



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:28 am BST

PDB ID : 2GLM
Title : Crystal structure of (3R)-Hydroxyacyl-Acyl Carrier Protein Dehydratase(FabZ) from Helicobacter pylori complexed with Compound 2
Authors : Zhang, L.; Liu, W.; Shen, X.; Jiang, H.
Deposited on : 2006-04-05
Resolution : 2.60 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 : 2.11
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) : 2.11

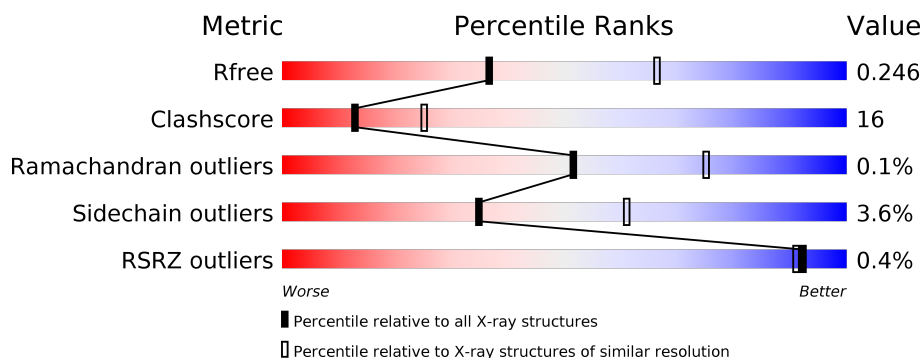
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	171	
1	B	171	
1	C	171	
1	D	171	
1	E	171	
1	F	171	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BEN	D	2006	-	-	-	X
4	SCB	A	3001	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7942 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 (3R)-hydroxymyristoyl-acyl carrier protein dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1225	803	203	214	5			
1	B	151	Total	C	N	O	S	0	0	0
			1217	797	202	213	5			
1	C	151	Total	C	N	O	S	0	0	0
			1217	797	202	213	5			
1	D	152	Total	C	N	O	S	0	0	0
			1225	803	203	214	5			
1	E	152	Total	C	N	O	S	0	0	0
			1225	803	203	214	5			
1	F	147	Total	C	N	O	S	0	0	0
			1181	778	194	204	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q5G940
A	-10	ARG	-	EXPRESSION TAG	UNP Q5G940
A	-9	GLY	-	EXPRESSION TAG	UNP Q5G940
A	-8	SER	-	EXPRESSION TAG	UNP Q5G940
A	-7	HIS	-	EXPRESSION TAG	UNP Q5G940
A	-6	HIS	-	EXPRESSION TAG	UNP Q5G940
A	-5	HIS	-	EXPRESSION TAG	UNP Q5G940
A	-4	HIS	-	EXPRESSION TAG	UNP Q5G940
A	-3	HIS	-	EXPRESSION TAG	UNP Q5G940
A	-2	HIS	-	EXPRESSION TAG	UNP Q5G940
A	-1	GLY	-	EXPRESSION TAG	UNP Q5G940
A	0	SER	-	EXPRESSION TAG	UNP Q5G940
B	-11	MET	-	EXPRESSION TAG	UNP Q5G940
B	-10	ARG	-	EXPRESSION TAG	UNP Q5G940
B	-9	GLY	-	EXPRESSION TAG	UNP Q5G940
B	-8	SER	-	EXPRESSION TAG	UNP Q5G940
B	-7	HIS	-	EXPRESSION TAG	UNP Q5G940

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP Q5G940
B	-5	HIS	-	EXPRESSION TAG	UNP Q5G940
B	-4	HIS	-	EXPRESSION TAG	UNP Q5G940
B	-3	HIS	-	EXPRESSION TAG	UNP Q5G940
B	-2	HIS	-	EXPRESSION TAG	UNP Q5G940
B	-1	GLY	-	EXPRESSION TAG	UNP Q5G940
B	0	SER	-	EXPRESSION TAG	UNP Q5G940
C	-11	MET	-	EXPRESSION TAG	UNP Q5G940
C	-10	ARG	-	EXPRESSION TAG	UNP Q5G940
C	-9	GLY	-	EXPRESSION TAG	UNP Q5G940
C	-8	SER	-	EXPRESSION TAG	UNP Q5G940
C	-7	HIS	-	EXPRESSION TAG	UNP Q5G940
C	-6	HIS	-	EXPRESSION TAG	UNP Q5G940
C	-5	HIS	-	EXPRESSION TAG	UNP Q5G940
C	-4	HIS	-	EXPRESSION TAG	UNP Q5G940
C	-3	HIS	-	EXPRESSION TAG	UNP Q5G940
C	-2	HIS	-	EXPRESSION TAG	UNP Q5G940
C	-1	GLY	-	EXPRESSION TAG	UNP Q5G940
C	0	SER	-	EXPRESSION TAG	UNP Q5G940
D	-11	MET	-	EXPRESSION TAG	UNP Q5G940
D	-10	ARG	-	EXPRESSION TAG	UNP Q5G940
D	-9	GLY	-	EXPRESSION TAG	UNP Q5G940
D	-8	SER	-	EXPRESSION TAG	UNP Q5G940
D	-7	HIS	-	EXPRESSION TAG	UNP Q5G940
D	-6	HIS	-	EXPRESSION TAG	UNP Q5G940
D	-5	HIS	-	EXPRESSION TAG	UNP Q5G940
D	-4	HIS	-	EXPRESSION TAG	UNP Q5G940
D	-3	HIS	-	EXPRESSION TAG	UNP Q5G940
D	-2	HIS	-	EXPRESSION TAG	UNP Q5G940
D	-1	GLY	-	EXPRESSION TAG	UNP Q5G940
D	0	SER	-	EXPRESSION TAG	UNP Q5G940
E	-11	MET	-	EXPRESSION TAG	UNP Q5G940
E	-10	ARG	-	EXPRESSION TAG	UNP Q5G940
E	-9	GLY	-	EXPRESSION TAG	UNP Q5G940
E	-8	SER	-	EXPRESSION TAG	UNP Q5G940
E	-7	HIS	-	EXPRESSION TAG	UNP Q5G940
E	-6	HIS	-	EXPRESSION TAG	UNP Q5G940
E	-5	HIS	-	EXPRESSION TAG	UNP Q5G940
E	-4	HIS	-	EXPRESSION TAG	UNP Q5G940
E	-3	HIS	-	EXPRESSION TAG	UNP Q5G940
E	-2	HIS	-	EXPRESSION TAG	UNP Q5G940
E	-1	GLY	-	EXPRESSION TAG	UNP Q5G940

