Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:53 PM GMT

PDB ID	:	1R0D
Title	:	HIP1R THATCH DOMAIN CORE
Authors	:	Brett, T.J.; Fremont, D.H.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2003-09-19
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

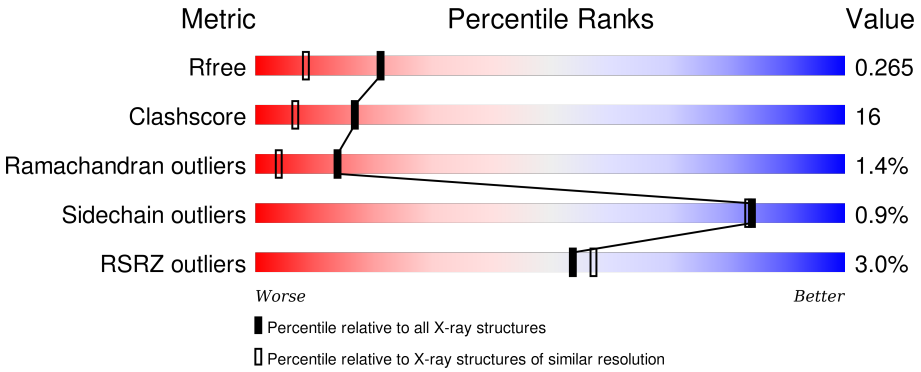
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 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 <=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	206	4% 69% 23% • 6%
1	B	206	2% 74% 17% • 8%
1	D	206	4% 74% 17% • 8%
1	E	206	2% 73% 17% • 8%
1	F	206	% 67% 23% • 8%

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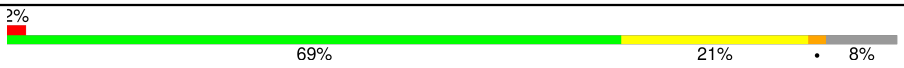
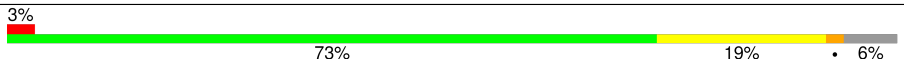
Mol	Chain	Length	Quality of chain
1	G	206	
1	H	206	
1	I	206	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12737 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 Huntingtin Interacting Protein 12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	Se	0	0	0
			1474	897	271	298	3	5			
1	B	190	Total	C	N	O	S	Se	0	0	0
			1440	878	264	291	3	4			
1	D	190	Total	C	N	O	S	Se	0	0	0
			1440	878	264	291	3	4			
1	E	190	Total	C	N	O	S	Se	0	0	0
			1440	878	264	291	3	4			
1	F	190	Total	C	N	O	S	Se	0	0	0
			1440	878	264	291	3	4			
1	G	190	Total	C	N	O	S	Se	0	0	0
			1440	878	264	291	3	4			
1	H	190	Total	C	N	O	S	Se	0	0	0
			1440	878	264	291	3	4			
1	I	194	Total	C	N	O	S	Se	0	0	0
			1474	897	271	298	3	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	766	GLY	-	CLONING ARTIFACT	UNP O75146
A	767	SER	-	CLONING ARTIFACT	UNP O75146
A	768	PRO	-	CLONING ARTIFACT	UNP O75146
A	769	GLU	-	CLONING ARTIFACT	UNP O75146
A	770	PHE	-	CLONING ARTIFACT	UNP O75146
A	787	MSE	MET	MODIFIED RESIDUE	UNP O75146
A	804	MSE	MET	MODIFIED RESIDUE	UNP O75146
A	805	MSE	MET	MODIFIED RESIDUE	UNP O75146
A	831	MSE	MET	MODIFIED RESIDUE	UNP O75146
A	966	MSE	MET	MODIFIED RESIDUE	UNP O75146
B	766	GLY	-	CLONING ARTIFACT	UNP O75146
B	767	SER	-	CLONING ARTIFACT	UNP O75146
B	768	PRO	-	CLONING ARTIFACT	UNP O75146

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Chain	Residue	Modelled	Actual	Comment	Reference
B	769	GLU	-	CLONING ARTIFACT	UNP O75146
B	770	PHE	-	CLONING ARTIFACT	UNP O75146
B	787	MSE	MET	MODIFIED RESIDUE	UNP O75146
B	804	MSE	MET	MODIFIED RESIDUE	UNP O75146
B	805	MSE	MET	MODIFIED RESIDUE	UNP O75146
B	831	MSE	MET	MODIFIED RESIDUE	UNP O75146
B	966	MSE	MET	MODIFIED RESIDUE	UNP O75146
D	766	GLY	-	CLONING ARTIFACT	UNP O75146
D	767	SER	-	CLONING ARTIFACT	UNP O75146
D	768	PRO	-	CLONING ARTIFACT	UNP O75146
D	769	GLU	-	CLONING ARTIFACT	UNP O75146
D	770	PHE	-	CLONING ARTIFACT	UNP O75146
D	787	MSE	MET	MODIFIED RESIDUE	UNP O75146
D	804	MSE	MET	MODIFIED RESIDUE	UNP O75146
D	805	MSE	MET	MODIFIED RESIDUE	UNP O75146
D	831	MSE	MET	MODIFIED RESIDUE	UNP O75146
D	966	MSE	MET	MODIFIED RESIDUE	UNP O75146
E	766	GLY	-	CLONING ARTIFACT	UNP O75146
E	767	SER	-	CLONING ARTIFACT	UNP O75146
E	768	PRO	-	CLONING ARTIFACT	UNP O75146
E	769	GLU	-	CLONING ARTIFACT	UNP O75146
E	770	PHE	-	CLONING ARTIFACT	UNP O75146
E	787	MSE	MET	MODIFIED RESIDUE	UNP O75146
E	804	MSE	MET	MODIFIED RESIDUE	UNP O75146
E	805	MSE	MET	MODIFIED RESIDUE	UNP O75146
E	831	MSE	MET	MODIFIED RESIDUE	UNP O75146
E	966	MSE	MET	MODIFIED RESIDUE	UNP O75146
F	766	GLY	-	CLONING ARTIFACT	UNP O75146
F	767	SER	-	CLONING ARTIFACT	UNP O75146
F	768	PRO	-	CLONING ARTIFACT	UNP O75146
F	769	GLU	-	CLONING ARTIFACT	UNP O75146
F	770	PHE	-	CLONING ARTIFACT	UNP O75146
F	787	MSE	MET	MODIFIED RESIDUE	UNP O75146
F	804	MSE	MET	MODIFIED RESIDUE	UNP O75146
F	805	MSE	MET	MODIFIED RESIDUE	UNP O75146
F	831	MSE	MET	MODIFIED RESIDUE	UNP O75146
F	966	MSE	MET	MODIFIED RESIDUE	UNP O75146
G	766	GLY	-	CLONING ARTIFACT	UNP O75146
G	767	SER	-	CLONING ARTIFACT	UNP O75146
G	768	PRO	-	CLONING ARTIFACT	UNP O75146
G	769	GLU	-	CLONING ARTIFACT	UNP O75146
G	770	PHE	-	CLONING ARTIFACT	UNP O75146

