Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 06:43 PM EDT

PDB ID	:	1TW9
Title	:	Glutathione Transferase-2, apo form, from the nematode Heligmosomoides polygyrus
Authors	:	Schuller, D.J.; Liu, Q.; Kriksunov, I.A.; Campbell, A.M.; Barrett, J.; Brophy, P.M.; Hao, Q.
Deposited on	:	2004-06-30
Resolution	:	1.71 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:

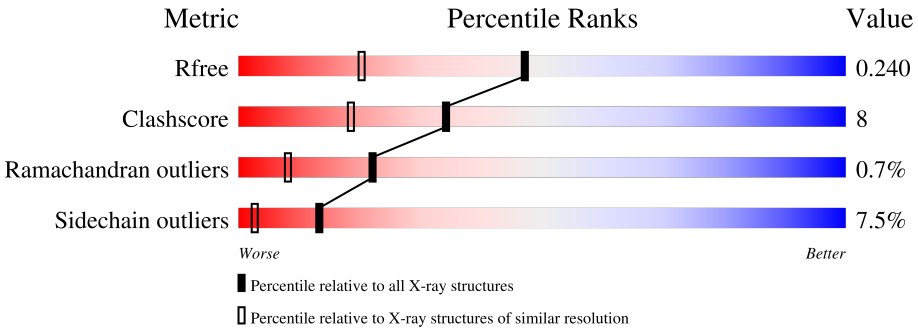
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)

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	206	75% 16% • 7%
1	B	206	74% 13% • • 9%
1	C	206	80% 13% • 6%
1	D	206	77% 15% • • 6%
1	E	206	73% 17% • • 6%
1	F	206	77% 18% •
1	G	206	75% 15% • 8%

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Mol	Chain	Length	Quality of chain
1	H	206	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14254 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 glutathione S-transferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1531	989	256	280	6			
1	B	188	Total	C	N	O	S	0	0	0
			1507	974	252	275	6			
1	C	194	Total	C	N	O	S	0	0	0
			1563	1013	260	284	6			
1	D	194	Total	C	N	O	S	0	0	0
			1559	1008	260	285	6			
1	E	193	Total	C	N	O	S	0	0	0
			1542	997	257	282	6			
1	F	205	Total	C	N	O	S	0	0	0
			1645	1066	271	301	7			
1	G	189	Total	C	N	O	S	0	0	0
			1516	980	254	276	6			
1	H	191	Total	C	N	O	S	0	0	0
			1531	989	256	280	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q9NJQ6
A	2	VAL	-	cloning artifact	UNP Q9NJQ6
A	21	VAL	ILE	conflict	UNP Q9NJQ6
A	40	VAL	ALA	conflict	UNP Q9NJQ6
A	91	LEU	PRO	conflict	UNP Q9NJQ6
A	108	THR	MET	conflict	UNP Q9NJQ6
A	120	PRO	LEU	conflict	UNP Q9NJQ6
A	140	LEU	PRO	conflict	UNP Q9NJQ6
B	1	MET	-	cloning artifact	UNP Q9NJQ6
B	2	VAL	-	cloning artifact	UNP Q9NJQ6
B	21	VAL	ILE	conflict	UNP Q9NJQ6
B	40	VAL	ALA	conflict	UNP Q9NJQ6
B	91	LEU	PRO	conflict	UNP Q9NJQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	108	THR	MET	conflict	UNP Q9NJQ6
B	120	PRO	LEU	conflict	UNP Q9NJQ6
B	140	LEU	PRO	conflict	UNP Q9NJQ6
C	1	MET	-	cloning artifact	UNP Q9NJQ6
C	2	VAL	-	cloning artifact	UNP Q9NJQ6
C	21	VAL	ILE	conflict	UNP Q9NJQ6
C	40	VAL	ALA	conflict	UNP Q9NJQ6
C	91	LEU	PRO	conflict	UNP Q9NJQ6
C	108	THR	MET	conflict	UNP Q9NJQ6
C	120	PRO	LEU	conflict	UNP Q9NJQ6
C	140	LEU	PRO	conflict	UNP Q9NJQ6
D	1	MET	-	cloning artifact	UNP Q9NJQ6
D	2	VAL	-	cloning artifact	UNP Q9NJQ6
D	21	VAL	ILE	conflict	UNP Q9NJQ6
D	40	VAL	ALA	conflict	UNP Q9NJQ6
D	91	LEU	PRO	conflict	UNP Q9NJQ6
D	108	THR	MET	conflict	UNP Q9NJQ6
D	120	PRO	LEU	conflict	UNP Q9NJQ6
D	140	LEU	PRO	conflict	UNP Q9NJQ6
E	1	MET	-	cloning artifact	UNP Q9NJQ6
E	2	VAL	-	cloning artifact	UNP Q9NJQ6
E	21	VAL	ILE	conflict	UNP Q9NJQ6
E	40	VAL	ALA	conflict	UNP Q9NJQ6
E	91	LEU	PRO	conflict	UNP Q9NJQ6
E	108	THR	MET	conflict	UNP Q9NJQ6
E	120	PRO	LEU	conflict	UNP Q9NJQ6
E	140	LEU	PRO	conflict	UNP Q9NJQ6
F	1	MET	-	cloning artifact	UNP Q9NJQ6
F	2	VAL	-	cloning artifact	UNP Q9NJQ6
F	21	VAL	ILE	conflict	UNP Q9NJQ6
F	40	VAL	ALA	conflict	UNP Q9NJQ6
F	91	LEU	PRO	conflict	UNP Q9NJQ6
F	108	THR	MET	conflict	UNP Q9NJQ6
F	120	PRO	LEU	conflict	UNP Q9NJQ6
F	140	LEU	PRO	conflict	UNP Q9NJQ6
G	1	MET	-	cloning artifact	UNP Q9NJQ6
G	2	VAL	-	cloning artifact	UNP Q9NJQ6
G	21	VAL	ILE	conflict	UNP Q9NJQ6
G	40	VAL	ALA	conflict	UNP Q9NJQ6
G	91	LEU	PRO	conflict	UNP Q9NJQ6
G	108	THR	MET	conflict	UNP Q9NJQ6
G	120	PRO	LEU	conflict	UNP Q9NJQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	140	LEU	PRO	conflict	UNP Q9NJQ6
H	1	MET	-	cloning artifact	UNP Q9NJQ6
H	2	VAL	-	cloning artifact	UNP Q9NJQ6
H	21	VAL	ILE	conflict	UNP Q9NJQ6
H	40	VAL	ALA	conflict	UNP Q9NJQ6
H	91	LEU	PRO	conflict	UNP Q9NJQ6
H	108	THR	MET	conflict	UNP Q9NJQ6
H	120	PRO	LEU	conflict	UNP Q9NJQ6
H	140	LEU	PRO	conflict	UNP Q9NJQ6