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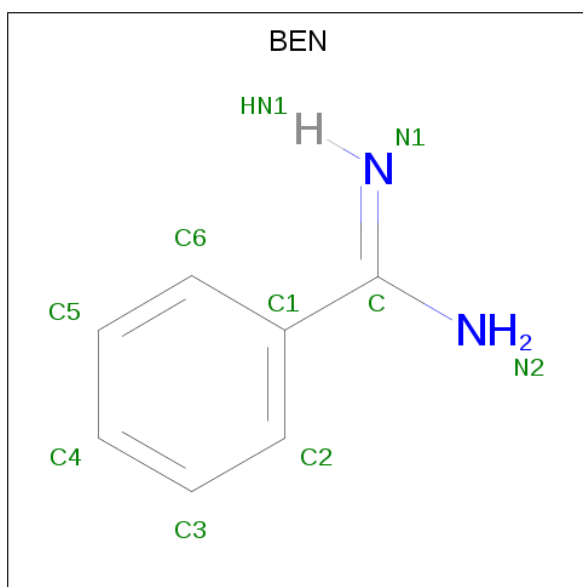
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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	SER	-	EXPRESSION TAG	UNP Q5G940
F	-11	MET	-	EXPRESSION TAG	UNP Q5G940
F	-10	ARG	-	EXPRESSION TAG	UNP Q5G940
F	-9	GLY	-	EXPRESSION TAG	UNP Q5G940
F	-8	SER	-	EXPRESSION TAG	UNP Q5G940
F	-7	HIS	-	EXPRESSION TAG	UNP Q5G940
F	-6	HIS	-	EXPRESSION TAG	UNP Q5G940
F	-5	HIS	-	EXPRESSION TAG	UNP Q5G940
F	-4	HIS	-	EXPRESSION TAG	UNP Q5G940
F	-3	HIS	-	EXPRESSION TAG	UNP Q5G940
F	-2	HIS	-	EXPRESSION TAG	UNP Q5G940
F	-1	GLY	-	EXPRESSION TAG	UNP Q5G940
F	0	SER	-	EXPRESSION TAG	UNP Q5G940

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

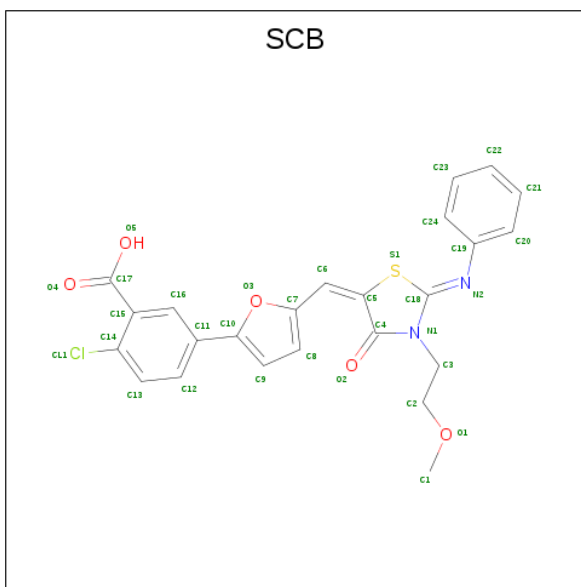
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	F	2	Total Cl 2 2	0	0

- Molecule 3 is BENZAMIDINE (three-letter code: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	7	2		
3	A	1	Total	C	N	0	0
			9	7	2		
3	B	1	Total	C	N	0	0
			9	7	2		
3	C	1	Total	C	N	0	0
			9	7	2		
3	C	1	Total	C	N	0	0
			9	7	2		
3	D	1	Total	C	N	0	0
			9	7	2		
3	E	1	Total	C	N	0	0
			9	7	2		

- Molecule 4 is 2-CHLORO-5-(5-{(E)-[(2Z)-3-(2-METHOXYETHYL)-4-OXO-2-(PHENYLIMINO)-1,3-THIAZOLIDIN-5-YLIDENE]METHYL}-2-FURYL)BENZOIC ACID (three-letter code: SCB) (formula: C₂₄H₁₉ClN₂O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	
			33	24	1	2	5	1	
								0	0



- Molecule 5 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total	O		
			124	124	0	0
5	B	88	Total	O		
			88	88	0	0
5	C	88	Total	O		
			88	88	0	0
5	D	76	Total	O		
			76	76	0	0
5	E	95	Total	O		
			95	95	0	0
5	F	79	Total	O		
			79	79	0	0

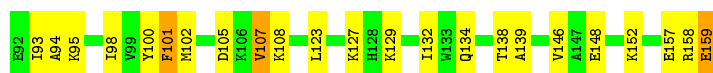
- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase



- Chain B:
-
- 29% 60% 27% 12%
- MET ARG GLY SER HIS HIS HIS HIS HIS GLY SER MET GLU GLN SER HIS GLN ASN LEU Q9 S10 Q11 R24 Y25 P26 I33 T34 E35 L36 Q37 I42 V43 M47 H58 F59 K62 G67 V68 L69 I70 V71 E72 G73 M74 A75 E92 I93 T96 K97 T98

- Chain C: 
- 

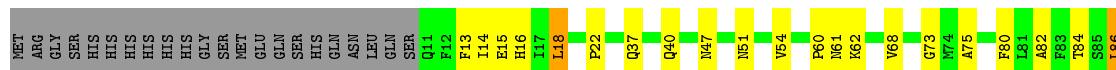
- Chain D: 
- | Label | Color |
|-------|--------|
| MET | Grey |
| ARG | Grey |
| GLY | Grey |
| SER | Grey |
| HIS | Grey |
| HIS | Grey |
| HIS | Grey |
| HIS | Grey |
| HIS | Grey |
| GLY | Grey |
| SER | Grey |
| MET | Grey |
| GLU | Grey |
| GLN | Grey |
| SER | Grey |
| HIS | Grey |
| GLN | Grey |
| ASN | Grey |
| L8 | Green |
| Q9 | Green |
| S10 | Green |
| Q11 | Green |
| F12 | Green |
| F13 | Green |
| I14 | Green |
| E15 | Green |
| H16 | Green |
| I17 | Green |
| L18 | Orange |
| R24 | Yellow |
| Y25 | Yellow |
| P26 | Yellow |
| L29 | Yellow |
| T34 | Yellow |
| E35 | Yellow |
| L36 | Yellow |
| M47 | Yellow |
| F50 | Yellow |
| H58 | Yellow |
| F59 | Yellow |
| K62 | Yellow |
| V68 | Yellow |
| M74 | Yellow |
| A75 | Yellow |
| Q76 | Yellow |
| L86 | Yellow |
| D90 | Yellow |
| D91 | Yellow |
| L92 | Yellow |
| L93 | Yellow |
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| L256 | Yellow |
| L257 | Yellow |
| | |



- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase



- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.05Å 100.53Å 186.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 39.06 – 2.60	Depositor EDS
% Data completeness (in resolution range)	85.7 (50.00-2.60) 85.7 (39.06-2.60)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	30.00 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.187 , 0.241 0.187 , 0.246	Depositor DCC
R_{free} test set	3733 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7942	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3023e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: CL, BEN, SCB

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	0/1256	0.63	0/1698
1	B	0.42	0/1248	0.60	0/1687
1	C	0.40	0/1248	0.62	0/1687
1	D	0.42	0/1256	0.63	0/1698
1	E	0.40	0/1256	0.63	0/1698
1	F	0.39	0/1212	0.63	0/1641
All	All	0.41	0/7476	0.62	0/10109

There are no bond length outliers.

