



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:06 AM GMT

PDB ID : 1R1Z  
Title : The Crystal structure of the Carbohydrate recognition domain of the glyco-protein sorting receptor p58/ERGIC-53 reveals a novel metal binding site and conformational changes associated with calcium ion binding  
Authors : Velloso, L.M.; Svensson, K.; Pettersson, R.F.; Lindqvist, Y.  
Deposited on : 2003-09-25  
Resolution : 2.40 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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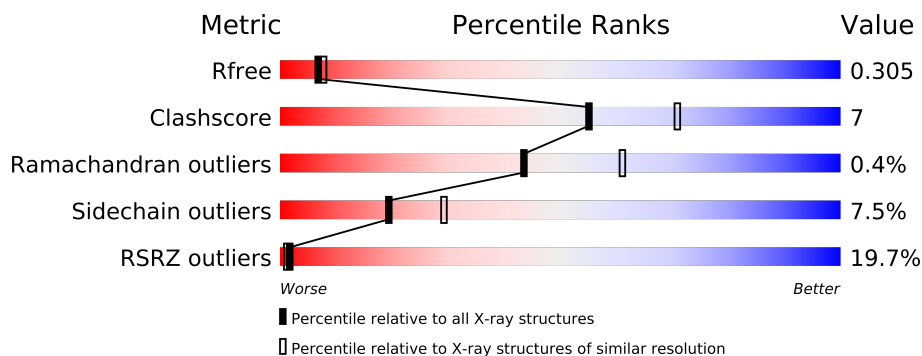
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	263	
1	B	263	
1	C	263	
1	D	263	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	B	315	-	X
2	CA	D	510	-	X
2	CA	D	515	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7793 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 ERGIC-53 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total 1898	C 1198	N 339	O 355	S 6	0	0	0
1	B	247	Total 1898	C 1198	N 339	O 355	S 6	0	0	0
1	C	247	Total 1898	C 1198	N 339	O 355	S 6	0	0	0
1	D	247	Total 1898	C 1198	N 339	O 355	S 6	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	CLONING ARTIFACT	UNP Q62902
A	23	GLY	-	CLONING ARTIFACT	UNP Q62902
A	24	SER	-	CLONING ARTIFACT	UNP Q62902
A	25	SER	-	CLONING ARTIFACT	UNP Q62902
A	26	HIS	-	CLONING ARTIFACT	UNP Q62902
A	27	HIS	-	CLONING ARTIFACT	UNP Q62902
A	28	HIS	-	CLONING ARTIFACT	UNP Q62902
A	29	HIS	-	CLONING ARTIFACT	UNP Q62902
A	30	HIS	-	CLONING ARTIFACT	UNP Q62902
A	31	HIS	-	CLONING ARTIFACT	UNP Q62902
A	32	SER	-	CLONING ARTIFACT	UNP Q62902
A	33	SER	-	CLONING ARTIFACT	UNP Q62902
A	34	GLY	-	CLONING ARTIFACT	UNP Q62902
A	35	LEU	-	CLONING ARTIFACT	UNP Q62902
A	36	VAL	-	CLONING ARTIFACT	UNP Q62902
A	37	PRO	-	CLONING ARTIFACT	UNP Q62902
A	38	ARG	-	CLONING ARTIFACT	UNP Q62902
A	39	GLY	-	CLONING ARTIFACT	UNP Q62902
A	40	SER	-	CLONING ARTIFACT	UNP Q62902
A	41	HIS	-	CLONING ARTIFACT	UNP Q62902
A	42	MET	-	CLONING ARTIFACT	UNP Q62902