- Molecule 2 is water.

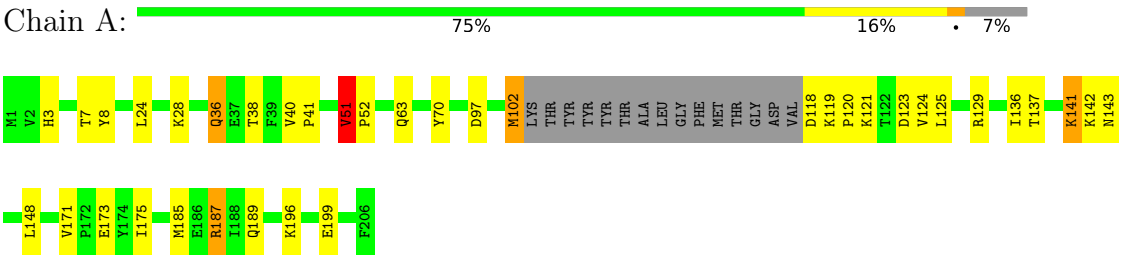
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	384	Total O 384 384	0	0
2	B	220	Total O 220 220	0	0
2	C	285	Total O 285 285	0	0
2	D	251	Total O 251 251	0	0
2	E	149	Total O 149 149	0	0
2	F	186	Total O 186 186	0	0
2	G	216	Total O 216 216	0	0
2	H	169	Total O 169 169	0	0

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.

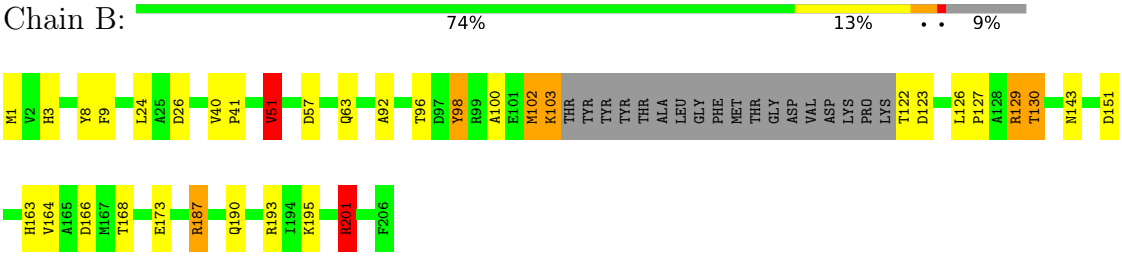
- Molecule 1: glutathione S-transferase 2

Chain A:



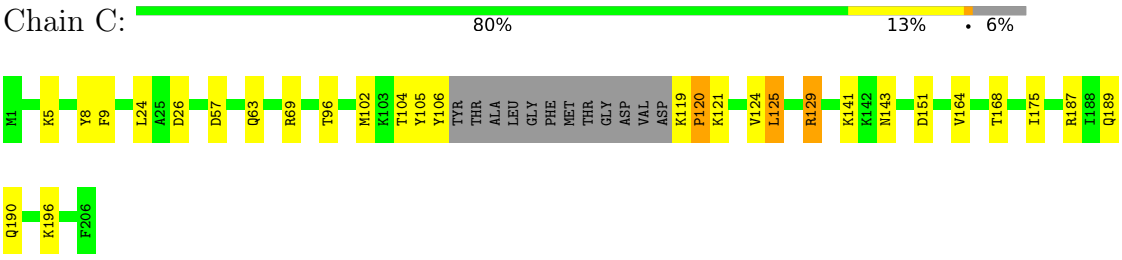
- Molecule 1: glutathione S-transferase 2