There are no bond angle outliers.

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	1225	0	1243	49	0
1	B	1217	0	1232	38	0
1	C	1217	0	1232	37	0
1	D	1225	0	1243	46	0
1	E	1225	0	1243	35	0
1	F	1181	0	1200	53	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	F	2	0	0	0	0
3	A	18	0	14	2	0
3	B	9	0	7	1	0
3	C	18	0	14	0	0
3	D	9	0	7	0	0
3	E	9	0	7	1	0
4	A	33	0	18	10	0
5	A	124	0	0	6	0
5	B	88	0	0	3	0
5	C	88	0	0	2	0
5	D	76	0	0	8	0
5	E	95	0	0	4	0
5	F	79	0	0	6	0
All	All	7942	0	7460	245	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 16.

All (245) 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)
4:A:3001:SCB:O2	4:A:3001:SCB:H8	1.59	1.02
4:A:3001:SCB:H20	4:A:3001:SCB:S1	2.03	0.98
1:D:13:PHE:H	1:D:16:HIS:HD2	1.13	0.92
1:A:40:GLN:HE21	3:A:2002:BEN:HN22	1.14	0.91
1:C:13:PHE:H	1:C:16:HIS:HD2	1.14	0.89
1:D:29:LEU:H	1:D:76:GLN:HE22	1.16	0.86
1:A:29:LEU:H	1:A:76:GLN:HE22	1.26	0.82
4:A:3001:SCB:O5	4:A:3001:SCB:CL1	2.35	0.82
1:F:37:GLN:HB3	1:F:40:GLN:HE21	1.45	0.80
1:C:47:ASN:HB3	1:E:47:ASN:HB3	1.62	0.80
4:A:3001:SCB:O2	4:A:3001:SCB:C8	2.30	0.79
1:D:13:PHE:H	1:D:16:HIS:CD2	2.01	0.79
1:E:107:VAL:CG2	1:F:104:ILE:HB	2.15	0.76
1:E:83:PHE:CZ	1:E:94:ALA:HB2	2.21	0.75
1:B:47:ASN:HB3	1:F:47:ASN:HB3	1.68	0.75
1:A:104:ILE:HG12	1:A:151:LEU:HD23	1.68	0.75
1:E:107:VAL:HG22	1:F:104:ILE:HB	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASN:HB3	1:D:47:ASN:HB3	1.69	0.74
1:F:15:GLU:HB3	5:F:1078:HOH:O	1.87	0.74
1:F:108:LYS:HB2	1:F:108:LYS:NZ	2.03	0.72
1:A:13:PHE:H	1:A:16:HIS:HD2	1.38	0.71
1:D:29:LEU:N	1:D:76:GLN:HE22	1.88	0.71
1:E:92:GLU:O	1:E:95:LYS:HG2	1.92	0.69
1:B:36:LEU:HD23	1:B:37:GLN:N	2.08	0.69
1:A:37:GLN:HG3	1:A:40:GLN:HB2	1.75	0.69
1:D:157:GLU:HG3	5:D:2069:HOH:O	1.92	0.68
4:A:3001:SCB:C20	4:A:3001:SCB:S1	2.80	0.67
1:C:104:ILE:HB	1:D:107:VAL:HG13	1.75	0.67
1:C:104:ILE:O	1:D:107:VAL:HG13	1.96	0.66
1:C:35:GLU:HG2	1:C:43:VAL:HB	1.77	0.66
1:C:11:GLN:HB2	5:C:2061:HOH:O	1.96	0.66
1:D:29:LEU:H	1:D:76:GLN:NE2	1.93	0.65
1:F:108:LYS:HB2	1:F:108:LYS:HZ3	1.62	0.64
1:C:9:GLN:HB2	1:C:12:PHE:CZ	2.32	0.64
1:D:36:LEU:C	1:D:36:LEU:HD23	2.17	0.64
1:C:13:PHE:N	1:C:16:HIS:HD2	1.93	0.64
1:F:155:ILE:HD13	1:F:156:ALA:N	2.12	0.64
1:B:103:THR:HG21	5:B:2068:HOH:O	1.97	0.64
1:D:11:GLN:HE22	1:D:34:THR:HA	1.63	0.64
1:E:98:ILE:H	1:E:98:ILE:HD13	1.63	0.63
4:A:3001:SCB:O1	1:B:100:TYR:HA	1.98	0.63
1:C:104:ILE:HB	1:D:107:VAL:CG1	2.29	0.63
1:E:104:ILE:HB	1:F:107:VAL:HG22	1.79	0.63
4:A:3001:SCB:H6	1:B:98:ILE:HD13	1.80	0.62
1:F:134:GLN:NE2	5:F:1065:HOH:O	2.32	0.62
1:B:33:ILE:HD12	1:B:42:ILE:HD11	1.82	0.61
1:F:131:MET:SD	1:F:155:ILE:HG23	2.41	0.61
1:A:9:GLN:HG3	1:A:10:SER:H	1.65	0.61
1:A:104:ILE:HG12	1:A:151:LEU:CD2	2.31	0.61
1:F:60:PRO:O	1:F:61:ASN:HB2	2.01	0.61
1:D:91:PRO:O	1:D:95:LYS:HG3	2.01	0.60
1:D:107:VAL:HA	1:D:148:GLU:O	2.01	0.60
1:F:37:GLN:HB3	1:F:40:GLN:NE2	2.15	0.60
1:C:13:PHE:H	1:C:16:HIS:CD2	2.07	0.59
1:D:157:GLU:C	1:D:159:GLU:H	2.06	0.59
1:F:13:PHE:H	1:F:16:HIS:HD2	1.50	0.59
1:D:14:ILE:O	1:D:18:LEU:HD22	2.03	0.58
1:E:98:ILE:HD13	1:E:156:ALA:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:GLU:HG3	5:F:1040:HOH:O	2.04	0.58
1:D:159:GLU:HG3	1:D:159:GLU:OXT	2.04	0.57
1:A:124:GLU:HG2	5:A:3111:HOH:O	2.05	0.56
1:E:107:VAL:HG21	1:F:104:ILE:HB	1.87	0.56
1:F:97:LYS:NZ	1:F:157:GLU:OE1	2.32	0.56
4:A:3001:SCB:H13A	5:B:2055:HOH:O	2.05	0.56
1:A:157:GLU:HG3	5:A:3010:HOH:O	2.06	0.56
1:E:98:ILE:N	1:E:98:ILE:HD13	2.21	0.56
1:A:40:GLN:HB3	3:A:2002:BEN:HN22	1.72	0.55
1:E:15:GLU:HG2	5:E:2072:HOH:O	2.07	0.55
1:F:95:LYS:HB3	5:F:1047:HOH:O	2.05	0.55
1:D:90:ASP:CG	1:D:93:ILE:HG22	2.27	0.55
1:C:122:HIS:O	1:C:137:GLY:HA3	2.06	0.55
1:B:99:VAL:HB	3:B:2001:BEN:C	2.36	0.55
1:C:103:THR:HG22	1:D:108:LYS:HG2	1.88	0.55
1:A:29:LEU:HD22	1:A:46:LYS:HE3	1.89	0.54
1:A:66:PRO:HB2	1:A:69:LEU:HG	1.90	0.54
1:B:127:LYS:HD2	1:B:134:GLN:OE1	2.08	0.54
1:C:103:THR:O	1:C:104:ILE:HD13	2.08	0.54
1:B:101:PHE:CE2	1:B:153:ALA:HB2	2.42	0.54
