



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2016 – 02:26 PM EDT

PDB ID : 4ZGV  
Title : The Crystal Structure of the Ferredoxin Receptor FusA from *Pectobacterium atrosepticum* SCRI1043  
Authors : Grinter, R.; Josts, I.; Roszak, A.W.; Cogdell, R.J.; Walker, D.  
Deposited on : 2015-04-24  
Resolution : 3.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028320  
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) : rb-20028320

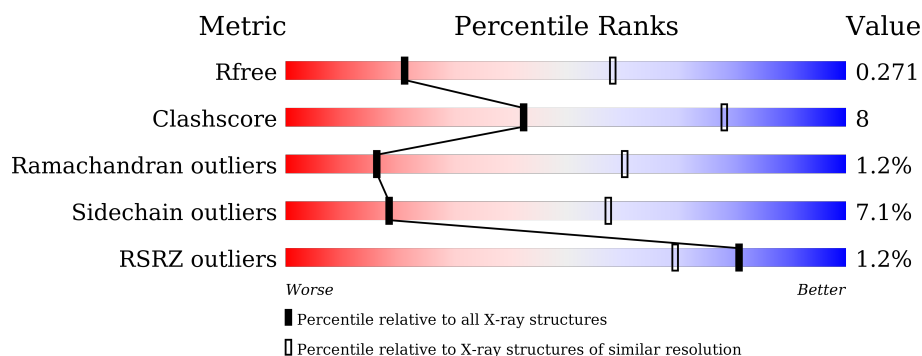
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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  $\geq 3$ , 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	868	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>• 7%</div> </div> </div>
1	B	868	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>• 7%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LDA	A	901[A]	-	-	-	X
2	LDA	A	901[B]	-	-	-	X
3	BOG	A	903	-	-	-	X
3	BOG	A	904	-	-	-	X
3	BOG	A	905	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13030 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 Ferredoxin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	809	Total	C	N	O	S	0	0	0
			6450	4062	1090	1279	19			
1	B	809	Total	C	N	O	S	0	0	0
			6450	4062	1090	1279	19			

There are 42 discrepancies between the modelled and reference sequences:

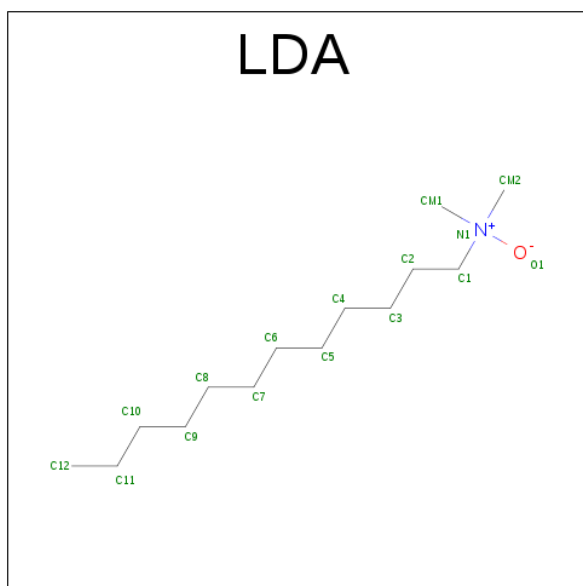
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q6D8U4
A	1	GLY	-	expression tag	UNP Q6D8U4
A	2	SER	-	expression tag	UNP Q6D8U4
A	3	SER	-	expression tag	UNP Q6D8U4
A	4	HIS	-	expression tag	UNP Q6D8U4
A	5	HIS	-	expression tag	UNP Q6D8U4
A	6	HIS	-	expression tag	UNP Q6D8U4
A	7	HIS	-	expression tag	UNP Q6D8U4
A	8	HIS	-	expression tag	UNP Q6D8U4
A	9	HIS	-	expression tag	UNP Q6D8U4
A	10	SER	-	expression tag	UNP Q6D8U4
A	11	SER	-	expression tag	UNP Q6D8U4
A	12	GLY	-	expression tag	UNP Q6D8U4
A	13	LEU	-	expression tag	UNP Q6D8U4
A	14	VAL	-	expression tag	UNP Q6D8U4
A	15	PRO	-	expression tag	UNP Q6D8U4
A	16	ARG	-	expression tag	UNP Q6D8U4
A	17	GLY	-	expression tag	UNP Q6D8U4
A	18	SER	-	expression tag	UNP Q6D8U4
A	19	HIS	-	expression tag	UNP Q6D8U4
A	20	MET	-	expression tag	UNP Q6D8U4
B	0	MET	-	initiating methionine	UNP Q6D8U4
B	1	GLY	-	expression tag	UNP Q6D8U4
B	2	SER	-	expression tag	UNP Q6D8U4
B	3	SER	-	expression tag	UNP Q6D8U4