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Chain	Residue	Modelled	Actual	Comment	Reference
G	787	MSE	MET	MODIFIED RESIDUE	UNP O75146
G	804	MSE	MET	MODIFIED RESIDUE	UNP O75146
G	805	MSE	MET	MODIFIED RESIDUE	UNP O75146
G	831	MSE	MET	MODIFIED RESIDUE	UNP O75146
G	966	MSE	MET	MODIFIED RESIDUE	UNP O75146
H	766	GLY	-	CLONING ARTIFACT	UNP O75146
H	767	SER	-	CLONING ARTIFACT	UNP O75146
H	768	PRO	-	CLONING ARTIFACT	UNP O75146
H	769	GLU	-	CLONING ARTIFACT	UNP O75146
H	770	PHE	-	CLONING ARTIFACT	UNP O75146
H	787	MSE	MET	MODIFIED RESIDUE	UNP O75146
H	804	MSE	MET	MODIFIED RESIDUE	UNP O75146
H	805	MSE	MET	MODIFIED RESIDUE	UNP O75146
H	831	MSE	MET	MODIFIED RESIDUE	UNP O75146
H	966	MSE	MET	MODIFIED RESIDUE	UNP O75146
I	766	GLY	-	CLONING ARTIFACT	UNP O75146
I	767	SER	-	CLONING ARTIFACT	UNP O75146
I	768	PRO	-	CLONING ARTIFACT	UNP O75146
I	769	GLU	-	CLONING ARTIFACT	UNP O75146
I	770	PHE	-	CLONING ARTIFACT	UNP O75146
I	787	MSE	MET	MODIFIED RESIDUE	UNP O75146
I	804	MSE	MET	MODIFIED RESIDUE	UNP O75146
I	805	MSE	MET	MODIFIED RESIDUE	UNP O75146
I	831	MSE	MET	MODIFIED RESIDUE	UNP O75146
I	966	MSE	MET	MODIFIED RESIDUE	UNP O75146

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	153	Total O 153 153	0	0
2	B	150	Total O 150 150	0	0
2	D	150	Total O 150 150	0	0
2	E	163	Total O 163 163	0	0
2	F	108	Total O 108 108	0	0
2	G	154	Total O 154 154	0	0
2	H	122	Total O 122 122	0	0

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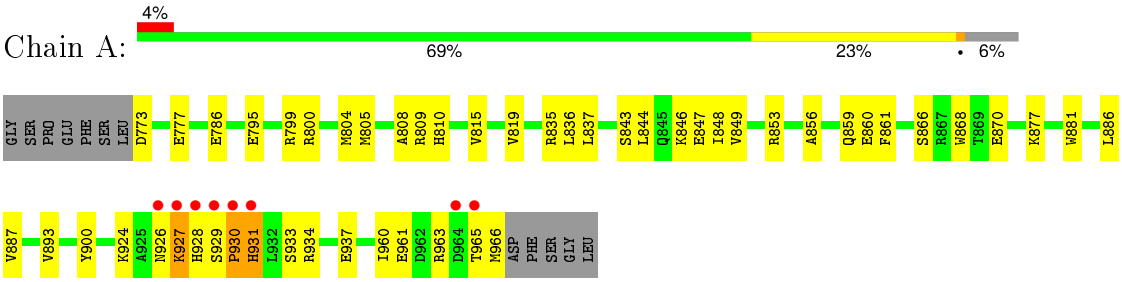
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	149	Total	O	0	0
			149	149		

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 (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.

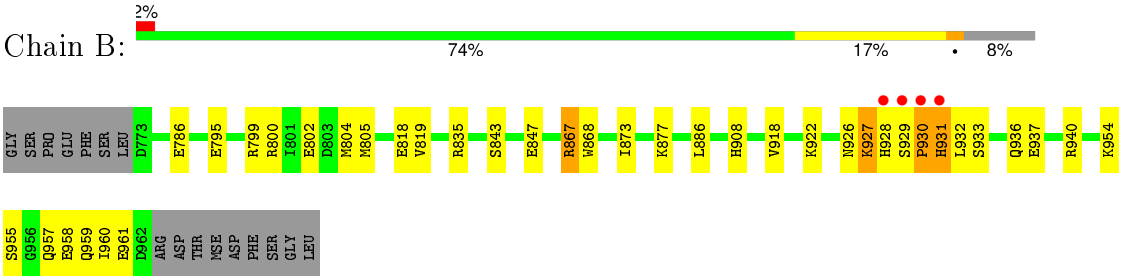
- Molecule 1: Huntingtin Interacting Protein 12

Chain A:



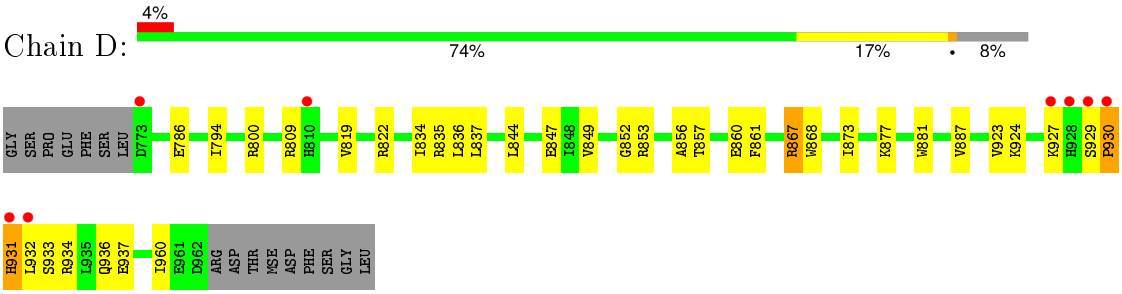
- Molecule 1: Huntingtin Interacting Protein 12

Chain B:



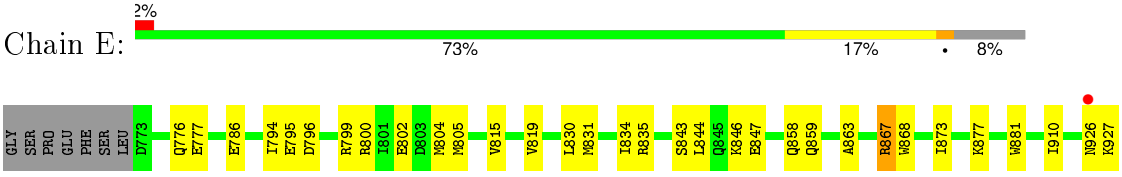
- Molecule 1: Huntingtin Interacting Protein 12

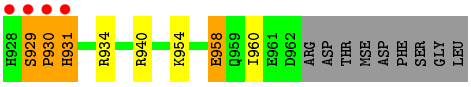
Chain D:



- Molecule 1: Huntingtin Interacting Protein 12

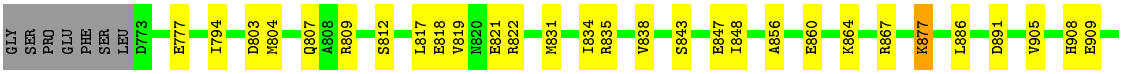
Chain E:

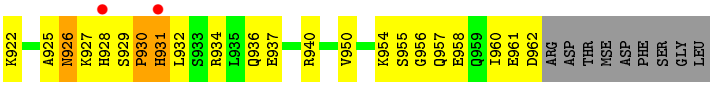




• Molecule 1: Huntingtin Interacting Protein 12

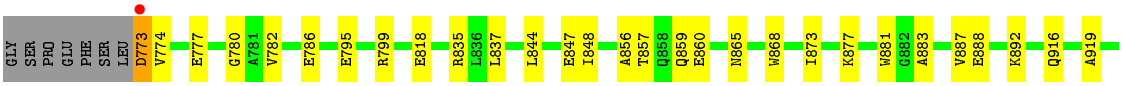
Chain F:

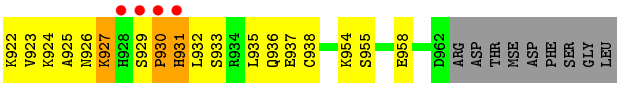




• Molecule 1: Huntingtin Interacting Protein 12

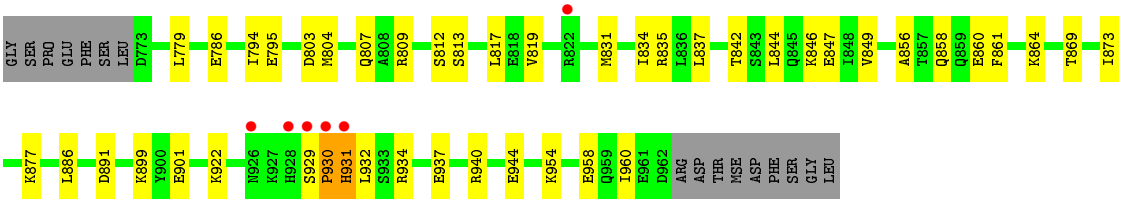
Chain G:





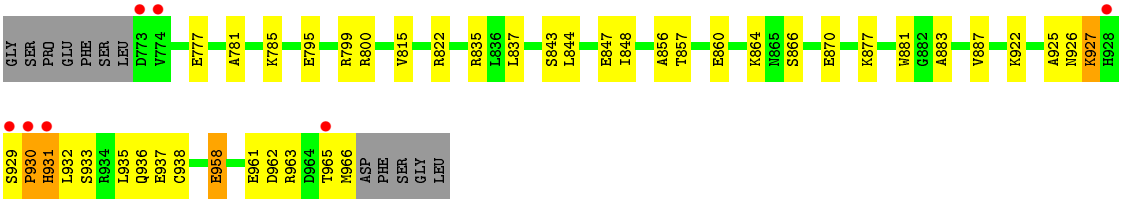
• Molecule 1: Huntingtin Interacting Protein 12

Chain H:



• Molecule 1: Huntingtin Interacting Protein 12

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.20Å 165.90Å 109.80Å 90.00° 132.40° 90.00°	Depositor
Resolution (Å)	19.88 – 1.90 45.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.8 (19.88-1.90) 89.7 (45.68-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.269 0.221 , 0.265	Depositor DCC
R_{free} test set	6709 reflections (4.88%)	DCC
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.7	EDS
Estimated twinning fraction	0.000 for -h,h+2*l,1/2*h+1/2*k 0.000 for -h,-h-2*l,1/2*h-1/2*k 0.487 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	7 of 299844 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12737	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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 39.28 % 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 3.2511e-04.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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.49	0/1481	0.61	0/1988
1	B	0.48	0/1448	0.59	0/1946
1	D	0.50	0/1448	0.58	0/1946
1	E	0.48	0/1448	0.58	0/1946
1	F	0.43	1/1448 (0.1%)	0.56	0/1946
1	G	0.47	0/1448	0.61	0/1946
1	H	0.44	0/1448	0.57	0/1946
1	I	0.44	0/1481	0.59	0/1988
All	All	0.47	1/11650 (0.0%)	0.59	0/15652

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	831	MSE	SE-CE	-5.32	1.64	1.95

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	1474	0	1481	71	0
1	B	1440	0	1448	44	0
1	D	1440	0	1448	42	0
1	E	1440	0	1448	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1440	0	1448	53	0
1	G	1440	0	1448	45	0
1	H	1440	0	1448	41	0
1	I	1474	0	1481	62	0
2	A	153	0	0	5	0
2	B	150	0	0	2	0
2	D	150	0	0	3	0
2	E	163	0	0	4	0
2	F	108	0	0	4	0
2	G	154	0	0	6	0
2	H	122	0	0	2	0
2	I	149	0	0	5	0
All	All	12737	0	11650	380	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 16.

