



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:13 AM GMT

PDB ID : 2X03  
Title : THE X-RAY STRUCTURE OF THE STREPTOMYCES COELICOLOR A3  
CHONDROITIN AC LYASE Y253 MUTANT  
Authors : Elmabrouk, Z.H.; Taylor, E.J.; Vincent, F.; Smith, N.L.; Turkenburg, J.P.;  
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Deposited on : 2009-12-04  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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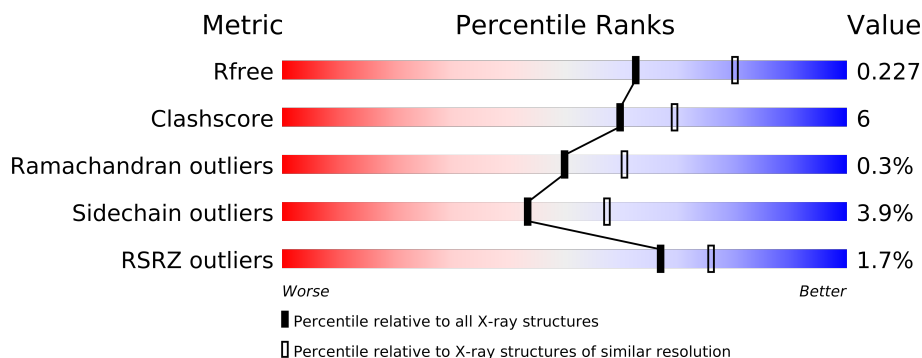
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	765	
1	B	765	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12283 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PUTATIVE SECRETED LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	742	Total	C	N	O	S	0	5	0
			5719	3587	1064	1048	20			
1	B	743	Total	C	N	O	S	0	4	0
			5722	3587	1065	1050	20			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP O86516
A	2	GLY	-	EXPRESSION TAG	UNP O86516
A	3	SER	-	EXPRESSION TAG	UNP O86516
A	4	SER	-	EXPRESSION TAG	UNP O86516
A	5	HIS	-	EXPRESSION TAG	UNP O86516
A	6	HIS	-	EXPRESSION TAG	UNP O86516
A	7	HIS	-	EXPRESSION TAG	UNP O86516
A	8	HIS	-	EXPRESSION TAG	UNP O86516
A	9	HIS	-	EXPRESSION TAG	UNP O86516
A	10	HIS	-	EXPRESSION TAG	UNP O86516
A	11	SER	-	EXPRESSION TAG	UNP O86516
A	12	SER	-	EXPRESSION TAG	UNP O86516
A	13	GLY	-	EXPRESSION TAG	UNP O86516
A	14	LEU	-	EXPRESSION TAG	UNP O86516
A	15	VAL	-	EXPRESSION TAG	UNP O86516
A	16	PRO	-	EXPRESSION TAG	UNP O86516
A	17	ARG	-	EXPRESSION TAG	UNP O86516
A	18	GLY	-	EXPRESSION TAG	UNP O86516
A	19	SER	-	EXPRESSION TAG	UNP O86516
A	20	HIS	-	EXPRESSION TAG	UNP O86516
A	21	MET	-	EXPRESSION TAG	UNP O86516
A	253	ALA	TYR	ENGINEERED MUTATION	UNP O86516
B	1	MET	-	EXPRESSION TAG	UNP O86516
B	2	GLY	-	EXPRESSION TAG	UNP O86516
B	3	SER	-	EXPRESSION TAG	UNP O86516

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	SER	-	EXPRESSION TAG	UNP O86516
B	5	HIS	-	EXPRESSION TAG	UNP O86516
B	6	HIS	-	EXPRESSION TAG	UNP O86516
B	7	HIS	-	EXPRESSION TAG	UNP O86516
B	8	HIS	-	EXPRESSION TAG	UNP O86516
B	9	HIS	-	EXPRESSION TAG	UNP O86516
B	10	HIS	-	EXPRESSION TAG	UNP O86516
B	11	SER	-	EXPRESSION TAG	UNP O86516
B	12	SER	-	EXPRESSION TAG	UNP O86516
B	13	GLY	-	EXPRESSION TAG	UNP O86516
B	14	LEU	-	EXPRESSION TAG	UNP O86516
B	15	VAL	-	EXPRESSION TAG	UNP O86516
B	16	PRO	-	EXPRESSION TAG	UNP O86516
B	17	ARG	-	EXPRESSION TAG	UNP O86516
B	18	GLY	-	EXPRESSION TAG	UNP O86516
B	19	SER	-	EXPRESSION TAG	UNP O86516
B	20	HIS	-	EXPRESSION TAG	UNP O86516
B	21	MET	-	EXPRESSION TAG	UNP O86516
B	253	ALA	TYR	ENGINEERED MUTATION	UNP O86516

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is water.

