Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:29 AM GMT

PDB ID	:	3EUV
Title	:	Crystal structure of FTase(ALPHA-subunit; BETA-subunit DELTA C10, W102T, Y154T) in complex with BiotinGPP
Authors	:	Guo, Z.; Nguyen, U.T.T.; Delon, C.; Bon, R.S.; Blankenfeldt, W.; Goody, R.S.; Waldmann, H.; Wolters, D.; Alexandrov, K.
Deposited on	:	2008-10-11
Resolution	:	2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

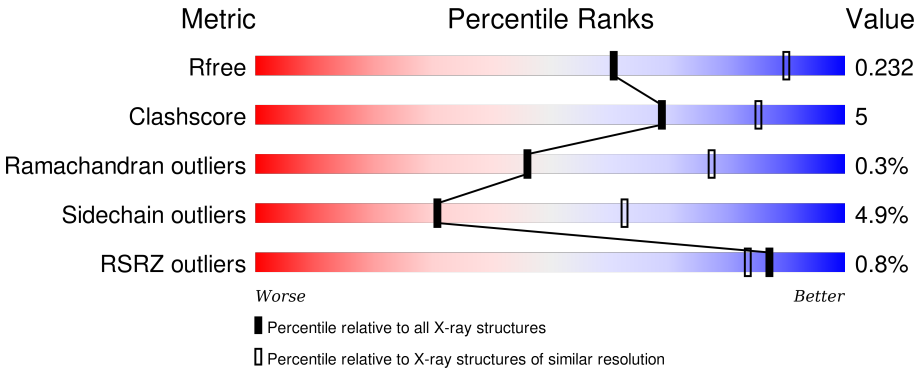
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	377	% 71% 10% • 16%
2	B	427	81% 12% •• 6%

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
4	GBO	B	429	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5966 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 Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2688	1712	473	498	5			

- Molecule 2 is a protein called Protein farnesyltransferase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	2	0
			3159	2014	543	579	23			

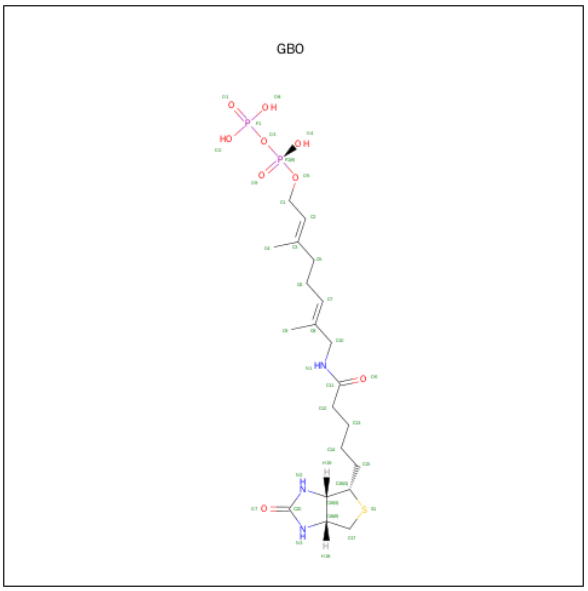
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	102	THR	TRP	ENGINEERED	UNP Q02293
B	154	THR	TYR	ENGINEERED	UNP Q02293

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (2E,6E)-3,7-DIMETHYL-8-({5-[(3AS,4S,6AR)-2-OXOHEXAHYDRO-1H-THIENO[3,4-D]IMIDAZOL-4-YL]PENTANOYL}AMINO)OCTA-2,6-DIEN-1-YL TRIHYDROGEN DIPHOSPHATE (three-letter code: GBO) (formula: $C_{20}H_{35}N_3O_9P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	0	0
			35	20	3	9	2	1		

- Molecule 5 is water.