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Chain	Residue	Modelled	Actual	Comment	Reference
B	19	MET	-	CLONING ARTIFACT	UNP Q62902
B	20	GLY	-	CLONING ARTIFACT	UNP Q62902
B	21	SER	-	CLONING ARTIFACT	UNP Q62902
B	22	SER	-	CLONING ARTIFACT	UNP Q62902
B	26	HIS	-	CLONING ARTIFACT	UNP Q62902
B	27	HIS	-	CLONING ARTIFACT	UNP Q62902
B	28	HIS	-	CLONING ARTIFACT	UNP Q62902
B	26	HIS	-	CLONING ARTIFACT	UNP Q62902
B	27	HIS	-	CLONING ARTIFACT	UNP Q62902
B	28	HIS	-	CLONING ARTIFACT	UNP Q62902
B	29	SER	-	CLONING ARTIFACT	UNP Q62902
B	30	SER	-	CLONING ARTIFACT	UNP Q62902
B	31	GLY	-	CLONING ARTIFACT	UNP Q62902
B	32	LEU	-	CLONING ARTIFACT	UNP Q62902
B	33	VAL	-	CLONING ARTIFACT	UNP Q62902
B	34	PRO	-	CLONING ARTIFACT	UNP Q62902
B	35	ARG	-	CLONING ARTIFACT	UNP Q62902
B	36	GLY	-	CLONING ARTIFACT	UNP Q62902
B	37	SER	-	CLONING ARTIFACT	UNP Q62902
B	38	HIS	-	CLONING ARTIFACT	UNP Q62902
B	39	MET	-	CLONING ARTIFACT	UNP Q62902
C	19	MET	-	CLONING ARTIFACT	UNP Q62902
C	20	GLY	-	CLONING ARTIFACT	UNP Q62902
C	21	SER	-	CLONING ARTIFACT	UNP Q62902
C	22	SER	-	CLONING ARTIFACT	UNP Q62902
C	26	HIS	-	CLONING ARTIFACT	UNP Q62902
C	27	HIS	-	CLONING ARTIFACT	UNP Q62902
C	28	HIS	-	CLONING ARTIFACT	UNP Q62902
C	26	HIS	-	CLONING ARTIFACT	UNP Q62902
C	27	HIS	-	CLONING ARTIFACT	UNP Q62902
C	28	HIS	-	CLONING ARTIFACT	UNP Q62902
C	29	SER	-	CLONING ARTIFACT	UNP Q62902
C	30	SER	-	CLONING ARTIFACT	UNP Q62902
C	31	GLY	-	CLONING ARTIFACT	UNP Q62902
C	32	LEU	-	CLONING ARTIFACT	UNP Q62902
C	33	VAL	-	CLONING ARTIFACT	UNP Q62902
C	34	PRO	-	CLONING ARTIFACT	UNP Q62902
C	35	ARG	-	CLONING ARTIFACT	UNP Q62902
C	36	GLY	-	CLONING ARTIFACT	UNP Q62902
C	37	SER	-	CLONING ARTIFACT	UNP Q62902
C	38	HIS	-	CLONING ARTIFACT	UNP Q62902
C	39	MET	-	CLONING ARTIFACT	UNP Q62902

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Chain	Residue	Modelled	Actual	Comment	Reference
D	19	MET	-	CLONING ARTIFACT	UNP Q62902
D	20	GLY	-	CLONING ARTIFACT	UNP Q62902
D	21	SER	-	CLONING ARTIFACT	UNP Q62902
D	22	SER	-	CLONING ARTIFACT	UNP Q62902
D	26	HIS	-	CLONING ARTIFACT	UNP Q62902
D	27	HIS	-	CLONING ARTIFACT	UNP Q62902
D	28	HIS	-	CLONING ARTIFACT	UNP Q62902
D	26	HIS	-	CLONING ARTIFACT	UNP Q62902
D	27	HIS	-	CLONING ARTIFACT	UNP Q62902
D	28	HIS	-	CLONING ARTIFACT	UNP Q62902
D	29	SER	-	CLONING ARTIFACT	UNP Q62902
D	30	SER	-	CLONING ARTIFACT	UNP Q62902
D	31	GLY	-	CLONING ARTIFACT	UNP Q62902
D	32	LEU	-	CLONING ARTIFACT	UNP Q62902
D	33	VAL	-	CLONING ARTIFACT	UNP Q62902
D	34	PRO	-	CLONING ARTIFACT	UNP Q62902
D	35	ARG	-	CLONING ARTIFACT	UNP Q62902
D	36	GLY	-	CLONING ARTIFACT	UNP Q62902
D	37	SER	-	CLONING ARTIFACT	UNP Q62902
D	38	HIS	-	CLONING ARTIFACT	UNP Q62902
D	39	MET	-	CLONING ARTIFACT	UNP Q62902