1:F:155:ILE:C	1:F:155:ILE:HD13	2.27	0.54
1:F:13:PHE:H	1:F:16:HIS:CD2	2.25	0.54
1:C:151:LEU:N	1:C:151:LEU:HD12	2.23	0.54
1:A:122:HIS:O	1:A:137:GLY:HA3	2.08	0.54
1:F:111:ILE:HB	1:F:146:VAL:HG12	1.89	0.53
1:C:36:LEU:HD11	1:C:84:THR:OG1	2.08	0.53
1:D:86:LEU:HD23	5:D:2065:HOH:O	2.09	0.53
4:A:3001:SCB:H21A	4:A:3001:SCB:O2	2.08	0.52
1:B:114:THR:HB	1:B:115:PRO:HD2	1.90	0.52
1:C:36:LEU:HD23	1:C:36:LEU:C	2.30	0.52
1:E:87:TRP:CH2	1:E:97:LYS:HE3	2.44	0.52
1:E:16:HIS:HB3	1:E:89:PHE:CE1	2.45	0.52
1:B:103:THR:CG2	1:B:104:ILE:N	2.72	0.52
1:B:75:ALA:HB1	1:B:101:PHE:CE1	2.45	0.52
1:E:130:GLY:HA2	3:E:2007:BEN:N2	2.25	0.52
1:E:119:LEU:HD11	1:E:139:ALA:HB1	1.92	0.51
1:F:108:LYS:HD2	1:F:110:ARG:NH2	2.25	0.51
1:A:36:LEU:HD13	1:A:37:GLN:N	2.25	0.51
1:E:11:GLN:HE21	1:E:13:PHE:HE1	1.58	0.51
1:F:125:VAL:HA	1:F:135:VAL:HG12	1.92	0.51
1:B:96:THR:HG22	1:B:97:LYS:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LYS:O	1:B:158:ARG:NH2	2.43	0.51
1:C:108:LYS:HB2	1:C:148:GLU:HG2	1.93	0.51
1:A:68:VAL:HB	1:B:68:VAL:HB	1.93	0.50
1:A:46:LYS:HE2	5:D:2018:HOH:O	2.10	0.50
1:A:108:LYS:HD3	1:A:110:ARG:NH1	2.25	0.50
1:F:131:MET:HB3	1:F:155:ILE:O	2.12	0.50
1:B:11:GLN:HB2	1:B:33:ILE:O	2.11	0.50
1:B:122:HIS:O	1:B:137:GLY:HA3	2.10	0.50
1:D:159:GLU:CG	1:D:159:GLU:OXT	2.59	0.50
1:E:104:ILE:HB	1:F:107:VAL:CG2	2.42	0.49
1:A:101:PHE:CE1	1:A:153:ALA:HB2	2.47	0.49
1:A:42:ILE:HG22	1:A:81:LEU:HD22	1.94	0.49
1:D:11:GLN:NE2	1:D:34:THR:HA	2.26	0.49
1:D:62:LYS:HA	5:D:2066:HOH:O	2.12	0.49
1:B:35:GLU:HB3	1:B:43:VAL:HB	1.95	0.49
1:F:138:THR:HG22	1:F:148:GLU:HB3	1.94	0.49
1:F:97:LYS:HD2	1:F:155:ILE:HD11	1.95	0.49
1:D:58:HIS:N	1:D:59:PHE:HA	2.27	0.49
1:A:107:VAL:HA	1:A:148:GLU:O	2.13	0.49
1:E:87:TRP:HH2	1:E:155:ILE:HD11	1.77	0.49
1:A:159:GLU:HG2	5:A:3117:HOH:O	2.12	0.49
1:B:114:THR:HB	1:B:115:PRO:CD	2.43	0.48
1:F:97:LYS:HB3	1:F:155:ILE:HD11	1.94	0.48
1:A:75:ALA:HB1	1:A:101:PHE:CE2	2.48	0.48
1:A:9:GLN:HG3	1:A:10:SER:N	2.28	0.48
1:A:134:GLN:HG2	1:A:152:LYS:HG3	1.94	0.48
1:B:62:LYS:HE3	1:B:62:LYS:HA	1.96	0.48
1:A:15:GLU:HG3	5:D:2066:HOH:O	2.14	0.47
1:D:102:MET:SD	1:D:132:ILE:HD12	2.53	0.47
1:A:13:PHE:H	1:A:16:HIS:CD2	2.26	0.47
1:E:131:MET:SD	1:E:155:ILE:HD11	2.54	0.47
1:C:60:PRO:O	1:C:61:ASN:HB2	2.15	0.47
1:F:22:PRO:HG3	1:F:98:ILE:HA	1.95	0.47
1:A:127:LYS:NZ	1:A:134:GLN:HE22	2.13	0.47
1:A:120:GLU:HG2	1:A:122:HIS:NE2	2.29	0.47
1:C:29:LEU:HD22	1:C:46:LYS:HE2	1.95	0.47
1:B:108:LYS:HD2	1:B:148:GLU:OE1	2.15	0.47
1:E:107:VAL:HA	1:E:148:GLU:O	2.15	0.47
1:B:93:ILE:O	1:B:96:THR:HB	2.14	0.46
1:B:98:ILE:CD1	1:B:158:ARG:HA	2.46	0.46
1:E:118:ARG:HD2	5:E:2032:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:THR:HG22	1:B:104:ILE:N	2.29	0.46
1:A:10:SER:HA	1:A:36:LEU:HB3	1.98	0.46
1:C:33:ILE:HD13	1:C:44:ALA:CB	2.46	0.46
1:C:51:ASN:ND2	5:C:2016:HOH:O	2.49	0.46
1:F:14:ILE:O	1:F:18:LEU:HD22	2.16	0.46
1:A:29:LEU:N	1:A:76:GLN:HE22	2.04	0.46
1:E:41:LYS:HE2	5:E:2081:HOH:O	2.15	0.46
1:F:86:LEU:HD13	1:F:133:TRP:CZ2	2.51	0.46
1:F:82:ALA:O	1:F:86:LEU:HB2	2.16	0.46
1:D:158:ARG:O	1:D:159:GLU:C	2.54	0.46
1:F:97:LYS:CG	1:F:155:ILE:HD11	2.46	0.46
1:A:36:LEU:C	1:A:36:LEU:CD1	2.84	0.45
1:D:134:GLN:HB2	5:D:2061:HOH:O	2.16	0.45
1:D:98:ILE:HG23	1:D:158:ARG:HG3	1.98	0.45
1:F:127:LYS:HD3	5:F:1073:HOH:O	2.15	0.45
1:E:107:VAL:HG22	1:F:104:ILE:CB	2.43	0.45
1:D:14:ILE:HG13	1:D:18:LEU:HD22	1.99	0.45
1:F:54:VAL:N	5:F:1027:HOH:O	2.44	0.45
1:B:126:LEU:HD11	1:B:150:GLU:HG2	1.97	0.45
1:D:98:ILE:HD11	1:D:100:TYR:HE1	1.81	0.45
1:F:87:TRP:HB3	1:F:93:ILE:HD12	1.99	0.45
1:A:15:GLU:CG	5:D:2066:HOH:O	2.64	0.45
1:C:36:LEU:HD23	1:C:37:GLN:N	2.32	0.45
1:D:11:GLN:HA	1:D:11:GLN:NE2	2.32	0.45
1:B:103:THR:HG22	5:B:2008:HOH:O	2.17	0.45
1:C:99:VAL:HG22	1:C:155:ILE:CD1	2.47	0.44
1:C:112:PRO:HB3	1:D:100:TYR:HE2	1.82	0.44
1:C:57:GLY:HA2	1:D:24:ARG:HB2	1.98	0.44
1:A:8:LEU:HD23	1:A:8:LEU:O	2.16	0.44
1:A:134:GLN:NE2	5:A:3114:HOH:O	2.51	0.44
1:B:58:HIS:N	1:B:59:PHE:HA	2.31	0.44
