



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:58 AM UTC

PDB ID : 8K9H / pdb_00008k9h
Title : Complex structure of Acetoacetate:butyrate/acetate coenzyme A transferase and Butyrate-acetoacetate CoA-transferase subunit B from Fusobacterium nucleatum ATCC 25586
Authors : Bai, X.; Zhao, Z.D.; Xu, Y.B.
Deposited on : 2023-08-01
Resolution : 2.73 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

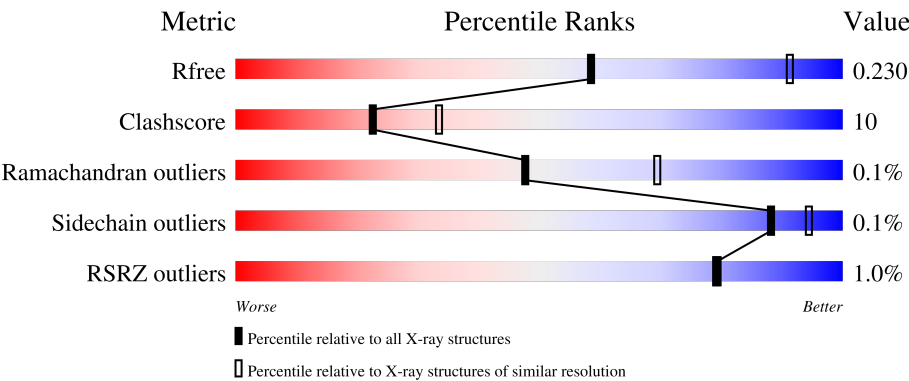
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	219	% 86%11%.
1	C	219	2% 81%14%5%
1	E	219	% 85%11%.
1	G	219	71%25%.

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Mol	Chain	Length	Quality of chain
2	B	225	73%22%5%
2	D	225	71%25%.
2	F	225	% 69%25%6%
2	H	225	% 81%15%.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12298 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 Butyrate-acetoacetate CoA-transferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1476	953	240	273	10			
1	C	209	Total	C	N	O	S	0	0	0
			1448	936	238	264	10			
1	E	212	Total	C	N	O	S	0	0	0
			1465	943	240	272	10			
1	G	212	Total	C	N	O	S	0	0	0
			1482	953	241	278	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q8RHY4
A	0	GLY	-	expression tag	UNP Q8RHY4
C	-1	MET	-	initiating methionine	UNP Q8RHY4
C	0	GLY	-	expression tag	UNP Q8RHY4
E	-1	MET	-	initiating methionine	UNP Q8RHY4
E	0	GLY	-	expression tag	UNP Q8RHY4
G	-1	MET	-	initiating methionine	UNP Q8RHY4
G	0	GLY	-	expression tag	UNP Q8RHY4

- Molecule 2 is a protein called Acetoacetate:butyrate/acetate coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1547	981	258	301	7			
2	D	216	Total	C	N	O	S	0	1	0
			1553	985	260	301	7			
2	F	212	Total	C	N	O	S	0	0	0
			1524	964	260	293	7			
2	H	216	Total	C	N	O	S	0	0	0
			1543	975	260	301	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	210	MET	-	initiating methionine	UNP Q8RHY3
B	211	GLY	-	expression tag	UNP Q8RHY3
B	212	HIS	-	expression tag	UNP Q8RHY3
B	213	HIS	-	expression tag	UNP Q8RHY3
B	214	HIS	-	expression tag	UNP Q8RHY3
B	215	HIS	-	expression tag	UNP Q8RHY3
B	216	HIS	-	expression tag	UNP Q8RHY3
B	217	HIS	-	expression tag	UNP Q8RHY3
D	210	MET	-	initiating methionine	UNP Q8RHY3
D	211	GLY	-	expression tag	UNP Q8RHY3
D	212	HIS	-	expression tag	UNP Q8RHY3
D	213	HIS	-	expression tag	UNP Q8RHY3
D	214	HIS	-	expression tag	UNP Q8RHY3
D	215	HIS	-	expression tag	UNP Q8RHY3
D	216	HIS	-	expression tag	UNP Q8RHY3
D	217	HIS	-	expression tag	UNP Q8RHY3
F	210	MET	-	initiating methionine	UNP Q8RHY3
F	211	GLY	-	expression tag	UNP Q8RHY3
F	212	HIS	-	expression tag	UNP Q8RHY3
F	213	HIS	-	expression tag	UNP Q8RHY3
F	214	HIS	-	expression tag	UNP Q8RHY3
F	215	HIS	-	expression tag	UNP Q8RHY3
F	216	HIS	-	expression tag	UNP Q8RHY3
F	217	HIS	-	expression tag	UNP Q8RHY3
H	210	MET	-	initiating methionine	UNP Q8RHY3
H	211	GLY	-	expression tag	UNP Q8RHY3
H	212	HIS	-	expression tag	UNP Q8RHY3
H	213	HIS	-	expression tag	UNP Q8RHY3
H	214	HIS	-	expression tag	UNP Q8RHY3
H	215	HIS	-	expression tag	UNP Q8RHY3
H	216	HIS	-	expression tag	UNP Q8RHY3
H	217	HIS	-	expression tag	UNP Q8RHY3

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	31	Total	O	0	0
			31	31		
4	C	32	Total	O	0	0
			32	32		
4	D	36	Total	O	0	0
			36	36		
4	E	40	Total	O	0	0
			40	40		
4	F	34	Total	O	0	0
			34	34		
4	G	16	Total	O	0	0
			16	16		
4	H	28	Total	O	0	0
			28	28		

3 Residue-property plots

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

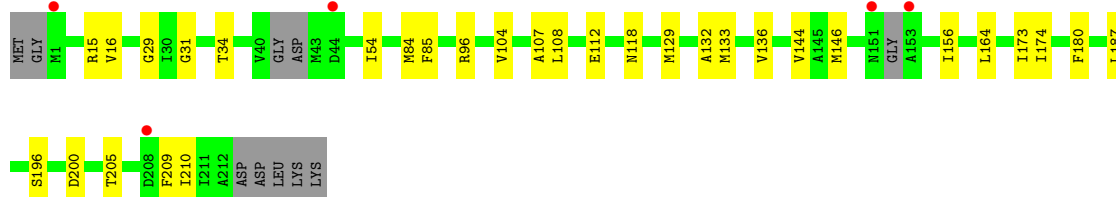
- Molecule 1: Butyrate-acetoacetate CoA-transferase subunit B