All (380) 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:E:929:SER:HA	1:E:931:HIS:H	1.12	1.15
1:A:929:SER:HA	1:A:931:HIS:N	1.62	1.12
1:B:929:SER:HA	1:B:931:HIS:N	1.65	1.12
1:I:929:SER:HA	1:I:931:HIS:H	0.97	1.11
1:G:847:GLU:HG2	1:G:929:SER:O	1.52	1.09
1:B:929:SER:HA	1:B:931:HIS:H	1.01	1.09
1:D:929:SER:HA	1:D:931:HIS:H	0.92	1.09
1:G:847:GLU:CB	1:G:930:PRO:HD3	1.82	1.08
1:H:929:SER:HA	1:H:931:HIS:H	0.94	1.08
1:I:847:GLU:HB2	1:I:930:PRO:HD3	1.29	1.07
1:G:929:SER:HA	1:G:931:HIS:H	0.94	1.07
1:G:847:GLU:HB2	1:G:930:PRO:HD3	1.39	1.03
1:D:929:SER:HA	1:D:931:HIS:N	1.72	1.02
1:H:929:SER:HA	1:H:931:HIS:N	1.73	1.02
1:E:929:SER:HA	1:E:931:HIS:N	1.75	1.02
1:A:934:ARG:HD3	1:I:931:HIS:HD2	1.20	1.01
1:D:867:ARG:HB3	1:D:867:ARG:HH11	1.22	1.01
1:G:929:SER:HA	1:G:931:HIS:N	1.75	1.00
1:F:929:SER:HA	1:F:931:HIS:N	1.77	1.00
1:B:929:SER:CA	1:B:931:HIS:H	1.76	0.99
1:I:847:GLU:CB	1:I:930:PRO:HD3	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:929:SER:HA	1:I:931:HIS:N	1.77	0.98
1:A:929:SER:CA	1:A:931:HIS:H	1.76	0.98
1:E:867:ARG:H	1:E:867:ARG:HD3	1.28	0.96
1:A:929:SER:HA	1:A:931:HIS:H	0.80	0.95
1:F:867:ARG:HB3	1:F:867:ARG:HH11	1.31	0.94
1:A:937:GLU:OE1	1:I:931:HIS:CD2	2.22	0.93
1:B:847:GLU:HG3	1:B:929:SER:O	1.69	0.92
1:I:932:LEU:HG	1:I:936:GLN:NE2	1.84	0.92
1:F:847:GLU:HB2	1:F:930:PRO:HD3	1.51	0.91
1:F:867:ARG:HB3	1:F:867:ARG:NH1	1.85	0.89
1:F:929:SER:HA	1:F:931:HIS:H	1.36	0.89
1:F:934:ARG:HH22	1:F:937:GLU:HG3	1.37	0.89
1:E:847:GLU:CB	1:E:930:PRO:HD3	2.02	0.89
1:I:844:LEU:HA	1:I:930:PRO:HD2	1.54	0.88
1:G:844:LEU:HA	1:G:930:PRO:HD2	1.53	0.87
1:H:931:HIS:HB2	1:H:934:ARG:HB2	1.53	0.87
1:B:847:GLU:HB2	1:B:930:PRO:HD3	1.56	0.87
1:D:867:ARG:HD2	1:D:867:ARG:H	1.38	0.87
1:D:847:GLU:HB2	1:D:930:PRO:HD3	1.56	0.86
1:A:934:ARG:HD3	1:I:931:HIS:CD2	2.11	0.85
1:A:934:ARG:HA	1:I:931:HIS:NE2	1.91	0.85
1:H:847:GLU:CB	1:H:930:PRO:HD3	2.07	0.85
1:E:847:GLU:HB2	1:E:930:PRO:HD3	1.60	0.84
1:A:847:GLU:HB2	1:A:930:PRO:HD3	1.60	0.83
1:I:962:ASP:HB3	1:I:966:MSE:HE2	1.61	0.82
1:B:908:HIS:NE2	1:I:965:THR:HG22	1.93	0.82
1:G:929:SER:CA	1:G:931:HIS:H	1.88	0.80
1:B:918:VAL:HG12	1:B:922:LYS:HE3	1.65	0.78
1:G:795:GLU:OE2	1:G:835:ARG:HD3	1.84	0.77
1:D:847:GLU:CB	1:D:930:PRO:HD3	2.15	0.77
1:A:819:VAL:HG21	1:A:960:ILE:HD11	1.65	0.77
1:H:847:GLU:HB2	1:H:930:PRO:HD3	1.67	0.77
1:I:929:SER:CA	1:I:931:HIS:H	1.90	0.75
1:A:934:ARG:CD	1:I:931:HIS:HD2	1.98	0.75
1:A:937:GLU:OE1	1:I:931:HIS:CG	2.40	0.74
1:G:932:LEU:HG	1:G:936:GLN:NE2	2.02	0.74
1:F:955:SER:O	1:F:958:GLU:HG2	1.88	0.74
1:I:795:GLU:OE2	1:I:835:ARG:HD3	1.88	0.73
1:E:831:MSE:HE1	1:E:910:ILE:HD13	1.69	0.73
1:G:926:ASN:O	1:G:927:LYS:HG2	1.88	0.73
1:F:928:HIS:HB2	2:F:1047:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:963:ARG:HA	1:I:966:MSE:HE3	1.70	0.73
1:F:929:SER:CA	1:F:931:HIS:H	2.01	0.72
1:F:934:ARG:NH2	1:F:937:GLU:HG3	2.03	0.71
1:D:931:HIS:HB2	1:D:934:ARG:HB3	1.73	0.71
1:G:922:LYS:HB3	1:G:932:LEU:HD11	1.72	0.71
1:G:848:ILE:HD11	1:G:925:ALA:HB2	1.73	0.70
1:D:819:VAL:HG21	1:D:960:ILE:HD11	1.72	0.70
1:B:867:ARG:H	1:B:867:ARG:HE	1.38	0.70
1:A:937:GLU:OE2	1:I:931:HIS:ND1	2.24	0.70
1:I:877:LYS:HE3	1:I:881:TRP:CE2	2.27	0.70
1:B:867:ARG:HG2	1:B:868:TRP:N	2.05	0.70
1:I:932:LEU:HG	1:I:936:GLN:HE21	1.54	0.69
1:A:795:GLU:OE2	1:A:835:ARG:HD3	1.92	0.69
1:B:847:GLU:HB2	1:B:930:PRO:CD	2.22	0.69
1:E:844:LEU:HA	1:E:930:PRO:HD2	1.75	0.69
1:D:867:ARG:CB	1:D:867:ARG:HH11	2.02	0.69
1:F:847:GLU:CB	1:F:930:PRO:HD3	2.23	0.69
1:A:934:ARG:CA	1:I:931:HIS:NE2	2.55	0.69
1:H:812:SER:O	1:H:817:LEU:HD12	1.93	0.69
1:G:847:GLU:HB3	1:G:930:PRO:HD3	1.73	0.68
1:E:867:ARG:HH11	1:E:867:ARG:N	1.92	0.68
1:A:926:ASN:HB3	1:A:928:HIS:CD2	2.28	0.68
1:H:922:LYS:HG3	1:H:932:LEU:HD11	1.74	0.68
1:B:922:LYS:HG2	1:B:932:LEU:HD11	1.74	0.68
1:H:804:MSE:HE1	1:H:891:ASP:HB2	1.74	0.68
1:E:867:ARG:NH1	1:E:868:TRP:H	1.91	0.68
1:B:933:SER:O	1:B:937:GLU:HG3	1.93	0.68
1:F:934:ARG:HH22	1:F:937:GLU:CG	2.07	0.67
1:F:835:ARG:HG3	2:F:998:HOH:O	1.94	0.67
1:E:877:LYS:HE3	1:E:881:TRP:CE2	2.30	0.67
1:B:867:ARG:HG2	1:B:868:TRP:H	1.60	0.66
1:F:819:VAL:HG21	1:F:960:ILE:HD11	1.77	0.66
1:B:802:GLU:HA	1:B:805:MSE:HE2	1.78	0.66
1:G:857:THR:OG1	1:G:860:GLU:HG3	1.95	0.66
1:H:860:GLU:O	1:H:864:LYS:HG2	1.96	0.66
1:A:961:GLU:HB3	1:F:954:LYS:HE2	1.76	0.66
1:B:929:SER:HB2	1:B:930:PRO:HA	1.77	0.65
1:H:809:ARG:HA	1:H:817:LEU:HD11	1.78	0.65
1:I:961:GLU:O	1:I:965:THR:HG23	1.96	0.65
1:A:846:LYS:HD2	2:A:1087:HOH:O	1.96	0.65
1:A:805:MSE:HB2	1:E:805:MSE:HE1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:940:ARG:NH1	1:E:940:ARG:HB3	2.11	0.64
1:H:844:LEU:HA	1:H:930:PRO:HD2	1.78	0.64
1:I:847:GLU:HB2	1:I:930:PRO:CD	2.18	0.64
1:E:786:GLU:HG3	1:E:873:ILE:HG23	1.80	0.64
1:H:795:GLU:OE2	1:H:835:ARG:NH1	2.23	0.64
1:G:919:ALA:HA	1:G:922:LYS:NZ	2.13	0.63
1:I:847:GLU:CG	1:I:930:PRO:HD3	2.27	0.63
1:D:931:HIS:HB2	1:D:934:ARG:CB	2.28	0.63
1:B:918:VAL:CG1	1:B:922:LYS:HE3	2.28	0.63
1:G:774:VAL:HG21	1:G:782:VAL:HG21	1.82	0.62
1:E:867:ARG:CD	1:E:867:ARG:H	2.08	0.62
1:A:847:GLU:CB	1:A:930:PRO:HD3	2.28	0.62
1:I:857:THR:OG1	1:I:860:GLU:HG3	2.00	0.62
1:H:931:HIS:CB	1:H:934:ARG:HB2	2.29	0.61
1:B:955:SER:O	1:B:959:GLN:HG3	2.00	0.61
1:D:849:VAL:HG22	1:D:861:PHE:CD2	2.35	0.61
1:F:931:HIS:HB3	1:F:934:ARG:H	1.65	0.61
1:B:926:ASN:O	1:B:928:HIS:N	2.33	0.61
1:A:926:ASN:O	1:A:928:HIS:N	2.32	0.61
1:F:877:LYS:HG2	2:F:1065:HOH:O	1.99	0.61
1:A:815:VAL:HG12	1:A:963:ARG:NH1	2.16	0.60
1:A:849:VAL:HG22	1:A:861:PHE:CD2	2.36	0.60
1:E:929:SER:HB2	1:E:930:PRO:HA	1.82	0.60
1:I:785:LYS:HG3	2:I:996:HOH:O	2.01	0.60
1:E:940:ARG:HB3	1:E:940:ARG:HH11	1.66	0.60
1:F:929:SER:CA	1:F:931:HIS:N	2.59	0.60
1:H:819:VAL:HG21	1:H:960:ILE:HD11	1.81	0.60