1:F:62:LYS:HG3	1:F:62:LYS:O	2.17	0.44
1:A:36:LEU:C	1:A:36:LEU:HD13	2.37	0.44
1:C:12:PHE:HB3	1:C:16:HIS:HB2	1.99	0.44
1:C:35:GLU:CG	1:C:43:VAL:HB	2.46	0.44
1:D:14:ILE:HG13	1:D:18:LEU:CD2	2.48	0.44
1:A:134:GLN:CG	1:A:152:LYS:HG3	2.47	0.44
1:D:139:ALA:O	1:D:146:VAL:HG22	2.18	0.44
1:C:158:ARG:HG2	1:C:159:GLU:N	2.33	0.44
1:E:12:PHE:HB2	1:E:33:ILE:HB	1.99	0.44
1:E:33:ILE:HD12	1:E:42:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HG21	1:B:72:GLU:HB2	2.00	0.43
1:B:70:ILE:O	1:B:74:MET:HG3	2.18	0.43
1:F:131:MET:SD	1:F:155:ILE:CG2	3.06	0.43
1:A:99:VAL:HB	5:A:3094:HOH:O	2.17	0.43
1:A:28:LEU:HD23	1:D:50:PHE:CD2	2.54	0.43
1:C:84:THR:O	1:C:88:GLY:N	2.50	0.43
1:D:102:MET:HB2	1:D:152:LYS:O	2.19	0.43
1:D:127:LYS:NZ	1:D:129:LYS:NZ	2.67	0.43
1:A:58:HIS:N	1:A:59:PHE:HA	2.34	0.43
1:A:42:ILE:HB	1:A:81:LEU:HD13	2.00	0.43
1:F:122:HIS:O	1:F:137:GLY:HA3	2.19	0.43
1:B:98:ILE:HG13	1:B:158:ARG:HA	2.00	0.42
1:F:131:MET:HB3	1:F:155:ILE:CG2	2.49	0.42
1:E:60:PRO:O	1:E:61:ASN:HB2	2.19	0.42
1:E:72:GLU:HG3	1:E:76:GLN:NE2	2.34	0.42
1:B:10:SER:OG	1:B:11:GLN:N	2.52	0.42
1:C:15:GLU:O	1:C:19:GLN:HG3	2.18	0.42
1:D:138:THR:HG22	1:D:148:GLU:HG2	2.02	0.42
1:F:102:MET:HB2	1:F:152:LYS:O	2.19	0.42
1:C:98:ILE:HG13	1:C:158:ARG:HA	2.01	0.42
1:A:57:GLY:HA3	1:B:24:ARG:O	2.18	0.42
1:E:101:PHE:HB3	1:F:109:PHE:CD1	2.54	0.42
1:C:150:GLU:C	1:C:151:LEU:HD12	2.39	0.42
1:C:80:PHE:CE2	1:C:84:THR:HG21	2.54	0.42
1:B:111:ILE:HB	1:B:146:VAL:HG12	2.02	0.42
1:E:120:GLU:HG2	1:E:122:HIS:CD2	2.55	0.42
1:F:97:LYS:CB	1:F:155:ILE:HD11	2.50	0.42
1:B:100:TYR:CZ	1:B:154:MET:HG2	2.55	0.42
1:A:108:LYS:CD	1:A:110:ARG:NH1	2.83	0.42
1:A:122:HIS:C	1:A:123:LEU:HD22	2.40	0.42
1:A:72:GLU:O	1:A:76:GLN:HG3	2.20	0.42
1:C:33:ILE:HD13	1:C:44:ALA:HB2	2.01	0.42
1:D:157:GLU:C	1:D:159:GLU:N	2.71	0.42
1:D:15:GLU:HG2	1:D:15:GLU:H	1.55	0.42
1:E:122:HIS:O	1:E:137:GLY:HA3	2.20	0.42
1:F:86:LEU:HD13	1:F:133:TRP:HZ2	1.85	0.42
1:F:146:VAL:O	1:F:147:ALA:HB2	2.19	0.42
1:F:138:THR:HA	1:F:148:GLU:HA	2.02	0.42
1:B:97:LYS:NZ	1:B:157:GLU:OE1	2.34	0.41
1:D:9:GLN:HB2	1:D:12:PHE:CZ	2.55	0.41
1:D:75:ALA:HB2	1:D:101:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:PHE:CE1	1:E:87:TRP:CE3	3.08	0.41
1:A:16:HIS:HB3	1:A:89:PHE:CE1	2.55	0.41
1:B:69:LEU:HA	1:B:69:LEU:HD23	1.88	0.41
1:C:72:GLU:HB2	1:D:68:VAL:HG11	2.02	0.41
1:F:108:LYS:NZ	1:F:108:LYS:CB	2.79	0.41
1:A:106:LYS:HE3	5:A:3055:HOH:O	2.19	0.41
1:E:25:TYR:CE1	1:E:26:PRO:HB3	2.56	0.41
1:A:25:TYR:HA	1:A:26:PRO:HA	1.85	0.41
4:A:3001:SCB:C2	4:A:3001:SCB:O2	2.69	0.41
1:F:75:ALA:HB2	1:F:101:PHE:CZ	2.56	0.41
1:F:73:GLY:HA3	1:F:121:TYR:CZ	2.56	0.41
5:E:2014:HOH:O	1:F:68:VAL:HG22	2.20	0.41
1:B:92:GLU:CD	1:B:92:GLU:H	2.23	0.41
1:C:158:ARG:CG	1:C:159:GLU:N	2.84	0.41
1:C:33:ILE:HD12	1:C:42:ILE:HD11	2.02	0.40
1:E:139:ALA:HB3	1:E:147:ALA:HB3	2.03	0.40
1:B:67:GLY:O	1:B:71:VAL:HG23	2.21	0.40
1:D:74:MET:HB3	1:D:123:LEU:HD11	2.04	0.40
1:F:14:ILE:HG13	1:F:18:LEU:HD22	2.02	0.40
1:D:94:ALA:HB2	5:D:2068:HOH:O	2.21	0.40
1:E:72:GLU:HG3	1:E:76:GLN:HE21	1.87	0.40
1:E:97:LYS:HG2	1:E:155:ILE:HD13	2.03	0.40
1:F:80:PHE:CE2	1:F:84:THR:HG21	2.57	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	150/171 (88%)	139 (93%)	11 (7%)	0	100	100
1	B	149/171 (87%)	141 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	149/171 (87%)	140 (94%)	9 (6%)	0	100	100
1	D	150/171 (88%)	138 (92%)	12 (8%)	0	100	100
1	E	150/171 (88%)	142 (95%)	8 (5%)	0	100	100
1	F	145/171 (85%)	137 (94%)	7 (5%)	1 (1%)	22	43
All	All	893/1026 (87%)	837 (94%)	55 (6%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	51	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	131/148 (88%)	127 (97%)	4 (3%)	40	66
1	B	130/148 (88%)	126 (97%)	4 (3%)	40	66
1	C	130/148 (88%)	125 (96%)	5 (4%)	33	59
1	D	131/148 (88%)	125 (95%)	6 (5%)	27	51
1	E	131/148 (88%)	127 (97%)	4 (3%)	40	66
1	F	126/148 (85%)	121 (96%)	5 (4%)	31	57
All	All	779/888 (88%)	751 (96%)	28 (4%)	35	61