Chain A: 



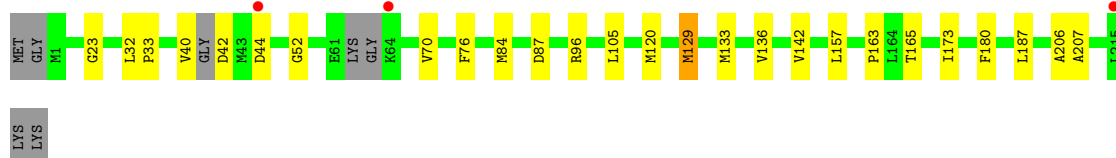
- Molecule 1: Butyrate-acetoacetate CoA-transferase subunit B

Chain C: 



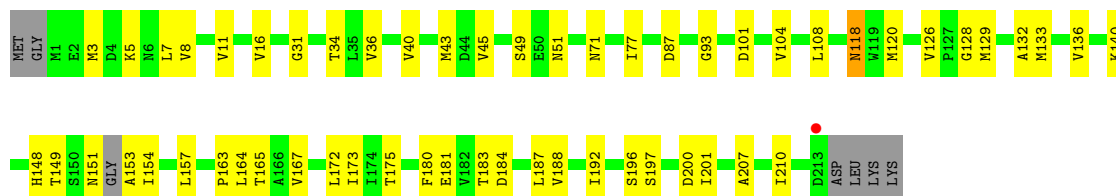
- Molecule 1: Butyrate-acetoacetate CoA-transferase subunit B

Chain E: 



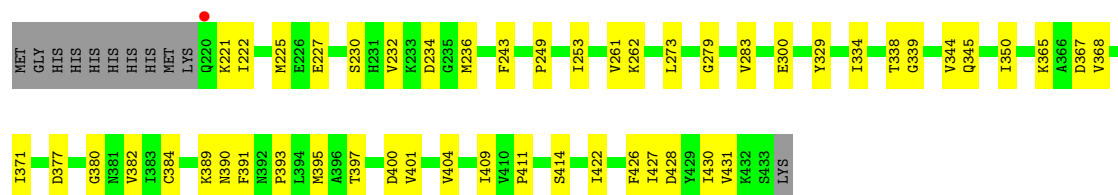
- Molecule 1: Butyrate-acetoacetate CoA-transferase subunit B

Chain G: 



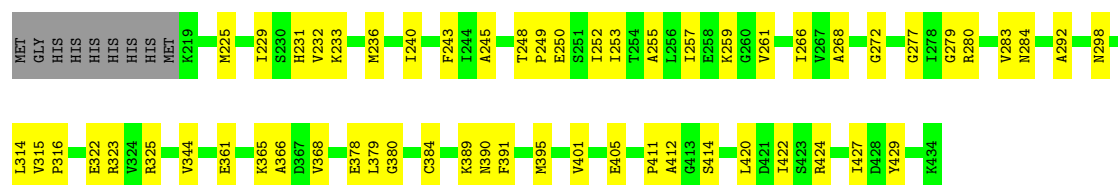
- Molecule 2: Acetoacetate:butyrate/acetate coenzyme A transferase

Chain B:  73% 22% 5%



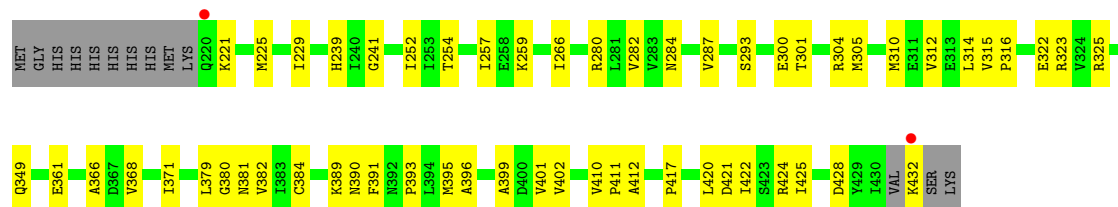
- Molecule 2: Acetoacetate:butyrate/acetate coenzyme A transferase

Chain D:  71% 25% 4%



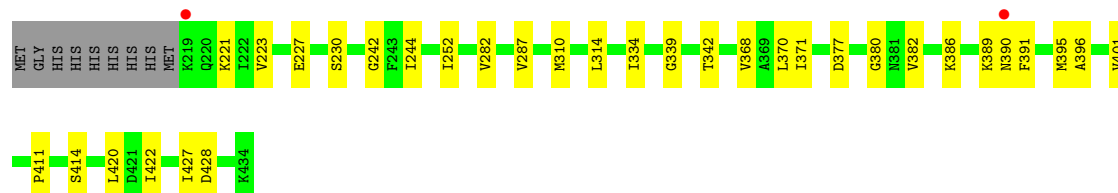
- Molecule 2: Acetoacetate:butyrate/acetate coenzyme A transferase

Chain F:  69% 25% 6%



- Molecule 2: Acetoacetate:butyrate/acetate coenzyme A transferase

Chain H:  81% 15% 4%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	166.52Å 166.52Å 191.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.07 – 2.73 48.07 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.07-2.73) 99.9 (48.07-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.195 , 0.228 0.197 , 0.230	Depositor DCC
R_{free} test set	1982 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.071 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12298	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/1499	0.59	0/2046
1	C	0.40	0/1471	0.59	0/2009
1	E	0.41	0/1488	0.60	1/2033 (0.0%)
1	G	0.40	0/1506	0.62	0/2056
2	B	0.39	0/1565	0.58	0/2127
2	D	0.42	0/1571	0.62	0/2137
2	F	0.42	0/1541	0.62	0/2094
2	H	0.41	0/1561	0.65	0/2125
All	All	0.41	0/12202	0.61	1/16627 (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	E	129	MET	CA-CB-CG	-6.01	102.08	114.10

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	1476	0	1414	22	0
1	C	1448	0	1396	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1465	0	1393	23	0
1	G	1482	0	1425	38	0
2	B	1547	0	1561	35	0
2	D	1553	0	1560	49	0
2	F	1524	0	1523	57	0
2	H	1543	0	1538	30	0
3	C	5	0	0	0	0
3	H	5	0	0	0	0
4	A	33	0	0	2	2
4	B	31	0	0	2	0
4	C	32	0	0	2	1
4	D	36	0	0	6	0
4	E	40	0	0	5	1
4	F	34	0	0	4	0
4	G	16	0	0	1	2
4	H	28	0	0	5	0
All	All	12298	0	11810	250	3

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 10.