1:A:800:ARG:HG2	1:A:887:VAL:CG1	2.31	0.60
1:A:934:ARG:CD	1:I:931:HIS:CD2	2.80	0.59
1:I:877:LYS:HE3	1:I:881:TRP:CZ2	2.37	0.59
1:E:795:GLU:OE2	1:E:835:ARG:NH1	2.35	0.59
1:A:877:LYS:HE3	1:A:881:TRP:NE1	2.17	0.59
1:F:929:SER:HB2	1:F:930:PRO:HA	1.84	0.59
1:H:817:LEU:C	1:H:817:LEU:HD23	2.22	0.59
1:B:931:HIS:HA	2:B:1092:HOH:O	2.01	0.59
1:G:795:GLU:OE2	1:G:835:ARG:CD	2.50	0.59
1:I:800:ARG:HG2	1:I:887:VAL:CG1	2.33	0.59
1:G:786:GLU:HG3	1:G:873:ILE:HG23	1.85	0.59
1:D:867:ARG:HG2	1:D:868:TRP:N	2.19	0.58
1:G:932:LEU:C	1:G:936:GLN:HE21	2.06	0.58
1:A:815:VAL:HG11	1:A:963:ARG:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:813:SER:HB3	2:H:995:HOH:O	2.04	0.58
1:F:926:ASN:O	1:F:927:LYS:HG2	2.04	0.57
1:A:795:GLU:OE2	1:A:835:ARG:CD	2.52	0.57
1:A:877:LYS:HE3	1:A:881:TRP:CE2	2.40	0.57
1:G:777:GLU:OE2	1:G:777:GLU:N	2.33	0.57
1:E:844:LEU:HA	1:E:930:PRO:CD	2.33	0.57
1:B:847:GLU:CB	1:B:930:PRO:HD3	2.33	0.57
1:A:877:LYS:HD2	2:A:1042:HOH:O	2.03	0.57
1:E:794:ILE:HD13	1:E:834:ILE:HG22	1.87	0.57
1:I:837:LEU:C	1:I:837:LEU:HD23	2.26	0.56
1:F:809:ARG:HA	1:F:817:LEU:HD11	1.87	0.56
1:A:843:SER:HB3	1:A:930:PRO:HG2	1.86	0.56
1:F:867:ARG:CB	1:F:867:ARG:HH11	2.12	0.56
1:G:818:GLU:HG2	2:G:1019:HOH:O	2.03	0.56
1:D:877:LYS:HE3	1:D:881:TRP:CE2	2.40	0.56
1:I:815:VAL:H	1:I:963:ARG:NH1	2.03	0.56
1:A:966:MSE:HG3	1:A:966:MSE:O	2.05	0.56
1:B:937:GLU:HG2	1:B:940:ARG:HH12	1.71	0.55
1:B:929:SER:CA	1:B:931:HIS:N	2.49	0.55
1:F:860:GLU:O	1:F:864:LYS:HG2	2.06	0.55
1:F:812:SER:O	1:F:817:LEU:HD12	2.06	0.55
1:B:847:GLU:CG	1:B:929:SER:O	2.50	0.55
1:F:847:GLU:HB2	1:F:930:PRO:CD	2.32	0.55
1:H:835:ARG:HG3	2:H:1001:HOH:O	2.07	0.55
1:E:929:SER:CA	1:E:931:HIS:H	2.03	0.55
1:B:843:SER:HB3	1:B:930:PRO:HG2	1.88	0.55
1:H:849:VAL:HG11	1:H:858:GLN:HG2	1.89	0.54
1:B:795:GLU:OE2	1:B:835:ARG:NH1	2.39	0.54
1:G:932:LEU:O	1:G:936:GLN:HG3	2.07	0.54
1:G:847:GLU:HB2	1:G:930:PRO:CD	2.27	0.54
1:I:777:GLU:N	1:I:777:GLU:OE1	2.37	0.54
1:D:844:LEU:HA	1:D:930:PRO:HD2	1.91	0.53
1:B:922:LYS:HG2	1:B:932:LEU:CD1	2.37	0.53
1:A:886:LEU:C	1:A:886:LEU:HD23	2.29	0.53
1:I:781:ALA:HA	2:I:1120:HOH:O	2.08	0.53
1:E:846:LYS:HD2	2:E:1099:HOH:O	2.08	0.53
1:E:830:LEU:HG	1:E:831:MSE:HE2	1.89	0.53
1:D:867:ARG:HB3	1:D:867:ARG:NH1	2.07	0.53
1:E:847:GLU:HB3	1:E:930:PRO:HD3	1.88	0.53
1:G:837:LEU:C	1:G:837:LEU:HD23	2.29	0.53
1:A:937:GLU:CD	1:I:931:HIS:CG	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:929:SER:CB	1:F:931:HIS:H	2.21	0.53
1:A:815:VAL:CG1	1:A:963:ARG:HD3	2.39	0.53
1:F:817:LEU:C	1:F:817:LEU:HD23	2.29	0.53
1:I:958:GLU:HG3	2:I:979:HOH:O	2.09	0.53
1:A:933:SER:O	1:A:937:GLU:HG3	2.08	0.52
1:E:926:ASN:O	1:E:927:LYS:HG2	2.09	0.52
1:A:844:LEU:HA	1:A:930:PRO:HD2	1.91	0.52
1:A:800:ARG:HG3	1:A:804:MSE:HE3	1.92	0.52
1:E:927:LYS:O	1:E:927:LYS:HG3	2.10	0.52
1:E:843:SER:C	1:E:930:PRO:HG3	2.29	0.52
1:D:867:ARG:HD2	1:D:867:ARG:N	2.17	0.52
1:F:957:GLN:O	1:F:961:GLU:HG3	2.10	0.52
1:A:800:ARG:HG2	1:A:887:VAL:HG11	1.91	0.52
1:A:886:LEU:O	1:A:886:LEU:HD23	2.09	0.52
1:E:954:LYS:O	1:E:958:GLU:HG2	2.09	0.51
1:I:795:GLU:O	1:I:799:ARG:HG3	2.11	0.51
1:D:800:ARG:HG2	1:D:887:VAL:CG1	2.39	0.51
1:H:847:GLU:HB3	1:H:930:PRO:HD3	1.89	0.51
1:G:868:TRP:HD1	1:G:923:VAL:HB	1.76	0.51
1:D:794:ILE:HD13	1:D:834:ILE:HG22	1.92	0.51
1:F:932:LEU:O	1:F:936:GLN:HG3	2.10	0.51
1:E:867:ARG:HH11	1:E:867:ARG:H	1.56	0.51
1:D:847:GLU:HG3	1:D:930:PRO:HD3	1.93	0.51
1:I:799:ARG:HD2	2:I:1057:HOH:O	2.10	0.51
1:I:877:LYS:HE3	1:I:881:TRP:NE1	2.25	0.50
1:B:928:HIS:HB3	2:B:1064:HOH:O	2.10	0.50
1:G:919:ALA:HA	1:G:922:LYS:HZ3	1.75	0.50
1:E:819:VAL:HG21	1:E:960:ILE:HG13	1.93	0.50
1:G:856:ALA:HB1	1:G:860:GLU:HB2	1.92	0.50
1:A:805:MSE:SE	1:E:805:MSE:HE3	2.62	0.50
1:A:847:GLU:HG3	1:A:929:SER:O	2.11	0.50
1:A:934:ARG:HA	1:I:931:HIS:CD2	2.47	0.50
1:B:929:SER:CB	1:B:931:HIS:H	2.23	0.50
1:E:858:GLN:NE2	2:E:1045:HOH:O	2.45	0.50
1:A:844:LEU:O	1:A:848:ILE:HG13	2.11	0.50
1:I:843:SER:HB3	1:I:930:PRO:HG2	1.92	0.50
1:A:937:GLU:OE2	1:I:931:HIS:CE1	2.65	0.50
1:A:847:GLU:CG	1:A:929:SER:O	2.60	0.49
1:G:922:LYS:HE2	2:G:1025:HOH:O	2.12	0.49
1:E:877:LYS:HD2	2:E:997:HOH:O	2.12	0.49
1:G:865:ASN:OD1	1:G:924:LYS:NZ	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:ALA:HB1	1:A:860:GLU:HB2	1.94	0.49
1:G:888:GLU:OE2	1:G:892:LYS:HE2	2.11	0.49
1:H:934:ARG:O	1:H:937:GLU:HB2	2.13	0.49
1:E:867:ARG:HD3	1:E:867:ARG:N	2.12	0.49
1:D:857:THR:HG23	1:D:860:GLU:OE2	2.12	0.49
1:D:931:HIS:HB3	1:D:934:ARG:H	1.77	0.49
1:F:934:ARG:NH2	1:F:937:GLU:CG	2.71	0.49
1:I:800:ARG:HG2	1:I:887:VAL:HG11	1.93	0.49
1:F:777:GLU:HB2	2:F:1004:HOH:O	2.12	0.49
1:E:800:ARG:HB2	2:E:1087:HOH:O	2.13	0.49
1:H:934:ARG:HG3	1:H:934:ARG:HH11	1.77	0.49
1:B:786:GLU:HG3	1:B:873:ILE:HG23	1.95	0.49
1:I:795:GLU:OE2	1:I:835:ARG:CD	2.60	0.48
1:B:802:GLU:CA	1:B:805:MSE:HE2	2.42	0.48
1:G:877:LYS:HE3	1:G:881:TRP:CE2	2.48	0.48
1:I:847:GLU:HG3	1:I:930:PRO:HD3	1.94	0.48
1:B:957:GLN:O	1:B:961:GLU:HG3	2.13	0.48
1:B:936:GLN:O	1:B:940:ARG:HG3	2.12	0.48
1:I:822:ARG:HH11	1:I:822:ARG:HG3	1.78	0.48
1:D:877:LYS:HE3	1:D:881:TRP:NE1	2.29	0.48
1:E:844:LEU:HD12	1:E:930:PRO:HD2	1.96	0.47
1:H:804:MSE:CE	1:H:891:ASP:HB2	2.42	0.47
1:H:779:LEU:HB3	1:H:869:THR:HG21	1.96	0.47
1:E:931:HIS:HB3	1:E:934:ARG:H	1.78	0.47
1:I:926:ASN:O	1:I:927:LYS:HB3	2.14	0.47
1:F:804:MSE:HE2	1:F:891:ASP:HB2	1.96	0.47
1:D:847:GLU:CG	1:D:930:PRO:HD3	2.43	0.47
1:E:800:ARG:HG3	1:E:804:MSE:HE3	1.96	0.47
1:A:859:GLN:HG3	2:A:994:HOH:O	2.14	0.47
1:G:932:LEU:HG	1:G:936:GLN:HE21	1.77	0.47
1:B:800:ARG:HG3	1:B:804:MSE:CE	2.45	0.47
1:F:819:VAL:CG2	1:F:960:ILE:HD11	2.44	0.47
1:A:853:ARG:NH1	1:A:856:ALA:O	2.42	0.47
1:E:776:GLN:NE2	1:E:863:ALA:O	2.47	0.47
1:G:933:SER:O	1:G:937:GLU:HG3	2.15	0.47
