Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 08:07 PM EDT

PDB ID	:	1T5R
Title	:	STRUCTURE OF THE PANTON-VALENTINE LEUCOCIDIN S COMPONENT FROM STAPHYLOCOCCUS AUREUS
Authors	:	Guillet, V.; Roblin, P.; Keller, D.; Prevost, G.; Mourey, L.
Deposited on	:	2004-05-05
Resolution	:	2.00 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:

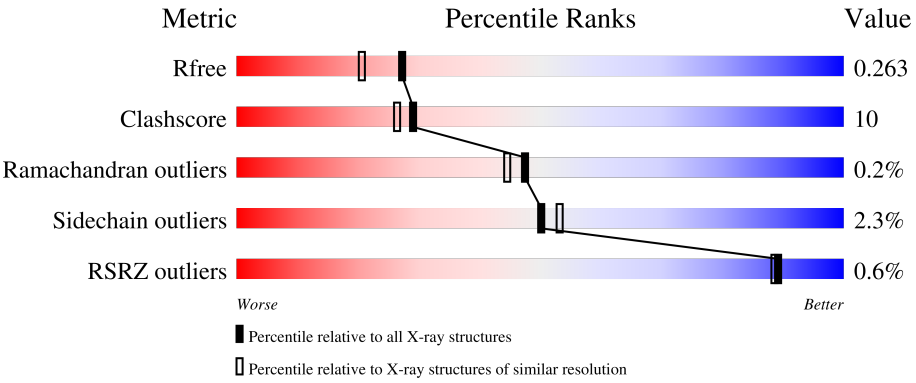
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	284	75% 18% 7%
1	B	284	76% 18% • 5%
1	C	284	% 77% 17% • 5%
1	D	284	77% 15% • 6%
1	E	284	% 71% 23% • 5%

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Mol	Chain	Length	Quality of chain
1	F	284	
1	G	284	
1	H	284	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17913 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 LukS-PV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2106	1331	361	410	4			
1	B	271	Total	C	N	O	S	0	0	0
			2151	1354	375	418	4			
1	C	269	Total	C	N	O	S	0	0	0
			2150	1356	373	417	4			
1	D	267	Total	C	N	O	S	0	0	0
			2127	1343	368	412	4			
1	E	271	Total	C	N	O	S	0	0	0
			2137	1346	373	414	4			
1	F	269	Total	C	N	O	S	0	0	0
			2144	1355	375	410	4			
1	G	269	Total	C	N	O	S	0	0	0
			2147	1357	374	412	4			
1	H	270	Total	C	N	O	S	0	0	0
			2130	1345	368	413	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	116	Total	O	0	0
			116	116		
2	B	105	Total	O	0	0
			105	105		
2	C	122	Total	O	0	0
			122	122		
2	D	123	Total	O	0	0
			123	123		
2	E	70	Total	O	0	0
			70	70		
2	F	103	Total	O	0	0
			103	103		

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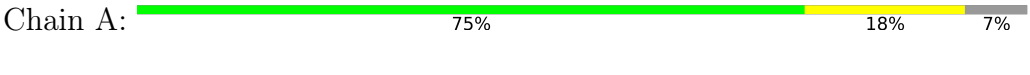
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	74	Total O 74 74	0	0
2	H	108	Total O 108 108	0	0

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.

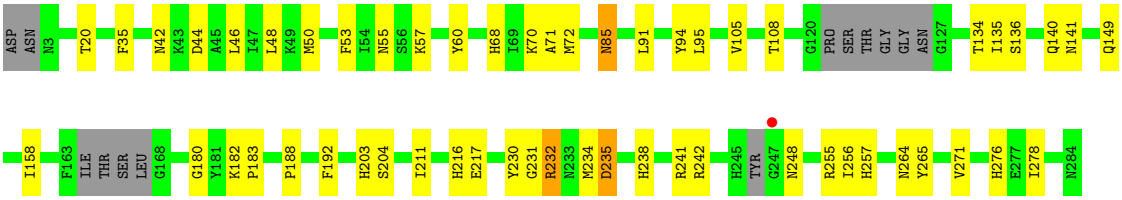
• Molecule 1: LukS-PV

Chain A:



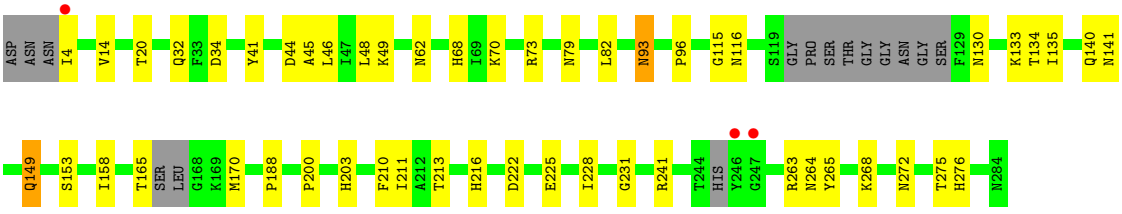
• Molecule 1: LukS-PV

Chain B:



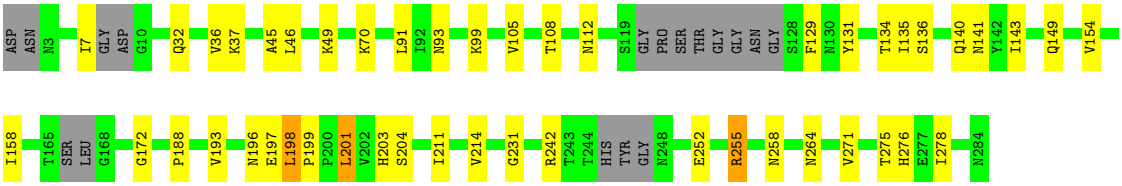
• Molecule 1: LukS-PV

Chain C:



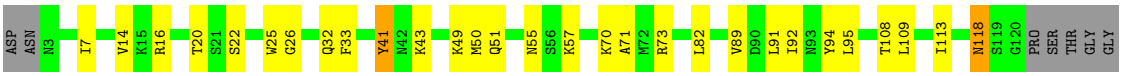
• Molecule 1: LukS-PV

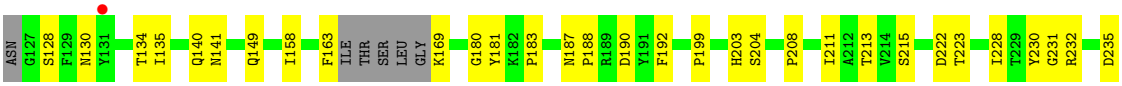
Chain D:

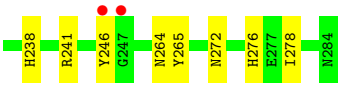


• Molecule 1: LukS-PV

Chain E:

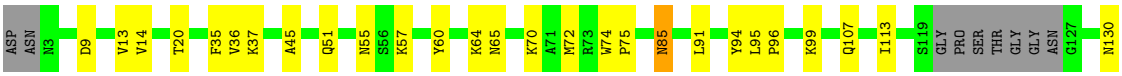


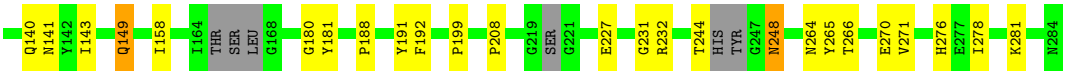




• Molecule 1: LukS-PV

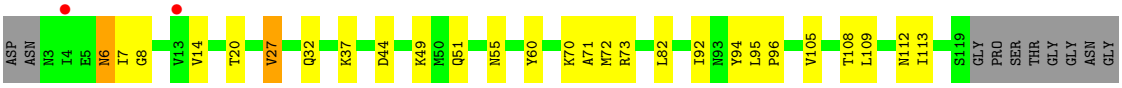
Chain F:

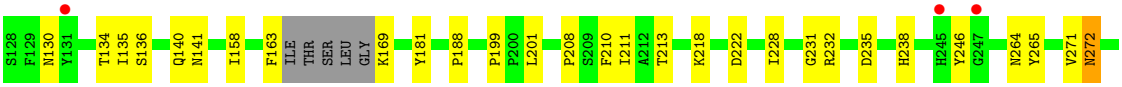




• Molecule 1: LukS-PV

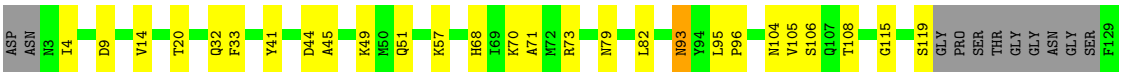
Chain G:

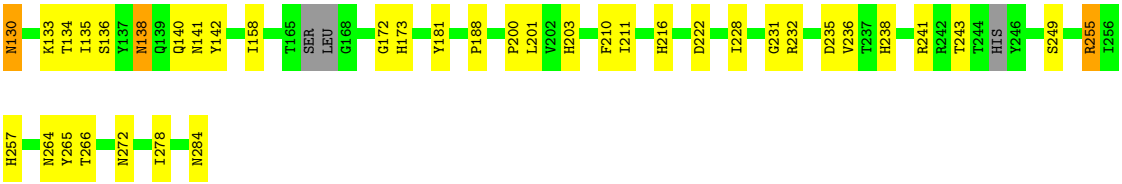




• Molecule 1: LukS-PV

Chain H:




N130
K133
T134
I135
S136
Y137
N138
Q139
Q140
N141
Y142
I158
T165
SER
LEU
G168
G172
H173
Y181
P188
P200
L201
V202
H203
F210
I211
H216
D222
I228
G231
R232
D235
V236
T237
H238
R241
R242
T243
T244
HIS
Y246
S249
R255
I256
H257
N264
Y265
T266
N272
I278
N284

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	94.85Å 94.85Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.50 – 2.00 35.49 – 2.00	Depositor EDS
% Data completeness (in resolution range)	75.6 (35.50-2.00) 93.5 (35.49-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.247 0.227 , 0.263	Depositor DCC
R_{free} test set	16823 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.487 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17913	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 36.93 % 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 4.6352e-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, 0.333 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	0.36	0/2158	0.64	0/2929
1	B	0.35	0/2204	0.62	0/2987
1	C	0.35	0/2204	0.63	0/2989
1	D	0.35	0/2179	0.64	0/2953
1	E	0.34	0/2192	0.61	0/2977
1	F	0.35	0/2196	0.62	0/2972
1	G	0.34	0/2203	0.61	0/2989
1	H	0.35	0/2184	0.63	0/2965
All	All	0.35	0/17520	0.63	0/23761

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	2106	0	1929	34	0
1	B	2151	0	1988	35	0
1	C	2150	0	1989	36	0
1	D	2127	0	1969	31	0
1	E	2137	0	1958	48	0
1	F	2144	0	2010	40	0
1	G	2147	0	1995	48	0
1	H	2130	0	1948	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	116	0	0	1	0
2	B	105	0	0	0	0
2	C	122	0	0	3	0
2	D	123	0	0	2	0
2	E	70	0	0	1	0
2	F	103	0	0	1	0
2	G	74	0	0	2	0
2	H	108	0	0	2	0
All	All	17913	0	15786	317	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 10.

