



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:51 PM GMT

PDB ID : 4GAA
Title : Structure of Leukotriene A4 hydrolase from *Xenopus laevis* complexed with inhibitor bestatin
Authors : Stsiapanava, A.; Kumar, R.B.; Haeggstrom, J.Z.; Rinaldo-Matthis, A.
Deposited on : 2012-07-25
Resolution : 2.26 Å(reported)

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

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

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

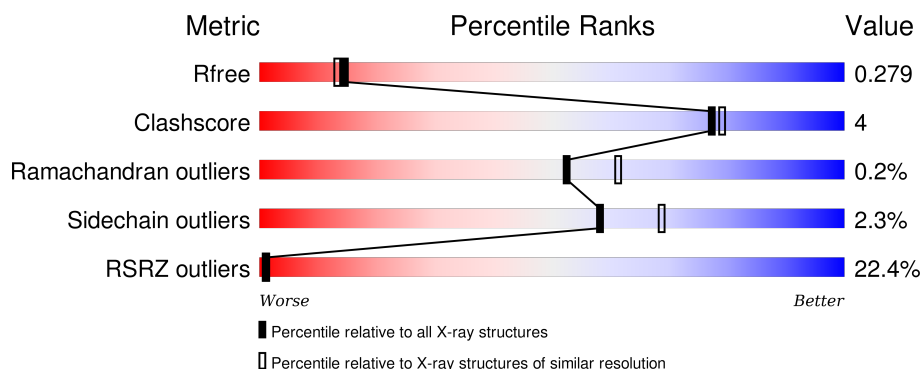
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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

Mol	Chain	Length	Quality of chain
1	A	609	<div> <div>11%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	B	609	<div> <div>34%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9859 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.

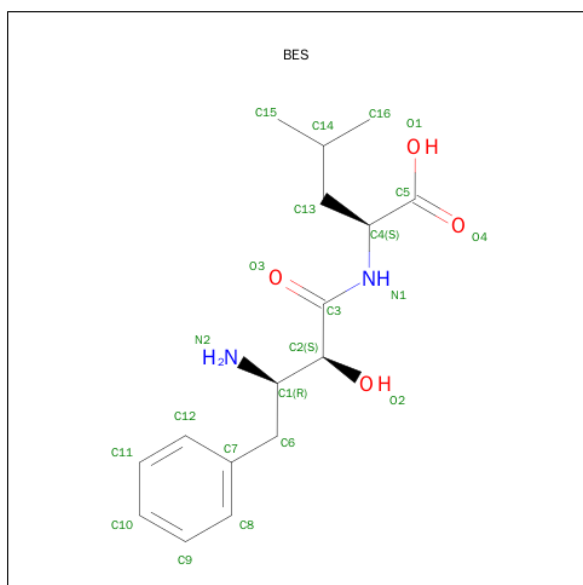
- Molecule 1 is a protein called MGC78867 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	0	2	0
			4861	3136	807	898	20			
1	B	605	Total	C	N	O	S	0	2	0
			4857	3133	807	897	20			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (three-letter code: BES) (formula: C₁₆H₂₄N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	16	2	4		
3	B	1	Total	C	N	O	0	0
			22	16	2	4		

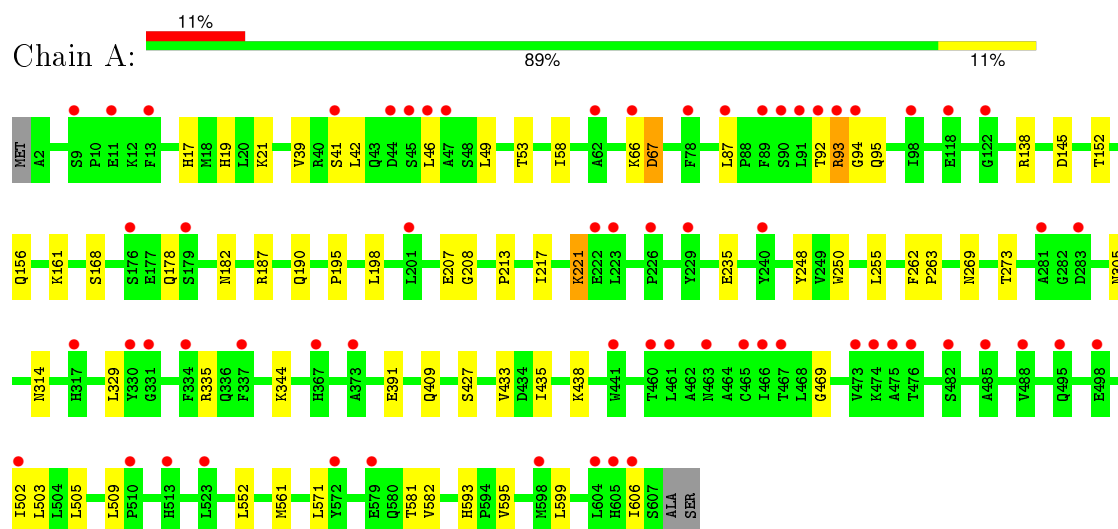
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	1
			58	58		
4	B	36	Total	O	0	1
			37	37		