1:H:940:ARG:O	1:H:944:GLU:HG3	2.13	0.47
1:G:916:GLN:HG2	2:G:1047:HOH:O	2.15	0.47
1:E:931:HIS:ND1	1:E:934:ARG:NH2	2.63	0.47
1:F:956:GLY:O	1:F:960:ILE:HG13	2.15	0.47
1:D:800:ARG:HG2	1:D:887:VAL:HG11	1.96	0.47
1:I:815:VAL:HB	1:I:963:ARG:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:848:ILE:HD11	1:I:925:ALA:HB2	1.97	0.46
1:B:954:LYS:O	1:B:958:GLU:HG2	2.16	0.46
1:F:905:VAL:O	1:F:909:GLU:HG3	2.15	0.46
1:G:935:LEU:O	1:G:938:CYS:HB2	2.15	0.46
1:F:926:ASN:HB3	1:F:928:HIS:NE2	2.30	0.46
1:G:955:SER:O	1:G:958:GLU:HG2	2.15	0.46
1:D:867:ARG:HG2	1:D:868:TRP:H	1.80	0.46
1:H:856:ALA:HB1	1:H:860:GLU:HB2	1.97	0.46
1:D:837:LEU:HD23	1:D:837:LEU:C	2.36	0.46
1:A:809:ARG:HG3	1:A:809:ARG:HH11	1.80	0.46
1:A:937:GLU:CD	1:I:931:HIS:CE1	2.90	0.46
1:G:926:ASN:C	1:G:927:LYS:HG2	2.37	0.46
1:F:794:ILE:CD1	1:F:838:VAL:HG21	2.46	0.45
1:D:819:VAL:CG2	1:D:960:ILE:HD11	2.45	0.45
1:A:805:MSE:HB2	1:E:805:MSE:CE	2.44	0.45
1:H:842:THR:O	1:H:846:LYS:HG2	2.16	0.45
1:A:965:THR:HG21	1:F:950:VAL:HG11	1.98	0.45
1:G:799:ARG:HD2	2:G:1068:HOH:O	2.16	0.45
1:I:864:LYS:HB2	2:I:1027:HOH:O	2.16	0.45
1:H:931:HIS:HB2	1:H:934:ARG:CB	2.37	0.45
1:I:856:ALA:HB1	1:I:860:GLU:HB2	1.98	0.45
1:A:786:GLU:OE1	1:A:877:LYS:HD3	2.17	0.45
1:F:886:LEU:HD23	1:F:886:LEU:C	2.36	0.45
1:I:935:LEU:O	1:I:938:CYS:HB2	2.17	0.45
1:D:927:LYS:O	1:D:927:LYS:HG3	2.17	0.45
1:G:868:TRP:CD1	1:G:923:VAL:HB	2.52	0.45
1:I:847:GLU:HG3	1:I:929:SER:O	2.17	0.44
1:E:777:GLU:O	1:E:859:GLN:NE2	2.48	0.44
1:A:937:GLU:OE2	1:I:931:HIS:CG	2.69	0.44
1:G:847:GLU:CG	1:G:930:PRO:HD3	2.44	0.44
1:B:927:LYS:HG3	1:B:927:LYS:O	2.16	0.44
1:B:886:LEU:HD23	1:B:886:LEU:C	2.38	0.44
1:B:937:GLU:HA	1:B:940:ARG:NH1	2.33	0.44
1:B:819:VAL:HG21	1:B:960:ILE:HG13	1.98	0.44
1:D:933:SER:O	1:D:937:GLU:HG3	2.17	0.44
1:A:929:SER:CA	1:A:931:HIS:N	2.55	0.44
1:I:866:SER:O	1:I:870:GLU:HG3	2.18	0.44
1:D:923:VAL:HG12	1:D:924:LYS:HG3	2.00	0.44
1:F:931:HIS:HB3	1:F:934:ARG:CB	2.48	0.43
1:H:831:MSE:HE2	1:H:831:MSE:HA	2.00	0.43
1:D:847:GLU:HG3	1:D:929:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:963:ARG:CA	1:I:966:MSE:HE3	2.43	0.43
1:F:927:LYS:O	1:F:927:LYS:HG3	2.17	0.43
1:I:847:GLU:HG3	1:I:929:SER:C	2.38	0.43
1:H:831:MSE:HE2	1:H:831:MSE:CA	2.49	0.43
1:D:835:ARG:HD2	2:D:1031:HOH:O	2.18	0.43
1:A:849:VAL:HG22	1:A:861:PHE:HD2	1.82	0.43
1:I:883:ALA:O	1:I:887:VAL:HG23	2.18	0.43
1:H:849:VAL:CG1	1:H:858:GLN:HG2	2.48	0.43
1:A:799:ARG:NH1	1:E:799:ARG:NH1	2.67	0.43
1:H:837:LEU:HD23	1:H:837:LEU:C	2.39	0.43
1:D:849:VAL:HG22	1:D:861:PHE:HD2	1.83	0.43
1:A:819:VAL:CG2	1:A:960:ILE:HD11	2.41	0.43
1:A:808:ALA:C	1:A:810:HIS:H	2.21	0.43
1:A:931:HIS:HB2	1:A:934:ARG:HB3	2.01	0.43
1:H:819:VAL:CG2	1:H:960:ILE:HD11	2.46	0.42
1:D:786:GLU:HG3	1:D:873:ILE:HG23	2.00	0.42
1:B:929:SER:HB2	1:B:930:PRO:CA	2.46	0.42
1:E:877:LYS:HE3	1:E:881:TRP:NE1	2.34	0.42
1:I:932:LEU:O	1:I:936:GLN:HG3	2.20	0.42
1:F:877:LYS:HE3	1:F:877:LYS:HA	2.01	0.42
1:A:773:ASP:N	2:A:1097:HOH:O	2.52	0.42
1:F:843:SER:HB3	1:F:930:PRO:HG2	2.01	0.42
1:D:822:ARG:HH11	1:D:822:ARG:HG2	1.85	0.42
1:H:794:ILE:HD13	1:H:834:ILE:HG22	2.02	0.42
1:D:853:ARG:HD2	1:D:856:ALA:O	2.18	0.42
1:F:794:ILE:HD13	1:F:834:ILE:HG22	2.02	0.42
1:A:965:THR:HG22	1:F:908:HIS:CE1	2.54	0.42
1:H:886:LEU:HD23	1:H:886:LEU:C	2.39	0.42
1:A:868:TRP:CG	1:A:924:LYS:HG3	2.54	0.42
1:A:866:SER:O	1:A:870:GLU:HG3	2.19	0.42
1:I:933:SER:O	1:I:937:GLU:HG3	2.19	0.42
1:A:926:ASN:OD1	1:A:927:LYS:HG2	2.19	0.42
1:F:922:LYS:HG3	1:F:932:LEU:HD11	2.02	0.42
1:A:777:GLU:HB2	2:A:976:HOH:O	2.19	0.42
1:D:852:GLY:O	2:D:1041:HOH:O	2.22	0.42
1:F:856:ALA:HB1	1:F:860:GLU:HG2	2.02	0.42
1:B:818:GLU:OE1	1:B:818:GLU:HA	2.20	0.42
1:F:803:ASP:O	1:F:807:GLN:HG3	2.20	0.42
1:A:929:SER:HB2	1:A:930:PRO:HA	2.03	0.41
1:B:954:LYS:NZ	1:I:965:THR:HG21	2.35	0.41
1:H:804:MSE:HE2	1:H:891:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:848:ILE:HD11	1:F:925:ALA:HB2	2.02	0.41
1:D:927:LYS:HA	1:D:932:LEU:HD23	2.03	0.41
1:I:922:LYS:HE3	1:I:932:LEU:HD21	2.02	0.41
1:B:958:GLU:H	1:B:958:GLU:HG2	1.66	0.41
1:D:809:ARG:HG3	1:D:809:ARG:O	2.21	0.41
1:G:954:LYS:HE2	2:G:1049:HOH:O	2.20	0.41
1:H:849:VAL:HG22	1:H:861:PHE:CD2	2.55	0.41
1:F:931:HIS:CB	1:F:934:ARG:HB2	2.50	0.41
1:A:815:VAL:HG12	1:A:963:ARG:HH11	1.85	0.41
1:F:936:GLN:O	1:F:940:ARG:HG3	2.21	0.41
1:G:773:ASP:N	2:G:1073:HOH:O	2.53	0.41
1:G:780:GLY:H	1:G:859:GLN:HE22	1.68	0.41
1:B:795:GLU:O	1:B:799:ARG:HG3	2.20	0.41
1:H:899:LYS:HE2	1:H:901:GLU:OE1	2.20	0.41
1:H:877:LYS:HB3	1:H:877:LYS:HE2	1.88	0.41
1:A:837:LEU:HD23	1:A:837:LEU:C	2.41	0.41
1:A:836:LEU:HA	1:A:836:LEU:HD12	1.88	0.41
1:D:936:GLN:NE2	2:D:1025:HOH:O	2.54	0.41
1:E:802:GLU:HA	1:E:805:MSE:HE2	2.04	0.40
1:F:817:LEU:O	1:F:821:GLU:HG2	2.22	0.40
1:D:836:LEU:HD12	1:D:836:LEU:HA	1.89	0.40
1:G:883:ALA:O	1:G:887:VAL:HG23	2.21	0.40
1:H:786:GLU:HG3	1:H:873:ILE:HG23	2.02	0.40
1:B:918:VAL:O	1:B:922:LYS:HG3	2.21	0.40
1:G:922:LYS:HB3	1:G:932:LEU:CD1	2.47	0.40
1:D:819:VAL:HG21	1:D:960:ILE:CD1	2.45	0.40
1:E:815:VAL:O	1:E:819:VAL:HG22	2.22	0.40
1:A:893:VAL:HG21	1:A:900:TYR:CD1	2.56	0.40
1:F:818:GLU:CD	1:F:822:ARG:HH21	2.24	0.40
1:H:954:LYS:O	1:H:958:GLU:HG3	2.21	0.40
1:H:803:ASP:O	1:H:807:GLN:HG3	2.22	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	192/206 (93%)	184 (96%)	5 (3%)	3 (2%)	12	3
1	B	188/206 (91%)	183 (97%)	2 (1%)	3 (2%)	12	3
1	D	188/206 (91%)	181 (96%)	5 (3%)	2 (1%)	17	6
1	E	188/206 (91%)	182 (97%)	3 (2%)	3 (2%)	12	3
1	F	188/206 (91%)	180 (96%)	5 (3%)	3 (2%)	12	3
1	G	188/206 (91%)	184 (98%)	2 (1%)	2 (1%)	17	6
1	H	188/206 (91%)	180 (96%)	6 (3%)	2 (1%)	17	6
1	I	192/206 (93%)	185 (96%)	4 (2%)	3 (2%)	12	3
All	All	1512/1648 (92%)	1459 (96%)	32 (2%)	21 (1%)	14	4