All (317) 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:141:ASN:HD22	1:E:199:PRO:HB3	1.30	0.94
1:F:85:ASN:H	1:F:85:ASN:HD22	1.18	0.90
1:C:231:GLY:HA3	1:C:264:ASN:HD22	1.38	0.88
1:F:248:ASN:HD22	1:F:248:ASN:H	1.23	0.87
1:H:231:GLY:HA3	1:H:264:ASN:HD22	1.45	0.81
1:C:34:ASP:OD1	1:C:133:LYS:HE2	1.82	0.79
1:E:141:ASN:ND2	1:E:199:PRO:HB3	1.96	0.79
1:H:130:ASN:HD22	1:H:130:ASN:N	1.84	0.75
1:C:231:GLY:HA3	1:C:264:ASN:ND2	2.01	0.75
1:B:85:ASN:H	1:B:85:ASN:HD22	1.37	0.73
1:F:37:LYS:HE2	1:F:276:HIS:CE1	2.25	0.72
1:F:85:ASN:H	1:F:85:ASN:ND2	1.88	0.70
1:E:113:ILE:HG12	1:E:130:ASN:OD1	1.92	0.70
1:H:243:THR:HG22	1:H:249:SER:OG	1.92	0.69
1:C:79:ASN:HD22	1:C:264:ASN:HD21	1.41	0.69
1:F:36:VAL:HG13	1:F:45:ALA:HB3	1.73	0.69
1:C:62:ASN:OD1	1:C:188:PRO:HG3	1.93	0.68
1:D:37:LYS:HE3	1:D:276:HIS:CE1	2.29	0.68
1:H:231:GLY:HA3	1:H:264:ASN:ND2	2.07	0.68
1:B:183:PRO:O	1:B:241:ARG:HD3	1.93	0.68
1:F:36:VAL:CG1	1:F:45:ALA:HB3	2.23	0.68
1:F:85:ASN:HD22	1:F:85:ASN:N	1.87	0.68
1:E:14:VAL:HG21	1:E:276:HIS:CE1	2.28	0.67
1:E:14:VAL:HG21	1:E:276:HIS:ND1	2.10	0.67
1:B:232:ARG:HG3	1:B:234:MET:SD	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:LEU:HD12	1:C:228:ILE:HG12	1.77	0.65
1:H:73:ARG:HD3	2:H:346:HOH:O	1.96	0.65
1:A:257:HIS:HE1	2:A:330:HOH:O	1.80	0.64
1:E:141:ASN:HD22	1:E:199:PRO:CB	2.04	0.64
1:E:231:GLY:HA3	1:E:264:ASN:OD1	1.97	0.64
1:B:235:ASP:OD2	1:B:257:HIS:HD2	1.80	0.64
1:C:4:ILE:HD13	1:C:14:VAL:HA	1.79	0.64
1:C:4:ILE:CD1	1:C:14:VAL:HG22	2.28	0.64
1:H:235:ASP:OD2	1:H:257:HIS:HD2	1.80	0.64
1:H:172:GLY:O	1:H:255:ARG:NH2	2.27	0.63
1:G:14:VAL:HG21	1:G:276:HIS:CE1	2.34	0.63
1:E:70:LYS:HD3	1:E:188:PRO:HA	1.81	0.62
1:E:94:TYR:C	1:E:95:LEU:HD12	2.20	0.62
1:G:92:ILE:HD11	1:G:213:THR:HG22	1.82	0.61
1:G:94:TYR:C	1:G:95:LEU:HD12	2.20	0.61
1:D:203:HIS:HD2	1:D:204:SER:OG	1.84	0.61
1:H:95:LEU:HD21	1:H:119:SER:HB2	1.81	0.61
1:F:55:ASN:O	1:F:232:ARG:HD3	2.01	0.60
1:G:70:LYS:HD3	1:G:188:PRO:HA	1.83	0.60
1:D:135:ILE:CG2	1:D:211:ILE:HG13	2.31	0.60
1:G:231:GLY:HA3	1:G:264:ASN:OD1	2.00	0.60
1:B:70:LYS:HD3	1:B:188:PRO:HA	1.83	0.60
1:H:79:ASN:HD22	1:H:264:ASN:HD21	1.50	0.60
1:F:70:LYS:HD3	1:F:188:PRO:HA	1.84	0.60
1:A:70:LYS:HD3	1:A:188:PRO:HA	1.84	0.60
1:B:158:ILE:HD12	1:B:158:ILE:N	2.17	0.59
1:G:6:ASN:HD22	1:G:7:ILE:N	2.01	0.59