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Ca 2 2	0	0
2	A	2	Total Ca 2 2	0	0
2	D	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	89	Total O 89 89	0	0
3	B	58	Total O 58 58	0	0
3	C	28	Total O 28 28	0	0

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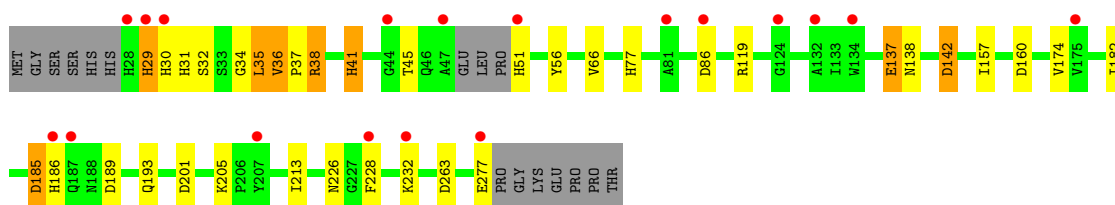
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	18	Total	O	0	0
			18	18		

### 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.

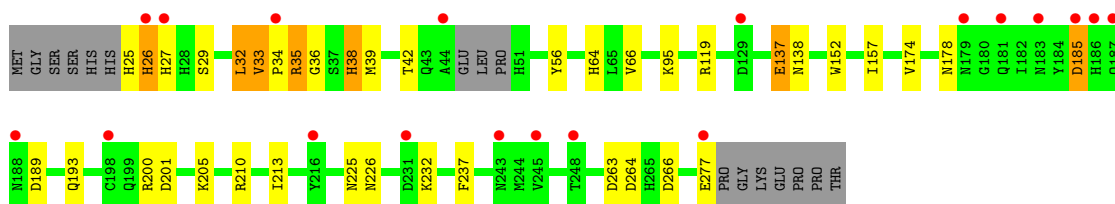
#### • Molecule 1: ERGIC-53 protein

Chain A: 



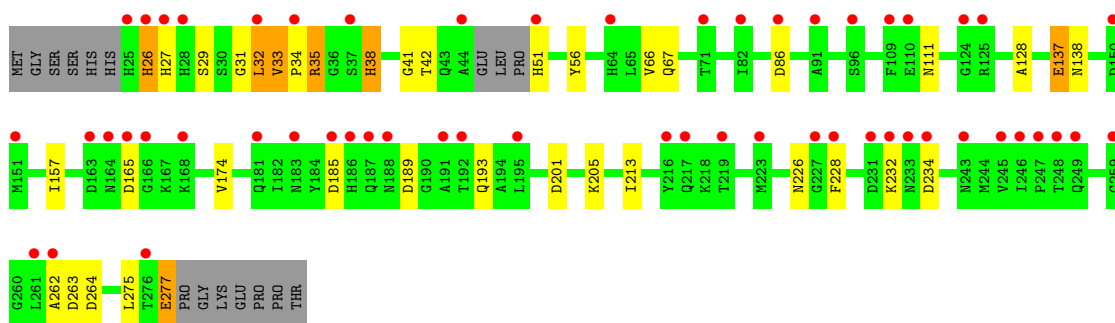
#### • Molecule 1: ERGIC-53 protein

Chain B: 



#### • Molecule 1: ERGIC-53 protein

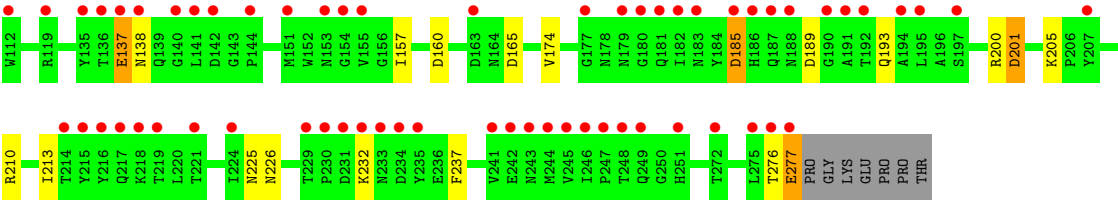
Chain C: 



#### • Molecule 1: ERGIC-53 protein

Chain D: 







