Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 02:23 AM EDT

PDB ID	:	3ISR
Title	:	The Crystal Structure of a Putative Cysteine Protease from Cytophaga hutchinsonii to 1.9A
Authors	:	Stein, A.J.; Bigelow, L.; Trevino, D.; Buck, K.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2009-08-27
Resolution	:	1.90 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:

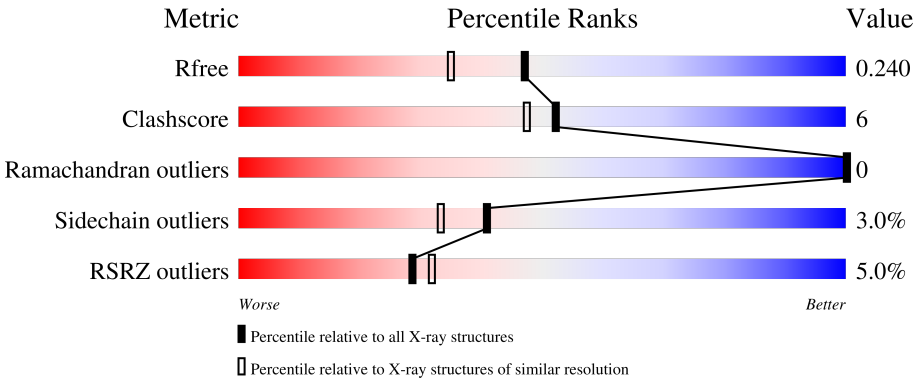
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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% 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	293	4% 86% 11%
1	B	293	6% 86% 12%
1	C	293	2% 83% 14%
1	D	293	8% 86% 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9509 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 Transglutaminase-like enzymes, putative cysteine protease.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	Se	0	4	0
			2228	1436	362	421	5	4			
1	B	289	Total	C	N	O	S	Se	0	0	0
			2234	1437	364	424	5	4			
1	C	285	Total	C	N	O	S	Se	0	1	0
			2228	1430	364	425	5	4			
1	D	289	Total	C	N	O	S	Se	0	0	0
			2254	1451	368	427	5	3			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP Q11RW0
A	-9	THR	-	expression tag	UNP Q11RW0
A	-8	GLU	-	expression tag	UNP Q11RW0
A	-7	ASN	-	expression tag	UNP Q11RW0
A	-6	LEU	-	expression tag	UNP Q11RW0
A	-5	TYR	-	expression tag	UNP Q11RW0
A	-4	PHE	-	expression tag	UNP Q11RW0
A	-3	GLN	-	expression tag	UNP Q11RW0
A	-2	SER	-	expression tag	UNP Q11RW0
A	-1	ASN	-	expression tag	UNP Q11RW0
A	0	ALA	-	expression tag	UNP Q11RW0
B	-10	GLY	-	expression tag	UNP Q11RW0
B	-9	THR	-	expression tag	UNP Q11RW0
B	-8	GLU	-	expression tag	UNP Q11RW0
B	-7	ASN	-	expression tag	UNP Q11RW0
B	-6	LEU	-	expression tag	UNP Q11RW0
B	-5	TYR	-	expression tag	UNP Q11RW0
B	-4	PHE	-	expression tag	UNP Q11RW0
B	-3	GLN	-	expression tag	UNP Q11RW0
B	-2	SER	-	expression tag	UNP Q11RW0
B	-1	ASN	-	expression tag	UNP Q11RW0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP Q11RW0
C	-10	GLY	-	expression tag	UNP Q11RW0
C	-9	THR	-	expression tag	UNP Q11RW0
C	-8	GLU	-	expression tag	UNP Q11RW0
C	-7	ASN	-	expression tag	UNP Q11RW0
C	-6	LEU	-	expression tag	UNP Q11RW0
C	-5	TYR	-	expression tag	UNP Q11RW0
C	-4	PHE	-	expression tag	UNP Q11RW0
C	-3	GLN	-	expression tag	UNP Q11RW0
C	-2	SER	-	expression tag	UNP Q11RW0
C	-1	ASN	-	expression tag	UNP Q11RW0
C	0	ALA	-	expression tag	UNP Q11RW0
D	-10	GLY	-	expression tag	UNP Q11RW0
D	-9	THR	-	expression tag	UNP Q11RW0
D	-8	GLU	-	expression tag	UNP Q11RW0
D	-7	ASN	-	expression tag	UNP Q11RW0
D	-6	LEU	-	expression tag	UNP Q11RW0
D	-5	TYR	-	expression tag	UNP Q11RW0
D	-4	PHE	-	expression tag	UNP Q11RW0
D	-3	GLN	-	expression tag	UNP Q11RW0
D	-2	SER	-	expression tag	UNP Q11RW0
D	-1	ASN	-	expression tag	UNP Q11RW0
D	0	ALA	-	expression tag	UNP Q11RW0