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	54	VAL
1	A	151	LEU
1	A	157	GLU
1	B	26	PRO
1	B	62	LYS

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Mol	Chain	Res	Type
1	B	151	LEU
1	B	158	ARG
1	C	11	GLN
1	C	51	ASN
1	C	105	ASP
1	C	111	ILE
1	C	123	LEU
1	D	18	LEU
1	D	26	PRO
1	D	101	PHE
1	D	105	ASP
1	D	107	VAL
1	D	159	GLU
1	E	8	LEU
1	E	69	LEU
1	E	98	ILE
1	E	101	PHE
1	F	18	LEU
1	F	86	LEU
1	F	101	PHE
1	F	107	VAL
1	F	155	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	40	GLN
1	A	47	ASN
1	A	51	ASN
1	A	76	GLN
1	A	134	GLN
1	B	9	GLN
1	B	40	GLN
1	B	47	ASN
1	B	51	ASN
1	C	16	HIS
1	C	40	GLN
1	C	47	ASN
1	C	51	ASN
1	C	61	ASN
1	D	11	GLN

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Mol	Chain	Res	Type
1	D	16	HIS
1	D	76	GLN
1	D	140	GLN
1	F	11	GLN
1	F	16	HIS
1	F	37	GLN
1	F	39	ASN
1	F	40	GLN
1	F	51	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BEN	B	2001	-	9,9,9	1.59	3 (33%)	7,11,11	0.60	0
3	BEN	C	2005	-	9,9,9	1.65	3 (33%)	7,11,11	0.59	0
3	BEN	A	2002	-	9,9,9	1.48	1 (11%)	7,11,11	0.60	0
3	BEN	E	2007	-	9,9,9	1.84	3 (33%)	7,11,11	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BEN	A	2003	-	9,9,9	2.15	4 (44%)	7,11,11	0.64	0
3	BEN	D	2006	-	9,9,9	2.00	3 (33%)	7,11,11	0.56	0
4	SCB	A	3001	-	29,36,36	2.36	9 (31%)	39,50,50	1.87	8 (20%)
3	BEN	C	2004	-	9,9,9	1.96	4 (44%)	7,11,11	0.52	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
3	BEN	B	2001	-	-	4/4/4/4	0/1/1/1
3	BEN	C	2005	-	-	4/4/4/4	0/1/1/1
3	BEN	A	2002	-	-	4/4/4/4	0/1/1/1
3	BEN	E	2007	-	-	4/4/4/4	0/1/1/1
3	BEN	A	2003	-	-	4/4/4/4	0/1/1/1
3	BEN	D	2006	-	-	4/4/4/4	0/1/1/1
4	SCB	A	3001	-	-	10/12/36/36	0/4/4/4
3	BEN	C	2004	-	-	4/4/4/4	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3001	SCB	C15-C17	5.86	1.53	1.47
4	A	3001	SCB	C19-N2	-5.11	1.33	1.42
4	A	3001	SCB	C4-C5	-4.83	1.39	1.48
4	A	3001	SCB	C6-C5	4.80	1.40	1.34
4	A	3001	SCB	C11-C10	-4.42	1.38	1.46
4	A	3001	SCB	C18-N2	3.55	1.33	1.27
3	A	2003	BEN	C6-C1	3.24	1.44	1.39
3	D	2006	BEN	C6-C1	2.92	1.44	1.39
3	A	2003	BEN	C2-C1	2.89	1.44	1.39
3	E	2007	BEN	C6-C1	2.76	1.44	1.39
4	A	3001	SCB	C18-S1	-2.73	1.68	1.75
3	C	2004	BEN	C6-C1	2.68	1.43	1.39
3	C	2004	BEN	C2-C1	2.68	1.43	1.39
3	C	2004	BEN	C1-C	2.65	1.52	1.47
3	E	2007	BEN	C2-C1	2.47	1.43	1.39
3	D	2006	BEN	C2-C1	2.43	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2003	BEN	C1-C	2.42	1.51	1.47
3	B	2001	BEN	C2-C1	2.33	1.43	1.39
3	D	2006	BEN	C-N2	2.31	1.39	1.33
3	C	2005	BEN	C2-C1	2.29	1.43	1.39
3	A	2003	BEN	C-N2	2.27	1.39	1.33
4	A	3001	SCB	C4-N1	-2.24	1.34	1.39
3	C	2005	BEN	C6-C1	2.23	1.43	1.39
3	B	2001	BEN	C6-C1	2.23	1.43	1.39
3	C	2005	BEN	C-N2	2.21	1.39	1.33
3	E	2007	BEN	C1-C	2.20	1.51	1.47
3	B	2001	BEN	C-N2	2.20	1.39	1.33
3	C	2004	BEN	C-N2	2.13	1.39	1.33
3	A	2002	BEN	C2-C1	2.07	1.42	1.39
4	A	3001	SCB	C18-N1	-2.02	1.34	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3001	SCB	C6-C5-C4	6.14	126.78	120.40
4	A	3001	SCB	C5-C4-N1	4.39	114.81	110.16
4	A	3001	SCB	C14-C15-C17	-3.86	117.27	125.09
4	A	3001	SCB	C4-C5-S1	-3.41	106.46	110.58
4	A	3001	SCB	C18-S1-C5	3.09	94.99	90.75
4	A	3001	SCB	C9-C8-C7	2.62	108.56	106.30
4	A	3001	SCB	O2-C4-C5	-2.28	122.91	126.46
4	A	3001	SCB	C12-C11-C10	-2.00	117.89	120.42