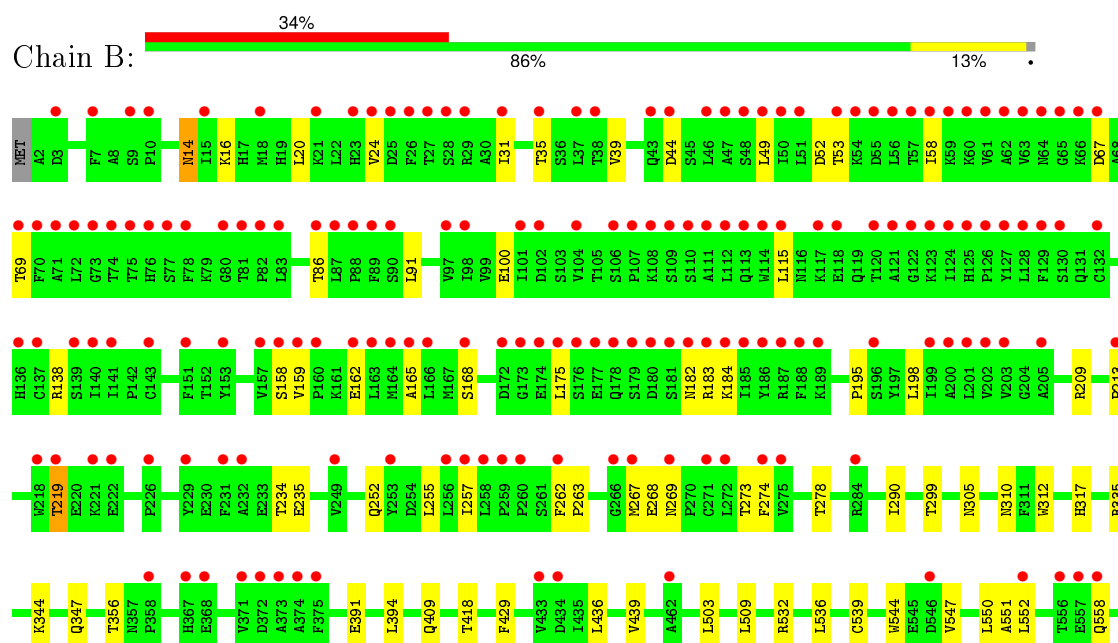
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: MGC78867 protein



• Molecule 1: MGC78867 protein



Y568	Y571	Y572	N573	F574	E575	K576	A577	R578	E579	Q580	T581	V582	M583	T584	F585	L586	K587	N588	R589	S590	F591	N592	H593	P594	V595	T596	E597	N598	L599	W600	A601	K602	D603	L604	H605	I606	SER	ALA	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	222.12Å 52.17Å 109.90Å 90.00° 111.58° 90.00°	Depositor
Resolution (Å)	29.30 – 2.26 29.23 – 2.26	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.30-2.26) 97.4 (29.23-2.26)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.26Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.222 , 0.250 0.242 , 0.279	Depositor DCC
R_{free} test set	2726 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 79.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 53926 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9859	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BES, 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	0.47	0/4991	0.64	0/6776
1	B	0.45	0/4987	0.63	0/6771
All	All	0.46	0/9978	0.63	0/13547

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

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	4861	0	4862	33	0
1	B	4857	0	4855	41	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	0	23	0	0
3	B	22	0	22	0	0
4	A	58	0	0	0	0
4	B	37	0	0	0	0
All	All	9859	0	9762	73	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 4.