- Molecule 2 is water.

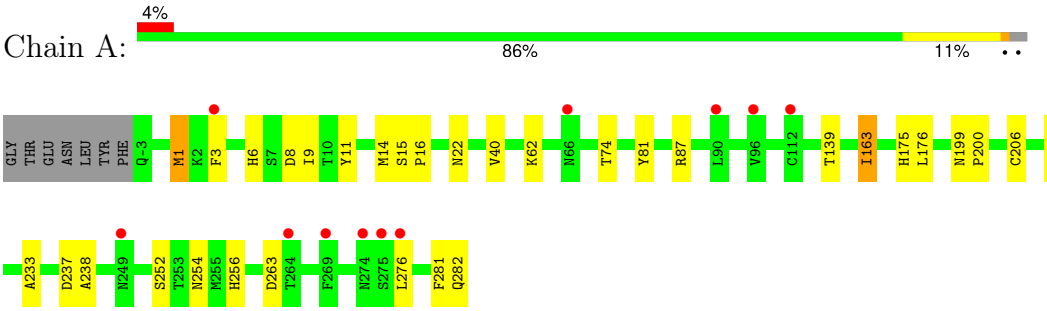
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	160	Total O 160 160	0	0
2	B	152	Total O 152 152	0	0
2	C	138	Total O 138 138	0	0
2	D	115	Total O 115 115	0	0

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 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.

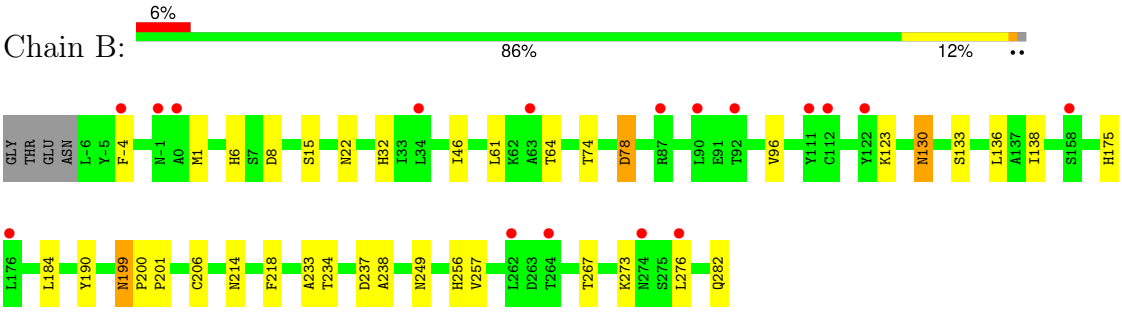
• Molecule 1: Transglutaminase-like enzymes, putative cysteine protease

Chain A:



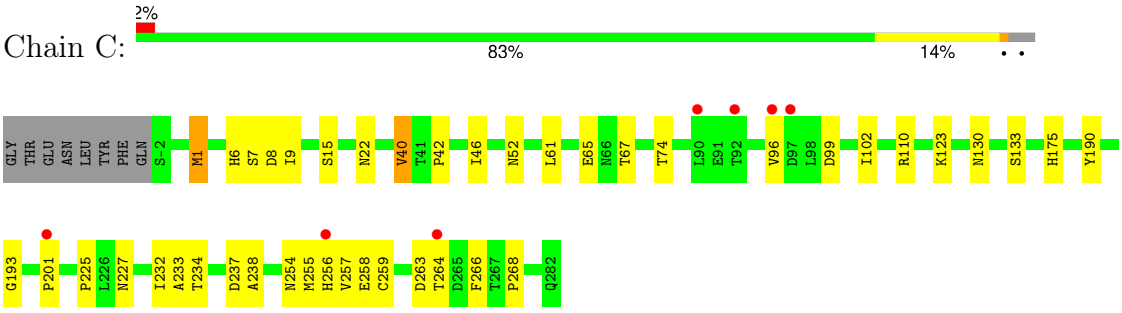
• Molecule 1: Transglutaminase-like enzymes, putative cysteine protease