All (250) 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)
2:F:254:THR:HG22	2:F:280:ARG:HH22	1.22	0.98
2:F:391:PHE:CB	2:F:395:MET:HE2	2.06	0.86
2:D:390:ASN:N	4:D:501:HOH:O	2.03	0.85
2:B:391:PHE:HB2	2:B:395:MET:HE3	1.58	0.85
2:F:282:VAL:HG11	2:F:301:THR:HG22	1.60	0.82
2:H:390:ASN:O	4:H:601:HOH:O	1.96	0.82
2:F:241:GLY:HA2	2:F:395:MET:HE1	1.61	0.80
2:H:227:GLU:O	2:H:230:SER:OG	1.98	0.80
1:A:119:TRP:CZ2	1:A:120:MET:HE2	2.16	0.80
2:F:391:PHE:HB2	2:F:395:MET:HE2	1.62	0.80
2:F:287:VAL:HB	2:F:310:MET:HE2	1.62	0.79
2:F:390:ASN:N	4:F:502:HOH:O	2.15	0.79
1:C:133:MET:HE1	2:D:344:VAL:HG21	1.66	0.78
1:A:52:GLY:O	4:A:301:HOH:O	2.02	0.77
2:H:282:VAL:HG13	2:H:310:MET:HE1	1.67	0.76
1:E:120:MET:HG2	1:E:163:PRO:HG2	1.66	0.76
2:B:391:PHE:CB	2:B:395:MET:HE3	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ALA:HB3	1:C:146:MET:HE3	1.69	0.75
2:F:241:GLY:HA2	2:F:395:MET:CE	2.18	0.73
1:A:84:MET:HE3	2:H:420:LEU:HB3	1.69	0.73
2:F:254:THR:HG22	2:F:280:ARG:NH2	2.01	0.71
2:F:391:PHE:HB3	2:F:395:MET:HE2	1.73	0.71
1:C:129:MET:HG2	4:D:503:HOH:O	1.92	0.69
2:B:367:ASP:OD1	4:B:501:HOH:O	2.11	0.68
2:D:368:VAL:HG22	2:D:401:VAL:HB	1.75	0.68
2:F:384:CYS:HB2	2:F:389:LYS:HB3	1.76	0.68
1:G:151:ASN:O	1:G:153:ALA:N	2.28	0.67
2:D:322:GLU:OE1	2:F:325:ARG:NH2	2.29	0.66
1:E:52:GLY:O	4:E:301:HOH:O	2.12	0.66
1:G:133:MET:HE2	2:H:339:GLY:HA2	1.76	0.66
1:A:212:ALA:O	1:A:214:ASP:N	2.29	0.66
2:B:368:VAL:HG22	2:B:401:VAL:HB	1.78	0.65
1:G:154:ILE:HD12	1:G:154:ILE:H	1.62	0.65
1:A:120:MET:HG2	1:A:163:PRO:HG2	1.78	0.65
2:D:391:PHE:O	2:D:395:MET:HG3	1.97	0.65
1:A:133:MET:CE	2:B:339:GLY:HA2	2.27	0.63
1:A:133:MET:HE3	2:B:339:GLY:HA2	1.79	0.63
1:G:133:MET:HE3	2:H:342:THR:HG21	1.80	0.63
1:C:129:MET:SD	1:C:133:MET:HE2	2.39	0.63
2:H:244:ILE:HG22	2:H:244:ILE:O	1.97	0.63
1:C:108:LEU:HG	1:C:118:ASN:HA	1.82	0.62
2:D:322:GLU:CD	2:F:325:ARG:HH22	2.08	0.61
1:C:112:GLU:HA	1:C:187:LEU:HD13	1.83	0.61
1:E:133:MET:HE1	2:F:316:PRO:HG3	1.83	0.60
2:D:250:GLU:OE2	2:D:277:GLY:N	2.34	0.59
1:E:42:ASP:N	4:E:303:HOH:O	2.33	0.59
2:F:432:LYS:N	4:F:505:HOH:O	2.34	0.59
1:G:108:LEU:HG	1:G:118:ASN:HA	1.84	0.59
2:B:283:VAL:HG12	2:B:300:GLU:HG2	1.86	0.58
2:D:225:MET:O	2:D:229:ILE:HG12	2.04	0.58
2:D:232:VAL:HA	2:D:236:MET:HE2	1.86	0.58
1:E:87:ASP:HA	2:F:389:LYS:O	2.03	0.58
1:C:196:SER:OG	1:C:200:ASP:OD2	2.22	0.58
1:G:196:SER:OG	1:G:200:ASP:OD2	2.20	0.58
2:H:386:LYS:O	2:H:389:LYS:NZ	2.36	0.58
1:A:10:GLU:HG3	1:A:39:TYR:OH	2.03	0.57
2:H:287:VAL:HB	2:H:310:MET:HE2	1.85	0.57
1:E:133:MET:CE	2:F:316:PRO:HG3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:ASP:HB2	4:H:601:HOH:O	2.04	0.57
2:B:384:CYS:O	2:B:389:LYS:NZ	2.38	0.57
2:D:257:ILE:HG23	2:D:284:ASN:ND2	2.20	0.57
2:F:382:VAL:HB	2:F:422:ILE:HB	1.86	0.56
1:G:49:SER:OG	1:G:51:ASN:OD1	2.22	0.56
2:H:368:VAL:HG22	2:H:401:VAL:HB	1.87	0.56
1:A:84:MET:HE3	2:H:420:LEU:CB	2.34	0.56
1:C:107:ALA:HA	1:C:118:ASN:HB2	1.88	0.56
2:F:282:VAL:HG13	2:F:310:MET:HE1	1.87	0.55
2:H:282:VAL:HG13	2:H:310:MET:CE	2.35	0.55
2:B:411:PRO:HG2	2:B:414:SER:HB2	1.88	0.55
2:F:379:LEU:HG	2:F:412:ALA:HB1	1.89	0.55
1:G:164:LEU:HD13	1:G:167:VAL:HG12	1.89	0.54
2:D:379:LEU:HD22	2:D:424:ARG:NH1	2.23	0.54
1:C:173:ILE:HB	1:C:180:PHE:HB2	1.89	0.54
2:D:378:GLU:HB2	2:D:412:ALA:HB2	1.89	0.53
2:D:322:GLU:CD	2:F:325:ARG:NH2	2.66	0.53
2:B:377:ASP:OD2	4:B:502:HOH:O	2.19	0.53
1:G:133:MET:HG2	1:G:165:THR:O	2.09	0.53
1:C:132:ALA:O	1:C:136:VAL:HG22	2.10	0.52
2:D:325:ARG:HH22	2:F:322:GLU:CD	2.17	0.52
1:E:70:VAL:HG12	1:E:76:PHE:HA	1.92	0.52
2:B:234:ASP:OD1	2:B:261:VAL:HG23	2.09	0.52
2:D:277:GLY:O	2:D:280:ARG:HG3	2.10	0.52
2:B:411:PRO:O	2:B:414:SER:HB3	2.09	0.52
2:F:266:ILE:HG12	2:F:287:VAL:HG13	1.92	0.51
2:H:221:LYS:HG2	2:H:428:ASP:O	2.10	0.51
1:E:40:VAL:O	1:E:42:ASP:N	2.43	0.51
2:H:287:VAL:O	2:H:310:MET:HE2	2.10	0.51
1:C:129:MET:CE	2:D:314:LEU:HB3	2.40	0.51
2:D:384:CYS:HB2	2:D:389:LYS:HB3	1.92	0.51
1:G:192:ILE:HG23	1:G:201:ILE:HD11	1.93	0.51
2:D:315:VAL:N	4:D:508:HOH:O	2.42	0.51
1:E:96:ARG:NH2	4:F:504:HOH:O	2.44	0.51
2:F:393:PRO:HD3	4:F:502:HOH:O	2.11	0.51
2:D:225:MET:HE2	2:D:255:ALA:HB3	1.93	0.51
2:F:393:PRO:HA	2:F:422:ILE:HG12	1.93	0.51