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.35Å 81.07Å 82.31Å 91.05° 94.14° 94.99°	Depositor
Resolution (Å)	10.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.5 (10.00-2.40) 95.9 (10.00-2.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.72 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.223 , 0.241 0.300 , 0.305	Depositor DCC
$R_{free}$ test set	1069 reflections (2.54%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.50 , 51.3	EDS
Estimated twinning fraction	0.015 for -h,-l,-k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 42111 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	7793	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% 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: CA

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	0.64	0/1951	0.81	6/2651 (0.2%)
1	B	0.60	1/1951 (0.1%)	0.80	5/2651 (0.2%)
1	C	0.55	0/1951	0.76	6/2651 (0.2%)
1	D	0.46	0/1951	0.75	5/2651 (0.2%)
All	All	0.57	1/7804 (0.0%)	0.78	22/10604 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	277	GLU	CG-CD	5.11	1.59	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ASP	CB-CG-OD2	7.13	124.72	118.30
1	D	189	ASP	CB-CG-OD2	6.53	124.18	118.30
1	A	189	ASP	CB-CG-OD2	6.44	124.10	118.30
1	D	160	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	86	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	185	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	185	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	189	ASP	CB-CG-OD2	6.17	123.85	118.30
1	C	86	ASP	CB-CG-OD2	6.03	123.72	118.30
1	B	189	ASP	CB-CG-OD2	5.95	123.66	118.30
1	B	264	ASP	CB-CG-OD2	5.85	123.57	118.30
1	D	165	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	266	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	263	ASP	CB-CG-OD2	5.42	123.17	118.30
1	C	165	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	263	ASP	CB-CG-OD2	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ASP	CB-CG-OD2	5.34	123.11	118.30
1	D	185	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	142	ASP	CB-CG-OD2	5.15	122.94	118.30
1	D	201	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	264	ASP	CB-CG-OD2	5.02	122.81	118.30
1	C	234	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1898	0	1765	34	0
1	B	1898	0	1765	25	0
1	C	1898	0	1765	39	0
1	D	1898	0	1765	17	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	89	0	0	10	0
3	B	58	0	0	12	0
3	C	28	0	0	7	1
3	D	18	0	0	3	0
All	All	7793	0	7060	98	1

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 7.

All (98) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:36:GLY:HA3	3:B:361:HOH:O	1.14	1.30
1:D:98:ARG:HD2	3:D:525:HOH:O	1.28	1.24

