



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:53 PM GMT

PDB ID : 1R1Z
Title : The Crystal structure of the Carbohydrate recognition domain of the glycoprotein 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 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

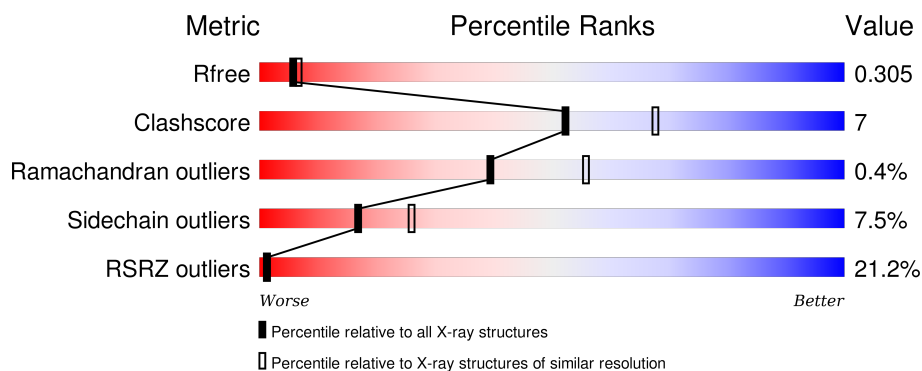
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 ≥ 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	263	
1	B	263	
1	C	263	
1	D	263	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	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 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 ERGIC-53 protein.

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

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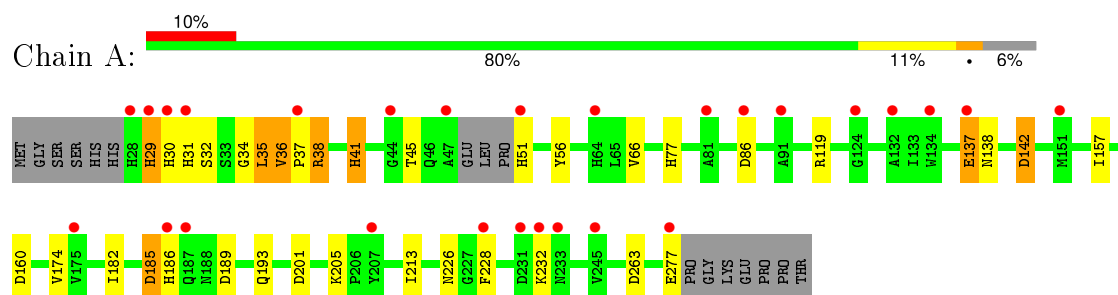
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	18	Total	O	0	0
			18	18		

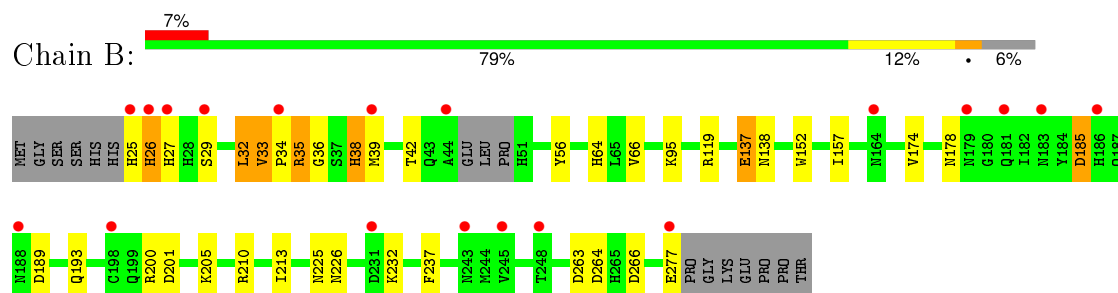
3 Residue-property plots [i](#)