Chain B:



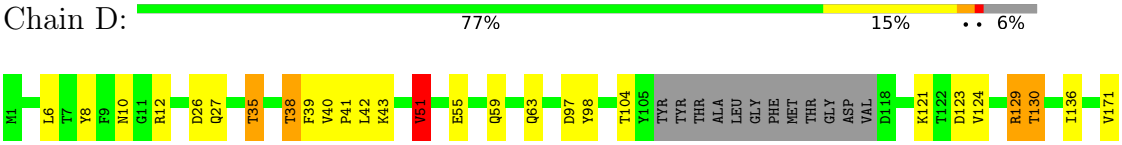
- Molecule 1: glutathione S-transferase 2

Chain C:



- Molecule 1: glutathione S-transferase 2

Chain D:

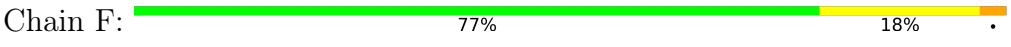


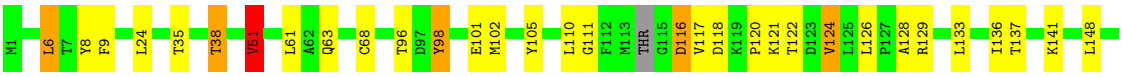
• Molecule 1: glutathione S-transferase 2

Chain E:

• Molecule 1: glutathione S-transferase 2

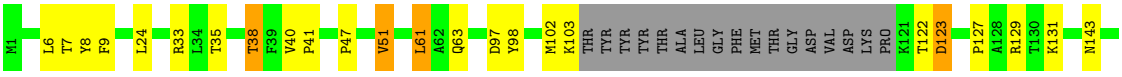
Chain F:

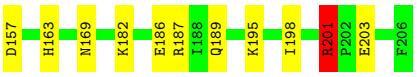




• Molecule 1: glutathione S-transferase 2

Chain G:





• Molecule 1: glutathione S-transferase 2

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.68Å 74.03Å 88.57Å 79.09° 80.08° 81.55°	Depositor
Resolution (Å)	25.00 – 1.71 24.26 – 1.71	Depositor EDS
% Data completeness (in resolution range)	95.2 (25.00-1.71) 95.2 (24.26-1.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.180 , 0.232 0.189 , 0.240	Depositor DCC
R_{free} test set	4568 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14254	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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 (i)

5.1 Standard geometry (i)

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	1.05	2/1568 (0.1%)	1.11	6/2120 (0.3%)
1	B	0.88	0/1543	1.00	8/2086 (0.4%)
1	C	0.96	0/1602	1.01	6/2166 (0.3%)
1	D	0.95	0/1597	0.99	5/2159 (0.2%)
1	E	0.94	2/1579 (0.1%)	0.98	8/2136 (0.4%)
1	F	0.97	2/1686 (0.1%)	1.04	6/2280 (0.3%)
1	G	0.88	0/1552	1.06	8/2097 (0.4%)
1	H	0.87	1/1568 (0.1%)	1.02	7/2120 (0.3%)
All	All	0.94	7/12695 (0.1%)	1.03	54/17164 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	199	GLU	CD-OE2	17.71	1.45	1.25
1	E	199	GLU	CD-OE1	8.35	1.34	1.25
1	H	68	CYS	CB-SG	-5.76	1.72	1.81
1	A	70	TYR	CD2-CE2	-5.55	1.31	1.39
1	A	70	TYR	CD1-CE1	-5.39	1.31	1.39
1	F	68	CYS	CB-SG	-5.06	1.73	1.81
1	F	161	ALA	CA-CB	5.01	1.62	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	201	ARG	NE-CZ-NH1	14.00	127.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	187	ARG	NE-CZ-NH1	13.65	127.13	120.30
1	B	201	ARG	NE-CZ-NH1	11.89	126.24	120.30
1	A	187	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	F	201	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	G	201	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	A	187	ARG	NE-CZ-NH2	-10.55	115.03	120.30
1	F	201	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	185	MET	CG-SD-CE	-9.25	85.40	100.20
1	C	187	ARG	NE-CZ-NH2	-9.03	115.79	120.30
1	A	51	VAL	CG1-CB-CG2	7.44	122.81	110.90
1	E	201	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	H	123	ASP	CB-CG-OD2	6.99	124.59	118.30
1	E	97	ASP	CB-CG-OD2	6.93	124.54	118.30
1	B	201	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	H	118	ASP	CB-CG-OD2	6.64	124.28	118.30
1	F	187	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	D	201	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	G	187	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	E	201	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	123	ASP	CB-CG-OD2	6.32	123.98	118.30
1	E	51	VAL	CG1-CB-CG2	6.24	120.88	110.90
1	B	51	VAL	CG1-CB-CG2	6.18	120.80	110.90
1	B	51	VAL	CB-CA-C	6.11	123.01	111.40
1	G	201	ARG	CD-NE-CZ	6.08	132.11	123.60
1	F	116	ASP	CB-CG-OD2	6.07	123.76	118.30
1	D	185	MET	CG-SD-CE	-6.03	90.55	100.20
1	D	123	ASP	CB-CG-OD2	5.91	123.62	118.30
1	F	6	LEU	CB-CG-CD2	5.77	120.81	111.00
1	B	151	ASP	CB-CG-OD2	5.62	123.36	118.30
1	F	51	VAL	CB-CA-C	5.61	122.06	111.40
1	C	69	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	26	ASP	CB-CG-OD1	5.56	123.30	118.30
1	G	97	ASP	CB-CG-OD2	5.53	123.28	118.30
1	G	61	LEU	CB-CG-CD2	5.50	120.34	111.00
1	H	6	LEU	CB-CG-CD2	5.48	120.32	111.00
1	B	187	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	129	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	H	201	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	G	157	ASP	CB-CG-OD1	5.39	123.16	118.30
1	A	51	VAL	CB-CA-C	5.36	121.58	111.40
1	E	51	VAL	N-CA-CB	-5.33	99.77	111.50
1	D	97	ASP	CB-CG-OD2	5.26	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	93	ASP	CB-CG-OD2	5.22	123.00	118.30
1	H	33	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	G	33	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	57	ASP	CB-CG-OD2	5.18	122.96	118.30
1	H	166	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	123	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	51	VAL	CB-CA-C	5.12	121.12	111.40
1	E	199	GLU	OE1-CD-OE2	5.12	129.44	123.30
1	B	166	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	5	LYS	CD-CE-NZ	-5.05	100.07	111.70
1	H	193	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	102	MET	Peptide

