86,87,88,89	0
5	SO4	D	1395	5/5	0.84	0.18	89,89,90,91	0
5	SO4	C	1397	5/5	0.87	0.16	84,84,85,86	0
5	SO4	A	1398	5/5	0.87	0.21	71,78,79,81	0
5	SO4	A	1400	5/5	0.88	0.20	60,60,69,75	0
5	SO4	B	1399	5/5	0.88	0.21	78,78,80,81	0
5	SO4	A	1396	5/5	0.89	0.13	31,39,50,57	0
5	SO4	B	1404	5/5	0.89	0.26	77,77,79,82	0
5	SO4	A	1395	5/5	0.89	0.15	46,54,58,59	0
5	SO4	B	1396	5/5	0.90	0.14	45,49,57,63	0
6	COA	A	1402	48/48	0.90	0.12	21,32,63,131	0
6	COA	B	1401	48/48	0.91	0.12	20,36,80,112	0
5	SO4	B	1402	5/5	0.92	0.12	75,75,76,76	0
5	SO4	D	1396	5/5	0.92	0.16	52,59,70,71	0
5	SO4	A	1397	5/5	0.93	0.17	47,48,56,56	0
8	NA	D	1398	1/1	0.93	0.10	38,38,38,38	0
7	CL	C	1396	1/1	0.93	0.14	58,58,58,58	0
5	SO4	B	1398	5/5	0.94	0.14	45,51,56,57	0
8	NA	C	1394	1/1	0.94	0.10	34,34,34,34	0
5	SO4	A	1394	5/5	0.95	0.11	41,43,48,48	0
5	SO4	B	1395	5/5	0.97	0.11	47,50,52,55	0
7	CL	B	1400	1/1	0.99	0.03	28,28,28,28	0
5	SO4	A	1401	5/5	0.99	0.36	28,44,49,50	0

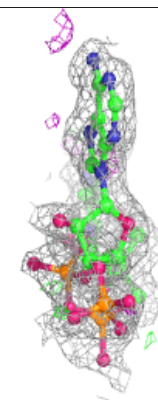
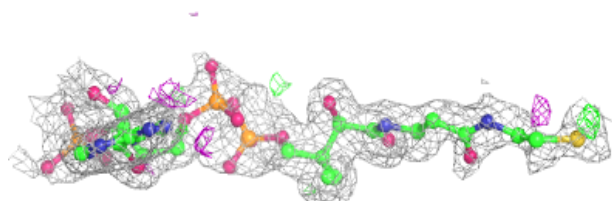
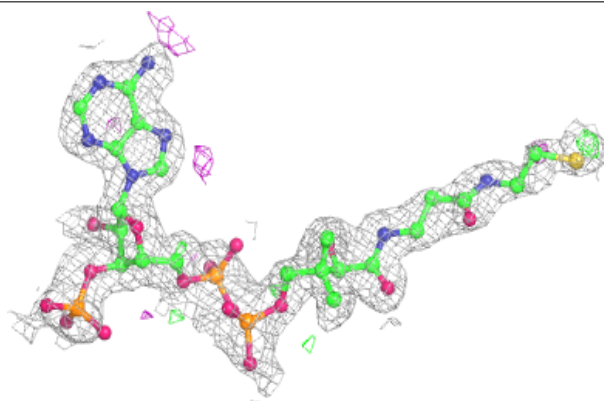
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA A 1402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around COA B 1401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.