2:D:379:LEU:HG	2:D:412:ALA:HB1	1.93	0.50
1:G:188:VAL:HG22	1:G:210:ILE:HG12	1.92	0.50
2:B:222:ILE:HD13	2:B:409:ILE:HD13	1.93	0.50
2:D:249:PRO:O	2:D:253:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:ASN:HB3	1:G:77:ILE:HG21	1.93	0.50
2:H:382:VAL:HB	2:H:422:ILE:HB	1.94	0.50
2:B:243:PHE:N	2:B:390:ASN:ND2	2.60	0.50
1:A:133:MET:HB3	2:B:338:THR:HG23	1.92	0.50
2:B:273:LEU:O	2:B:279:GLY:HA3	2.12	0.50
2:B:382:VAL:HB	2:B:422:ILE:HB	1.94	0.50
2:H:227:GLU:OE1	4:H:602:HOH:O	2.19	0.50
2:D:268:ALA:O	2:D:292:ALA:HA	2.13	0.49
1:E:142:VAL:HG13	4:E:332:HOH:O	2.13	0.49
1:E:33:PRO:HG2	1:E:105:LEU:HA	1.94	0.49
2:F:424:ARG:HG3	2:F:425:ILE:N	2.27	0.49
1:C:133:MET:HE3	2:D:316:PRO:HB3	1.95	0.49
2:B:371:ILE:HG13	2:B:404:VAL:HG23	1.94	0.48
2:F:381:ASN:HB3	2:F:420:LEU:HD22	1.95	0.48
1:G:31:GLY:O	1:G:34:THR:OG1	2.31	0.48
1:G:3:MET:HE2	1:G:8:VAL:HG12	1.93	0.48
2:D:279:GLY:O	2:D:283:VAL:HG23	2.13	0.48
2:H:252:ILE:HG21	2:H:370:LEU:HD22	1.94	0.48
2:F:305:MET:HB2	2:F:312:VAL:HG21	1.96	0.48
2:F:229:ILE:HD12	2:F:259:LYS:HB2	1.95	0.48
2:F:323:ARG:HD2	2:F:361:GLU:HB3	1.96	0.48
1:C:54:ILE:HG12	2:F:425:ILE:HD13	1.96	0.48
1:E:129:MET:CB	1:E:133:MET:HE2	2.44	0.47
2:D:240:ILE:HD11	2:D:266:ILE:HD12	1.96	0.47
2:D:322:GLU:OE2	2:F:325:ARG:NH2	2.46	0.47
1:G:148:HIS:HB2	1:G:175:THR:HB	1.95	0.47
2:H:411:PRO:O	2:H:414:SER:HB3	2.14	0.47
1:A:96:ARG:NH2	4:A:302:HOH:O	2.39	0.47
2:B:334:ILE:HG22	2:H:334:ILE:HG22	1.96	0.47
1:G:120:MET:HE3	1:G:126:VAL:HG13	1.97	0.47
2:B:249:PRO:O	2:B:253:ILE:HG13	2.14	0.47
2:D:323:ARG:HD2	2:D:361:GLU:HB3	1.97	0.47
2:D:259:LYS:HG2	2:D:261:VAL:HG22	1.97	0.47
2:F:410:VAL:HG13	2:F:411:PRO:HD2	1.97	0.47
1:G:157:LEU:O	1:G:207:ALA:HB2	2.15	0.47
2:D:233:LYS:O	2:D:236:MET:HG3	2.15	0.47
2:D:236:MET:HE1	2:D:368:VAL:CG2	2.44	0.47
1:C:144:VAL:HG12	1:C:146:MET:HG2	1.95	0.47
1:C:31:GLY:O	1:C:34:THR:OG1	2.31	0.46
1:C:133:MET:HE1	2:D:344:VAL:CG2	2.43	0.46
1:G:184:ASP:OD1	1:G:184:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:245:ALA:HA	2:D:248:THR:OG1	2.16	0.46
2:H:390:ASN:C	4:H:601:HOH:O	2.53	0.46
2:B:365:LYS:HE2	2:B:400:ASP:OD1	2.16	0.46
2:D:411:PRO:O	2:D:414:SER:OG	2.28	0.46
1:G:172:LEU:HD23	1:G:172:LEU:HA	1.67	0.46
1:G:132:ALA:O	1:G:136:VAL:HG22	2.16	0.46
2:F:300:GLU:O	2:F:304:ARG:HG3	2.15	0.46
2:H:380:GLY:O	2:H:427:ILE:HG13	2.15	0.46
2:F:287:VAL:HB	2:F:310:MET:CE	2.39	0.45
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.74	0.45
1:A:12:ILE:HG23	1:A:174:ILE:HG22	1.98	0.45
2:B:380:GLY:HA2	2:B:430:ILE:HD11	1.99	0.45
2:B:380:GLY:O	2:B:427:ILE:HG13	2.17	0.45
2:F:380:GLY:O	2:F:382:VAL:HG23	2.16	0.45
2:D:325:ARG:NH2	2:F:322:GLU:OE1	2.50	0.45
1:G:40:VAL:HA	1:G:43:MET:HE3	1.97	0.45
1:A:146:MET:SD	1:A:155:LYS:HE2	2.56	0.45
2:B:232:VAL:HA	2:B:236:MET:CE	2.46	0.45
1:E:129:MET:SD	1:E:133:MET:CE	3.04	0.45
2:D:231:HIS:CD2	2:D:429:TYR:CE2	3.04	0.45
2:D:252:ILE:HG13	2:D:405:GLU:OE1	2.17	0.45
1:E:23:GLY:N	1:E:44:ASP:O	2.46	0.45
2:H:287:VAL:HB	2:H:310:MET:CE	2.45	0.45
2:H:391:PHE:O	2:H:395:MET:HG2	2.17	0.45
2:B:225:MET:HE1	2:B:431:VAL:HG21	1.99	0.45
1:C:84:MET:HE3	2:F:420:LEU:CB	2.47	0.45
2:F:349:GLN:HA	4:H:608:HOH:O	2.17	0.45
1:C:84:MET:HE3	2:F:420:LEU:HB3	1.98	0.44
2:D:225:MET:HE2	2:D:255:ALA:CB	2.47	0.44
1:E:32:LEU:HB3	1:E:33:PRO:HD3	1.98	0.44
1:C:96:ARG:NH2	4:C:404:HOH:O	2.49	0.44
1:G:163:PRO:HD3	4:G:305:HOH:O	2.17	0.44
1:A:133:MET:HE1	2:B:344:VAL:HG21	2.00	0.44
1:A:84:MET:HG3	2:H:420:LEU:HB2	2.00	0.44
1:A:104:VAL:O	1:A:105:LEU:HD12	2.18	0.44
2:B:329:TYR:CD2	1:G:93:GLY:HA3	2.53	0.44
2:D:389:LYS:HA	4:D:501:HOH:O	2.17	0.44
1:A:50:GLU:H	1:A:50:GLU:HG3	1.59	0.44
2:F:221:LYS:HG2	2:F:428:ASP:O	2.16	0.44
1:G:173:ILE:HB	1:G:180:PHE:HB2	2.00	0.44
2:B:397:THR:HG22	2:B:426:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:VAL:O	1:G:40:VAL:HG13	2.17	0.44
1:E:157:LEU:HA	1:E:206:ALA:HB3	2.00	0.43
1:C:129:MET:HE1	2:D:314:LEU:HB3	2.00	0.43
2:F:225:MET:CE	2:F:252:ILE:HG12	2.48	0.43
1:E:133:MET:HG2	1:E:165:THR:O	2.18	0.43
2:F:384:CYS:N	2:F:421:ASP:OD2	2.44	0.43
2:H:221:LYS:O	2:H:223:VAL:HG13	2.19	0.43
2:F:287:VAL:O	2:F:310:MET:HE2	2.18	0.43
2:F:314:LEU:HD23	2:F:314:LEU:HA	1.80	0.43