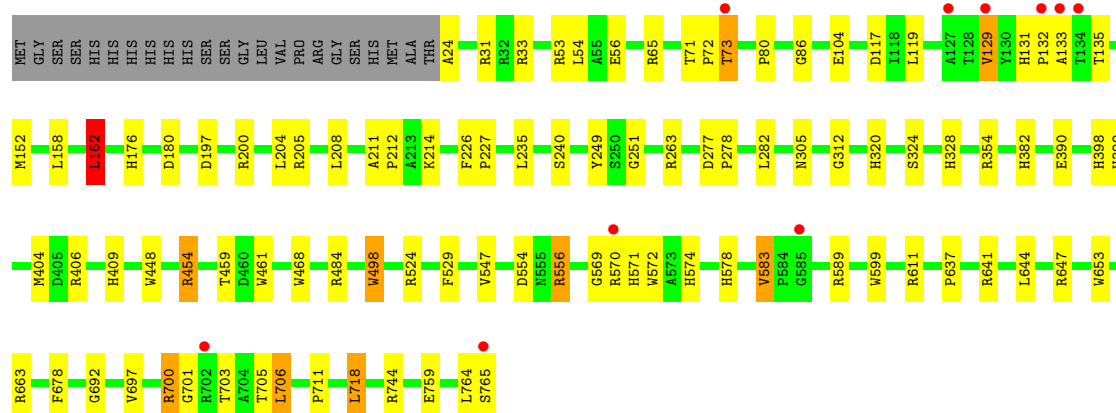
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	419	Total O 419 419	0	0
3	B	422	Total O 422 422	0	0

### 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.

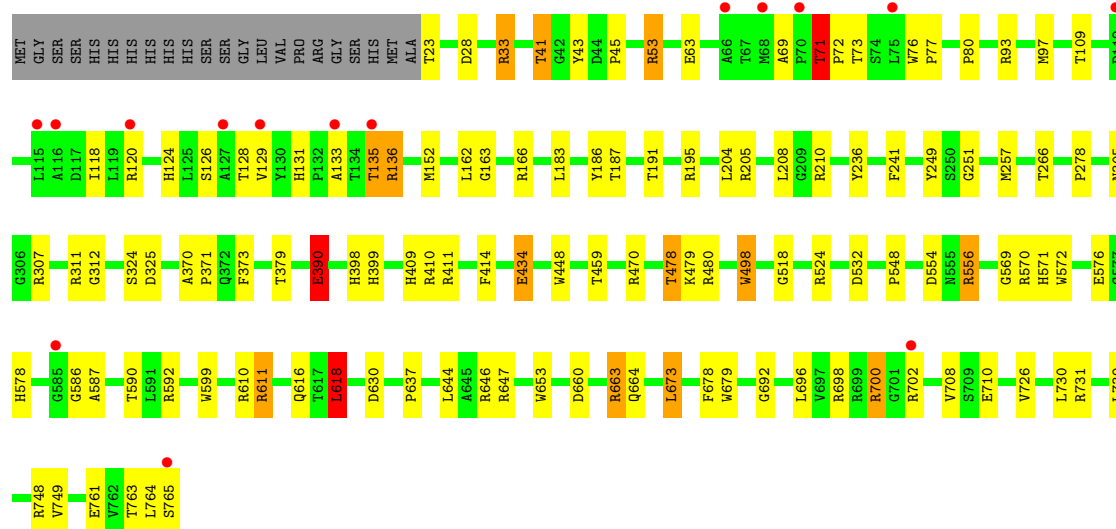
#### • Molecule 1: PUTATIVE SECRETED LYASE

Chain A: 