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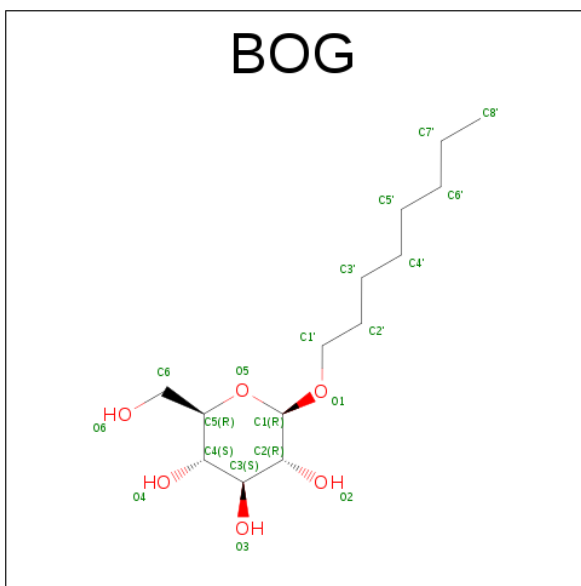
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	HIS	-	expression tag	UNP Q6D8U4
B	5	HIS	-	expression tag	UNP Q6D8U4
B	6	HIS	-	expression tag	UNP Q6D8U4
B	7	HIS	-	expression tag	UNP Q6D8U4
B	8	HIS	-	expression tag	UNP Q6D8U4
B	9	HIS	-	expression tag	UNP Q6D8U4
B	10	SER	-	expression tag	UNP Q6D8U4
B	11	SER	-	expression tag	UNP Q6D8U4
B	12	GLY	-	expression tag	UNP Q6D8U4
B	13	LEU	-	expression tag	UNP Q6D8U4
B	14	VAL	-	expression tag	UNP Q6D8U4
B	15	PRO	-	expression tag	UNP Q6D8U4
B	16	ARG	-	expression tag	UNP Q6D8U4
B	17	GLY	-	expression tag	UNP Q6D8U4
B	18	SER	-	expression tag	UNP Q6D8U4
B	19	HIS	-	expression tag	UNP Q6D8U4
B	20	MET	-	expression tag	UNP Q6D8U4

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			32	28	2	2		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 3 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		

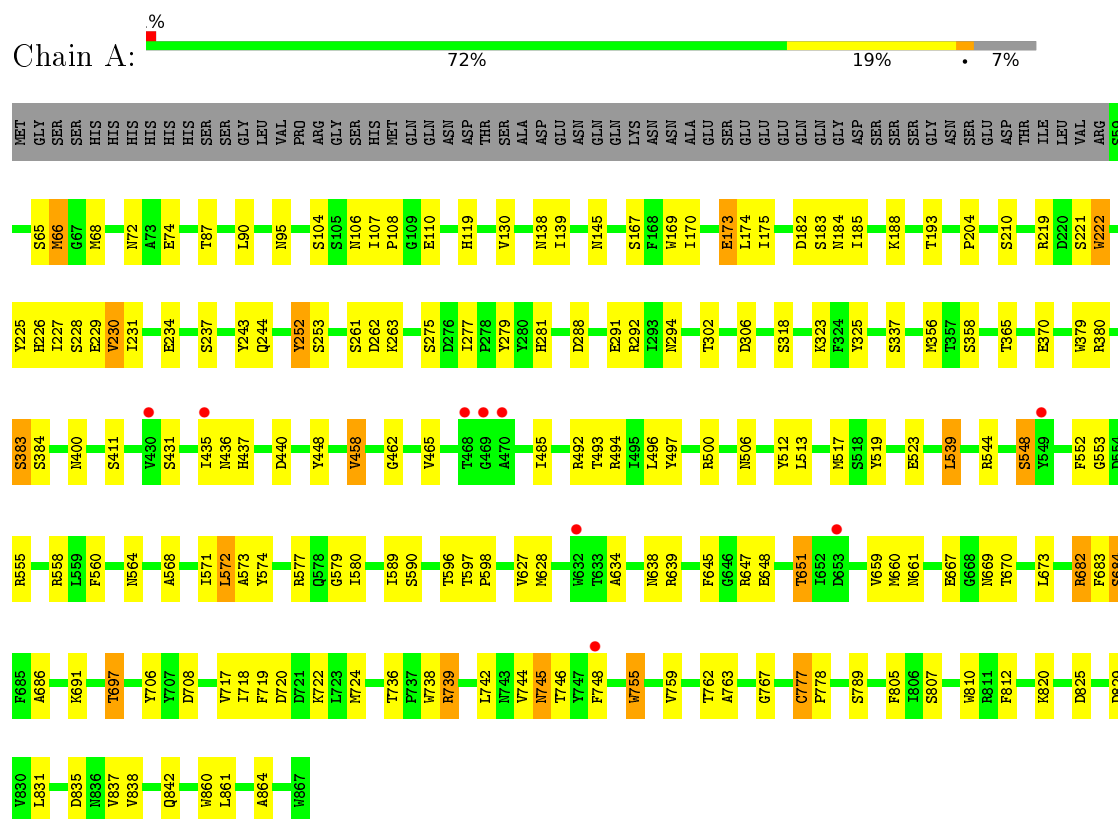
- Molecule 4 is water.