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

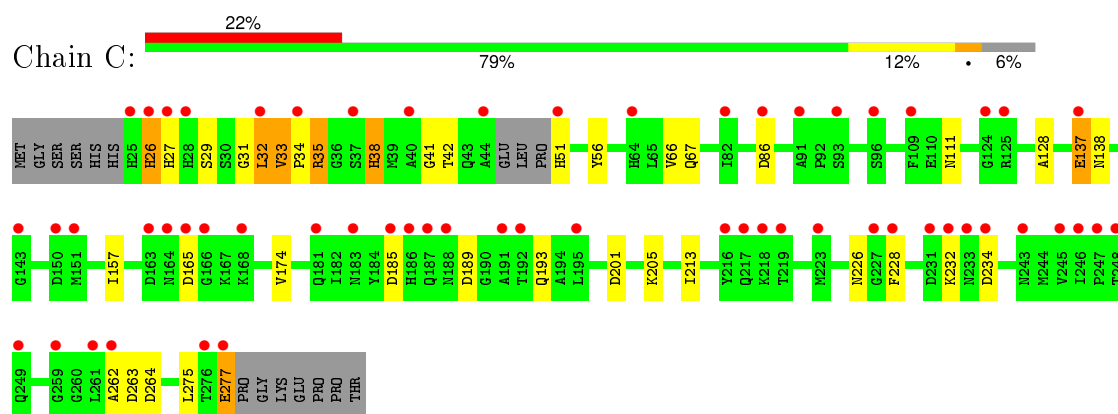
- Molecule 1: ERGIC-53 protein



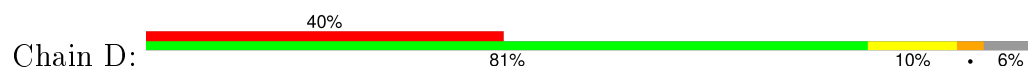
- Molecule 1: ERGIC-53 protein

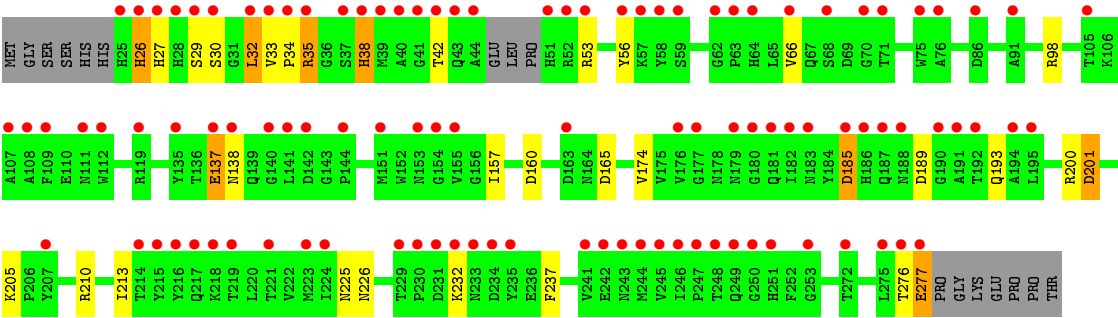


- Molecule 1: ERGIC-53 protein



- Molecule 1: ERGIC-53 protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 95.1 (10.00-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	35.9	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.50 , 66.9	EDS
Estimated twinning fraction	0.015 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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: 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 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	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

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 7.

All (98) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:HIS:HE1	3:B:336:HOH:O	1.86	0.58
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

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	243/263 (92%)	234 (96%)	8 (3%)	1 (0%)	39	56
1	B	243/263 (92%)	236 (97%)	6 (2%)	1 (0%)	39	56
1	C	243/263 (92%)	237 (98%)	5 (2%)	1 (0%)	39	56
1	D	243/263 (92%)	236 (97%)	6 (2%)	1 (0%)	39	56
All	All	972/1052 (92%)	943 (97%)	25 (3%)	4 (0%)	39	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	B	26	HIS
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%)	16	24
1	B	193/215 (90%)	180 (93%)	13 (7%)	20	31
1	C	193/215 (90%)	179 (93%)	14 (7%)	17	27
1	D	193/215 (90%)	177 (92%)	16 (8%)	14	21
All	All	772/860 (90%)	714 (92%)	58 (8%)	17	26

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

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Mol	Chain	Res	Type
1	B	27	HIS
1	B	29	SER
1	B	32	LEU
1	B	33	VAL
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 [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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.

No monomer is involved in short contacts.