All (73) 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:B:571:LEU:HB3	1:B:581:THR:HG21	1.65	0.77
1:A:571:LEU:HB3	1:A:581:THR:HG21	1.64	0.77
1:B:312:TRP:HE1	1:B:418:THR:CG2	2.04	0.71
1:B:52:ASP:HB3	1:B:138:ARG:HG2	1.75	0.67
1:A:161:LYS:HE3	1:A:182:ASN:HA	1.77	0.65
1:B:312:TRP:HE1	1:B:418:THR:HG21	1.62	0.64
1:B:158:SER:HB3	1:B:183:ARG:HD2	1.84	0.59
1:B:195:PRO:HD2	1:B:198:LEU:HD12	1.85	0.59
1:B:159:VAL:HG11	1:B:165:ALA:HB2	1.86	0.57
1:A:195:PRO:HD2	1:A:198:LEU:HD12	1.87	0.56
1:B:310:ASN:OD1	1:B:418:THR:HG23	2.07	0.55
1:A:469:GLY:HA3	1:A:502:ILE:HD11	1.89	0.55
1:B:335:ARG:NH2	1:B:391:GLU:OE1	2.39	0.55
1:A:41:SER:O	1:A:94:GLY:HA2	2.07	0.55
1:A:335:ARG:NH2	1:A:391:GLU:OE1	2.41	0.54
1:A:138:ARG:HH21	1:A:145:ASP:HB3	1.72	0.54
1:B:532:ARG:HH22	1:B:550:LEU:HD22	1.72	0.54
1:B:267:MET:HB3	1:B:274:PHE:HB2	1.90	0.54
1:A:344:LYS:HD2	1:A:502:ILE:HG22	1.88	0.53
1:B:503:LEU:HD22	1:B:509:LEU:HD11	1.91	0.53
1:A:582:VAL:HG13	1:A:606:ILE:HD11	1.91	0.52
1:A:503:LEU:HD22	1:A:509:LEU:HD11	1.90	0.52
1:A:49:LEU:HD13	1:A:87:LEU:HD11	1.91	0.51
1:B:312:TRP:HE1	1:B:418:THR:HG22	1.76	0.50
1:B:213:PRO:HD2	1:B:235:GLU:HG3	1.95	0.49
1:A:213:PRO:HD2	1:A:235:GLU:HG3	1.94	0.48
1:B:234:THR:HG21	1:B:255:LEU:HD11	1.94	0.48
1:B:39:VAL:HG11	1:B:49:LEU:HD11	1.96	0.47
1:B:24:VAL:HG12	1:B:31:ILE:HG12	1.97	0.47
1:B:593:HIS:ND1	1:B:594:PRO:HD2	2.30	0.47
1:A:39:VAL:HG11	1:A:49:LEU:HD11	1.96	0.47
1:B:601:ALA:HA	1:B:606:ILE:HD13	1.97	0.46
1:A:92:THR:O	1:A:95:GLN:HB2	2.16	0.46
1:B:234:THR:HG22	1:B:290:ILE:HG21	1.98	0.46
1:A:156:GLN:HG2	1:A:187:ARG:HG2	1.97	0.46
1:B:219:THR:HG23	1:B:257:ILE:HB	1.97	0.45
1:B:20:LEU:HD23	1:B:35:THR:HG23	1.99	0.44
1:B:344:LYS:HA	1:B:347:GLN:HG2	1.99	0.44
1:A:207:GLU:HG3	1:A:221:LYS:HG3	1.99	0.44
1:A:53:THR:HG21	1:A:58:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409[B]:GLN:CD	1:B:409:GLN:HG2	2.37	0.44
1:A:262:PHE:CD1	1:A:263:PRO:HD2	2.53	0.44
1:A:255:LEU:HD23	1:A:273:THR:HB	2.00	0.43
1:A:66:LYS:O	1:A:67:ASP:HB2	2.17	0.43
1:A:152:THR:HG23	1:A:190:GLN:O	2.19	0.43
1:B:69:THR:HG23	1:B:86:THR:HG23	1.99	0.43
1:B:262:PHE:CD1	1:B:263:PRO:HD2	2.54	0.43
1:A:248:TYR:CZ	1:A:250:TRP:HB2	2.53	0.43
1:B:168:SER:HB3	1:B:269:ASN:HB3	2.01	0.43
1:A:593:HIS:CE1	1:A:595:VAL:HG23	2.54	0.43
1:A:593:HIS:HE1	1:A:595:VAL:HG23	1.84	0.43
1:A:208:GLY:HA2	1:A:217:ILE:O	2.19	0.43
1:B:552:LEU:HD21	1:B:581:THR:HG22	2.01	0.42
1:A:17:HIS:ND1	1:A:152:THR:HG22	2.34	0.42
1:B:255:LEU:HD23	1:B:273:THR:HB	2.01	0.42
1:B:394:LEU:HD13	1:B:429:PHE:CE1	2.54	0.42
1:B:536:LEU:HD13	1:B:551:ALA:HA	2.02	0.42
1:A:19:HIS:ND1	1:A:21:LYS:HE2	2.35	0.41
1:B:436:LEU:O	1:B:439:VAL:HG13	2.21	0.41
1:B:568:TYR:CZ	1:B:585:PHE:HD1	2.38	0.41
1:B:544:TRP:O	1:B:547:VAL:HG12	2.21	0.41
1:B:53:THR:HG21	1:B:58:ILE:HD11	2.01	0.41
1:A:561:MET:SD	1:A:599:LEU:HD12	2.60	0.41
1:A:168:SER:HB3	1:A:269:ASN:HB3	2.03	0.41
1:B:159:VAL:O	1:B:184:LYS:N	2.54	0.41
1:B:299:THR:HG21	1:B:317:HIS:HB3	2.03	0.41
1:B:539:CYS:HG	1:B:544:TRP:HE3	1.69	0.41
1:B:14:ASN:HB3	1:B:16:LYS:HE2	2.02	0.41
1:B:278:THR:HG22	1:B:558:GLN:HG2	2.03	0.41
1:A:435:ILE:HA	1:A:438:LYS:HD2	2.03	0.41
1:A:552:LEU:HD21	1:A:581:THR:HG22	2.02	0.40
1:A:42:LEU:C	1:A:93:ARG:HG3	2.41	0.40
1:B:278:THR:HG22	1:B:558:GLN:HE21	1.87	0.40