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

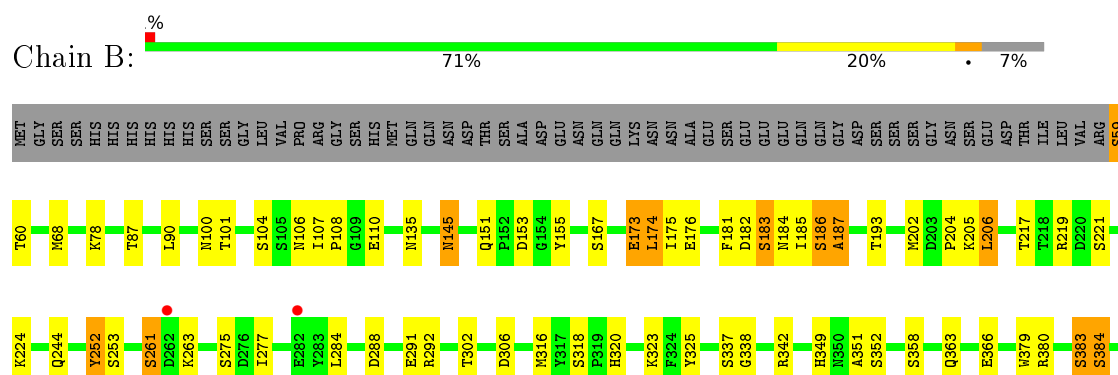
### 3 Residue-property plots

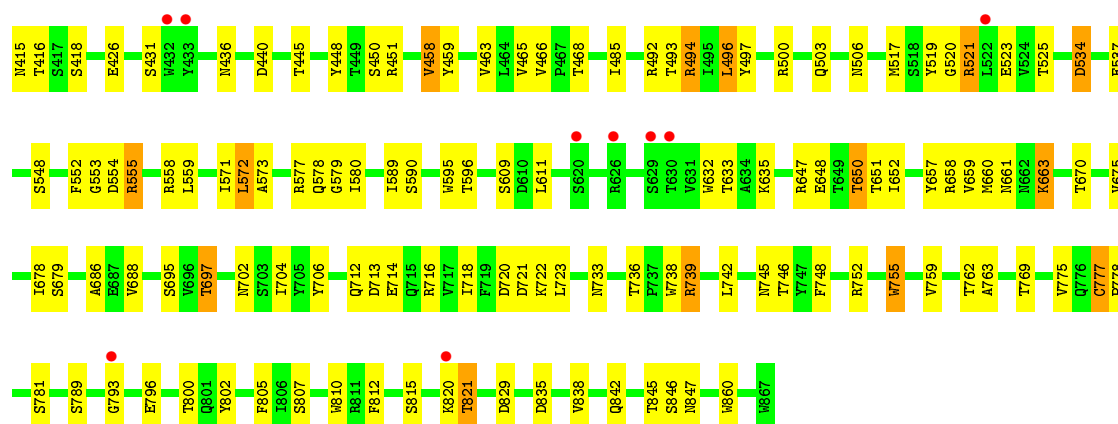
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Ferredoxin receptor



#### • Molecule 1: Ferredoxin receptor







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.27Å 79.89Å 137.91Å 90.00° 90.71° 90.00°	Depositor
Resolution (Å)	48.95 – 3.20 48.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.95-3.20) 99.9 (48.95-3.20)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.218 , 0.271 0.222 , 0.271	Depositor DCC
$R_{free}$ test set	2511 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.4	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.006 for l,k,-h 0.026 for h,-k,-l 0.014 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	13030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

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

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	0.59	0/6625	0.76	1/9003 (0.0%)
1	B	0.58	0/6625	0.78	3/9003 (0.0%)
All	All	0.59	0/13250	0.77	4/18006 (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	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	723	LEU	CA-CB-CG	6.57	130.41	115.30
1	B	572	LEU	CA-CB-CG	6.16	129.47	115.30
1	B	284	LEU	N-CA-C	-5.51	96.13	111.00
1	A	684	SER	N-CA-C	5.47	125.77	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	683	PHE	Peptide
1	A	777	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	552	PHE	Peptide
1	B	777	CYS	Peptide

## 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	6450	0	6024	109	0
1	B	6450	0	6024	102	0
2	A	48	0	93	0	0
3	A	60	0	84	0	0
3	B	20	0	28	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	13030	0	12253	210	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 8.