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	1531	0	1527	26	0
1	B	1507	0	1503	27	0
1	C	1563	0	1561	20	0
1	D	1559	0	1556	28	0
1	E	1542	0	1527	29	0
1	F	1645	0	1634	36	1
1	G	1516	0	1516	16	0
1	H	1531	0	1527	27	0
2	A	384	0	0	12	1
2	B	220	0	0	10	0
2	C	285	0	0	8	0
2	D	251	0	0	8	1
2	E	149	0	0	11	1
2	F	186	0	0	8	0
2	G	216	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	169	0	0	4	0
All	All	14254	0	12351	207	2

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 8.

All (207) 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:G:195:LYS:NZ	2:G:268:HOH:O	1.73	1.18
1:E:2:VAL:HB	2:E:1781:HOH:O	0.96	1.12
1:C:106:TYR:C	2:C:1685:HOH:O	1.88	1.10
1:B:96:THR:HG22	2:B:337:HOH:O	1.52	1.08
1:E:143:ASN:CG	2:E:1376:HOH:O	1.95	1.03
1:A:196:LYS:HD2	2:A:400:HOH:O	1.59	1.00
1:F:187:ARG:HB2	2:F:318:HOH:O	1.69	0.91
1:E:143:ASN:ND2	2:E:1376:HOH:O	2.02	0.90
1:D:186:GLU:OE2	2:D:220:HOH:O	1.95	0.83
1:B:190:GLN:HE22	1:B:195:LYS:HE2	1.44	0.82
1:B:193:ARG:NE	2:B:343:HOH:O	2.12	0.82
2:G:240:HOH:O	1:H:138:LYS:HE3	1.78	0.82
1:D:104:THR:HG21	2:D:426:HOH:O	1.79	0.81
1:F:176:GLU:OE1	2:F:351:HOH:O	1.97	0.81
1:E:40:VAL:HG23	2:E:1569:HOH:O	1.79	0.81
1:B:26:ASP:HB2	1:B:193:ARG:NH1	1.98	0.79
1:B:98:TYR:OH	1:B:163:HIS:HE1	1.66	0.79
1:G:195:LYS:HD3	2:G:412:HOH:O	1.79	0.79
1:A:38:THR:HG21	2:A:257:HOH:O	1.82	0.78
1:F:133:LEU:HA	1:F:136:ILE:HG22	1.64	0.78
1:E:47:PRO:O	2:E:1716:HOH:O	2.03	0.77
1:D:193:ARG:CZ	2:D:447:HOH:O	2.32	0.76
1:C:151:ASP:OD2	2:C:638:HOH:O	2.03	0.76
1:B:193:ARG:CZ	2:B:343:HOH:O	2.32	0.76
1:A:199:GLU:OE2	2:A:403:HOH:O	2.05	0.74
2:G:240:HOH:O	1:H:138:LYS:CE	2.33	0.74
1:F:116:ASP:OD1	1:F:118:ASP:HB2	1.88	0.73
1:D:182:LYS:NZ	1:D:186:GLU:OE1	2.22	0.72
1:E:97:ASP:HB2	2:E:1473:HOH:O	1.90	0.72
1:H:164:VAL:HG12	1:H:185:MET:CE	2.20	0.72
1:B:201:ARG:HD3	2:B:283:HOH:O	1.91	0.71
1:B:130:THR:HG21	2:B:251:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:PRO:O	2:G:240:HOH:O	2.08	0.71
1:F:164:VAL:O	1:F:168:THR:HG23	1.90	0.70
1:H:120:PRO:O	1:H:124:VAL:HG12	1.92	0.70
1:D:175:ILE:HG12	1:D:182:LYS:HB2	1.74	0.70
1:G:201:ARG:HD3	2:G:208:HOH:O	1.91	0.69
1:D:129:ARG:HH11	1:D:130:THR:HG22	1.57	0.69
1:D:10:ASN:OD1	2:D:405:HOH:O	2.10	0.68
1:C:164:VAL:O	1:C:168:THR:HG23	1.94	0.67
1:B:190:GLN:NE2	1:B:195:LYS:HE2	2.08	0.67
1:E:97:ASP:OD2	2:E:1486:HOH:O	2.12	0.67
1:D:193:ARG:NE	2:D:447:HOH:O	2.27	0.67
1:H:101:GLU:N	1:H:101:GLU:OE1	2.28	0.67
1:F:102:MET:HA	1:F:124:VAL:HG23	1.78	0.65
1:F:133:LEU:HA	1:F:136:ILE:CG2	2.27	0.65
1:H:3:HIS:HE1	1:H:30:GLU:OE2	1.78	0.65
1:H:8:TYR:CD1	1:H:51:VAL:HG13	2.32	0.65
1:H:164:VAL:O	1:H:168:THR:HG23	1.97	0.65
1:A:3:HIS:HD2	2:A:277:HOH:O	1.79	0.65
1:A:199:GLU:OE1	2:A:405:HOH:O	2.14	0.65
1:D:26:ASP:OD1	2:D:241:HOH:O	2.14	0.64
1:B:187:ARG:HD3	2:B:489:HOH:O	1.97	0.64
1:E:133:LEU:O	1:E:136:ILE:HG22	1.96	0.64
1:F:157:ASP:OD1	1:F:184:HIS:HE1	1.81	0.64
1:D:104:THR:HG23	1:D:104:THR:O	1.97	0.63
1:C:119:LYS:NZ	2:C:854:HOH:O	2.31	0.63
1:F:186:GLU:OE2	2:F:334:HOH:O	2.15	0.62
1:C:119:LYS:CE	2:H:893:HOH:O	2.47	0.62
1:H:35:THR:OG1	1:H:38:THR:HG23	2.00	0.61