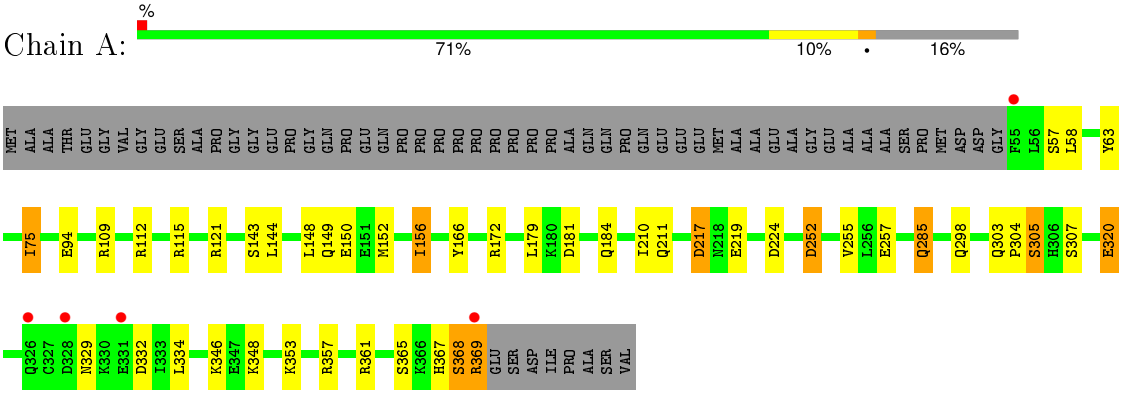
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total	O	0	0
			33	33		
5	B	50	Total	O	0	0
			50	50		

3 Residue-property plots (i)

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

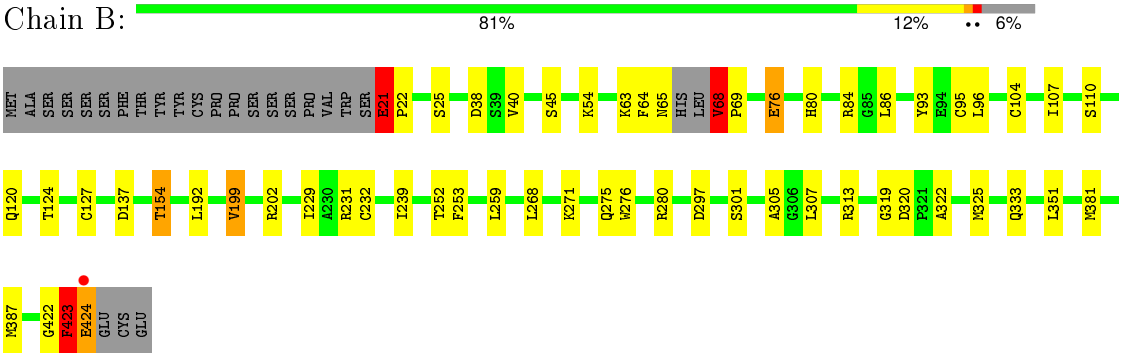
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

Chain A:



- Molecule 2: Protein farnesyltransferase subunit beta

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	174.78Å 174.78Å 70.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 2.75 29.97 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.97-2.75) 99.9 (29.97-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	6.14 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.169 , 0.231 0.179 , 0.232	Depositor DCC
R_{free} test set	1613 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.7	EDS
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 32102 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5966	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.99	4/2754 (0.1%)	0.85	1/3738 (0.0%)
2	B	0.92	5/3247 (0.2%)	0.85	2/4407 (0.0%)
All	All	0.95	9/6001 (0.1%)	0.85	3/8145 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
2	B	0	3
All	All	1	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	104	CYS	CB-SG	-9.80	1.65	1.82
2	B	127	CYS	CB-SG	-8.27	1.68	1.82
1	A	150	GLU	CG-CD	6.41	1.61	1.51
2	B	76	GLU	CG-CD	5.94	1.60	1.51
2	B	275	GLN	CG-CD	5.71	1.64	1.51
1	A	94	GLU	CD-OE1	5.55	1.31	1.25
1	A	166	TYR	CE2-CZ	5.47	1.45	1.38
1	A	320	GLU	CG-CD	5.45	1.60	1.51
2	B	21	GLU	CB-CG	5.44	1.62	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	423	PHE	N-CA-C	-6.79	92.68	111.00
1	A	285	GLN	CB-CA-C	5.50	121.40	110.40
2	B	154	THR	CB-CA-C	-5.34	97.18	111.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	285	GLN	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	368	SER	Peptide
2	B	21	GLU	Peptide
2	B	423	PHE	Peptide
2	B	68	VAL	Peptide

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	2688	0	2614	26	0
2	B	3159	0	3086	29	0
3	B	1	0	0	0	0
4	B	35	0	32	1	0
5	A	33	0	0	1	0
5	B	50	0	0	4	0
All	All	5966	0	5732	53	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 5.