All (210) 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:110:GLU:OE2	1:A:292:ARG:NH1	1.82	1.12
1:A:261:SER:HB2	1:A:263:LYS:H	1.51	0.75
1:B:521:ARG:HD2	1:B:553:GLY:HA2	1.69	0.73
1:B:523:GLU:OE1	1:B:548:SER:HB3	1.89	0.73
1:A:523:GLU:OE1	1:A:548:SER:HB3	1.89	0.72
1:A:574:TYR:CD1	1:A:660:MET:HE3	2.26	0.70
1:A:574:TYR:CE1	1:A:660:MET:HE2	2.28	0.68
1:A:219:ARG:HB2	1:A:221:SER:O	1.93	0.68
1:A:682:ARG:O	1:A:684:SER:HA	1.93	0.68
1:A:572:LEU:HD23	1:A:572:LEU:C	2.15	0.67
1:A:647:ARG:NH1	1:A:708:ASP:O	2.29	0.66
1:B:182:ASP:OD2	1:B:183:SER:OG	2.11	0.66
1:A:226:HIS:CD2	1:A:837:VAL:HG22	2.31	0.65
1:A:574:TYR:CD1	1:A:660:MET:CE	2.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:670:THR:HG22	1:B:697:THR:HG22	1.77	0.64
1:A:66:MET:HG3	1:A:560:PHE:CZ	2.33	0.64
1:B:78:LYS:HB3	1:B:745:ASN:HD22	1.61	0.63
1:A:670:THR:HG22	1:A:697:THR:HG22	1.80	0.63
1:B:739:ARG:HB2	1:B:762:THR:HG23	1.82	0.62
1:B:173:GLU:O	1:B:175:ILE:HG22	1.98	0.62
1:B:87:THR:HA	1:B:90:LEU:HD13	1.82	0.62
1:A:87:THR:HA	1:A:90:LEU:HD13	1.82	0.62
1:A:139:ILE:HA	1:A:572:LEU:CD2	2.30	0.61
1:B:648:GLU:HG3	1:B:661:ASN:HB3	1.83	0.61
1:A:745:ASN:N	1:A:745:ASN:HD22	1.99	0.60
1:B:261:SER:HB2	1:B:263:LYS:H	1.66	0.60
1:B:186:SER:O	1:B:187:ALA:CB	2.47	0.60
1:B:571:ILE:O	1:B:572:LEU:HB3	2.00	0.60
1:A:138:ASN:O	1:A:572:LEU:HD22	2.02	0.59
1:B:500:ARG:NH1	1:B:579:GLY:HA3	2.17	0.59
1:A:500:ARG:NH1	1:A:579:GLY:HA3	2.18	0.59
1:B:647:ARG:HD2	1:B:658:ARG:HD3	1.85	0.59
1:B:204:PRO:HG2	1:B:302:THR:HG23	1.83	0.58
1:B:217:THR:HG21	1:B:219:ARG:HH12	1.68	0.58
1:B:186:SER:O	1:B:187:ALA:HB3	2.02	0.58
1:B:555:ARG:CZ	1:B:555:ARG:HB2	2.33	0.58
1:A:574:TYR:CE1	1:A:660:MET:CE	2.86	0.58
1:A:648:GLU:HG3	1:A:661:ASN:HB3	1.85	0.58
1:A:108:PRO:O	1:A:244:GLN:OE1	2.22	0.58
1:A:718:ILE:O	1:A:722:LYS:O	2.22	0.58
1:A:229:GLU:O	1:A:231:ILE:N	2.37	0.57
1:B:755:TRP:HH2	1:B:810:TRP:CE2	2.22	0.57
1:A:755:TRP:HH2	1:A:810:TRP:CE2	2.22	0.57
1:A:500:ARG:HH12	1:A:579:GLY:HA3	1.70	0.57
1:A:173:GLU:O	1:A:175:ILE:HG22	2.03	0.57
1:A:572:LEU:HD23	1:A:572:LEU:O	2.04	0.57
1:A:596:THR:O	1:A:598:PRO:HD3	2.05	0.56
1:B:500:ARG:HH12	1:B:579:GLY:HA3	1.71	0.56
1:A:139:ILE:O	1:A:573:ALA:HB2	2.06	0.56
1:A:193:THR:HG23	1:A:568:ALA:HB2	1.88	0.55
1:A:458:VAL:HG22	1:A:497:TYR:HB2	1.88	0.55
1:A:227:ILE:O	1:A:227:ILE:HG22	2.07	0.55
1:B:244:GLN:HG2	1:B:277:ILE:HG21	1.88	0.55
1:B:217:THR:HG21	1:B:219:ARG:NH1	2.22	0.55
1:A:138:ASN:O	1:A:571:ILE:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:720:ASP:O	1:B:722:LYS:N	2.38	0.55
1:B:829:ASP:HB2	1:B:860:TRP:HB2	1.88	0.54
1:A:539:LEU:HD12	1:A:539:LEU:C	2.27	0.54
1:A:139:ILE:HA	1:A:572:LEU:HD22	1.89	0.54
1:B:185:ILE:HG22	1:B:186:SER:H	1.72	0.54
1:B:176:GLU:HG2	1:B:202:MET:HA	1.90	0.54
1:B:342:ARG:HE	1:B:363:GLN:HE21	1.57	0.53
1:A:65:SER:HA	1:A:68:MET:HG2	1.91	0.53
1:A:261:SER:HB2	1:A:263:LYS:N	2.24	0.53
1:A:400:ASN:ND2	1:A:400:ASN:O	2.41	0.53
1:B:688:VAL:HG12	1:B:746:THR:HG23	1.90	0.52
1:A:244:GLN:HG2	1:A:277:ILE:HG21	1.91	0.52
1:A:106:ASN:HB2	1:A:107:ILE:HG13	1.92	0.52
1:B:173:GLU:O	1:B:175:ILE:N	2.42	0.52
1:A:744:VAL:C	1:A:745:ASN:HD22	2.12	0.52