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, 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	247/263 (93%)	0.93	27 (10%) 7 7	11, 20, 29, 38	0
1	B	247/263 (93%)	0.80	19 (7%) 16 16	11, 20, 29, 38	0
1	C	247/263 (93%)	1.30	59 (23%) 1 1	11, 20, 29, 38	0
1	D	247/263 (93%)	2.14	104 (42%) 0 0	11, 20, 31, 70	0
All	All	988/1052 (93%)	1.29	209 (21%) 1 1	11, 20, 30, 70	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	40	ALA	10.2
1	D	28	HIS	8.7
1	D	44	ALA	8.0
1	D	219	THR	7.8
1	D	29	SER	7.6
1	D	249	GLN	7.3
1	D	233	ASN	7.3
1	D	27	HIS	6.6
1	D	245	VAL	6.4
1	D	33	VAL	6.1
1	D	275	LEU	6.1
1	D	215	TYR	5.9
1	D	41	GLY	5.9
1	D	234	ASP	5.6
1	C	44	ALA	5.6
1	C	243	ASN	5.6
1	D	248	THR	5.6
1	D	34	PRO	5.4
1	D	190	GLY	5.3
1	D	229	THR	5.3
1	D	38	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	219	THR	5.2
1	A	30	HIS	5.1
1	D	214	THR	5.1
1	D	108	ALA	5.1
1	D	246	ILE	5.1
1	D	230	PRO	5.0
1	D	185	ASP	5.0
1	B	245	VAL	4.9
1	D	62	GLY	4.8
1	C	262	ALA	4.8
1	D	39	MET	4.8
1	D	218	LYS	4.7
1	B	27	HIS	4.7
1	D	153	ASN	4.7
1	C	259	GLY	4.6
1	D	70	GLY	4.6
1	D	247	PRO	4.5
1	C	124	GLY	4.5
1	D	183	ASN	4.5
1	C	186	HIS	4.5
1	D	244	MET	4.5
1	A	47	ALA	4.4
1	A	44	GLY	4.4
1	D	137	GLU	4.4
1	C	25	HIS	4.4
1	D	105	THR	4.3
1	D	86	ASP	4.3
1	B	26	HIS	4.2
1	D	25	HIS	4.2
1	D	64	HIS	4.2
1	C	276	THR	4.2
1	D	242	GLU	4.2
1	D	182	ILE	4.1
1	C	27	HIS	4.1
1	C	164	ASN	4.1
1	D	216	TYR	4.1
1	C	248	THR	4.1
1	C	192	THR	4.0
1	D	138	ASN	4.0
1	A	29	HIS	4.0
1	D	195	LEU	4.0
1	D	231	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	35	ARG	3.9
1	C	233	ASN	3.8
1	D	52	ARG	3.8
1	D	177	GLY	3.8
1	C	228	PHE	3.8
1	D	232	LYS	3.7
1	D	109	PHE	3.7
1	D	32	LEU	3.7
1	C	234	ASP	3.7
1	C	28	HIS	3.6
1	C	245	VAL	3.6
1	C	26	HIS	3.6
1	B	34	PRO	3.5
1	A	187	GLN	3.5
1	D	217	GLN	3.5
1	D	241	VAL	3.5
1	D	277	GLU	3.4
1	D	243	ASN	3.4
1	C	232	LYS	3.4
1	D	188	ASN	3.4
1	C	187	GLN	3.4
1	B	186	HIS	3.3
1	D	207	TYR	3.3
1	B	248	THR	3.3
1	D	180	GLY	3.3
1	D	58	TYR	3.2
1	D	144	PRO	3.2
1	D	194	ALA	3.2
1	C	151	MET	3.2
1	A	124	GLY	3.2
1	D	37	SER	3.2
1	D	154	GLY	3.2
1	B	44	ALA	3.2
1	D	51	HIS	3.2
1	D	26	HIS	3.2
1	D	192	THR	3.2
1	D	191	ALA	3.1
1	C	185	ASP	3.1
1	D	53	ARG	3.1
1	C	96	SER	3.0
1	D	155	VAL	3.0
1	D	181	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	82	ILE	2.9
1	D	111	ASN	2.9
1	C	34	PRO	2.9