All (53) 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)
1:A:156:ILE:HD13	1:A:172:ARG:HH12	1.33	0.92
1:A:368:SER:O	1:A:369:ARG:HG2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:LEU:HD23	2:B:199:VAL:HG23	1.75	0.69
1:A:303:GLN:O	1:A:307:SER:HB2	1.93	0.67
1:A:149:GLN:HE22	1:A:184:GLN:HE22	1.44	0.65
1:A:368:SER:C	1:A:369:ARG:HG2	2.14	0.61
2:B:231:ARG:HD3	5:B:451:HOH:O	2.00	0.61
1:A:156:ILE:CD1	1:A:172:ARG:HH12	2.09	0.60
1:A:152:MET:O	1:A:156:ILE:CG1	2.52	0.57
2:B:76:GLU:OE2	2:B:80[B]:HIS:NE2	2.38	0.56
2:B:93:TYR:HD2	2:B:96:LEU:HD12	1.71	0.55
1:A:210:ILE:HD11	1:A:219:GLU:OE1	2.07	0.54
1:A:152:MET:O	1:A:156:ILE:HG12	2.09	0.53
2:B:325:MET:HB3	2:B:381:MET:HG3	1.91	0.52
1:A:353:LYS:O	1:A:357:ARG:HG3	2.10	0.51
1:A:152:MET:O	1:A:156:ILE:HG13	2.11	0.51
2:B:301:SER:O	2:B:305:ALA:HB3	2.11	0.51
5:A:469:HOH:O	2:B:95:CYS:HB3	2.11	0.49
2:B:64:PHE:O	2:B:65:ASN:O	2.30	0.49
1:A:156:ILE:HD13	1:A:172:ARG:NH1	2.16	0.49
1:A:252:ASP:HB3	1:A:255:VAL:HB	1.94	0.49
1:A:361:ARG:NH2	2:B:322:ALA:O	2.45	0.48
2:B:229:ILE:O	2:B:232:CYS:HB2	2.15	0.47
2:B:319:GLY:O	2:B:320:ASP:C	2.53	0.47
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.97	0.46
2:B:259:LEU:HD12	2:B:268:LEU:HD11	1.98	0.46
2:B:253:PHE:HA	2:B:307:LEU:HD21	1.97	0.45
2:B:68:VAL:N	2:B:69:PRO:CD	2.78	0.45
2:B:76:GLU:OE2	2:B:80[B]:HIS:CD2	2.70	0.45
2:B:333:GLN:HG3	2:B:387:MET:SD	2.56	0.45
2:B:64:PHE:CB	5:B:456:HOH:O	2.66	0.44
1:A:334:LEU:HD22	1:A:367:HIS:O	2.18	0.44
2:B:38:ASP:O	2:B:40:VAL:HG23	2.18	0.44
1:A:320:GLU:OE1	2:B:271:LYS:NZ	2.43	0.44
1:A:75:ILE:HD13	1:A:115:ARG:NH2	2.33	0.44
2:B:239:ILE:HB	2:B:252:THR:HA	1.99	0.44
2:B:68:VAL:N	2:B:69:PRO:HD3	2.32	0.44
1:A:334:LEU:CD2	1:A:367:HIS:O	2.65	0.43
2:B:423:PHE:CA	2:B:424:GLU:C	2.86	0.43
1:A:217:ASP:OD2	1:A:217:ASP:N	2.51	0.43
2:B:276:TRP:O	2:B:280:ARG:HG2	2.19	0.42
1:A:304:PRO:O	1:A:305:SER:CB	2.68	0.42
2:B:64:PHE:HB3	5:B:456:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:HD23	1:A:63:TYR:CE1	2.54	0.42
1:A:148:LEU:HB2	1:A:179:LEU:HD21	2.02	0.42
1:A:121:ARG:HG2	1:A:121:ARG:O	2.12	0.41
1:A:112:ARG:O	1:A:144:LEU:HD21	2.20	0.41
2:B:422:GLY:O	2:B:423:PHE:HD1	2.04	0.41
2:B:86:LEU:HB2	2:B:107:ILE:HG21	2.01	0.41
1:A:181:ASP:OD1	1:A:181:ASP:C	2.59	0.41
2:B:63:LYS:O	5:B:500:HOH:O	2.22	0.41
2:B:202:ARG:HD2	4:B:429:GBO:H13	2.02	0.41
2:B:297:ASP:OD1	2:B:297:ASP:C	2.58	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	313/377 (83%)	291 (93%)	20 (6%)	2 (1%)	30 62
2	B	400/427 (94%)	379 (95%)	21 (5%)	0	100 100
All	All	713/804 (89%)	670 (94%)	41 (6%)	2 (0%)	46 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	SER
1	A	252	ASP