1:B:648:GLU:OE2	1:B:663:LYS:NZ	2.37	0.52
1:B:573:ALA:O	1:B:577:ARG:HD2	2.09	0.51
1:B:650:THR:HG23	1:B:657:TYR:HB2	1.91	0.51
1:A:221:SER:O	1:A:222:TRP:CB	2.59	0.51
1:A:589:ILE:HG13	1:A:590:SER:N	2.25	0.50
1:A:221:SER:O	1:A:222:TRP:CD1	2.64	0.50
1:A:755:TRP:CZ3	1:A:812:PHE:CZ	2.99	0.50
1:B:755:TRP:CZ3	1:B:812:PHE:CZ	2.99	0.50
1:A:436:ASN:O	1:A:517:MET:HA	2.11	0.50
1:B:78:LYS:HB3	1:B:745:ASN:ND2	2.27	0.50
1:A:173:GLU:O	1:A:175:ILE:N	2.45	0.50
1:B:100:ASN:OD1	1:B:733:ASN:OD1	2.30	0.50
1:A:767:GLY:HA3	1:A:842:GLN:OE1	2.11	0.50
1:A:288:ASP:HB3	1:A:325:TYR:CZ	2.46	0.49
1:A:448:TYR:CZ	1:A:506:ASN:HB2	2.47	0.49
1:A:596:THR:OG1	1:A:597:THR:N	2.44	0.49
1:B:151:GLN:HG2	1:B:155:TYR:CE2	2.47	0.49
1:A:739:ARG:HB2	1:A:762:THR:HG23	1.94	0.49
1:A:571:ILE:O	1:A:572:LEU:HD22	2.11	0.49
1:A:738:TRP:CE2	1:A:763:ALA:HB2	2.46	0.49
1:A:204:PRO:HG2	1:A:302:THR:HG23	1.93	0.49
1:A:745:ASN:ND2	1:A:745:ASN:N	2.60	0.49
1:B:416:THR:HG22	1:B:450:SER:OG	2.12	0.49
1:B:555:ARG:NH1	1:B:555:ARG:HB2	2.26	0.49
1:B:738:TRP:CE2	1:B:763:ALA:HB2	2.47	0.49
1:B:534:ASP:O	1:B:537:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:ARG:NH1	1:B:815:SER:O	2.46	0.49
1:A:188:LYS:HG3	1:A:512:TYR:CZ	2.48	0.49
1:A:130:VAL:HG11	1:A:170:ILE:HD12	1.95	0.48
1:A:107:ILE:CG2	1:A:110:GLU:HG3	2.44	0.48
1:B:458:VAL:HG22	1:B:497:TYR:HB2	1.96	0.48
1:A:370:GLU:HG3	1:A:411:SER:HB3	1.95	0.47
1:B:291:GLU:HB2	1:B:323:LYS:HB3	1.96	0.47
1:A:252:TYR:CD1	1:A:252:TYR:N	2.80	0.47
1:B:712:GLN:C	1:B:713:ASP:O	2.51	0.47
1:B:320:HIS:NE2	1:B:338:GLY:O	2.48	0.47
1:B:686:ALA:HB2	1:B:748:PHE:CD1	2.49	0.47
1:B:145:ASN:OD1	1:B:706:TYR:HB3	2.15	0.47
1:B:835:ASP:O	1:B:835:ASP:CG	2.53	0.47
1:A:742:LEU:HB3	1:A:759:VAL:HG12	1.97	0.47
1:B:577:ARG:O	1:B:580:ILE:HG22	2.15	0.47
1:B:802:TYR:OH	1:B:842:GLN:NE2	2.48	0.47
1:A:686:ALA:HB2	1:A:748:PHE:CD1	2.49	0.46
1:A:119:HIS:HD2	1:A:670:THR:CG2	2.28	0.46
1:B:106:ASN:HB2	1:B:107:ILE:HG13	1.97	0.46
1:B:100:ASN:O	1:B:101:THR:HG23	2.16	0.46
1:A:169:TRP:HE3	1:A:294:ASN:HD21	1.62	0.46
1:A:435:ILE:HG13	1:A:437:HIS:CE1	2.51	0.46
1:B:845:THR:OG1	1:B:847:ASN:HB3	2.16	0.46
1:B:100:ASN:OD1	1:B:733:ASN:HA	2.16	0.46
1:B:755:TRP:CE3	1:B:812:PHE:CE1	3.04	0.46
1:A:651:THR:O	1:A:651:THR:HG22	2.14	0.46
1:A:829:ASP:HB2	1:A:860:TRP:HB2	1.96	0.46
1:A:72:ASN:ND2	1:A:74:GLU:HG2	2.30	0.46
1:B:135:ASN:O	1:B:135:ASN:CG	2.54	0.46
1:B:181:PHE:CD1	1:B:181:PHE:N	2.83	0.46
1:A:95:ASN:ND2	1:A:182:ASP:OD2	2.48	0.45
1:A:227:ILE:O	1:A:229:GLU:N	2.48	0.45
1:A:221:SER:O	1:A:222:TRP:CG	2.70	0.45
1:B:820:LYS:O	1:B:821:THR:HG22	2.17	0.45
1:A:107:ILE:HA	1:A:244:GLN:OE1	2.17	0.45
1:B:805:PHE:CD2	1:B:838:VAL:HG11	2.52	0.45
1:A:234:GLU:O	1:A:237:SER:OG	2.31	0.44
1:B:275:SER:HB3	1:B:292:ARG:HB2	1.98	0.44
1:A:279:TYR:HE2	1:A:281:HIS:CE1	2.35	0.44
1:A:719:PHE:CD2	1:A:724:MET:HE3	2.51	0.44
1:B:451:ARG:HG2	1:B:503:GLN:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:VAL:O	1:B:793:GLY:HA2	2.17	0.44
1:A:755:TRP:HH2	1:A:810:TRP:CD2	2.35	0.44
1:B:695:SER:OG	1:B:739:ARG:NH1	2.50	0.44
1:B:553:GLY:O	1:B:555:ARG:N	2.41	0.44
1:A:139:ILE:HG12	1:A:572:LEU:HD21	1.98	0.44