1	D	141	LEU	2.9
1	B	179	ASN	2.9
1	B	188	ASN	2.9
1	C	223	MET	2.9
1	D	43	GLN	2.9
1	A	232	LYS	2.9
1	C	188	ASN	2.8
1	A	186	HIS	2.8
1	C	195	LEU	2.8
1	C	231	ASP	2.8
1	D	75	TRP	2.8
1	C	163	ASP	2.8
1	D	71	THR	2.8
1	D	63	PRO	2.8
1	D	221	THR	2.7
1	D	66	VAL	2.7
1	C	125	ARG	2.7
1	A	207	TYR	2.7
1	C	37	SER	2.7
1	A	134	TRP	2.7
1	C	168	LYS	2.7
1	C	261	LEU	2.7
1	C	143	GLY	2.7
1	A	277	GLU	2.6
1	A	37	PRO	2.6
1	D	42	THR	2.6
1	A	86	ASP	2.6
1	C	93	SER	2.6
1	D	135	TYR	2.6
1	D	57	LYS	2.6
1	C	165	ASP	2.6
1	C	51	HIS	2.6
1	C	91	ALA	2.6
1	B	181	GLN	2.6
1	D	59	SER	2.5
1	C	246	ILE	2.5
1	D	276	THR	2.5
1	A	132	ALA	2.5
1	B	277	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	151	MET	2.5
1	B	243	ASN	2.5
1	D	30	SER	2.5
1	A	175	VAL	2.5
1	C	247	PRO	2.5
1	A	28	HIS	2.5
1	C	64	HIS	2.5
1	D	119	ARG	2.5
1	D	187	GLN	2.5
1	A	51	HIS	2.4
1	D	179	ASN	2.4
1	A	81	ALA	2.4
1	B	231	ASP	2.4
1	C	183	ASN	2.4
1	C	166	GLY	2.4
1	D	68	SER	2.4
1	C	109	PHE	2.4
1	A	91	ALA	2.4
1	D	253	GLY	2.3
1	D	112	TRP	2.3
1	B	29	SER	2.3
1	C	217	GLN	2.3
1	C	227	GLY	2.3
1	C	216	TYR	2.3
1	D	235	TYR	2.3
1	D	251	HIS	2.3
1	D	224	ILE	2.3
1	D	142	ASP	2.3
1	B	25	HIS	2.2
1	A	228	PHE	2.2
1	C	32	LEU	2.2
1	A	245	VAL	2.2
1	D	56	TYR	2.2
1	D	186	HIS	2.2
1	C	191	ALA	2.2
1	D	107	ALA	2.2
1	C	181	GLN	2.2
1	C	249	GLN	2.2
1	A	64	HIS	2.2
1	D	91	ALA	2.2
1	A	151	MET	2.2
1	D	140	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	76	ALA	2.1
1	D	272	THR	2.1
1	D	223	MET	2.1
1	A	233	ASN	2.1
1	B	183	ASN	2.1
1	A	31	HIS	2.1
1	C	150	ASP	2.1
1	D	176	VAL	2.1
1	B	39	MET	2.1
1	C	137	GLU	2.1
1	C	277	GLU	2.1
1	C	86	ASP	2.1
1	B	198	CYS	2.1
1	A	231	ASP	2.1
1	A	137	GLU	2.0
1	C	218	LYS	2.0
1	B	164	ASN	2.0
1	C	40	ALA	2.0
1	D	250	GLY	2.0
1	D	163	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, 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(Å ²)	Q<0.9
2	CA	B	315	1/1	0.85	0.51	8.82	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	D	515	1/1	0.68	0.43	4.20	61,61,61,61	0
2	CA	D	510	1/1	0.92	0.35	2.61	48,48,48,48	0
2	CA	B	310	1/1	0.86	0.32	1.41	45,45,45,45	0
2	CA	A	286	1/1	0.94	0.23	0.88	34,34,34,34	0
2	CA	C	410	1/1	0.72	0.37	0.74	59,59,59,59	0
2	CA	A	285	1/1	0.90	0.24	0.53	32,32,32,32	0
2	CA	C	415	1/1	0.62	0.31	0.13	66,66,66,66	0

6.5 Other polymers

There are no such residues in this entry.