Chain B:



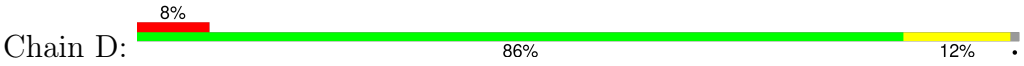
• Molecule 1: Transglutaminase-like enzymes, putative cysteine protease

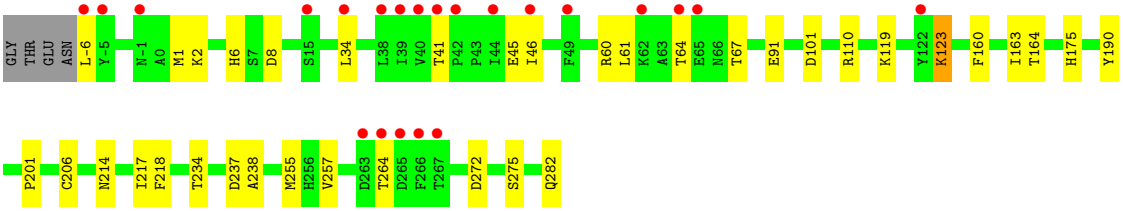
Chain C:



• Molecule 1: Transglutaminase-like enzymes, putative cysteine protease

Chain D:




GLY
THR
GLU
ASN
L-6
Y-5
N-1
A0
M1
K2
H6
S7
D8
S15
L34
L38
I39
V40
T41
P42
P43
I44
E45
I46
F49
R60
L61
K62
A63
T64
E65
N66
T67
E91
D101
R110
K119
Y122
K123
F160
I163
T164
H175
Y190
P201
C206
N214
I217
F218
T234
D237
A238
M255
H256
V257
D263
T264
D265
F266
T267
D272
S275
Q282

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.72Å 115.24Å 131.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.28 – 1.90 48.28 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.28-1.90) 99.3 (48.28-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 1.90Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0102	Depositor
R, R_{free}	0.187 , 0.220 0.210 , 0.240	Depositor DCC
R_{free} test set	5394 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9509	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2201e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.57	0/2291	0.63	0/3118
1	B	0.55	0/2287	0.60	0/3116
1	C	0.52	0/2282	0.59	0/3103
1	D	0.52	0/2307	0.60	0/3139
All	All	0.54	0/9167	0.61	0/12476

There are no bond length outliers.

There are no bond angle outliers.