#### • Molecule 1: PUTATIVE SECRETED LYASE

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	317.10Å 317.10Å 82.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	158.55 – 2.30 56.11 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (158.55-2.30) 99.9 (56.11-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.194 , 0.228 0.195 , 0.227	Depositor DCC
$R_{free}$ test set	6932 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 17.4	EDS
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 138075 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12283	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	1.14	5/5874 (0.1%)	0.96	10/8026 (0.1%)
1	B	1.16	7/5877 (0.1%)	1.04	21/8032 (0.3%)
All	All	1.15	12/11751 (0.1%)	1.00	31/16058 (0.2%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	547	VAL	CB-CG1	6.42	1.66	1.52
1	A	759	GLU	CG-CD	5.88	1.60	1.51
1	B	434	GLU	CB-CG	5.85	1.63	1.52
1	B	390	GLU	CG-CD	5.84	1.60	1.51
1	A	56	GLU	CG-CD	5.66	1.60	1.51
1	B	236	TYR	CG-CD1	5.64	1.46	1.39
1	A	583	VAL	CB-CG1	-5.58	1.41	1.52
1	B	726	VAL	CB-CG2	-5.56	1.41	1.52
1	A	468	TRP	CE3-CZ3	5.48	1.47	1.38
1	B	576	GLU	CG-CD	5.47	1.60	1.51
1	B	710	GLU	CG-CD	5.26	1.59	1.51
1	B	698	ARG	CZ-NH1	5.09	1.39	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	THR	C-N-CD	-22.63	70.81	120.60
1	B	195	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	A	354	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	B	325	ASP	CB-CG-OD1	8.45	125.90	118.30
1	B	660	ASP	CB-CG-OD1	7.90	125.41	118.30
1	B	646	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	B	618	LEU	CA-CB-CG	7.70	133.01	115.30
1	A	718	LEU	CB-CG-CD1	-7.45	98.33	111.00
1	B	480	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	611	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	470	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	532	ASP	CB-CG-OD1	5.85	123.56	118.30
1	B	673	LEU	CB-CG-CD2	-5.74	101.24	111.00
1	B	311	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	263	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	454	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	B	610	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	195	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	480	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	696	LEU	CA-CB-CG	5.39	127.69	115.30
1	B	663	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	129	VAL	CB-CA-C	-5.28	101.37	111.40
1	A	589	ARG	CG-CD-NE	-5.22	100.83	111.80
1	A	484	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	162	LEU	CA-CB-CG	5.15	127.14	115.30
1	B	28	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	210	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	197	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	31	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	B	630	ASP	CB-CG-OD1	5.04	122.83	118.30
1	B	33	ARG	CG-CD-NE	-5.01	101.28	111.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	571[B]	HIS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	764	LEU	Peptide



## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5719	0	5531	61	0
1	B	5722	0	5540	75	0
2	B	1	0	0	0	0
3	A	419	0	0	10	0
3	B	422	0	0	5	0
All	All	12283	0	11071	136	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (136) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:152:MET:CE	1:A:208:LEU:HD12	1.62	1.30
1:A:152:MET:HE3	1:A:208:LEU:HD12	1.24	1.10
1:B:152:MET:HE3	1:B:208:LEU:HD12	1.33	1.06
1:B:390:GLU:HA	1:B:390:GLU:OE1	1.54	1.01
1:A:24:ALA:HB3	3:A:2001:HOH:O	1.58	1.01
1:A:700:ARG:HH11	1:A:700:ARG:HG2	1.23	0.98
1:B:53[B]:ARG:NH2	1:B:370:ALA:O	1.98	0.96
1:A:571[B]:HIS:CD2	1:A:571[B]:HIS:N	2.27	0.95
1:A:556[B]:ARG:HE	1:A:578:HIS:HD2	1.18	0.91
1:A:152:MET:HE3	1:A:208:LEU:CD1	2.02	0.89
1:B:556[B]:ARG:HE	1:B:578:HIS:HD2	1.20	0.88
1:A:570:ARG:CA	1:A:571[B]:HIS:N	2.40	0.84
1:B:152:MET:CE	1:B:208:LEU:HD12	2.06	0.84
1:B:592:ARG:HH21	1:B:616:GLN:HE21	1.26	0.83
1:B:478:THR:HB	1:B:548:PRO:O	1.79	0.82
1:A:152:MET:CE	1:A:208:LEU:CD1	2.54	0.80
1:A:570:ARG:CA	1:A:571[A]:HIS:N	2.45	0.79
1:A:569:GLY:HA3	1:A:572:TRP:CE2	2.18	0.77
1:A:556[A]:ARG:HD3	1:A:578:HIS:HD2	1.49	0.77
1:A:556[A]:ARG:HD3	1:A:578:HIS:CD2	2.21	0.76
1:B:478:THR:HG23	3:B:2032:HOH:O	1.88	0.74
1:A:152:MET:HE1	1:A:208:LEU:HD12	1.70	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:556[B]:ARG:HE	1:A:578:HIS:CD2	2.07	0.71
1:B:478:THR:CG2	3:B:2032:HOH:O	2.37	0.71
1:B:586:GLY:HA2	3:B:2287:HOH:O	1.91	0.71
1:A:705:THR:HG23	3:A:2378:HOH:O	1.91	0.70
1:A:700:ARG:HG2	1:A:700:ARG:NH1	2.02	0.67
1:B:163:GLY:H	1:B:166:ARG:HH11	1.42	0.67
1:A:700:ARG:HH11	1:A:700:ARG:CG	2.03	0.65
1:A:132:PRO:HA	1:A:176:HIS:CD2	2.32	0.65
1:B:570:ARG:O	1:B:571:HIS:HB2	1.96	0.64
1:B:590:THR:HG22	1:B:618:LEU:HD13	1.80	0.63
1:B:312:GLY:HA3	1:B:599:TRP:CD2	2.33	0.62
1:B:556[B]:ARG:HE	1:B:578:HIS:CD2	2.10	0.62
1:B:390:GLU:OE1	1:B:390:GLU:CA	2.42	0.61
1:B:700:ARG:HH11	1:B:700:ARG:HG2	1.65	0.61
1:A:399:HIS:HD2	3:A:2102:HOH:O	1.83	0.60
1:A:312:GLY:HA3	1:A:599:TRP:CD2	2.37	0.60
1:B:556[A]:ARG:CD	1:B:578:HIS:HD2	2.15	0.57
1:A:556[A]:ARG:HH11	1:A:578:HIS:HD2	1.53	0.57
1:B:128:THR:O	1:B:131:HIS:HE1	1.88	0.57
1:A:382:HIS:HD2	3:A:2155:HOH:O	1.88	0.55
1:A:152:MET:HE2	1:A:204:LEU:HB3	1.89	0.55
1:B:592:ARG:HE	1:B:616:GLN:NE2	2.04	0.55
1:A:569:GLY:HA3	1:A:572:TRP:CZ2	2.42	0.55
1:B:186:TYR:CE1	1:B:191:THR:HA	2.42	0.55
1:B:730:LEU:HD21	1:B:763:THR:CG2	2.37	0.55
1:B:572:TRP:CE3	1:B:644:LEU:HD23	2.42	0.54
1:A:65:ARG:HD2	1:A:117:ASP:OD2	2.08	0.54
1:A:697:VAL:HG22	1:A:706:LEU:HG	1.88	0.54
1:B:76:TRP:CD1	1:B:93:ARG:NH1	2.76	0.54
1:B:647:ARG:HD2	1:B:653:TRP:CE2	2.43	0.54
1:B:448:TRP:CE3	1:B:637:PRO:HB3	2.43	0.54
1:B:324:SER:HB2	1:B:459:THR:HG23	1.90	0.53
1:B:592:ARG:HH21	1:B:616:GLN:NE2	2.01	0.53
1:A:574:HIS:CD2	1:A:641:ARG:HA	2.44	0.53
1:B:312:GLY:HA3	1:B:599:TRP:CE2	2.44	0.52
1:B:556[A]:ARG:HD3	1:B:578:HIS:HD2	1.73	0.52
1:B:664:GLN:NE2	1:B:679:TRP:HE1	2.08	0.52
1:A:398:HIS:HD2	1:A:409:HIS:ND1	2.07	0.52
1:A:158:LEU:O	1:A:162:LEU:HD22	2.09	0.52
1:B:590:THR:HG22	1:B:618:LEU:CD1	2.39	0.52
1:A:572:TRP:CE3	1:A:644:LEU:HD23	2.45	0.52
1:A:390:GLU:HA	1:A:390:GLU:OE1	2.09	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:33:ARG:NH1	1:B:266:THR:O	2.39	0.51
1:B:479:LYS:HE2	1:B:518:GLY:O	2.10	0.51
1:B:399:HIS:HD2	3:B:2099:HOH:O	1.92	0.51