1:A:519:TYR:CG	1:A:519:TYR:O	2.70	0.44
1:A:231:ILE:HD13	1:A:243:TYR:OH	2.17	0.44
1:A:825:ASP:HB2	1:A:864:ALA:HB3	1.98	0.44
1:A:230:VAL:HG22	1:A:231:ILE:N	2.33	0.43
1:B:108:PRO:O	1:B:244:GLN:OE1	2.36	0.43
1:B:379:TRP:CE2	1:B:485:ILE:HD11	2.53	0.43
1:A:462:GLY:HA3	1:A:493:THR:OG1	2.18	0.43
1:B:494:ARG:HB3	1:B:595:TRP:CZ3	2.53	0.43
1:A:107:ILE:HG22	1:A:110:GLU:CG	2.49	0.43
1:B:718:ILE:HB	1:B:796:GLU:HA	2.00	0.43
1:A:719:PHE:HD2	1:A:724:MET:HE3	1.84	0.43
1:B:205:LYS:O	1:B:206:LEU:CB	2.66	0.43
1:A:379:TRP:CE2	1:A:485:ILE:HD11	2.54	0.43
1:B:366:GLU:HG3	1:B:415:ASN:HB3	2.01	0.43
1:A:183:SER:O	1:A:184:ASN:C	2.56	0.43
1:B:383:SER:O	1:B:384:SER:C	2.57	0.43
1:B:652:ILE:HG22	1:B:652:ILE:O	2.18	0.43
1:A:638:ASN:HD22	1:A:669:ASN:ND2	2.16	0.43
1:A:746:THR:HB	1:A:755:TRP:HB3	2.01	0.43
1:B:379:TRP:CD2	1:B:485:ILE:HD11	2.54	0.43
1:B:448:TYR:CZ	1:B:506:ASN:HB2	2.54	0.43
1:A:275:SER:HB3	1:A:292:ARG:HB2	2.00	0.43
1:A:383:SER:O	1:A:384:SER:C	2.56	0.43
1:A:755:TRP:CE3	1:A:812:PHE:CE1	3.07	0.42
1:B:632:TRP:CG	1:B:675:VAL:HG12	2.55	0.42
1:B:805:PHE:CG	1:B:838:VAL:HG11	2.54	0.42
1:A:661:ASN:C	1:A:661:ASN:OD1	2.57	0.42
1:B:745:ASN:N	1:B:745:ASN:OD1	2.53	0.42
1:B:205:LYS:O	1:B:206:LEU:HG	2.20	0.42
1:B:523:GLU:OE2	1:B:525:THR:CG2	2.67	0.42
1:B:769:THR:HG21	1:B:846:SER:HA	2.01	0.42
1:B:288:ASP:HB3	1:B:325:TYR:CZ	2.54	0.42
1:B:519:TYR:O	1:B:520:GLY:C	2.58	0.42
1:B:589:ILE:HG13	1:B:590:SER:N	2.34	0.42
1:B:742:LEU:HB3	1:B:759:VAL:HG12	2.00	0.42
1:B:755:TRP:HH2	1:B:810:TRP:CD2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ALA:HB2	1:A:673:LEU:CD1	2.50	0.42
1:A:645:PHE:HA	1:A:661:ASN:O	2.19	0.42
1:A:831:LEU:HA	1:A:831:LEU:HD23	1.90	0.42
1:A:835:ASP:O	1:A:835:ASP:CG	2.58	0.42
1:B:746:THR:HB	1:B:755:TRP:HB3	2.02	0.42
1:A:435:ILE:HG22	1:A:519:TYR:HD1	1.85	0.42
1:B:380:ARG:HD3	1:B:383:SER:CB	2.50	0.42
1:B:349:HIS:CE1	1:B:351:ALA:HB2	2.55	0.41
1:A:262:ASP:HA	1:B:652:ILE:CD1	2.50	0.41
1:A:553:GLY:O	1:A:555:ARG:N	2.42	0.41
1:A:805:PHE:CD2	1:A:838:VAL:HG21	2.55	0.41
1:B:261:SER:HB2	1:B:263:LYS:N	2.34	0.41
1:B:611:LEU:HD21	1:B:660:MET:HB3	2.01	0.41
1:B:702:ASN:HB3	1:B:704:ILE:H	1.85	0.41
1:B:718:ILE:O	1:B:722:LYS:O	2.39	0.41
1:A:706:TYR:CE2	1:A:708:ASP:HB2	2.56	0.41
1:B:463:VAL:HG22	1:B:493:THR:HG23	2.03	0.41
1:A:627:VAL:HG13	1:A:628:MET:N	2.36	0.41
1:B:252:TYR:N	1:B:252:TYR:CD1	2.88	0.41
1:A:544:ARG:HD3	1:A:564:ASN:HB3	2.02	0.41
1:B:107:ILE:CG2	1:B:110:GLU:HG3	2.51	0.41
1:A:291:GLU:HB2	1:A:323:LYS:HB3	2.03	0.41
1:A:577:ARG:O	1:A:580:ILE:HG22	2.21	0.41
1:B:59:SER:OG	1:B:60:THR:N	2.51	0.41
1:A:225:TYR:O	1:A:226:HIS:ND1	2.54	0.40
1:B:459:TYR:CE1	1:B:496:LEU:HG	2.55	0.40
1:A:193:THR:O	1:A:639:ARG:NH1	2.54	0.40
1:B:436:ASN:O	1:B:517:MET:HA	2.22	0.40
1:A:380:ARG:HD3	1:A:383:SER:HB3	2.04	0.40
1:B:183:SER:O	1:B:184:ASN:C	2.59	0.40
1:B:466:VAL:O	1:B:468:THR:HG23	2.21	0.40
1:B:534:ASP:O	1:B:537:GLU:CG	2.69	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	807/868 (93%)	743 (92%)	55 (7%)	9 (1%)	17	62
1	B	807/868 (93%)	740 (92%)	56 (7%)	11 (1%)	14	57
All	All	1614/1736 (93%)	1483 (92%)	111 (7%)	20 (1%)	16	60