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3001	SCB	C2-C3-N1-C18
4	A	3001	SCB	C4-C5-C6-C7
4	A	3001	SCB	S1-C5-C6-C7
4	A	3001	SCB	N1-C18-N2-C19
4	A	3001	SCB	O1-C2-C3-N1
4	A	3001	SCB	S1-C18-N2-C19
4	A	3001	SCB	C3-C2-O1-C1
4	A	3001	SCB	C20-C19-N2-C18
4	A	3001	SCB	C2-C3-N1-C4
4	A	3001	SCB	C24-C19-N2-C18
3	B	2001	BEN	N2-C-C1-C2

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Mol	Chain	Res	Type	Atoms
3	B	2001	BEN	N2-C-C1-C6
3	C	2005	BEN	N2-C-C1-C2
3	C	2005	BEN	N2-C-C1-C6
3	A	2002	BEN	N2-C-C1-C2
3	A	2002	BEN	N2-C-C1-C6
3	A	2003	BEN	N2-C-C1-C2
3	A	2003	BEN	N2-C-C1-C6
3	D	2006	BEN	N2-C-C1-C2
3	D	2006	BEN	N2-C-C1-C6
3	E	2007	BEN	N2-C-C1-C2
3	E	2007	BEN	N2-C-C1-C6
3	C	2004	BEN	N2-C-C1-C2
3	C	2004	BEN	N2-C-C1-C6
3	B	2001	BEN	N1-C-C1-C2
3	B	2001	BEN	N1-C-C1-C6
3	C	2005	BEN	N1-C-C1-C2
3	C	2005	BEN	N1-C-C1-C6
3	A	2002	BEN	N1-C-C1-C2
3	A	2002	BEN	N1-C-C1-C6
3	A	2003	BEN	N1-C-C1-C2
3	A	2003	BEN	N1-C-C1-C6
3	D	2006	BEN	N1-C-C1-C2
3	D	2006	BEN	N1-C-C1-C6
3	E	2007	BEN	N1-C-C1-C2
3	E	2007	BEN	N1-C-C1-C6
3	C	2004	BEN	N1-C-C1-C2
3	C	2004	BEN	N1-C-C1-C6

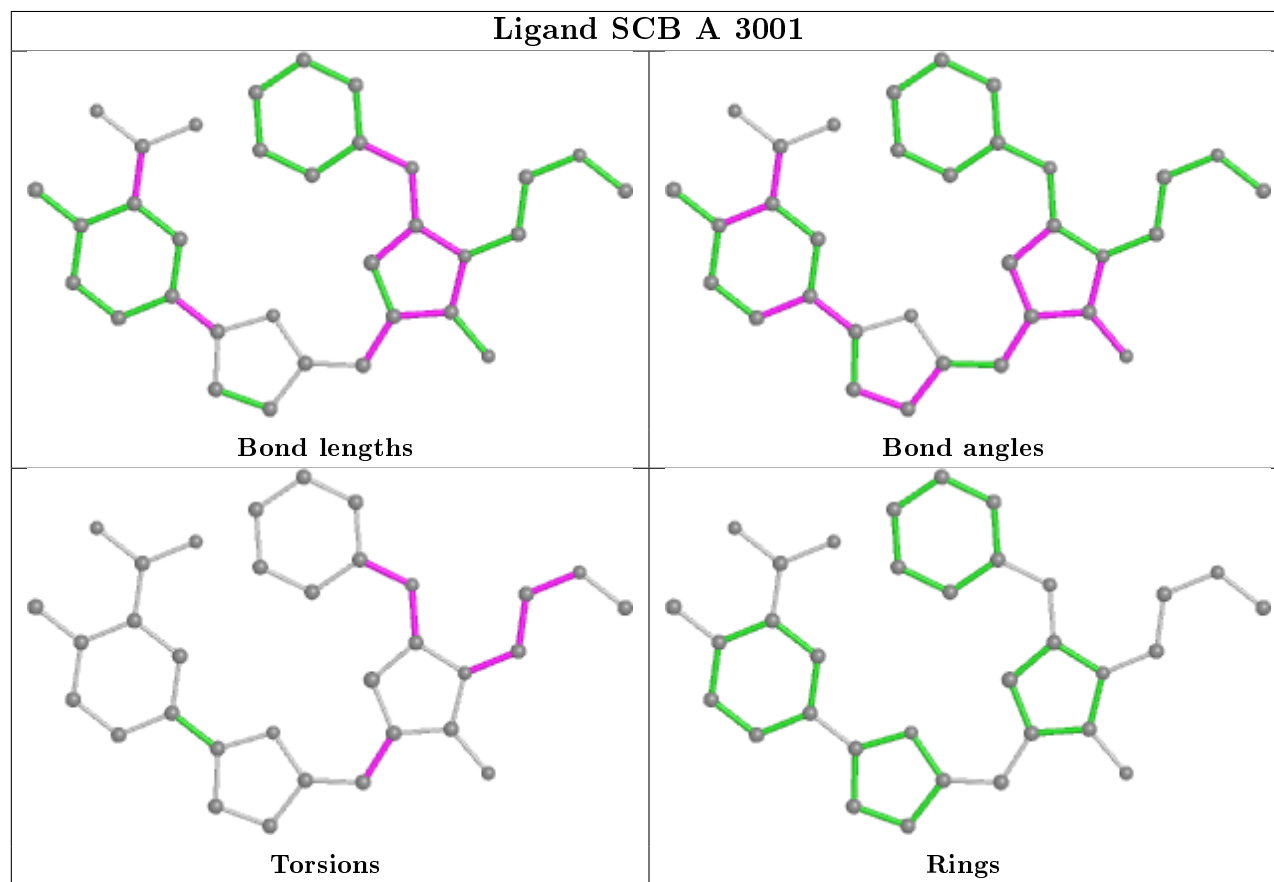
There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	BEN	1	0
3	A	2002	BEN	2	0
3	E	2007	BEN	1	0
4	A	3001	SCB	10	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	152/171 (88%)	-0.77	0 100 100	5, 13, 27, 39	0
1	B	151/171 (88%)	-0.63	3 (1%) 65 60	6, 13, 27, 54	0
1	C	151/171 (88%)	-0.75	0 100 100	4, 13, 26, 44	0
1	D	152/171 (88%)	-0.66	0 100 100	5, 13, 29, 46	0
1	E	152/171 (88%)	-0.77	1 (0%) 87 86	6, 13, 26, 42	0
1	F	147/171 (85%)	-0.68	0 100 100	6, 14, 25, 30	0
All	All	905/1026 (88%)	-0.71	4 (0%) 92 91	4, 13, 27, 54	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9	GLN	3.2
1	B	10	SER	2.9
1	E	8	LEU	2.5
1	B	159	GLU	2.3