2:B:345:GLN:NE2	2:B:350:ILE:HD11	2.34	0.43
1:G:5:LYS:O	1:G:8:VAL:HG22	2.18	0.43
1:C:129:MET:SD	1:C:133:MET:CE	3.07	0.43
2:D:325:ARG:HD2	4:D:526:HOH:O	2.19	0.43
2:B:227:GLU:O	2:B:230:SER:OG	2.31	0.43
2:F:368:VAL:HA	2:F:401:VAL:O	2.19	0.43
1:A:102:ALA:HA	1:A:141:LYS:O	2.18	0.43
1:C:146:MET:HE2	4:C:414:HOH:O	2.18	0.43
2:D:240:ILE:CD1	2:D:266:ILE:HD12	2.49	0.43
1:G:43:MET:HB3	1:G:45:VAL:HG23	2.00	0.43
2:F:239:HIS:HB3	2:F:395:MET:SD	2.59	0.43
2:F:371:ILE:HD13	2:F:396:ALA:HB2	2.00	0.43
2:H:368:VAL:HA	2:H:401:VAL:O	2.19	0.43
2:D:243:PHE:HB3	4:D:517:HOH:O	2.19	0.42
2:F:257:ILE:HG23	2:F:284:ASN:ND2	2.33	0.42
2:B:221:LYS:HG2	2:B:428:ASP:O	2.18	0.42
1:G:181:GLU:HG2	1:G:183:THR:HG23	2.01	0.42
1:C:129:MET:CG	1:C:133:MET:HE2	2.49	0.42
1:C:156:ILE:HB	1:C:205:THR:HG23	2.00	0.42
2:D:365:LYS:HG3	2:D:366:ALA:N	2.34	0.42
2:D:420:LEU:HB2	1:E:84:MET:HG3	2.01	0.42
2:B:234:ASP:OD2	2:B:262:LYS:HG2	2.20	0.42
2:F:293:SER:HA	2:F:315:VAL:O	2.19	0.42
1:C:209:PHE:C	1:C:210:ILE:HD13	2.45	0.42
2:D:272:GLY:O	2:D:298:ASN:HB2	2.20	0.42
1:G:197:SER:O	1:G:200:ASP:N	2.51	0.42
2:H:371:ILE:HD13	2:H:396:ALA:HB2	2.01	0.42
1:E:173:ILE:HB	1:E:180:PHE:HB2	2.02	0.41
2:F:225:MET:HE1	2:F:252:ILE:HA	2.02	0.41
1:G:129:MET:HE3	1:G:129:MET:HB3	1.93	0.41
1:G:149:THR:HG23	1:G:153:ALA:O	2.20	0.41
2:F:396:ALA:O	2:F:402:VAL:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:VAL:O	1:G:43:MET:HE3	2.19	0.41
2:H:377:ASP:OD1	2:H:377:ASP:C	2.63	0.41
2:F:381:ASN:HB3	2:F:420:LEU:CD2	2.51	0.41
1:C:164:LEU:HD12	1:C:164:LEU:H	1.85	0.41
1:E:105:LEU:HG	4:E:332:HOH:O	2.19	0.41
1:G:101:ASP:OD1	1:G:140:LYS:HE3	2.20	0.41
2:D:422:ILE:C	1:E:84:MET:HE1	2.45	0.41
2:B:232:VAL:HA	2:B:236:MET:HE1	2.02	0.41
1:C:15:ARG:HG3	1:C:174:ILE:HD13	2.03	0.41
2:D:325:ARG:NH2	2:F:322:GLU:CD	2.78	0.41
2:D:380:GLY:O	2:D:427:ILE:HG13	2.21	0.41
1:E:136:VAL:HG12	4:E:332:HOH:O	2.19	0.41
1:A:133:MET:HE1	2:B:339:GLY:HA2	2.01	0.41
1:C:16:VAL:HG11	1:C:104:VAL:HG11	2.03	0.41
1:C:29:GLY:O	1:C:34:THR:HG23	2.20	0.41
1:G:16:VAL:HG11	1:G:104:VAL:HG11	2.03	0.41
2:H:242:GLY:H	2:H:390:ASN:HD22	1.69	0.41
1:E:157:LEU:O	1:E:207:ALA:HB2	2.21	0.40
2:F:241:GLY:HA2	2:F:395:MET:HE3	2.01	0.40
1:G:128:GLY:HA2	2:H:314:LEU:HD13	2.03	0.40
1:G:187:LEU:HD23	1:G:187:LEU:HA	1.80	0.40
2:F:366:ALA:O	2:F:399:ALA:HA	2.22	0.40
1:G:7:LEU:O	1:G:11:VAL:HG22	2.22	0.40
1:A:112:GLU:HG2	1:A:158:LYS:O	2.21	0.40
2:B:389:LYS:O	2:B:393:PRO:HD3	2.21	0.40
1:C:85:PHE:CD2	2:F:417:PRO:HB2	2.56	0.40
2:D:368:VAL:HA	2:D:401:VAL:O	2.22	0.40
1:A:196:SER:OG	1:A:197:SER:N	2.54	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:424:HOH:O	4:E:318:HOH:O[5_655]	1.87	0.33
4:A:331:HOH:O	4:G:313:HOH:O[5_555]	1.89	0.31
4:A:323:HOH:O	4:G:315:HOH:O[5_555]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	208/219 (95%)	199 (96%)	9 (4%)	0	100	100
1	C	203/219 (93%)	190 (94%)	13 (6%)	0	100	100
1	E	206/219 (94%)	201 (98%)	5 (2%)	0	100	100
1	G	208/219 (95%)	199 (96%)	8 (4%)	1 (0%)	24	40
2	B	212/225 (94%)	205 (97%)	7 (3%)	0	100	100
2	D	215/225 (96%)	205 (95%)	10 (5%)	0	100	100
2	F	209/225 (93%)	199 (95%)	10 (5%)	0	100	100
2	H	214/225 (95%)	203 (95%)	11 (5%)	0	100	100
All	All	1675/1776 (94%)	1601 (96%)	73 (4%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	118	ASN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	136/171 (80%)	136 (100%)	0	100	100
1	C	134/171 (78%)	134 (100%)	0	100	100
1	E	135/171 (79%)	134 (99%)	1 (1%)	76	85
1	G	140/171 (82%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	162/186 (87%)	162 (100%)	0	100	100
2	D	161/186 (87%)	161 (100%)	0	100	100
2	F	156/186 (84%)	156 (100%)	0	100	100
2	H	160/186 (86%)	160 (100%)	0	100	100
All	All	1184/1428 (83%)	1183 (100%)	1 (0%)	88	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	187	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	390	ASN
1	C	27	ASN
1	C	38	ASN
2	D	306	GLN
1	G	6	ASN
1	G	38	ASN
2	H	390	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands 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	$\# Z > 2$
3	SO4	C	301	-	4,4,4	0.38	0	6,6,6	0.39	0
3	SO4	H	501	-	4,4,4	0.36	0	6,6,6	0.31	0