There are no symmetry-related clashes.

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	606/609 (100%)	581 (96%)	23 (4%)	2 (0%)	46	52
1	B	605/609 (99%)	584 (96%)	20 (3%)	1 (0%)	52	61
All	All	1211/1218 (99%)	1165 (96%)	43 (4%)	3 (0%)	52	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	221	LYS
1	B	268	GLU

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	538/538 (100%)	529 (98%)	9 (2%)	68	79
1	B	537/538 (100%)	521 (97%)	16 (3%)	48	59
All	All	1075/1076 (100%)	1050 (98%)	25 (2%)	58	69

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	93	ARG
1	A	178	GLN

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Mol	Chain	Res	Type
1	A	305	ASN
1	A	314	ASN
1	A	329	LEU
1	A	427	SER
1	A	433	VAL
1	A	505	LEU
1	B	14	ASN
1	B	44	ASP
1	B	67	ASP
1	B	91	LEU
1	B	100	GLU
1	B	115	LEU
1	B	162	GLU
1	B	175	LEU
1	B	182	ASN
1	B	209	ARG
1	B	219	THR
1	B	252	GLN
1	B	305	ASN
1	B	356	THR
1	B	592	MET
1	B	597	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	A	314	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	BES	A	702	2	19,22,22	0.85	0	19,29,29	1.31	4 (21%)
3	BES	B	702	2	19,22,22	0.71	0	19,29,29	0.76	1 (5%)

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	BES	A	702	2	-	0/20/24/24	0/1/1/1
3	BES	B	702	2	-	0/20/24/24	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	BES	C13-C4-N1	-2.94	103.14	110.48
3	A	702	BES	C2-C3-N1	-2.62	112.60	116.33
3	B	702	BES	C13-C4-N1	-2.16	105.09	110.48
3	A	702	BES	C4-N1-C3	2.30	127.02	123.43
3	A	702	BES	O2-C2-C1	2.44	114.60	109.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	606/609 (99%)	0.61	64 (10%) 8 8	32, 74, 127, 141	0
1	B	605/609 (99%)	1.70	207 (34%) 0 0	36, 105, 164, 185	0
All	All	1211/1218 (99%)	1.16	271 (22%) 1 1	32, 83, 156, 185	0