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:35:LEU:HD23	3:A:375:HOH:O	1.37	1.23
1:C:128:ALA:O	3:C:422:HOH:O	1.57	1.19
1:B:32:LEU:HD23	3:B:324:HOH:O	1.42	1.17
3:B:330:HOH:O	1:C:32:LEU:HD23	1.43	1.15
1:D:98:ARG:CD	3:D:525:HOH:O	1.86	1.10
1:C:38:HIS:NE2	3:C:435:HOH:O	1.87	1.06
1:A:35:LEU:CD2	3:A:375:HOH:O	2.00	1.02
1:C:262:ALA:HA	3:C:422:HOH:O	1.58	1.00
1:B:95:LYS:H	1:C:67:GLN:HE22	1.00	1.00
1:A:228:PHE:CE2	1:C:228:PHE:CZ	2.51	0.97
1:C:31:GLY:HA3	3:C:441:HOH:O	1.66	0.95
1:C:41:GLY:HA3	3:C:437:HOH:O	1.66	0.93
1:A:142:ASP:OD2	3:A:327:HOH:O	1.89	0.90
1:B:39:MET:CE	3:B:368:HOH:O	2.25	0.84
1:B:95:LYS:N	1:C:67:GLN:HE22	1.77	0.81
1:B:95:LYS:H	1:C:67:GLN:NE2	1.77	0.81
1:A:186:HIS:HB2	3:A:326:HOH:O	1.86	0.75
1:A:34:GLY:HA3	3:A:325:HOH:O	1.88	0.74
1:A:228:PHE:CE2	1:C:228:PHE:CE2	2.76	0.73
3:B:372:HOH:O	1:C:32:LEU:HD22	1.88	0.72
1:A:228:PHE:CE1	1:C:228:PHE:CD1	2.77	0.72
1:A:228:PHE:CZ	1:C:228:PHE:CD2	2.80	0.70
1:A:228:PHE:CZ	1:C:228:PHE:CE2	2.82	0.68
1:B:32:LEU:H	1:B:32:LEU:HD23	1.57	0.68
1:B:32:LEU:CD2	3:B:324:HOH:O	2.15	0.66
1:A:35:LEU:H	1:A:35:LEU:HD23	1.61	0.66
1:A:228:PHE:CD2	1:C:228:PHE:CZ	2.83	0.65
1:C:32:LEU:H	1:C:32:LEU:HD23	1.63	0.63
1:A:201:ASP:O	1:A:205:LYS:NZ	2.32	0.63
1:C:157:ILE:HD13	1:C:213:ILE:HD13	1.81	0.63
1:B:185:ASP:H	1:B:193:GLN:HE22	1.45	0.63
1:D:157:ILE:HD13	1:D:213:ILE:HD13	1.81	0.62
1:D:98:ARG:HD3	3:D:525:HOH:O	1.76	0.62
1:A:185:ASP:H	1:A:193:GLN:HE22	1.49	0.61
1:D:32:LEU:H	1:D:32:LEU:HD23	1.64	0.61
1:A:228:PHE:CD2	1:C:228:PHE:CE1	2.89	0.61
1:A:228:PHE:CE1	1:C:228:PHE:CG	2.89	0.61
1:B:119:ARG:HD3	3:B:325:HOH:O	1.99	0.60
1:B:64:HIS:ND1	3:B:340:HOH:O	2.30	0.60
1:A:157:ILE:HD13	1:A:213:ILE:HD13	1.83	0.60
1:B:152:TRP:CE2	1:B:178:ASN:HB2	2.38	0.58
1:B:25:HIS:HE1	3:B:336:HOH:O	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:32:LEU:HB2	1:B:34:PRO:HD2	1.85	0.58
1:B:157:ILE:HD13	1:B:213:ILE:HD13	1.85	0.58
1:B:201:ASP:O	1:B:205:LYS:NZ	2.37	0.57
1:A:228:PHE:CG	1:C:228:PHE:CE1	2.93	0.56
1:C:201:ASP:O	1:C:205:LYS:NZ	2.39	0.56
1:A:228:PHE:CZ	1:C:228:PHE:CG	2.94	0.56
1:D:185:ASP:H	1:D:193:GLN:HE22	1.52	0.56
1:D:32:LEU:HB2	1:D:34:PRO:HD2	1.88	0.55
1:D:201:ASP:O	1:D:205:LYS:NZ	2.39	0.55
1:A:31:HIS:CD2	3:A:305:HOH:O	2.59	0.55
1:C:185:ASP:H	1:C:193:GLN:HE22	1.53	0.55
1:C:35:ARG:NH2	3:C:435:HOH:O	2.40	0.54
1:A:182:ILE:HD11	3:A:288:HOH:O	2.09	0.53
1:B:119:ARG:NH2	3:B:362:HOH:O	2.21	0.53
1:A:137:GLU:OE1	1:A:138:ASN:ND2	2.42	0.52
1:C:35:ARG:HD2	1:C:56:TYR:OH	2.10	0.52
1:A:228:PHE:CD1	1:C:228:PHE:CD1	2.98	0.52
1:A:228:PHE:CZ	1:C:228:PHE:CZ	2.98	0.52
1:C:32:LEU:HB2	1:C:34:PRO:HD2	1.91	0.52
1:B:38:HIS:NE2	3:B:369:HOH:O	1.60	0.51
1:A:35:LEU:HB2	1:A:37:PRO:HD2	1.91	0.51
1:A:228:PHE:CE2	1:C:228:PHE:CE1	2.98	0.51
1:D:32:LEU:HD12	1:D:34:PRO:HG2	1.93	0.50
1:D:210:ARG:HB2	1:D:225:ASN:HB3	1.92	0.50
1:B:200:ARG:NH2	1:B:237:PHE:O	2.46	0.49
1:D:137:GLU:OE1	1:D:138:ASN:ND2	2.46	0.48
1:A:36:VAL:HG23	1:A:37:PRO:HD3	1.94	0.48
1:C:33:VAL:HG23	1:C:34:PRO:HD3	1.95	0.48
1:B:39:MET:HE2	3:B:368:HOH:O	2.00	0.48
1:A:38:ARG:HD2	1:A:56:TYR:OH	2.14	0.48
1:B:137:GLU:OE1	1:B:138:ASN:ND2	2.47	0.47
1:C:277:GLU:O	1:C:277:GLU:HG3	2.14	0.47
1:C:137:GLU:OE1	1:C:138:ASN:ND2	2.48	0.47
1:B:33:VAL:HG23	1:B:34:PRO:HD3	1.97	0.47
1:C:111:ASN:HB2	1:C:275:LEU:O	2.15	0.46
1:B:210:ARG:HB2	1:B:225:ASN:HB3	1.97	0.46
1:A:119:ARG:NH1	3:A:314:HOH:O	2.18	0.46
1:B:35:ARG:HA	1:B:38:HIS:HB3	1.96	0.45
1:D:200:ARG:NH2	1:D:237:PHE:O	2.49	0.45
1:D:35:ARG:HA	1:D:38:HIS:HB3	1.98	0.45
1:C:35:ARG:HA	1:C:38:HIS:HB3	1.99	0.44
1:C:51:HIS:O	1:C:275:LEU:HA	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:32:LEU:HD12	1:D:34:PRO:HD2	2.00	0.44
1:A:77:HIS:HD2	3:A:301:HOH:O	2.01	0.44
1:A:228:PHE:CD1	1:C:228:PHE:CE1	3.07	0.42
1:A:119:ARG:HD3	3:A:314:HOH:O	2.18	0.42
1:C:185:ASP:H	1:C:193:GLN:NE2	2.18	0.42
1:A:185:ASP:H	1:A:193:GLN:NE2	2.16	0.42
1:B:35:ARG:HD2	1:B:56:TYR:OH	2.20	0.41
1:A:38:ARG:HA	1:A:41:HIS:HB3	2.01	0.41
1:D:32:LEU:HD12	1:D:34:PRO:CG	2.51	0.41
1:D:277:GLU:O	1:D:277:GLU:HG3	2.21	0.41
1:C:31:GLY:CA	3:C:441:HOH:O	2.45	0.41
1:D:35:ARG:HD2	1:D:56:TYR:OH	2.20	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:30:SER:OG	3:C:430:HOH:O[1_545]	1.92	0.28