1:B:152:MET:HE2	1:B:204:LEU:C	2.30	0.51
1:B:71:THR:O	1:B:124:HIS:CE1	2.63	0.51
1:A:54:LEU:HD13	1:A:104:GLU:O	2.11	0.51
1:B:739:LEU:HD11	1:B:748:ARG:HB2	1.93	0.50
1:B:569:GLY:HA3	1:B:572:TRP:CE2	2.45	0.50
1:B:673:LEU:HD23	1:B:673:LEU:C	2.31	0.50
1:B:731:ARG:NH2	1:B:761:GLU:OE1	2.45	0.49
1:B:556[A]:ARG:HD3	1:B:578:HIS:CD2	2.47	0.49
1:A:324:SER:HB2	1:A:459:THR:HG23	1.95	0.49
1:B:586:GLY:O	1:B:587:ALA:HB3	2.12	0.48
1:B:611:ARG:NH1	3:B:2320:HOH:O	2.38	0.48
1:A:454:ARG:NH1	3:A:2199:HOH:O	2.17	0.48
1:A:448:TRP:CE3	1:A:637:PRO:HB3	2.49	0.48
1:B:556[A]:ARG:HD2	1:B:578:HIS:HD2	1.78	0.48
1:B:128:THR:O	1:B:131:HIS:CE1	2.66	0.48
1:A:320:HIS:HE1	3:A:2306:HOH:O	1.97	0.47
1:B:664:GLN:HE21	1:B:679:TRP:HE1	1.63	0.47
1:B:708:VAL:HG11	1:B:749:VAL:HG21	1.95	0.47
1:B:69:ALA:O	1:B:71:THR:HG23	2.14	0.47
1:B:241:PHE:CZ	1:B:257[B]:MET:HG3	2.50	0.47
1:A:71:THR:O	1:A:73:THR:N	2.48	0.47
1:A:647:ARG:HD2	1:A:653:TRP:CE2	2.50	0.47
1:A:312:GLY:HA3	1:A:599:TRP:CE2	2.49	0.47
1:A:461:TRP:CE2	1:A:611:ARG:HG3	2.51	0.46
1:B:43:TYR:O	1:B:45:PRO:HD3	2.16	0.46
1:A:200:ARG:O	1:A:204:LEU:HD23	2.15	0.46
1:A:556[A]:ARG:CD	1:A:578:HIS:HD2	2.20	0.46
1:A:409:HIS:CE1	1:A:529:PHE:HB3	2.51	0.46
1:A:404:MET:O	1:A:406:ARG:HG2	2.16	0.46
1:A:328:HIS:HE1	3:A:2116:HOH:O	1.97	0.46
1:B:126:SER:O	1:B:131:HIS:HB3	2.16	0.46
1:A:744[B]:ARG:NH1	3:A:2405:HOH:O	2.26	0.45
1:A:556[A]:ARG:HH11	1:A:578:HIS:CD2	2.33	0.45
1:B:556[A]:ARG:CD	1:B:578:HIS:CD2	2.98	0.45
1:B:307:ARG:NE	1:B:434:GLU:OE1	2.48	0.44
1:B:135:THR:O	1:B:136:ARG:O	2.36	0.44
1:B:251:GLY:HA3	1:B:305:ASN:OD1	2.17	0.44
1:A:251:GLY:HA3	1:A:305:ASN:OD1	2.18	0.44
1:B:41:THR:O	1:B:379:THR:HG21	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:498:TRP:HE3	1:B:498:TRP:C	2.22	0.44
1:A:235:LEU:HD12	1:A:240:SER:O	2.18	0.43
1:A:211:ALA:HA	1:A:212:PRO:HD2	1.78	0.43
1:A:556[B]:ARG:NE	1:A:578:HIS:HD2	2.00	0.43
1:A:382:HIS:CD2	3:A:2155:HOH:O	2.69	0.43
1:A:498:TRP:CH2	1:A:711:PRO:HG2	2.54	0.43
1:B:398:HIS:HD2	1:B:409:HIS:ND1	2.17	0.42
1:B:524:ARG:HD2	1:B:679:TRP:CD2	2.54	0.42
1:A:277:ASP:HA	1:A:278:PRO:HD2	1.86	0.42
1:B:764:LEU:HD23	1:B:764:LEU:HA	1.81	0.42
1:B:76:TRP:HA	1:B:77:PRO:HD2	1.75	0.42
1:B:370:ALA:HA	1:B:371:PRO:HD3	1.83	0.42
1:B:73:THR:O	1:B:80:PRO:HA	2.19	0.42
1:B:93:ARG:O	1:B:97:MET:HG3	2.20	0.41
1:A:180:ASP:OD1	1:A:214:LYS:NZ	2.38	0.41
1:B:556[B]:ARG:NE	1:B:578:HIS:HD2	2.01	0.41
1:B:370:ALA:HB3	1:B:373:PHE:CD2	2.55	0.41
1:B:730:LEU:HD21	1:B:763:THR:HG23	2.02	0.41
1:B:678:PHE:O	1:B:692:GLY:HA2	2.20	0.41
1:B:131:HIS:CD2	1:B:133:ALA:HB3	2.55	0.41
1:A:524:ARG:NH1	3:A:2258:HOH:O	2.42	0.41
1:B:700:ARG:HG2	1:B:700:ARG:NH1	2.34	0.41
1:A:131:HIS:CE1	1:A:133:ALA:HB3	2.56	0.41
1:A:678:PHE:O	1:A:692:GLY:HA2	2.21	0.41
1:B:414:PHE:CB	1:B:637:PRO:HB2	2.51	0.41
1:B:131:HIS:NE2	1:B:133:ALA:HB3	2.37	0.40
1:B:97:MET:HE2	1:B:118:ILE:HG13	2.02	0.40
1:B:410:ARG:O	1:B:411:ARG:HD2	2.21	0.40
1:A:80:PRO:O	1:A:86:GLY:HA3	2.21	0.40
1:A:226:PHE:N	1:A:227:PRO:HD3	2.35	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	742/765 (97%)	712 (96%)	28 (4%)	2 (0%)	50	60
1	B	745/765 (97%)	703 (94%)	39 (5%)	3 (0%)	43	52
All	All	1487/1530 (97%)	1415 (95%)	67 (4%)	5 (0%)	50	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	136	ARG
1	A	72	PRO
1	B	71	THR
1	B	72	PRO
1	A	701	GLY

