Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 02:54 PM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

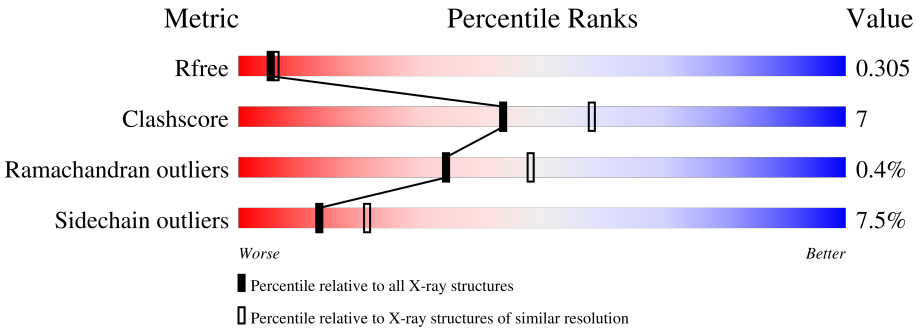
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	263	80% 11% · 6%
1	B	263	79% 12% · 6%
1	C	263	79% 12% · 6%
1	D	263	81% 10% · 6%

2 Entry composition (i)

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	A	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0
2	D	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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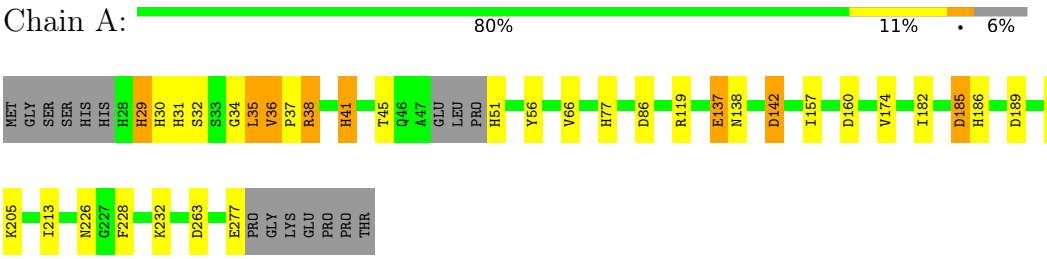
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	18	Total O 18 18	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

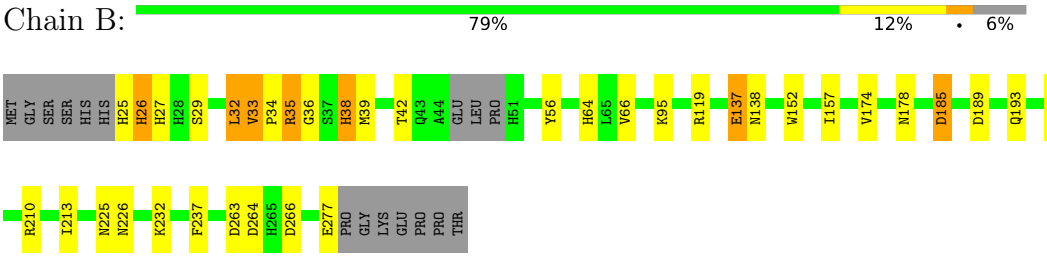
- Molecule 1: ERGIC-53 protein

Chain A:



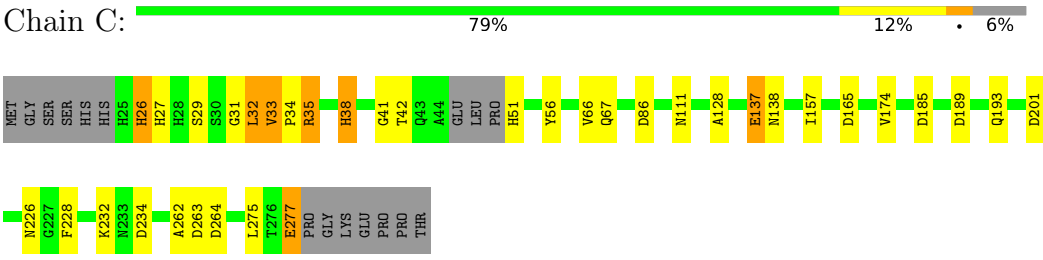
- Molecule 1: ERGIC-53 protein

Chain B:



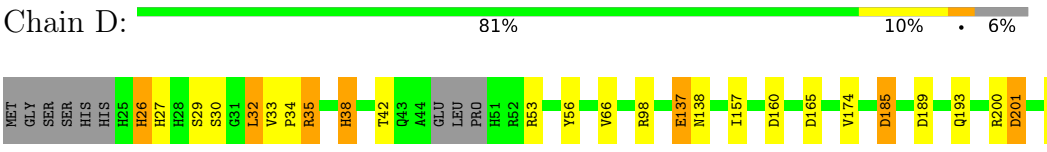
- Molecule 1: ERGIC-53 protein

Chain C:



- Molecule 1: ERGIC-53 protein

Chain D:




I213
N225
N226
K232
F237
T276
E277
PRO
GLY
LYS
GLU
PRO
PRO
THR

4 Data and refinement statistics (i)

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) 95.9 (10.00-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [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	1071 reflections (2.54%)	wwPDB-VP
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 , 67.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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:HD23	1:B:32:LEU:H	1.57	0.68
1:B:32:LEU:CD2	3:B:324:HOH:O	2.15	0.66
1:A:35:LEU:HD23	1:A:35:LEU:H	1.61	0.66
1:A:228:PHE:CD2	1:C:228:PHE:CZ	2.83	0.65
1:C:32:LEU:HD23	1:C:32:LEU:H	1.63	0.63
1:A:201:ASP:O	1:A:205:LYS:NZ	2.32	0.63
1:B:185:ASP:H	1:B:193:GLN:HE22	1.45	0.63
1:C:157:ILE:HD13	1:C:213:ILE:HD13	1.81	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:HD23	1:D:32:LEU:H	1.64	0.61
1:A:228:PHE:CE1	1:C:228:PHE:CG	2.89	0.61
1:A:228:PHE:CD2	1:C:228:PHE:CE1	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:A:31:HIS:CD2	3:A:305:HOH:O	2.59	0.55
1:D:201:ASP:O	1:D:205:LYS:NZ	2.39	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:CZ	1:C:228:PHE:CZ	2.98	0.52
1:A:228:PHE:CD1	1:C:228:PHE:CD1	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%)	34	48
1	B	243/263 (92%)	236 (97%)	6 (2%)	1 (0%)	34	48
1	C	243/263 (92%)	237 (98%)	5 (2%)	1 (0%)	34	48
1	D	243/263 (92%)	236 (97%)	6 (2%)	1 (0%)	34	48
All	All	972/1052 (92%)	943 (97%)	25 (3%)	4 (0%)	34	48

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 (i)

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%)	12	19
1	B	193/215 (90%)	180 (93%)	13 (7%)	16	26
1	C	193/215 (90%)	179 (93%)	14 (7%)	14	22
1	D	193/215 (90%)	177 (92%)	16 (8%)	11	17
All	All	772/860 (90%)	714 (92%)	58 (8%)	13	21

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

Sometimes 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 monosaccharides 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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.