## 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	243/263 (92%)	234 (96%)	8 (3%)	1 (0%)	43	61
1	B	243/263 (92%)	236 (97%)	6 (2%)	1 (0%)	43	61
1	C	243/263 (92%)	237 (98%)	5 (2%)	1 (0%)	43	61
1	D	243/263 (92%)	236 (97%)	6 (2%)	1 (0%)	43	61
All	All	972/1052 (92%)	943 (97%)	25 (3%)	4 (0%)	43	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	B	26	HIS

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Mol	Chain	Res	Type
1	C	26	HIS
1	D	26	HIS

### 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	193/215 (90%)	178 (92%)	15 (8%)	18	27
1	B	193/215 (90%)	180 (93%)	13 (7%)	23	35
1	C	193/215 (90%)	179 (93%)	14 (7%)	20	30
1	D	193/215 (90%)	177 (92%)	16 (8%)	16	24
All	All	772/860 (90%)	714 (92%)	58 (8%)	19	29

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	30	HIS
1	A	32	SER
1	A	35	LEU
1	A	36	VAL
1	A	38	ARG
1	A	41	HIS
1	A	45	THR
1	A	51	HIS
1	A	66	VAL
1	A	137	GLU
1	A	174	VAL
1	A	226	ASN
1	A	232	LYS
1	A	277	GLU
1	B	26	HIS
1	B	27	HIS
1	B	29	SER
1	B	32	LEU
1	B	33	VAL