### 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	566/581 (97%)	545 (96%)	21 (4%)	45	60
1	B	567/581 (98%)	541 (95%)	26 (5%)	37	48
All	All	1133/1162 (98%)	1086 (96%)	47 (4%)	43	55

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	53	ARG
1	A	73	THR
1	A	119	LEU
1	A	129	VAL
1	A	135	THR
1	A	162	LEU
1	A	205	ARG
1	A	249	TYR
1	A	282	LEU
1	A	498	TRP
1	A	554	ASP

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Mol	Chain	Res	Type
1	A	556[A]	ARG
1	A	556[B]	ARG
1	A	583	VAL
1	A	663	ARG
1	A	700	ARG
1	A	703	THR
1	A	706	LEU
1	A	718	LEU
1	A	765	SER
1	B	23	THR
1	B	41	THR
1	B	53[A]	ARG
1	B	53[B]	ARG
1	B	63	GLU
1	B	109	THR
1	B	120	ARG
1	B	129	VAL
1	B	135	THR
1	B	162	LEU
1	B	183	LEU
1	B	187	THR
1	B	205	ARG
1	B	249	TYR
1	B	278	PRO
1	B	390	GLU
1	B	478	THR
1	B	498	TRP
1	B	554	ASP
1	B	556[A]	ARG
1	B	556[B]	ARG
1	B	618	LEU
1	B	663	ARG
1	B	700	ARG
1	B	702	ARG
1	B	765	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	64	HIS
1	A	243	GLN
1	A	289	HIS

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Mol	Chain	Res	Type
1	A	320	HIS
1	A	328	HIS
1	A	382	HIS
1	A	398	HIS
1	A	399	HIS
1	A	578	HIS
1	B	79	HIS
1	B	131	HIS
1	B	243	GLN
1	B	328	HIS
1	B	398	HIS
1	B	399	HIS
1	B	578	HIS
1	B	616	GLN
1	B	664	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<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	742/765 (96%)	-0.39	10 (1%) 74 82	7, 21, 47, 57	1 (0%)
1	B	743/765 (97%)	-0.36	15 (2%) 62 72	8, 20, 59, 75	1 (0%)
All	All	1485/1530 (97%)	-0.37	25 (1%) 67 76	7, 21, 52, 75	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	ALA	4.6
1	B	116	ALA	3.9
1	A	765	SER	3.8
1	A	133	ALA	3.1
1	B	585	GLY	3.0
1	B	75	LEU	3.0
1	B	68	MET	2.9
1	B	70	PRO	2.8
1	B	765	SER	2.8
1	A	73	THR	2.8
1	B	112	PRO	2.7
1	B	127	ALA	2.6
1	B	120	ARG	2.6
1	B	115	LEU	2.6
1	B	702	ARG	2.4
1	A	132	PRO	2.3
1	A	129	VAL	2.2
1	B	66	ALA	2.2
1	B	129	VAL	2.2
1	A	570	ARG	2.1
1	A	702	ARG	2.1
1	A	585	GLY	2.1
1	A	127	ALA	2.1
1	B	135	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	134	THR	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<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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	1766	1/1	0.09	0.43	30,30,30,30	0

## 6.5 Other polymers

There are no such residues in this entry.