1:E:195:LYS:O	1:E:199:GLU:HG3	2.01	0.61
1:A:97:ASP:OD2	2:A:263:HOH:O	2.16	0.61
1:D:8:TYR:CD1	1:D:51:VAL:HG13	2.36	0.61
1:E:157:ASP:OD1	1:E:184:HIS:HE1	1.84	0.61
1:A:40:VAL:HB	1:A:41:PRO:HD3	1.83	0.60
1:F:133:LEU:CA	1:F:136:ILE:HG22	2.31	0.60
1:D:26:ASP:HB2	1:D:193:ARG:NH1	2.16	0.60
1:D:38:THR:O	1:D:42:LEU:HD13	2.02	0.60
1:A:36:GLN:O	1:A:40:VAL:HG23	2.02	0.59
1:F:195:LYS:NZ	1:F:199:GLU:OE2	2.35	0.59
1:H:187:ARG:O	2:H:918:HOH:O	2.16	0.58
1:C:119:LYS:HE2	2:H:893:HOH:O	2.04	0.58
1:E:35:THR:HG22	1:E:38:THR:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:LEU:O	1:F:136:ILE:HG22	2.04	0.57
1:E:2:VAL:HG22	1:H:2:VAL:HB	1.85	0.57
1:F:133:LEU:C	1:F:136:ILE:HG22	2.25	0.57
1:E:143:ASN:CB	2:E:1376:HOH:O	2.46	0.57
1:D:121:LYS:HD2	1:D:171:VAL:HG13	1.86	0.56
1:E:104:THR:HG22	1:E:124:VAL:HG21	1.87	0.56
1:A:142:LYS:NZ	2:A:443:HOH:O	2.38	0.55
1:F:120:PRO:HA	1:F:124:VAL:HG13	1.88	0.55
1:H:173:GLU:HA	1:H:176:GLU:HG3	1.89	0.55
1:F:96:THR:HG21	2:F:330:HOH:O	2.07	0.54
1:G:98:TYR:OH	1:G:163:HIS:HE1	1.90	0.54
1:E:40:VAL:O	2:E:1564:HOH:O	2.19	0.53
1:F:35:THR:H	1:F:38:THR:CG2	2.21	0.53
1:H:127:PRO:O	1:H:130:THR:HG22	2.09	0.53
1:F:136:ILE:HD11	1:F:148:LEU:HD21	1.90	0.53
1:F:98:TYR:O	1:F:101:GLU:HG2	2.09	0.53
1:B:103:LYS:N	2:B:497:HOH:O	2.25	0.52
1:F:35:THR:OG1	1:F:38:THR:HG22	2.09	0.52
1:A:187:ARG:HD3	2:A:409:HOH:O	2.09	0.52
1:D:129:ARG:NH1	1:D:130:THR:HG22	2.23	0.52
1:F:102:MET:HA	1:F:124:VAL:CG2	2.40	0.52
1:H:125:LEU:C	1:H:125:LEU:HD13	2.29	0.52
1:B:126:LEU:HB2	1:B:127:PRO:HD3	1.92	0.51
1:E:126:LEU:O	1:E:129:ARG:HG3	2.11	0.51
1:F:136:ILE:HG23	1:F:137:THR:N	2.24	0.51
1:B:96:THR:HG21	2:B:361:HOH:O	2.10	0.50
1:B:8:TYR:CD1	1:B:51:VAL:HG13	2.46	0.50
1:H:8:TYR:HD1	1:H:51:VAL:HG13	1.75	0.50
1:C:120:PRO:HD2	2:C:1264:HOH:O	2.11	0.50
1:B:8:TYR:HA	1:B:51:VAL:HG13	1.94	0.50
1:D:175:ILE:CG1	1:D:182:LYS:HB2	2.40	0.50
1:A:8:TYR:CD1	1:A:51:VAL:HG13	2.47	0.49
1:E:197:TRP:O	1:E:201:ARG:HB3	2.11	0.49
1:B:126:LEU:O	1:B:129:ARG:HG3	2.13	0.49
1:H:164:VAL:HG12	1:H:185:MET:HE2	1.93	0.49
1:D:104:THR:HG22	2:D:431:HOH:O	2.11	0.49
1:C:104:THR:HG22	2:C:763:HOH:O	2.13	0.49
1:A:196:LYS:CD	2:A:400:HOH:O	2.38	0.48
1:F:35:THR:H	1:F:38:THR:HG22	1.77	0.48
1:F:120:PRO:CA	1:F:124:VAL:HG13	2.43	0.48
1:H:120:PRO:HA	1:H:124:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:THR:H	1:G:38:THR:CG2	2.26	0.48
1:D:40:VAL:HB	1:D:41:PRO:HD3	1.95	0.48
1:F:184:HIS:HD2	2:F:328:HOH:O	1.96	0.48
1:H:102:MET:HA	1:H:124:VAL:HG22	1.96	0.48
1:E:11:GLY:HA2	1:E:204:THR:HG21	1.96	0.48
1:B:98:TYR:OH	1:B:163:HIS:CE1	2.57	0.47
1:E:104:THR:CG2	1:E:124:VAL:HG21	2.45	0.47
1:F:187:ARG:O	2:F:289:HOH:O	2.21	0.47
1:D:198:ILE:HA	1:D:201:ARG:HD2	1.96	0.47
1:C:190:GLN:NE2	2:C:813:HOH:O	2.43	0.46
1:D:8:TYR:HD1	1:D:51:VAL:HG13	1.76	0.46
1:F:136:ILE:CD1	1:F:148:LEU:HD21	2.44	0.46
1:G:8:TYR:CD1	1:G:51:VAL:HG13	2.50	0.46
1:B:92:ALA:O	1:B:96:THR:HG23	2.14	0.46
1:F:8:TYR:CD1	1:F:51:VAL:HG13	2.50	0.46
1:D:12:ARG:HD2	1:D:201:ARG:NH2	2.29	0.46
1:H:39:PHE:CZ	1:H:43:LYS:HG2	2.50	0.46
1:G:35:THR:H	1:G:38:THR:HG22	1.80	0.46
1:A:136:ILE:HG23	1:A:148:LEU:HD21	1.98	0.46