1:A:235:ASP:OD2	1:A:257:HIS:HD2	1.85	0.58
1:A:55:ASN:O	1:A:232:ARG:HD3	2.04	0.58
1:F:37:LYS:HE2	1:F:276:HIS:NE2	2.18	0.58
1:H:130:ASN:N	1:H:130:ASN:ND2	2.51	0.58
1:H:236:VAL:O	1:H:255:ARG:HG3	2.03	0.58
1:C:225:GLU:OE1	1:C:268:LYS:HE2	2.03	0.57
1:H:82:LEU:HD12	1:H:228:ILE:HG12	1.85	0.57
1:F:231:GLY:HA3	1:F:264:ASN:OD1	2.03	0.57
1:G:82:LEU:HD23	1:G:228:ILE:HG12	1.86	0.57
1:D:112:ASN:HD21	1:D:129:PHE:HA	1.69	0.57
1:G:141:ASN:OD1	1:G:199:PRO:HB3	2.04	0.57
1:B:85:ASN:H	1:B:85:ASN:ND2	2.00	0.57
1:A:189:ARG:O	1:A:189:ARG:HD3	2.04	0.56
1:B:46:LEU:HD21	1:B:48:LEU:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:PHE:O	1:E:169:LYS:HA	2.06	0.56
1:E:183:PRO:O	1:E:241:ARG:HD3	2.06	0.56
1:G:6:ASN:ND2	1:G:8:GLY:H	2.03	0.56
1:A:57:LYS:O	1:A:59:THR:HG23	2.05	0.56
1:B:94:TYR:C	1:B:95:LEU:HD12	2.26	0.56
1:F:57:LYS:HD2	1:F:232:ARG:NH1	2.21	0.56
1:E:158:ILE:N	1:E:158:ILE:HD12	2.21	0.55
1:F:158:ILE:HD12	1:F:158:ILE:N	2.21	0.55
1:F:64:LYS:HE3	1:F:65:ASN:HD21	1.72	0.55
1:A:231:GLY:HA3	1:A:264:ASN:OD1	2.07	0.55
1:A:158:ILE:N	1:A:158:ILE:HD12	2.22	0.55
1:C:4:ILE:HD12	1:C:14:VAL:HG22	1.88	0.55
1:A:46:LEU:HG	1:A:48:LEU:HD22	1.88	0.54
1:C:93:ASN:HD22	1:C:93:ASN:C	2.11	0.54
1:G:108:THR:HG23	1:G:134:THR:HG22	1.89	0.54
1:A:94:TYR:O	1:A:95:LEU:HD23	2.08	0.54
1:F:248:ASN:H	1:F:248:ASN:ND2	1.99	0.54
1:H:41:TYR:CD1	1:H:115:GLY:HA3	2.42	0.54
1:H:173:HIS:HA	1:H:255:ARG:NH2	2.23	0.54
1:F:94:TYR:C	1:F:95:LEU:HD12	2.27	0.54
1:A:242:ARG:HG2	1:A:242:ARG:HH11	1.72	0.54
1:B:140:GLN:O	1:B:141:ASN:HB2	2.07	0.54
1:D:158:ILE:HD12	1:D:158:ILE:N	2.23	0.54
1:G:20:THR:HG22	1:G:265:TYR:OH	2.08	0.53
1:G:163:PHE:O	1:G:169:LYS:HA	2.08	0.53
1:C:68:HIS:HB2	1:C:241:ARG:HB3	1.90	0.53
1:C:116:ASN:HB2	2:C:334:HOH:O	2.08	0.53
1:A:242:ARG:NE	1:A:252:GLU:OE1	2.41	0.53
1:C:130:ASN:N	1:C:130:ASN:HD22	2.07	0.52
1:D:242:ARG:HG2	1:D:242:ARG:HH11	1.72	0.52
1:E:20:THR:HG22	1:E:265:TYR:OH	2.09	0.52
1:G:7:ILE:HB	1:G:130:ASN:O	2.08	0.52
1:H:4:ILE:CD1	1:H:14:VAL:HG22	2.40	0.52
1:D:37:LYS:HE3	1:D:276:HIS:NE2	2.24	0.52
1:D:193:VAL:HG23	1:D:198:LEU:HD13	1.91	0.52
1:E:118:ASN:C	1:E:118:ASN:HD22	2.11	0.52
1:E:135:ILE:CG2	1:E:211:ILE:HG13	2.40	0.52
1:A:19:ASP:OD1	1:A:30:ASN:ND2	2.42	0.52
1:G:92:ILE:HD11	1:G:213:THR:CG2	2.40	0.52
1:F:14:VAL:CG2	1:F:37:LYS:HE3	2.39	0.52