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Mol	Chain	Res	Type
1	B	35	ARG
1	B	38	HIS
1	B	42	THR
1	B	66	VAL
1	B	137	GLU
1	B	174	VAL
1	B	226	ASN
1	B	232	LYS
1	C	26	HIS
1	C	27	HIS
1	C	29	SER
1	C	32	LEU
1	C	33	VAL
1	C	35	ARG
1	C	38	HIS
1	C	42	THR
1	C	66	VAL
1	C	137	GLU
1	C	174	VAL
1	C	226	ASN
1	C	232	LYS
1	C	277	GLU
1	D	26	HIS
1	D	27	HIS
1	D	29	SER
1	D	32	LEU
1	D	33	VAL
1	D	35	ARG
1	D	38	HIS
1	D	42	THR
1	D	53	ARG
1	D	66	VAL
1	D	137	GLU
1	D	174	VAL
1	D	226	ASN
1	D	232	LYS
1	D	276	THR
1	D	277	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	77	HIS
1	A	138	ASN
1	A	139	GLN
1	A	193	GLN
1	A	226	ASN
1	A	265	HIS
1	B	77	HIS
1	B	138	ASN
1	B	139	GLN
1	B	193	GLN
1	B	226	ASN
1	C	67	GLN
1	C	138	ASN
1	C	139	GLN
1	C	193	GLN
1	C	226	ASN
1	D	138	ASN
1	D	139	GLN
1	D	193	GLN
1	D	226	ASN