There are no bond length outliers.

There are no bond angle outliers.

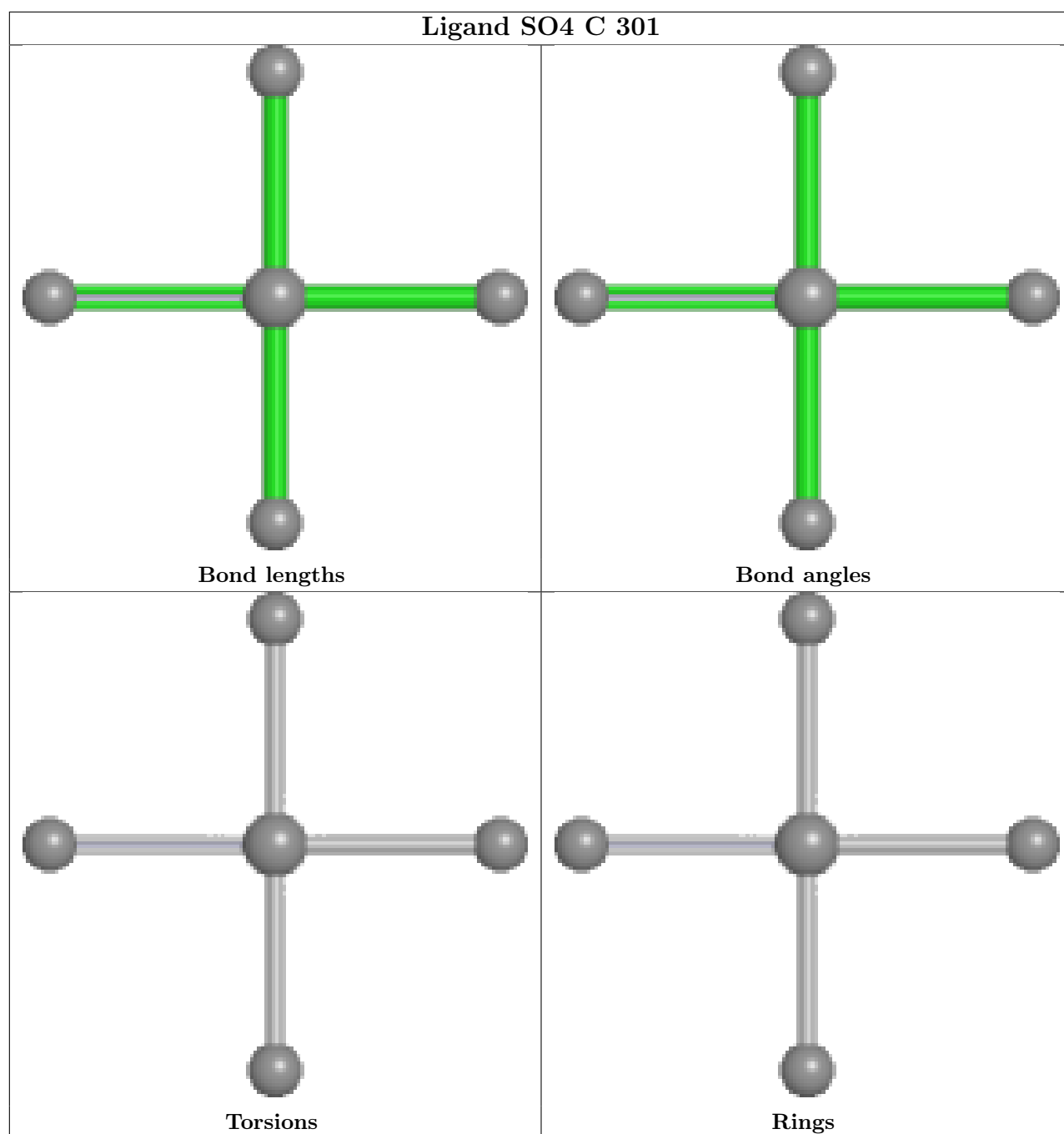
There are no chirality outliers.