1:E:128:SER:HB2	1:H:138:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:TYR:CE1	1:E:43:LYS:HB2	2.45	0.51
1:F:271:VAL:HG12	1:F:278:ILE:HD12	1.92	0.51
1:H:108:THR:OG1	1:H:134:THR:HG22	2.10	0.51
1:E:22:SER:HG	1:E:25:TRP:HD1	1.57	0.51
1:G:222:ASP:O	1:G:272:ASN:HA	2.10	0.51
1:G:108:THR:OG1	1:G:134:THR:HG22	2.11	0.51
1:B:20:THR:HG22	1:B:265:TYR:OH	2.11	0.51
1:B:95:LEU:HD12	1:B:95:LEU:N	2.26	0.51
1:G:271:VAL:HG12	1:G:278:ILE:HD12	1.93	0.51
1:F:248:ASN:HD22	1:F:248:ASN:N	2.02	0.51
1:G:14:VAL:HG21	1:G:276:HIS:ND1	2.25	0.50
1:B:108:THR:OG1	1:B:134:THR:HG22	2.11	0.50
1:G:27:VAL:CG2	1:G:265:TYR:HD1	2.24	0.50
1:A:140:GLN:O	1:A:141:ASN:HB2	2.11	0.50
1:E:7:ILE:HB	1:E:130:ASN:O	2.11	0.50
1:G:27:VAL:HG22	1:G:265:TYR:CD1	2.45	0.50
1:E:57:LYS:HD3	1:E:232:ARG:NH2	2.27	0.50
1:E:222:ASP:O	1:E:272:ASN:HA	2.12	0.50
1:H:57:LYS:HG3	1:H:232:ARG:NH1	2.27	0.50
1:D:231:GLY:HA3	1:D:264:ASN:OD1	2.12	0.50
1:G:135:ILE:CG2	1:G:211:ILE:HG13	2.42	0.50
1:B:57:LYS:HG3	1:B:232:ARG:CZ	2.42	0.50
1:D:108:THR:OG1	1:D:134:THR:HG22	2.12	0.50
1:G:140:GLN:O	1:G:141:ASN:HB2	2.12	0.50
1:H:70:LYS:HD3	1:H:188:PRO:HA	1.92	0.50
1:G:55:ASN:O	1:G:232:ARG:HD3	2.11	0.49
1:G:222:ASP:HB3	1:G:272:ASN:HD21	1.77	0.49
1:F:60:TYR:CE2	1:F:72:MET:HG3	2.48	0.49
1:A:70:LYS:HD3	1:A:188:PRO:CA	2.42	0.49
1:F:20:THR:HG22	1:F:265:TYR:OH	2.12	0.49
1:H:68:HIS:HB2	1:H:241:ARG:HB3	1.95	0.49
1:A:135:ILE:CG2	1:A:211:ILE:HG13	2.43	0.49
1:D:258:ASN:HA	2:D:302:HOH:O	2.13	0.49
1:H:135:ILE:CG2	1:H:211:ILE:HG13	2.43	0.49
1:H:235:ASP:OD2	1:H:257:HIS:CD2	2.64	0.49
1:H:4:ILE:HD12	1:H:14:VAL:HG22	1.94	0.49
1:G:201:LEU:HG	2:G:312:HOH:O	2.13	0.49
1:C:158:ILE:N	1:C:158:ILE:HD12	2.28	0.48
1:C:222:ASP:O	1:C:272:ASN:HA	2.12	0.48
1:F:227:GLU:HG2	1:F:266:THR:CG2	2.43	0.48
1:H:41:TYR:HE2	1:H:45:ALA:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:VAL:HG12	1:A:278:ILE:HD12	1.96	0.48
1:C:140:GLN:O	1:C:141:ASN:HB2	2.13	0.48
1:H:266:THR:H	1:H:284:ASN:HB2	1.78	0.48
1:B:53:PHE:HE2	1:B:55:ASN:OD1	1.95	0.48
1:B:248:ASN:H	1:B:248:ASN:HD22	1.59	0.48
1:C:41:TYR:HE2	1:C:45:ALA:HB2	1.79	0.48
1:B:50:MET:HB3	1:B:230:TYR:OH	2.14	0.48
1:G:158:ILE:N	1:G:158:ILE:HD12	2.29	0.48
1:H:4:ILE:HD13	1:H:14:VAL:HA	1.96	0.48
1:B:271:VAL:HG23	1:B:278:ILE:CD1	2.44	0.48