### 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 8 ligands modelled in this entry, 8 are 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	247/263 (93%)	0.89	18 (7%) 15 13	11, 20, 29, 38	0
1	B	247/263 (93%)	0.80	19 (7%) 13 12	11, 20, 29, 38	0
1	C	247/263 (93%)	1.28	55 (22%) 1 1	11, 20, 29, 38	0
1	D	247/263 (93%)	2.03	98 (39%) 1 0	11, 20, 31, 70	0
All	All	988/1052 (93%)	1.25	190 (19%) 2 1	11, 20, 30, 70	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	40	ALA	9.2
1	D	28	HIS	7.5
1	D	29	SER	7.2
1	D	233	ASN	6.9
1	D	44	ALA	6.9
1	D	219	THR	6.9
1	D	249	GLN	6.6
1	D	41	GLY	5.8
1	C	44	ALA	5.7
1	D	215	TYR	5.7
1	D	214	THR	5.6
1	D	248	THR	5.5
1	C	243	ASN	5.4
1	D	245	VAL	5.4
1	D	27	HIS	5.4
1	D	230	PRO	5.2
1	D	33	VAL	5.1
1	D	229	THR	5.0
1	C	262	ALA	4.9
1	D	183	ASN	4.9
1	D	275	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	108	ALA	4.8
1	D	218	LYS	4.8
1	D	70	GLY	4.8
1	D	153	ASN	4.7
1	D	234	ASP	4.7
1	D	247	PRO	4.7
1	D	34	PRO	4.6
1	A	30	HIS	4.6
1	D	64	HIS	4.6
1	D	185	ASP	4.6
1	C	219	THR	4.6
1	D	38	HIS	4.5
1	B	245	VAL	4.5
1	D	39	MET	4.4
1	D	137	GLU	4.4
1	C	248	THR	4.4
1	D	25	HIS	4.4
1	A	47	ALA	4.4
1	D	190	GLY	4.3
1	C	186	HIS	4.3
1	B	27	HIS	4.3
1	D	244	MET	4.2
1	B	26	HIS	4.2
1	D	246	ILE	4.2
1	D	231	ASP	4.1
1	D	32	LEU	4.1
1	D	105	THR	4.1
1	D	182	ILE	4.1
1	D	62	GLY	4.0
1	D	217	GLN	4.0
1	C	27	HIS	4.0
1	C	164	ASN	4.0
1	D	216	TYR	4.0
1	C	259	GLY	3.9
1	C	25	HIS	3.9
1	C	192	THR	3.9
1	C	276	THR	3.9
1	A	44	GLY	3.9
1	C	233	ASN	3.8
1	A	29	HIS	3.8
1	D	138	ASN	3.8
1	C	228	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	35	ARG	3.6
1	D	232	LYS	3.6
1	D	242	GLU	3.6
1	C	234	ASP	3.6
1	D	195	LEU	3.6
1	B	248	THR	3.5
1	C	124	GLY	3.5
1	C	245	VAL	3.4
1	D	63	PRO	3.4
1	C	26	HIS	3.4
1	D	52	ARG	3.4
1	C	28	HIS	3.4
1	A	187	GLN	3.4
1	D	177	GLY	3.4
1	D	86	ASP	3.3
1	C	185	ASP	3.3
1	D	51	HIS	3.3
1	D	188	ASN	3.3
1	D	58	TYR	3.3
1	D	43	GLN	3.2
1	D	53	ARG	3.2
1	D	207	TYR	3.2
1	C	151	MET	3.2
1	B	34	PRO	3.2
1	D	144	PRO	3.2
1	D	109	PHE	3.2
1	D	241	VAL	3.1
1	D	37	SER	3.1
1	D	111	ASN	3.1
1	B	44	ALA	3.1
1	D	154	GLY	3.1
1	D	192	THR	3.0
1	D	221	THR	3.0
1	D	26	HIS	3.0
1	C	246	ILE	2.9
1	A	232	LYS	2.9
1	C	232	LYS	2.9
1	B	186	HIS	2.9
1	B	188	ASN	2.9
1	D	71	THR	2.9
1	D	243	ASN	2.9
1	D	181	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	179	ASN	2.8
1	D	141	LEU	2.8
1	D	180	GLY	2.8
1	C	82	ILE	2.8
1	D	59	SER	2.7
1	C	188	ASN	2.7
1	D	142	ASP	2.7
1	C	187	GLN	2.7
1	B	181	GLN	2.7
1	C	125	ARG	2.7
1	C	231	ASP	2.7
1	A	186	HIS	2.7
1	C	32	LEU	2.7
1	C	261	LEU	2.7
1	C	216	TYR	2.6
1	D	135	TYR	2.6
1	D	151	MET	2.6
1	D	75	TRP	2.6
1	A	86	ASP	2.6
1	C	183	ASN	2.6
1	C	34	PRO	2.6
1	A	207	TYR	2.6
1	A	124	GLY	2.6
1	C	168	LYS	2.6
1	C	86	ASP	2.6
1	C	109	PHE	2.6
1	C	247	PRO	2.5
1	D	42	THR	2.5
1	D	191	ALA	2.5
1	D	277	GLU	2.5
1	C	96	SER	2.5
1	A	134	TRP	2.5
1	D	66	VAL	2.5
1	C	51	HIS	2.5
1	C	166	GLY	2.5
1	D	155	VAL	2.5
1	B	185	ASP	2.5
1	C	181	GLN	2.5
1	D	187	GLN	2.5
1	C	191	ALA	2.4
1	D	272	THR	2.4
1	A	277	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	30	SER	2.4
1	C	223	MET	2.4
1	C	195	LEU	2.4
1	D	224	ILE	2.4
1	C	217	GLN	2.3
1	D	112	TRP	2.3
1	A	175	VAL	2.3
1	C	163	ASP	2.3
1	C	165	ASP	2.3
1	C	64	HIS	2.3
1	C	110	GLU	2.3
1	B	231	ASP	2.3
1	B	277	GLU	2.3
1	A	81	ALA	2.2
1	B	243	ASN	2.2
1	D	179	ASN	2.2
1	C	91	ALA	2.2
1	B	198	CYS	2.2
1	D	140	GLY	2.2
1	D	235	TYR	2.2
1	D	57	LYS	2.2
1	A	228	PHE	2.2
1	D	276	THR	2.2
1	C	37	SER	2.2
1	C	150	ASP	2.2
1	D	194	ALA	2.2
1	D	119	ARG	2.1
1	A	51	HIS	2.1
1	D	251	HIS	2.1
1	A	28	HIS	2.1
1	C	71	THR	2.1
1	D	163	ASP	2.1
1	D	107	ALA	2.1
1	D	186	HIS	2.1
1	D	197	SER	2.1
1	B	187	GLN	2.1
1	C	249	GLN	2.0
1	C	227	GLY	2.0
1	D	136	THR	2.0
1	A	132	ALA	2.0
1	B	183	ASN	2.0
1	B	216	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	129	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<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	CA	B	315	1/1	0.49	7.68	59,59,59,59	0
2	CA	D	515	1/1	0.44	4.11	61,61,61,61	0
2	CA	D	510	1/1	0.34	2.28	48,48,48,48	0
2	CA	B	310	1/1	0.32	1.52	45,45,45,45	0
2	CA	A	286	1/1	0.24	1.39	34,34,34,34	0
2	CA	C	410	1/1	0.36	0.64	59,59,59,59	0
2	CA	A	285	1/1	0.23	0.35	32,32,32,32	0
2	CA	C	415	1/1	0.31	0.31	66,66,66,66	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.