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	927	LYS
1	B	930	PRO
1	B	931	HIS
1	F	930	PRO
1	F	931	HIS
1	H	931	HIS
1	I	927	LYS
1	A	931	HIS
1	B	927	LYS
1	D	931	HIS
1	E	931	HIS
1	F	926	ASN
1	G	931	HIS
1	I	931	HIS
1	A	930	PRO
1	D	930	PRO
1	E	930	PRO
1	G	930	PRO
1	H	930	PRO
1	I	930	PRO
1	E	929	SER

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	159/164 (97%)	159 (100%)	0	100	100
1	B	155/164 (94%)	153 (99%)	2 (1%)	76	73
1	D	155/164 (94%)	154 (99%)	1 (1%)	90	90
1	E	155/164 (94%)	152 (98%)	3 (2%)	65	59
1	F	155/164 (94%)	153 (99%)	2 (1%)	76	73
1	G	155/164 (94%)	153 (99%)	2 (1%)	76	73
1	H	155/164 (94%)	155 (100%)	0	100	100
1	I	159/164 (97%)	158 (99%)	1 (1%)	90	90
All	All	1248/1312 (95%)	1237 (99%)	11 (1%)	84	83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	867	ARG
1	B	877	LYS
1	D	867	ARG
1	E	796	ASP
1	E	867	ARG
1	E	958	GLU
1	F	877	LYS
1	F	962	ASP
1	G	773	ASP
1	G	927	LYS
1	I	958	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	885	GLN
1	A	957	GLN
1	B	885	GLN