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	2228	0	2147	29	0
1	B	2234	0	2116	22	0
1	C	2228	0	2142	29	0
1	D	2254	0	2157	22	0
2	A	160	0	0	1	0
2	B	152	0	0	1	0
2	C	138	0	0	1	0
2	D	115	0	0	1	0
All	All	9509	0	8562	97	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MSE:HE1	1:A:81:TYR:CE2	2.11	0.85
1:C:175:HIS:HE1	1:C:238:ALA:H	1.32	0.75
1:A:1:MSE:HE1	1:A:81:TYR:HE2	1.52	0.75
1:A:9:ILE:HD11	1:A:252:SER:HB2	1.69	0.74
1:D:175:HIS:HE1	1:D:238:ALA:H	1.35	0.74
1:A:175:HIS:HE1	1:A:238:ALA:H	1.33	0.73
1:B:175:HIS:HE1	1:B:238:ALA:H	1.34	0.72
1:A:214:ASN:HD22	1:A:282:GLN:HE22	1.37	0.72
1:A:214:ASN:ND2	1:A:282:GLN:HE22	1.89	0.70
1:B:199:ASN:HD22	1:B:200:PRO:HA	1.57	0.69
1:D:6:HIS:HE1	1:D:8:ASP:OD1	1.77	0.67
1:A:199:ASN:HD22	1:A:200:PRO:HA	1.61	0.65
1:B:214:ASN:HD22	1:B:282:GLN:HE22	1.45	0.63
1:B:214:ASN:ND2	1:B:282:GLN:HE22	1.96	0.63
1:B:6:HIS:HE1	1:B:8:ASP:OD1	1.81	0.63
1:A:6:HIS:HD2	1:A:74:THR:OG1	1.84	0.60
1:B:8:ASP:OD2	1:B:256:HIS:HD2	1.84	0.60
1:C:15:SER:HA	1:C:65:GLU:HB3	1.82	0.60
1:B:175:HIS:CE1	1:B:238:ALA:H	2.20	0.59
1:B:1:MSE:O	1:B:78:ASP:HA	2.02	0.58
1:B:136:LEU:HD21	1:B:273:LYS:HA	1.85	0.58
1:A:1:MSE:HB2	1:A:263:ASP:OD2	2.04	0.58
1:D:214:ASN:ND2	1:D:282:GLN:HE22	2.02	0.58
1:D:214:ASN:HD22	1:D:282:GLN:HE22	1.53	0.57
1:D:201:PRO:HB2	1:D:257:VAL:O	2.04	0.56
1:B:6:HIS:HD2	1:B:74:THR:OG1	1.89	0.56
1:B:32:HIS:HB2	1:B:78:ASP:OD2	2.05	0.56
1:C:1:MSE:HE3	1:C:266:PHE:HE1	1.71	0.56
1:C:1:MSE:HE2	1:C:227:ASN:O	2.05	0.56
1:A:163:ILE:HG12	1:A:176:LEU:HD11	1.87	0.55
1:C:22:ASN:HD21	1:C:233:ALA:HB2	1.72	0.54
1:C:99:ASP:HB2	1:C:102:ILE:HG12	1.88	0.54
1:A:175:HIS:CE1	1:A:237:ASP:HB2	2.43	0.54
1:C:1:MSE:HE3	1:C:266:PHE:CE1	2.41	0.54
1:D:175:HIS:CE1	1:D:238:ALA:H	2.22	0.54
1:B:46:ILE:HD12	1:B:61:LEU:HD23	1.90	0.53
1:A:9:ILE:HD12	1:A:254:ASN:O	2.08	0.53
1:A:1:MSE:HE1	1:A:81:TYR:CD2	2.44	0.52
1:B:201:PRO:HB2	1:B:257:VAL:O	2.10	0.52
1:C:6:HIS:HE1	1:C:8:ASP:OD1	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:HIS:CE1	1:B:237:ASP:HB2	2.46	0.51
1:A:175:HIS:CE1	1:A:238:ALA:H	2.22	0.51
1:D:6:HIS:CE1	1:D:8:ASP:OD1	2.62	0.51
1:A:175:HIS:HD2	2:A:296:HOH:O	1.94	0.51
1:C:175:HIS:HD2	2:C:287:HOH:O	1.94	0.51