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	ALA	17.5
1	B	179	SER	13.6
1	B	176	SER	13.3
1	B	175	LEU	12.8
1	B	122	GLY	11.4
1	B	26	PHE	11.1
1	B	73	GLY	9.6
1	B	83	LEU	9.2
1	B	123	LYS	8.8
1	B	61	VAL	8.8
1	B	585	PHE	8.6
1	B	59	LYS	8.5
1	B	62	ALA	8.3
1	B	27	THR	8.2
1	B	118	GLU	8.2
1	B	601	ALA	7.9
1	B	88	PRO	7.9
1	B	202	VAL	7.8
1	B	115	LEU	7.4
1	B	185	ILE	7.1
1	B	67	ASP	7.1
1	B	174	GLU	7.0
1	B	178	GLN	6.8
1	B	126	PRO	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	74	THR	6.7
1	B	181	SER	6.6
1	B	590	SER	6.6
1	B	129	PHE	6.5
1	B	107	PRO	6.3
1	B	186	TYR	6.2
1	B	591	PHE	5.8
1	B	114	TRP	5.6
1	B	203	VAL	5.6
1	B	106	SER	5.6
1	B	29	ARG	5.6
1	B	159	VAL	5.5
1	B	219	THR	5.5
1	A	488	VAL	5.5
1	B	54	LYS	5.5
1	B	86	THR	5.5
1	B	177	GLU	5.5
1	B	120	THR	5.5
1	B	7	PHE	5.5
1	B	182	ASN	5.4
1	A	229	TYR	5.4
1	B	113	GLN	5.4
1	B	163	LEU	5.4
1	B	124	ILE	5.3
1	B	128	LEU	5.3
1	B	201	LEU	5.3
1	B	78	PHE	5.2
1	B	588	ASN	5.2
1	B	75	THR	5.2
1	B	586	LEU	5.2
1	B	72	LEU	5.1
1	B	606	ILE	5.1
1	B	602	LYS	5.1
1	B	200	ALA	4.9
1	B	260	PRO	4.9
1	B	222	GLU	4.9
1	B	76	HIS	4.9
1	A	330	TYR	4.8
1	B	259	PRO	4.8
1	B	274	PHE	4.7
1	A	92	THR	4.7
1	B	165	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	183	ARG	4.7
1	B	64	ASN	4.6
1	B	184	LYS	4.5
1	B	180	ASP	4.5
1	B	574	PHE	4.5
1	B	130	SER	4.4
1	B	80	GLY	4.4
1	B	162	GLU	4.4
1	A	510	PRO	4.4
1	B	63	VAL	4.4
1	B	596	THR	4.3
1	A	91	LEU	4.3
1	B	56	LEU	4.3
1	B	173	GLY	4.3
1	B	58	ILE	4.2
1	B	605	HIS	4.2
1	B	25	ASP	4.2
1	B	77	SER	4.2
1	B	82	PRO	4.2
1	A	62	ALA	4.2
1	B	87	LEU	4.2
1	B	595	VAL	4.1
1	A	11	GLU	4.1
1	A	334	PHE	4.1
1	B	81	THR	4.1
1	B	172	ASP	4.0
1	B	127	TYR	4.0
1	B	28	SER	4.0
1	B	374	ALA	3.9
1	B	597	GLU	3.9
1	B	584	THR	3.9
1	B	572	TYR	3.9
1	B	157	VAL	3.9
1	B	592	MET	3.8
1	B	143	CYS	3.8
1	B	604	LEU	3.8
1	B	168	SER	3.8
1	B	373	ALA	3.8
1	B	368	GLU	3.7
1	A	90	SER	3.7
1	B	132	CYS	3.7
1	B	66	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	160	PRO	3.6
1	B	581	THR	3.6
1	B	568	TYR	3.6
1	A	281	ALA	3.5
1	A	66	LYS	3.5
1	A	283	ASP	3.5
1	B	109	SER	3.5
1	A	605	HIS	3.5
1	B	137	CYS	3.4
1	A	498	GLU	3.4
1	A	474	LYS	3.4
1	B	108	LYS	3.4
1	B	43	GLN	3.4
1	B	257	ILE	3.4
1	B	188	PHE	3.3
1	B	256	LEU	3.3
1	B	60	LYS	3.3
1	B	117	LYS	3.3
1	B	46	LEU	3.3
1	B	275	VAL	3.3
1	B	125	HIS	3.3
1	B	44	ASP	3.3
1	B	112	LEU	3.3
1	A	78	PHE	3.2
1	B	110	SER	3.2
1	A	460	THR	3.2
1	B	272	LEU	3.2
1	A	44	ASP	3.2
1	A	45	SER	3.2
1	A	223	LEU	3.2
1	A	604	LEU	3.2
1	B	102	ASP	3.2
1	B	229	TYR	3.1
1	B	367	HIS	3.1
1	B	594	PRO	3.1
1	A	87	LEU	3.1