1:A:102:MET:SD	1:A:102:MET:C	2.94	0.46
1:A:137:THR:HG22	1:A:141:LYS:HD2	1.98	0.46
1:D:55:GLU:HA	1:D:59:GLN:O	2.16	0.45
1:B:100:ALA:O	1:B:103:LYS:HB2	2.17	0.45
1:C:105:TYR:HB2	1:C:120:PRO:O	2.16	0.45
1:E:104:THR:CG2	1:E:124:VAL:HG11	2.47	0.45
1:F:133:LEU:O	1:F:136:ILE:CG2	2.65	0.45
1:E:8:TYR:CG	1:E:9:PHE:N	2.84	0.45
1:E:99:ARG:HD2	1:E:102:MET:SD	2.57	0.45
1:B:164:VAL:O	1:B:168:THR:HG23	2.17	0.45
1:D:35:THR:CG2	1:D:38:THR:HG22	2.47	0.45
1:F:101:GLU:HG3	1:F:128:ALA:CB	2.47	0.44
1:G:198:ILE:HA	1:G:201:ARG:HD2	1.99	0.44
1:F:105:TYR:CD1	1:F:105:TYR:C	2.90	0.44
1:B:193:ARG:NH2	2:B:343:HOH:O	2.48	0.44
1:D:35:THR:HG23	1:D:38:THR:HG22	1.98	0.44
1:A:36:GLN:O	1:A:36:GLN:NE2	2.51	0.43
1:E:55:GLU:HA	1:E:59:GLN:O	2.18	0.43
1:E:168:THR:HG22	1:E:175:ILE:HB	2.01	0.43
1:F:121:LYS:HE2	1:F:126:LEU:HD11	2.01	0.43
1:D:175:ILE:HG12	1:D:182:LYS:CB	2.47	0.43
1:C:196:LYS:HD3	2:C:1183:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:THR:HG21	2:C:613:HOH:O	2.17	0.43
1:H:122:THR:HA	1:H:126:LEU:HD12	2.00	0.43
1:F:121:LYS:CE	1:F:126:LEU:HD11	2.49	0.42
1:C:105:TYR:CD1	1:C:120:PRO:O	2.72	0.42
1:E:40:VAL:CG2	2:E:1569:HOH:O	2.51	0.42
1:E:170:ARG:HB3	2:E:1730:HOH:O	2.19	0.42
1:G:40:VAL:HB	1:G:41:PRO:HD3	2.00	0.42
1:H:127:PRO:HA	1:H:130:THR:HG22	2.00	0.42
1:A:141:LYS:CE	2:A:447:HOH:O	2.66	0.42
1:F:8:TYR:CG	1:F:9:PHE:N	2.87	0.42
1:G:103:LYS:NZ	2:G:422:HOH:O	2.52	0.42
1:G:123:ASP:O	1:G:127:PRO:HG2	2.18	0.42
1:H:99:ARG:O	1:H:101:GLU:N	2.53	0.42
1:E:8:TYR:CD1	1:E:51:VAL:HG13	2.54	0.42
1:C:105:TYR:HD1	1:C:120:PRO:O	2.02	0.42
1:F:141:LYS:HD2	2:F:348:HOH:O	2.19	0.42
1:H:101:GLU:N	1:H:101:GLU:CD	2.73	0.42
1:H:118:ASP:O	1:H:121:LYS:HB3	2.19	0.42
1:H:119:LYS:HE2	1:H:123:ASP:HB2	2.01	0.42
1:A:121:LYS:NZ	1:A:173:GLU:OE1	2.53	0.42
1:A:7:THR:O	1:A:52:PRO:HA	2.20	0.41
1:E:35:THR:H	1:E:38:THR:HG22	1.85	0.41
1:D:39:PHE:CE2	1:D:43:LYS:HG3	2.55	0.41
1:G:8:TYR:CG	1:G:9:PHE:N	2.89	0.41
1:G:182:LYS:NZ	1:G:186:GLU:OE2	2.50	0.41
1:A:119:LYS:HB3	1:A:120:PRO:CD	2.50	0.41
1:B:1:MET:HA	1:C:57:ASP:OD1	2.20	0.41
1:B:40:VAL:N	1:B:41:PRO:CD	2.84	0.41
1:F:110:LEU:HD11	1:F:170:ARG:HH22	1.86	0.41
1:A:8:TYR:HD1	1:A:51:VAL:HG13	1.86	0.41
1:A:119:LYS:HB3	1:A:120:PRO:HD3	2.02	0.41
1:B:3:HIS:HD2	2:B:403:HOH:O	2.02	0.41
1:C:8:TYR:CG	1:C:9:PHE:N	2.89	0.41
1:E:24:LEU:HD13	1:E:77:PHE:CE2	2.55	0.41
1:G:7:THR:O	1:G:51:VAL:HG22	2.21	0.41
1:H:40:VAL:N	1:H:41:PRO:HD2	2.35	0.41
1:A:121:LYS:HE2	1:A:171:VAL:HG13	2.03	0.41
1:B:98:TYR:CE2	1:B:163:HIS:CE1	3.09	0.41
1:C:119:LYS:N	1:C:120:PRO:CD	2.84	0.41
1:F:187:ARG:HD3	2:F:299:HOH:O	2.20	0.41
1:B:8:TYR:CG	1:B:9:PHE:N	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:NZ	2:A:447:HOH:O	2.17	0.40
1:A:175:ILE:HD12	1:A:175:ILE:HA	1.78	0.40
1:B:8:TYR:HD1	1:B:51:VAL:HG13	1.85	0.40
1:G:163:HIS:HD2	2:G:390:HOH:O	2.03	0.40
1:D:129:ARG:HD2	1:D:130:THR:N	2.37	0.40
1:A:118:ASP:N	2:A:427:HOH:O	2.53	0.40
1:C:105:TYR:CD2	1:C:125:LEU:HG	2.56	0.40
1:H:120:PRO:HD2	2:H:754:HOH:O	2.19	0.40
1:C:104:THR:HG23	1:C:124:VAL:HG11	2.03	0.40
1:C:175:ILE:HD12	1:C:175:ILE:HA	1.96	0.40
1:D:27:GLN:NE2	2:D:389:HOH:O	2.53	0.40