1:C:73:ARG:HD3	2:C:305:HOH:O	2.13	0.48
1:E:92:ILE:HD11	1:E:213:THR:HG22	1.95	0.48
1:E:55:ASN:O	1:E:232:ARG:HD3	2.13	0.47
1:E:128:SER:HB2	1:H:138:ASN:CG	2.35	0.47
1:F:95:LEU:HD12	1:F:95:LEU:N	2.29	0.47
1:H:173:HIS:HA	1:H:255:ARG:HH22	1.79	0.47
1:D:203:HIS:CD2	1:D:204:SER:OG	2.66	0.47
1:H:71:ALA:HB2	1:H:238:HIS:CD2	2.50	0.47
1:B:203:HIS:HD2	1:B:204:SER:OG	1.98	0.47
1:C:46:LEU:HD21	1:C:48:LEU:HD21	1.96	0.47
1:H:133:LYS:HD3	2:H:363:HOH:O	2.13	0.47
1:E:180:GLY:N	1:E:192:PHE:HA	2.30	0.47
1:E:92:ILE:HD11	1:E:213:THR:CG2	2.45	0.47
1:E:32:GLN:HB2	1:E:49:LYS:HB3	1.97	0.46
1:G:73:ARG:HD2	2:G:303:HOH:O	2.15	0.46
1:H:222:ASP:O	1:H:272:ASN:HA	2.14	0.46
1:B:135:ILE:CG2	1:B:211:ILE:HG13	2.45	0.46
1:C:32:GLN:OE1	1:C:49:LYS:HD3	2.15	0.46
1:G:7:ILE:O	1:G:130:ASN:HB3	2.16	0.46
1:D:70:LYS:HD3	1:D:188:PRO:HA	1.95	0.46
1:D:242:ARG:NE	1:D:252:GLU:OE1	2.46	0.46
1:F:96:PRO:HA	1:F:107:GLN:OE1	2.15	0.46
1:B:105:VAL:O	1:B:136:SER:HA	2.16	0.46
1:G:27:VAL:HG22	1:G:265:TYR:HD1	1.81	0.46
1:F:149:GLN:NE2	2:F:347:HOH:O	2.47	0.46
1:A:108:THR:OG1	1:A:134:THR:HG22	2.15	0.46
1:C:130:ASN:N	1:C:130:ASN:ND2	2.64	0.46
1:D:196:ASN:OD1	1:D:197:GLU:HG3	2.17	0.45
1:C:96:PRO:HD2	1:C:210:PHE:CD1	2.51	0.45
1:E:108:THR:OG1	1:E:134:THR:HG22	2.15	0.45
1:A:70:LYS:CD	1:A:188:PRO:HA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ASN:ND2	1:D:129:PHE:HA	2.32	0.45
1:G:113:ILE:HG12	1:G:130:ASN:CG	2.36	0.45
1:D:99:LYS:HD3	1:D:143:ILE:HD11	1.99	0.45
1:B:248:ASN:H	1:B:248:ASN:ND2	2.14	0.45
1:H:105:VAL:O	1:H:136:SER:HA	2.17	0.45
1:D:36:VAL:HB	1:D:45:ALA:HB3	1.99	0.45
1:E:33:PHE:CD2	1:E:278:ILE:HD13	2.51	0.45
1:C:4:ILE:HD11	1:C:14:VAL:HG13	1.98	0.45
1:F:14:VAL:HG21	1:F:37:LYS:HE3	1.97	0.45
1:H:20:THR:HG22	1:H:265:TYR:OH	2.16	0.45
1:C:135:ILE:CG2	1:C:211:ILE:HG13	2.47	0.45
1:F:113:ILE:HG12	1:F:130:ASN:ND2	2.32	0.45
1:G:222:ASP:HB3	1:G:272:ASN:ND2	2.32	0.45
1:H:140:GLN:O	1:H:141:ASN:HB2	2.17	0.45
1:C:20:THR:HG22	1:C:265:TYR:OH	2.16	0.45
1:C:49:LYS:HE3	1:C:134:THR:O	2.17	0.45
1:B:85:ASN:HD22	1:B:85:ASN:N	1.99	0.44
1:B:180:GLY:N	1:B:192:PHE:HA	2.32	0.44
1:H:158:ILE:N	1:H:158:ILE:HD12	2.32	0.44
1:D:7:ILE:HG21	1:D:131:TYR:HB2	1.99	0.44
1:D:140:GLN:O	1:D:141:ASN:HB2	2.17	0.44
1:E:51:GLN:HA	1:E:208:PRO:O	2.17	0.44
1:F:99:LYS:HD3	1:F:143:ILE:HD11	1.99	0.44