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	720	ASP
1	A	778	PRO
1	B	554	ASP
1	B	778	PRO
1	A	145	ASN
1	A	174	LEU
1	A	228	SER
1	A	820	LYS
1	B	145	ASN
1	B	174	LEU
1	B	187	ALA
1	B	206	LEU
1	B	384	SER
1	B	721	ASP
1	A	173	GLU
1	A	222	TRP
1	A	230	VAL
1	B	173	GLU
1	B	578	GLN
1	B	821	THR

### 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	702/754 (93%)	660 (94%)	42 (6%)	24	65
1	B	702/754 (93%)	645 (92%)	57 (8%)	15	51
All	All	1404/1508 (93%)	1305 (93%)	99 (7%)	18	57

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	MET
1	A	104	SER
1	A	167	SER
1	A	185	ILE
1	A	210	SER
1	A	252	TYR
1	A	253	SER
1	A	306	ASP
1	A	318	SER
1	A	337	SER
1	A	356	MET
1	A	358	SER
1	A	365	THR
1	A	383	SER
1	A	431	SER
1	A	440	ASP
1	A	458	VAL
1	A	465	VAL
1	A	492	ARG
1	A	494	ARG
1	A	496	LEU
1	A	513	LEU
1	A	539	LEU
1	A	548	SER
1	A	552	PHE
1	A	558	ARG
1	A	572	LEU
1	A	651	THR
1	A	659	VAL
1	A	667	GLU
1	A	682	ARG
1	A	691	LYS
1	A	697	THR
1	A	717	VAL
1	A	736	THR

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Mol	Chain	Res	Type
1	A	739	ARG
1	A	745	ASN
1	A	755	TRP
1	A	777	CYS
1	A	789	SER
1	A	807	SER
1	A	861	LEU
1	B	59	SER
1	B	68	MET
1	B	104	SER
1	B	153	ASP
1	B	167	SER
1	B	174	LEU
1	B	183	SER
1	B	186	SER
1	B	193	THR
1	B	221	SER
1	B	224	LYS
1	B	252	TYR
1	B	253	SER
1	B	261	SER
1	B	306	ASP
1	B	316	MET
1	B	318	SER
1	B	337	SER
1	B	352	SER
1	B	358	SER
1	B	383	SER
1	B	418	SER
1	B	426	GLU
1	B	431	SER
1	B	440	ASP
1	B	445	THR
1	B	458	VAL
1	B	465	VAL
1	B	492	ARG
1	B	494	ARG
1	B	496	LEU
1	B	521	ARG
1	B	534	ASP
1	B	555	ARG
1	B	558	ARG

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Mol	Chain	Res	Type
1	B	559	LEU
1	B	596	THR
1	B	609	SER
1	B	633	THR
1	B	635	LYS
1	B	650	THR
1	B	651	THR
1	B	659	VAL
1	B	663	LYS
1	B	678	ILE
1	B	679	SER
1	B	697	THR
1	B	714	GLU
1	B	716	ARG
1	B	736	THR
1	B	739	ARG
1	B	755	TRP
1	B	777	CYS
1	B	781	SER
1	B	789	SER
1	B	800	THR
1	B	807	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	400	ASN
1	A	437	HIS
1	A	514	GLN
1	A	665	HIS
1	A	669	ASN
1	A	745	ASN
1	A	801	GLN
1	B	95	ASN
1	B	100	ASN
1	B	363	GLN
1	B	400	ASN
1	B	437	HIS
1	B	514	GLN
1	B	662	ASN
1	B	745	ASN

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Mol	Chain	Res	Type
1	B	757	GLN
1	B	842	GLN