1	B	24	VAL	3.1
1	B	101	ILE	3.1
1	B	358	PRO	3.1
1	B	582	VAL	3.1
1	B	35	THR	3.1
1	B	556	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	176	SER	3.1
1	B	65	GLY	3.1
1	B	600	VAL	3.0
1	B	53	THR	3.0
1	B	57	THR	3.0
1	A	98	ILE	3.0
1	B	575	GLU	3.0
1	B	573	ASN	3.0
1	B	462	ALA	3.0
1	B	603	ASP	2.9
1	B	70	PHE	2.9
1	B	262	PHE	2.9
1	B	189	LYS	2.9
1	B	258	LEU	2.9
1	B	434	ASP	2.9
1	A	41	SER	2.9
1	B	139	SER	2.9
1	B	21	LYS	2.8
1	A	461	LEU	2.8
1	B	15	ILE	2.8
1	B	37	LEU	2.8
1	B	375	PHE	2.8
1	A	222	GLU	2.8
1	B	136	HIS	2.8
1	A	89	PHE	2.8
1	B	271	CYS	2.8
1	B	48	SER	2.7
1	B	121	ALA	2.7
1	A	226	PRO	2.7
1	B	141	ILE	2.7
1	A	373	ALA	2.7
1	A	502	ILE	2.7
1	B	3	ASP	2.7
1	B	89	PHE	2.7
1	B	218	TRP	2.7
1	B	97	VAL	2.7
1	B	578	ARG	2.6
1	B	31	ILE	2.6
1	B	49	LEU	2.6
1	B	284	ARG	2.6
1	B	253	TYR	2.6
1	A	513	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	13	PHE	2.6
1	B	226	PRO	2.6
1	A	579	GLU	2.6
1	B	213	PRO	2.5
1	A	47	ALA	2.5
1	B	51	LEU	2.5
1	A	367	HIS	2.5
1	B	55	ASP	2.5
1	A	465	CYS	2.5
1	A	475	ALA	2.5
1	B	583	ASN	2.5
1	B	140	ILE	2.5
1	B	104	VAL	2.4
1	B	579	GLU	2.4
1	B	433	VAL	2.4
1	B	269	ASN	2.4
1	A	485	ALA	2.4
1	B	205	ALA	2.4
1	B	10	PRO	2.4
1	B	9	SER	2.4
1	B	577	ALA	2.4
1	B	18	MET	2.4
1	B	267	MET	2.4
1	A	9	SER	2.4
1	B	231	PHE	2.4
1	B	221	LYS	2.4
1	B	576	LYS	2.4
1	A	179	SER	2.3
1	B	371	VAL	2.3
1	A	466	ILE	2.3
1	A	572	TYR	2.3
1	B	164	MET	2.3
1	A	240	TYR	2.3
1	B	153	TYR	2.3
1	A	463	ASN	2.3
1	A	337	PHE	2.3
1	A	94	GLY	2.3
1	B	98	ILE	2.3
1	B	546	ASP	2.3
1	B	266	GLY	2.2
1	B	166	LEU	2.2
1	B	47	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	372	ASP	2.2
1	B	593	HIS	2.2
1	B	587	LYS	2.2
1	B	599	LEU	2.2
1	A	598	MET	2.2
1	B	589	ARG	2.2
1	A	476	THR	2.2
1	B	199	ILE	2.2
1	B	187	ARG	2.2
1	A	93	ARG	2.1
1	A	122	GLY	2.1
1	A	523	LEU	2.1
1	B	69	THR	2.1
1	A	317	HIS	2.1
1	A	482	SER	2.1
1	B	23	HIS	2.1
1	A	46	LEU	2.1
1	A	467	THR	2.1
1	B	558	GLN	2.1
1	A	441	TRP	2.1
1	B	557	GLU	2.1
1	B	552	LEU	2.1
1	A	331	GLY	2.1
1	A	495	GLN	2.1
1	A	201	LEU	2.1
1	B	232	ALA	2.1
1	B	50	ILE	2.1
1	B	38	THR	2.0
1	B	196	SER	2.0
1	A	473	VAL	2.0
1	B	151	PHE	2.0
1	B	111	ALA	2.0
1	B	90	SER	2.0
1	B	158	SER	2.0
1	A	606	ILE	2.0
1	B	249	VAL	2.0
1	A	118	GLU	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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BES	B	702	22/22	0.85	0.27	1.79	48,66,76,78	0
3	BES	A	702	22/22	0.89	0.22	1.46	33,48,63,65	0
2	ZN	B	701	1/1	0.97	0.09	-2.38	55,55,55,55	0
2	ZN	A	701	1/1	0.92	0.10	-3.87	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.