1:D:46:ILE:HD13	1:D:61:LEU:HD23	1.93	0.50
1:A:9:ILE:HG12	1:A:11:TYR:CE2	2.47	0.50
1:A:1:MSE:CE	1:A:81:TYR:HE2	2.23	0.50
1:B:130:ASN:ND2	1:B:133:SER:H	2.10	0.50
1:C:46:ILE:HG22	1:C:61:LEU:HB3	1.94	0.49
1:C:6:HIS:HD2	1:C:74:THR:OG1	1.96	0.49
1:A:1:MSE:CE	1:A:81:TYR:CE2	2.91	0.48
1:A:139[A]:THR:HG21	1:A:218:PHE:HB3	1.94	0.48
1:B:190:TYR:O	1:B:234:THR:HA	2.13	0.48
1:C:9:ILE:HG12	1:C:255:MSE:HG3	1.95	0.48
1:C:1:MSE:HG3	1:C:263:ASP:OD2	2.14	0.48
1:C:96:VAL:HA	1:D:60:ARG:HD2	1.96	0.48
1:D:175:HIS:CE1	1:D:237:ASP:HB2	2.48	0.47
1:D:206:CYS:HB2	1:D:218:PHE:O	2.14	0.47
1:D:46:ILE:HD12	1:D:61:LEU:HB3	1.95	0.47
1:A:9:ILE:HD11	1:A:252:SER:CB	2.41	0.47
1:C:175:HIS:CE1	1:C:238:ALA:H	2.22	0.47
1:A:22:ASN:HD21	1:A:233:ALA:HB2	1.80	0.46
1:C:175:HIS:CE1	1:C:237:ASP:HB2	2.50	0.46
1:C:258:GLU:HG2	1:C:259:CYS:N	2.30	0.46
1:C:130:ASN:HB3	1:C:133:SER:HB2	1.98	0.46
1:D:64:THR:O	1:D:67:THR:OG1	2.23	0.46
1:C:201:PRO:HB2	1:C:257:VAL:O	2.16	0.46
1:C:52:ASN:HD21	1:D:101:ASP:HB3	1.80	0.45
1:C:40:VAL:HG23	1:C:42:PRO:O	2.16	0.45
1:B:138:ILE:HD11	1:B:184:LEU:HD12	1.98	0.45
1:C:1:MSE:HE1	1:C:227:ASN:HB2	1.99	0.45
1:D:2:LYS:HE3	1:D:34:LEU:HD11	1.98	0.44
1:D:175:HIS:HD2	2:D:285:HOH:O	2.01	0.44
1:A:8:ASP:OD2	1:A:256:HIS:HD2	2.00	0.43
1:A:1:MSE:HG3	1:A:3:PHE:CE2	2.54	0.43
1:B:175:HIS:HD2	2:B:306:HOH:O	2.03	0.42
1:A:217[B]:ILE:HD13	1:A:281:PHE:HE2	1.84	0.42
1:C:110:ARG:HA	1:D:110:ARG:HA	2.02	0.42
1:C:225:PRO:HB3	1:C:268:PRO:HB3	2.01	0.42
1:C:193:GLY:HA2	1:C:232:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:CYS:HB2	1:B:218:PHE:O	2.20	0.41
1:C:1:MSE:HE1	1:C:227:ASN:ND2	2.35	0.41
1:C:7:SER:HA	1:C:256:HIS:O	2.20	0.41
1:A:163:ILE:HG21	1:D:164:THR:HG22	2.02	0.41
1:D:190:TYR:O	1:D:234:THR:HA	2.20	0.41
1:A:206:CYS:HB2	1:A:218:PHE:O	2.20	0.41
1:B:15:SER:OG	1:B:249:ASN:HB2	2.20	0.41
1:C:190:TYR:O	1:C:234:THR:HA	2.20	0.41
1:A:15:SER:HB2	1:A:16:PRO:HD2	2.02	0.41
1:A:87:ARG:HG2	1:A:276:LEU:HD12	2.03	0.41
1:C:52:ASN:N	1:C:52:ASN:HD22	2.18	0.41
1:D:119:LYS:O	1:D:123:LYS:HD3	2.21	0.40
1:D:160:PHE:O	1:D:163:ILE:HG22	2.21	0.40
1:D:255:MSE:HE2	1:D:255:MSE:HB3	2.00	0.40
1:A:62:LYS:HD3	1:B:96:VAL:HG11	2.04	0.40
1:B:22:ASN:HD21	1:B:233:ALA:HB2	1.86	0.40