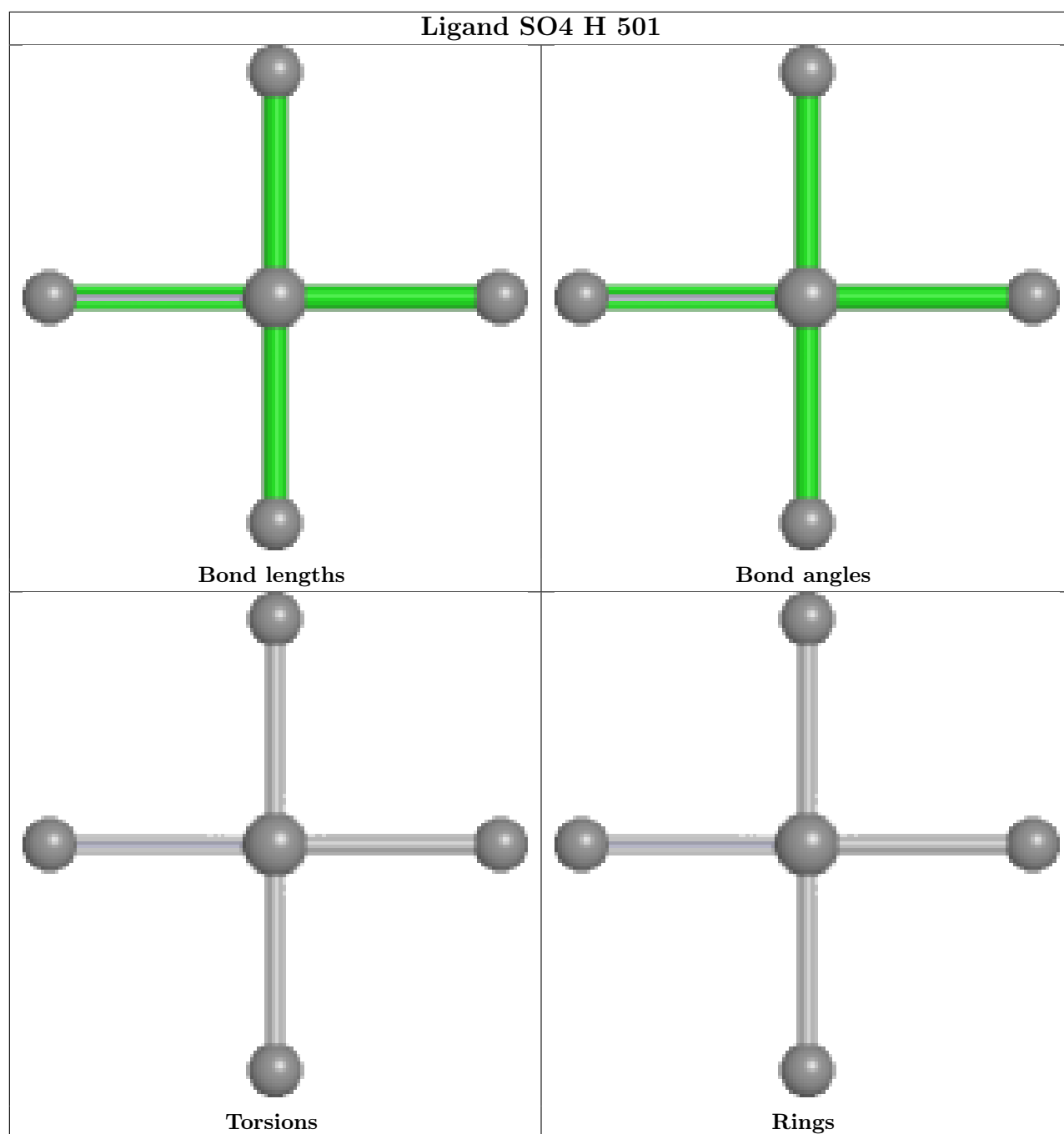
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	214/219 (97%)	-0.21	3 (1%) 73 72	36, 55, 72, 83	0
1	C	209/219 (95%)	0.01	5 (2%) 59 56	41, 60, 76, 88	0
1	E	212/219 (96%)	-0.26	3 (1%) 73 72	40, 55, 73, 87	0
1	G	212/219 (96%)	0.09	1 (0%) 87 87	41, 64, 81, 100	0
2	B	214/225 (95%)	-0.33	1 (0%) 87 87	35, 55, 71, 76	0
2	D	216/225 (96%)	-0.23	0 100 100	29, 56, 67, 75	1 (0%)
2	F	212/225 (94%)	-0.34	2 (0%) 81 81	38, 54, 70, 81	0
2	H	216/225 (96%)	-0.24	2 (0%) 81 81	35, 54, 67, 73	0
All	All	1705/1776 (96%)	-0.19	17 (0%) 79 79	29, 56, 74, 100	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	213	ASP	3.8
2	H	390	ASN	3.1
2	F	432	LYS	3.0
1	E	215	LEU	2.7
1	C	153	ALA	2.7
1	C	44	ASP	2.6
1	A	42	ASP	2.4
1	C	1	MET	2.4
1	A	62	LYS	2.4
1	E	44	ASP	2.3
2	F	220	GLN	2.3
1	C	151	ASN	2.2
2	B	220	GLN	2.2
1	A	44	ASP	2.1
1	E	64	LYS	2.1
1	C	208	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	219	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