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Mol	Chain	Res	Type
1	B	959	GLN
1	D	825	ASN
1	D	936	GLN
1	D	943	ASN
1	D	957	GLN
1	E	885	GLN
1	G	859	GLN
1	G	885	GLN
1	G	936	GLN
1	G	943	ASN
1	G	948	ASN
1	H	885	GLN
1	H	936	GLN
1	H	943	ASN
1	H	957	GLN
1	I	936	GLN
1	I	948	ASN
1	I	957	GLN

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 carbohydrates 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	189/206 (91%)	-0.05	8 (4%)	40	44	17, 30, 67, 104	0
1	B	186/206 (90%)	-0.25	4 (2%)	65	68	17, 29, 55, 94	0
1	D	186/206 (90%)	-0.07	8 (4%)	39	42	17, 30, 63, 92	0
1	E	186/206 (90%)	-0.22	5 (2%)	58	61	18, 30, 54, 83	0
1	F	186/206 (90%)	-0.09	2 (1%)	82	84	19, 34, 62, 94	0
1	G	186/206 (90%)	-0.11	5 (2%)	58	61	20, 32, 56, 89	0
1	H	186/206 (90%)	-0.07	6 (3%)	51	54	19, 34, 63, 93	0
1	I	189/206 (91%)	-0.12	7 (3%)	45	49	19, 32, 64, 90	0
All	All	1494/1648 (90%)	-0.12	45 (3%)	54	57	17, 32, 64, 104	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	930	PRO	8.6
1	A	929	SER	7.5
1	I	931	HIS	7.4
1	A	926	ASN	7.3
1	G	931	HIS	7.3
1	G	930	PRO	6.7
1	B	928	HIS	6.4
1	I	773	ASP	6.0
1	I	929	SER	5.9
1	I	930	PRO	5.9
1	F	928	HIS	5.8
1	G	929	SER	5.7
1	E	930	PRO	5.7
1	A	965	THR	5.4
1	E	931	HIS	5.2
1	A	930	PRO	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	929	SER	4.8
1	D	931	HIS	4.5
1	H	928	HIS	4.4
1	D	928	HIS	4.3
1	A	931	HIS	4.2
1	H	929	SER	3.9
1	H	930	PRO	3.9
1	B	930	PRO	3.9
1	E	929	SER	3.7
1	B	931	HIS	3.7
1	G	928	HIS	3.2
1	B	929	SER	3.1
1	A	964	ASP	3.1
1	E	926	ASN	3.0
1	A	928	HIS	2.9
1	H	931	HIS	2.8
1	D	810	HIS	2.7
1	I	928	HIS	2.7
1	A	927	LYS	2.7
1	E	928	HIS	2.6
1	D	927	LYS	2.5
1	D	773	ASP	2.5
1	G	773	ASP	2.4
1	F	931	HIS	2.3
1	H	926	ASN	2.3
1	I	965	THR	2.3
1	I	774	VAL	2.1
1	D	932	LEU	2.0
1	H	822	ARG	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.