There are no symmetry-related clashes.

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	288/293 (98%)	282 (98%)	6 (2%)	0	100	100
1	B	287/293 (98%)	279 (97%)	8 (3%)	0	100	100
1	C	284/293 (97%)	277 (98%)	7 (2%)	0	100	100
1	D	287/293 (98%)	282 (98%)	5 (2%)	0	100	100
All	All	1146/1172 (98%)	1120 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	238/251 (95%)	234 (98%)	4 (2%)	60	57
1	B	236/251 (94%)	228 (97%)	8 (3%)	37	28
1	C	240/251 (96%)	234 (98%)	6 (2%)	47	41
1	D	240/251 (96%)	230 (96%)	10 (4%)	30	20
All	All	954/1004 (95%)	926 (97%)	28 (3%)	41	35

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	14	MSE
1	A	40	VAL
1	A	163	ILE
1	B	-4	PHE
1	B	64	THR
1	B	78	ASP
1	B	123	LYS
1	B	130	ASN
1	B	199	ASN
1	B	267	THR
1	B	276	LEU
1	C	1	MSE
1	C	40	VAL
1	C	67	THR
1	C	123	LYS
1	C	254	ASN
1	C	264	THR
1	D	-6	LEU
1	D	1	MSE
1	D	41	THR
1	D	45	GLU
1	D	91	GLU
1	D	123	LYS

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Mol	Chain	Res	Type
1	D	217	ILE
1	D	264	THR
1	D	272	ASP
1	D	275	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	22	ASN
1	A	175	HIS
1	A	199	ASN
1	A	214	ASN
1	A	256	HIS
1	B	6	HIS
1	B	22	ASN
1	B	80	GLN
1	B	130	ASN
1	B	145	ASN
1	B	175	HIS
1	B	199	ASN
1	B	214	ASN
1	B	256	HIS
1	C	6	HIS
1	C	22	ASN
1	C	52	ASN
1	C	145	ASN
1	C	175	HIS
1	C	214	ASN
1	C	282	GLN
1	D	6	HIS
1	D	22	ASN
1	D	175	HIS
1	D	214	ASN
1	D	256	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{th} 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	282/293 (96%)	0.56	11 (3%)	39	42	3, 16, 22, 26	0
1	B	285/293 (97%)	0.44	17 (5%)	21	24	5, 16, 21, 27	0
1	C	281/293 (95%)	0.29	7 (2%)	57	60	4, 17, 23, 26	0
1	D	285/293 (97%)	0.57	22 (7%)	13	15	8, 17, 22, 25	0
All	All	1133/1172 (96%)	0.46	57 (5%)	28	32	3, 16, 22, 27	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	266	PHE	5.8
1	C	96	VAL	5.2
1	D	44	ILE	4.8
1	D	46	ILE	4.2
1	A	264	THR	3.7
1	B	0	ALA	3.4
1	D	38	LEU	3.4
1	C	90	LEU	3.3
1	D	40	VAL	3.3
1	D	263	ASP	3.3
1	D	64	THR	3.2
1	D	39	ILE	3.1
1	D	42	PRO	3.0
1	D	-6	LEU	3.0
1	C	97	ASP	3.0
1	B	90	LEU	2.9
1	A	66	ASN	2.9
1	A	274	ASN	2.9
1	C	201	PRO	2.9
1	D	65	GLU	2.9
1	A	96	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	276	LEU	2.7
1	A	269	PHE	2.7
1	B	158	SER	2.7
1	B	122	TYR	2.7
1	D	122	TYR	2.7
1	C	92	THR	2.6
1	D	267	THR	2.6
1	B	274	ASN	2.6
1	D	-1	ASN	2.6
1	B	262	LEU	2.5
1	A	90	LEU	2.4
1	A	275	SER	2.4
1	D	265	ASP	2.4
1	A	276	LEU	2.4
1	D	264	THR	2.3
1	C	264	THR	2.3
1	A	3	PHE	2.3
1	B	264	THR	2.2
1	D	15	SER	2.2
1	B	-4	PHE	2.2
1	B	112	CYS	2.2
1	B	92	THR	2.2
1	B	111	TYR	2.2
1	B	176	LEU	2.1
1	A	112	CYS	2.1
1	D	49	PHE	2.1
1	B	87	ARG	2.1
1	C	256	HIS	2.1
1	D	34	LEU	2.1
1	D	-5	TYR	2.1
1	B	63	ALA	2.1
1	B	34	LEU	2.1
1	D	62	LYS	2.0
1	A	249	ASN	2.0
1	B	-1	ASN	2.0
1	D	41	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.