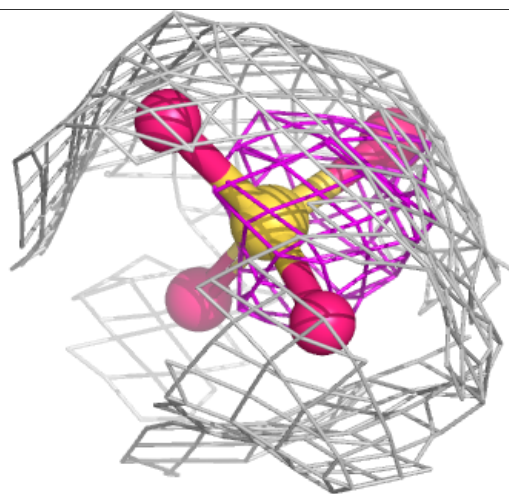
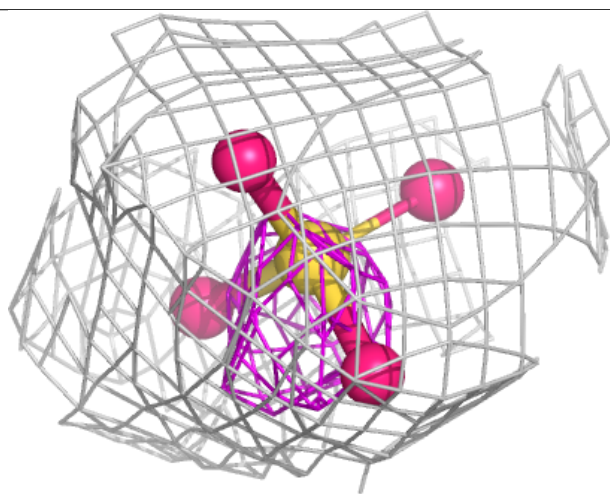
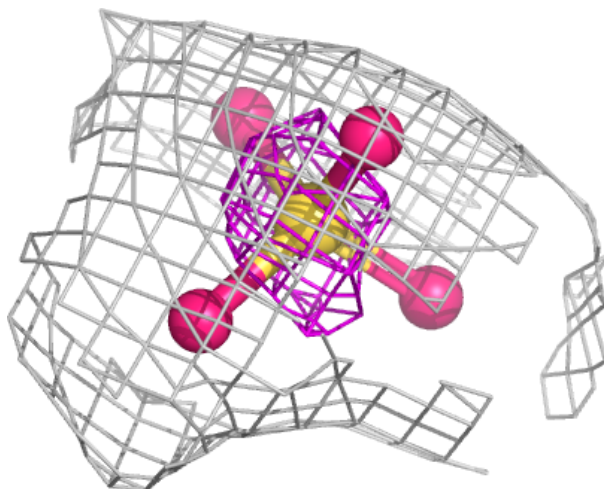
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	H	501	5/5	0.81	0.15	88,89,104,121	0
3	SO4	C	301	5/5	0.90	0.19	81,81,84,90	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.

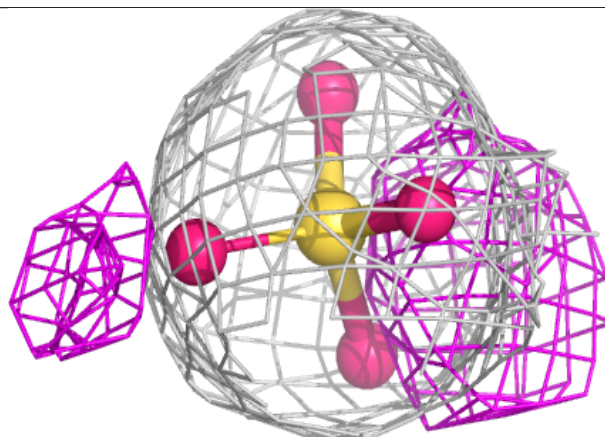
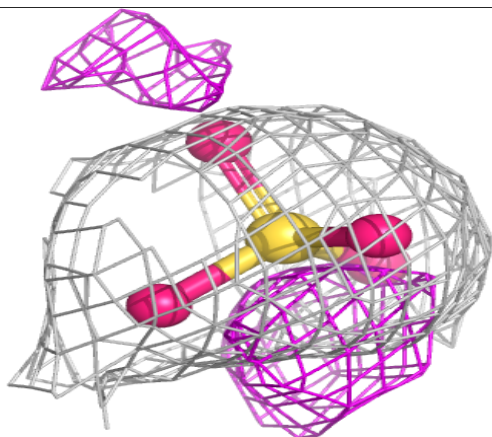
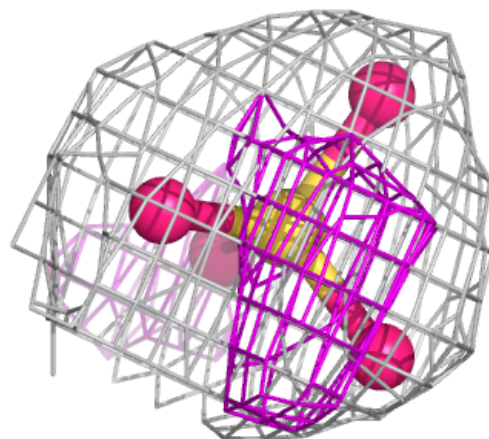
Electron density around SO4 H 501:

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



Electron density around SO4 C 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.