### 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 ⓘ

7 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$
2	LDA	A	901[A]	-	15,15,15	3.98	2 (13%)	16,17,17	0.87	1 (6%)
2	LDA	A	901[B]	-	15,15,15	4.06	2 (13%)	16,17,17	0.65	0
2	LDA	A	902	-	15,15,15	4.06	1 (6%)	16,17,17	0.82	1 (6%)
3	BOG	A	903	-	20,20,20	1.10	2 (10%)	25,25,25	1.75	6 (24%)
3	BOG	A	904	-	20,20,20	0.83	1 (5%)	25,25,25	1.83	2 (8%)
3	BOG	A	905	-	20,20,20	0.83	1 (5%)	25,25,25	2.19	4 (16%)
3	BOG	B	901	-	20,20,20	1.15	1 (5%)	25,25,25	2.93	6 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDA	A	901[A]	-	-	0/13/13/13	0/0/0/0
2	LDA	A	901[B]	-	-	0/13/13/13	0/0/0/0
2	LDA	A	902	-	-	0/13/13/13	0/0/0/0
3	BOG	A	903	-	-	0/11/31/31	0/1/1/1
3	BOG	A	904	-	-	0/11/31/31	0/1/1/1
3	BOG	A	905	-	-	0/11/31/31	0/1/1/1
3	BOG	B	901	-	-	0/11/31/31	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	LDA	O1-N1	-15.60	1.24	1.39
2	A	901[B]	LDA	O1-N1	-15.42	1.24	1.39
2	A	901[A]	LDA	O1-N1	-15.13	1.25	1.39
2	A	901[A]	LDA	C1-N1	-2.33	1.47	1.51
2	A	901[B]	LDA	C1-N1	-2.12	1.47	1.51
3	A	904	BOG	O1-C1	2.08	1.43	1.40
3	A	905	BOG	O1-C1	2.81	1.45	1.40
3	A	903	BOG	O5-C1	3.09	1.49	1.41
3	A	903	BOG	O1-C1	3.64	1.46	1.40
3	B	901	BOG	O1-C1	4.66	1.48	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	BOG	O5-C1-C2	-7.07	95.58	110.28
3	B	901	BOG	O5-C1-O1	-4.68	98.76	109.99
3	A	903	BOG	C4-C3-C2	-3.33	104.64	110.79
3	A	903	BOG	C1'-O1-C1	-2.61	109.43	114.00
2	A	901[A]	LDA	O1-N1-C1	-2.59	107.36	110.27
3	A	904	BOG	C1-O5-C5	-2.57	108.71	113.74
3	A	903	BOG	C1-C2-C3	-2.19	105.63	109.98
3	B	901	BOG	O3-C3-C2	-2.11	105.60	110.36
3	B	901	BOG	C1'-O1-C1	-2.09	110.35	114.00
2	A	902	LDA	O1-N1-C1	-2.05	107.97	110.27
3	A	905	BOG	C1-C2-C3	2.06	114.06	109.98
3	A	905	BOG	C3-C4-C5	2.09	113.96	110.23
3	A	903	BOG	O5-C5-C4	2.13	113.74	109.67
3	A	903	BOG	O5-C1-C2	2.81	116.12	110.28
3	B	901	BOG	C4-C3-C2	3.44	117.12	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	905	BOG	C1'-O1-C1	3.58	120.25	114.00
3	A	903	BOG	O1-C1-C2	5.25	114.46	108.00
3	A	904	BOG	O5-C1-C2	7.98	126.88	110.28
3	A	905	BOG	O1-C1-C2	9.31	119.45	108.00
3	B	901	BOG	O1-C1-C2	10.39	120.78	108.00

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	809/868 (93%)	-0.12	9 (1%) 82 72	42, 75, 114, 151	0
1	B	809/868 (93%)	-0.15	11 (1%) 78 65	46, 85, 120, 165	0
All	All	1618/1736 (93%)	-0.14	20 (1%) 81 69	42, 80, 118, 165	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	820	LYS	3.0
1	B	629	SER	2.9
1	B	433	TYR	2.9
1	A	470	ALA	2.8
1	A	430	VAL	2.7
1	A	469	GLY	2.6
1	B	262	ASP	2.6
1	B	620	SER	2.5
1	A	435	ILE	2.5
1	A	468	THR	2.4
1	A	549	TYR	2.4
1	B	522	LEU	2.4
1	B	793	GLY	2.3
1	A	632	TRP	2.3
1	B	630	THR	2.3
1	B	432	TRP	2.2
1	B	626	ARG	2.1
1	B	282	GLU	2.0
1	A	748	PHE	2.0
1	A	653	ASP	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	LDA	A	901[A]	16/16	0.74	0.39	6.79	70,94,103,105	16
2	LDA	A	901[B]	16/16	0.74	0.39	6.37	68,87,91,92	16
3	BOG	A	904	20/20	0.83	0.30	6.35	82,127,142,142	0
3	BOG	A	903	20/20	0.90	0.27	2.86	63,77,86,95	0
3	BOG	A	905	20/20	0.65	0.32	2.57	117,134,152,157	0
3	BOG	B	901	20/20	0.88	0.27	1.42	81,88,96,96	0
2	LDA	A	902	16/16	0.70	0.34	-	92,118,155,159	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.