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	294/338 (87%)	279 (95%)	15 (5%)	29	61
2	B	340/363 (94%)	324 (95%)	16 (5%)	32	64
All	All	634/701 (90%)	603 (95%)	31 (5%)	31	62

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	75	ILE
1	A	109	ARG
1	A	143	SER
1	A	156	ILE
1	A	211	GLN
1	A	217	ASP
1	A	224	ASP
1	A	257	GLU
1	A	285	GLN
1	A	298	GLN
1	A	346	LYS
1	A	348	LYS
1	A	365	SER
1	A	369	ARG
2	B	21	GLU
2	B	22	PRO
2	B	25	SER
2	B	45	SER
2	B	54	LYS
2	B	68	VAL
2	B	84	ARG
2	B	110	SER
2	B	120	GLN
2	B	124	THR
2	B	137	ASP
2	B	154	THR
2	B	199	VAL
2	B	313	ARG
2	B	351	LEU
2	B	424	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	221	GLN
1	A	225	GLN
1	A	303	GLN
1	A	325	ASN
2	B	56	GLN
2	B	170	ASN
2	B	275	GLN

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	GBO	B	429	-	31,36,36	2.34	12 (38%)	37,50,50	1.81	8 (21%)

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
4	GBO	B	429	-	-	0/31/52/52	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	429	GBO	O5-C1	-6.97	1.34	1.43
4	B	429	GBO	C1-C2	-3.63	1.37	1.49
4	B	429	GBO	C6-C7	-3.46	1.40	1.50
4	B	429	GBO	C5-C3	2.19	1.56	1.51
4	B	429	GBO	C18-N3	2.34	1.50	1.45
4	B	429	GBO	C4-C3	2.45	1.56	1.50
4	B	429	GBO	P1-O2	2.87	1.65	1.54
4	B	429	GBO	C19-N2	2.98	1.51	1.45
4	B	429	GBO	C2-C3	3.09	1.39	1.33
4	B	429	GBO	C7-C8	3.18	1.39	1.33
4	B	429	GBO	C12-C11	3.63	1.58	1.51
4	B	429	GBO	P1-O8	3.89	1.68	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	429	GBO	C6-C7-C8	-4.10	118.85	127.76
4	B	429	GBO	P2-O3-P1	-3.73	120.15	132.67
4	B	429	GBO	C10-N1-C11	-3.44	111.54	121.47
4	B	429	GBO	O3-P2-O5	-3.10	94.71	102.94
4	B	429	GBO	C5-C6-C7	2.03	117.00	111.69
4	B	429	GBO	C4-C3-C5	2.94	119.90	115.41
4	B	429	GBO	C17-S1-C16	2.98	96.90	90.33
4	B	429	GBO	N3-C20-N2	3.38	111.22	108.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	429	GBO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	315/377 (83%)	-0.41	5 (1%)	74	70	25, 58, 83, 97	0
2	B	402/427 (94%)	-0.37	1 (0%)	95	95	30, 50, 80, 117	0
All	All	717/804 (89%)	-0.39	6 (0%)	87	83	25, 55, 83, 117	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	369	ARG	4.1
1	A	55	PHE	2.7
1	A	326	GLN	2.6
1	A	331	GLU	2.6
2	B	424	GLU	2.3
1	A	328	ASP	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GBO	B	429	35/35	0.95	0.20	2.03	48,66,135,137	0
3	ZN	B	428	1/1	0.97	0.10	-	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.