All (2) 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)
2:A:240:HOH:O	2:E:1566:HOH:O[1_444]	1.76	0.44
1:F:180:GLU:OE1	2:D:367:HOH:O[1_665]	2.07	0.13

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	187/206 (91%)	184 (98%)	2 (1%)	1 (0%)	29 13
1	B	184/206 (89%)	180 (98%)	3 (2%)	1 (0%)	29 13
1	C	190/206 (92%)	186 (98%)	2 (1%)	2 (1%)	14 3
1	D	190/206 (92%)	187 (98%)	2 (1%)	1 (0%)	29 13
1	E	189/206 (92%)	185 (98%)	3 (2%)	1 (0%)	29 13
1	F	201/206 (98%)	197 (98%)	2 (1%)	2 (1%)	15 4
1	G	185/206 (90%)	181 (98%)	3 (2%)	1 (0%)	29 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	187/206 (91%)	180 (96%)	5 (3%)	2 (1%)	14 3
All	All	1513/1648 (92%)	1480 (98%)	22 (2%)	11 (1%)	22 8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	111	GLY
1	H	63	GLN
1	B	63	GLN
1	C	63	GLN
1	E	63	GLN
1	F	63	GLN
1	D	63	GLN
1	G	63	GLN
1	H	100	ALA
1	A	63	GLN
1	C	120	PRO