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 carbohydrates in this entry.

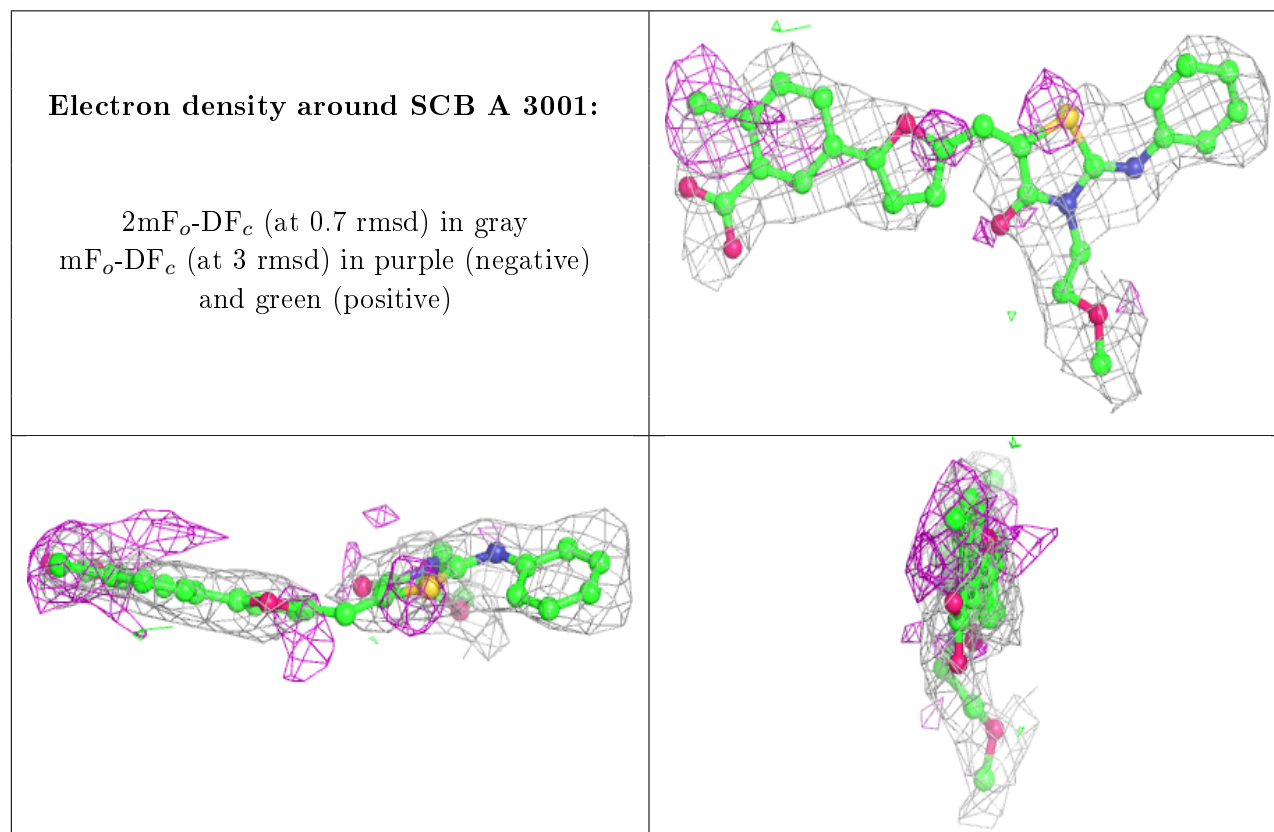
6.4 Ligands [i](#)

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
4	SCB	A	3001	33/33	0.69	0.40	43,49,51,53	0
3	BEN	A	2003	9/9	0.71	0.34	45,47,48,48	0
3	BEN	D	2006	9/9	0.76	0.47	50,51,53,53	0
3	BEN	C	2004	9/9	0.89	0.20	25,27,30,32	0
3	BEN	E	2007	9/9	0.92	0.24	22,26,27,28	0
3	BEN	B	2001	9/9	0.92	0.22	31,32,35,36	0
3	BEN	C	2005	9/9	0.92	0.24	29,30,33,34	0
2	CL	C	1003	1/1	0.96	0.14	25,25,25,25	0
2	CL	A	1001	1/1	0.96	0.09	22,22,22,22	0
2	CL	D	1004	1/1	0.96	0.12	33,33,33,33	0
3	BEN	A	2002	9/9	0.96	0.13	12,13,16,16	0
2	CL	F	1005	1/1	0.97	0.13	31,31,31,31	0
2	CL	B	1002	1/1	0.98	0.13	38,38,38,38	0
2	CL	F	1006	1/1	1.00	0.12	21,21,21,21	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.