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	162/174 (93%)	151 (93%)	11 (7%)	16 3
1	B	159/174 (91%)	147 (92%)	12 (8%)	13 3
1	C	165/174 (95%)	157 (95%)	8 (5%)	25 8
1	D	165/174 (95%)	153 (93%)	12 (7%)	14 3
1	E	161/174 (92%)	149 (92%)	12 (8%)	13 3
1	F	173/174 (99%)	161 (93%)	12 (7%)	15 3
1	G	160/174 (92%)	145 (91%)	15 (9%)	8 1
1	H	162/174 (93%)	146 (90%)	16 (10%)	8 1
All	All	1307/1392 (94%)	1209 (92%)	98 (8%)	13 3

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	28	LYS
1	A	36	GLN
1	A	51	VAL
1	A	102	MET
1	A	124	VAL
1	A	125	LEU
1	A	129	ARG
1	A	141	LYS
1	A	143	ASN
1	A	189	GLN
1	B	24	LEU
1	B	51	VAL
1	B	98	TYR
1	B	102	MET
1	B	103	LYS
1	B	122	THR
1	B	123	ASP
1	B	129	ARG
1	B	130	THR
1	B	143	ASN
1	B	173	GLU
1	B	201	ARG
1	C	24	LEU
1	C	102	MET
1	C	121	LYS
1	C	125	LEU
1	C	129	ARG
1	C	141	LYS
1	C	143	ASN
1	C	189	GLN
1	D	6	LEU
1	D	35	THR
1	D	38	THR
1	D	51	VAL
1	D	98	TYR
1	D	124	VAL
1	D	129	ARG
1	D	130	THR
1	D	136	ILE
1	D	189	GLN
1	D	201	ARG
1	D	203	GLU

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Mol	Chain	Res	Type
1	E	6	LEU
1	E	24	LEU
1	E	51	VAL
1	E	122	THR
1	E	124	VAL
1	E	129	ARG
1	E	131	LYS
1	E	136	ILE
1	E	189	GLN
1	E	190	GLN
1	E	192	PRO
1	E	201	ARG
1	F	6	LEU
1	F	24	LEU
1	F	38	THR
1	F	51	VAL
1	F	61	LEU
1	F	98	TYR
1	F	117	VAL
1	F	122	THR
1	F	124	VAL
1	F	129	ARG
1	F	189	GLN
1	F	201	ARG
1	G	6	LEU
1	G	24	LEU
1	G	38	THR
1	G	51	VAL
1	G	61	LEU
1	G	102	MET
1	G	122	THR
1	G	123	ASP
1	G	129	ARG
1	G	131	LYS
1	G	143	ASN
1	G	169	ASN
1	G	189	GLN
1	G	201	ARG
1	G	203	GLU
1	H	6	LEU
1	H	38	THR
1	H	51	VAL

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Mol	Chain	Res	Type
1	H	99	ARG
1	H	101	GLU
1	H	102	MET
1	H	118	ASP
1	H	119	LYS
1	H	122	THR
1	H	129	ARG
1	H	131	LYS
1	H	143	ASN
1	H	189	GLN
1	H	193	ARG
1	H	201	ARG
1	H	203	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	36	GLN
1	A	63	GLN
1	A	143	ASN
1	A	190	GLN
1	B	3	HIS
1	B	63	GLN
1	B	143	ASN
1	B	163	HIS
1	B	190	GLN
1	C	143	ASN
1	D	27	GLN
1	D	63	GLN
1	D	190	GLN
1	E	63	GLN
1	E	184	HIS
1	E	190	GLN
1	F	63	GLN
1	F	184	HIS
1	G	63	GLN
1	G	143	ASN
1	G	163	HIS
1	H	3	HIS
1	H	27	GLN
1	H	143	ASN

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

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.