1:H:93:ASN:C	1:H:93:ASN:HD22	2.19	0.44
1:H:96:PRO:HD2	1:H:210:PHE:CD1	2.52	0.44
1:A:235:ASP:OD2	1:A:257:HIS:CD2	2.67	0.44
1:A:32:GLN:HB2	1:A:49:LYS:HB3	2.00	0.44
1:A:57:LYS:HG3	1:A:232:ARG:NH1	2.32	0.44
1:G:70:LYS:HD3	1:G:188:PRO:CA	2.47	0.44
1:G:275:THR:O	1:G:276:HIS:HB2	2.18	0.44
1:H:44:ASP:HB2	1:H:216:HIS:HB3	2.00	0.44
1:C:41:TYR:CD1	1:C:115:GLY:HA3	2.52	0.44
1:E:108:THR:HG23	1:E:134:THR:HG22	2.00	0.44
1:A:163:PHE:O	1:A:169:LYS:HA	2.18	0.44
1:A:91:LEU:HA	1:A:214:VAL:HG12	2.00	0.44
1:A:242:ARG:HG2	1:A:242:ARG:NH1	2.33	0.44
1:E:70:LYS:HD3	1:E:188:PRO:CA	2.48	0.44
1:G:32:GLN:HB2	1:G:49:LYS:HB3	2.00	0.44
1:G:105:VAL:O	1:G:136:SER:HA	2.17	0.44
1:G:271:VAL:HG12	1:G:278:ILE:CD1	2.47	0.44
1:A:51:GLN:HG2	1:A:209:SER:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:VAL:HA	1:F:35:PHE:O	2.18	0.43
1:E:73:ARG:HD2	2:E:337:HOH:O	2.17	0.43
1:G:135:ILE:HG23	1:G:211:ILE:CD1	2.48	0.43
1:B:271:VAL:HG23	1:B:278:ILE:HD13	2.00	0.43
1:D:105:VAL:O	1:D:136:SER:HA	2.17	0.43
1:G:71:ALA:HB2	1:G:238:HIS:HD2	1.84	0.43
1:H:32:GLN:OE1	1:H:49:LYS:HD3	2.18	0.43
1:G:44:ASP:OD2	1:G:218:LYS:HG2	2.18	0.43
1:A:41:TYR:O	1:A:218:LYS:NZ	2.50	0.43
1:B:44:ASP:HB2	1:B:216:HIS:HB3	1.99	0.43
1:C:275:THR:O	1:C:276:HIS:HB2	2.18	0.43
1:D:242:ARG:HG2	1:D:242:ARG:NH1	2.33	0.43
1:H:49:LYS:HE3	1:H:134:THR:O	2.19	0.43
1:C:93:ASN:ND2	1:C:213:THR:HB	2.34	0.43
1:B:217:GLU:HA	1:B:217:GLU:OE1	2.18	0.43
1:C:149:GLN:HA	1:C:153:SER:O	2.19	0.43
1:C:200:PRO:HA	1:C:203:HIS:CE1	2.53	0.43
1:G:60:TYR:CE2	1:G:72:MET:HG3	2.54	0.43
1:G:71:ALA:HB2	1:G:238:HIS:CD2	2.54	0.43
1:H:71:ALA:HB2	1:H:238:HIS:HD2	1.84	0.43
1:B:60:TYR:CE2	1:B:72:MET:HG3	2.54	0.43
1:B:255:ARG:HG3	1:B:256:ILE:N	2.34	0.43
1:D:275:THR:O	1:D:276:HIS:HB2	2.18	0.43
1:G:70:LYS:CD	1:G:188:PRO:HA	2.48	0.43
1:D:70:LYS:CD	1:D:188:PRO:HA	2.49	0.42
1:D:91:LEU:HD21	1:D:154:VAL:HB	2.00	0.42
1:D:271:VAL:HG12	1:D:278:ILE:HD12	2.01	0.42
1:F:141:ASN:OD1	1:F:199:PRO:HB3	2.19	0.42
1:F:85:ASN:ND2	1:F:85:ASN:N	2.54	0.42
1:H:33:PHE:CD2	1:H:278:ILE:HD13	2.55	0.42
1:A:163:PHE:CD1	1:A:163:PHE:N	2.87	0.42
1:B:203:HIS:CD2	1:B:204:SER:OG	2.72	0.42
1:G:112:ASN:HA	1:G:130:ASN:OD1	2.19	0.42
1:C:70:LYS:HD3	1:C:188:PRO:HA	2.01	0.42
1:D:172:GLY:O	1:D:255:ARG:NH2	2.30	0.42
1:E:223:THR:HG22	1:E:272:ASN:HA	2.01	0.42
1:B:35:PHE:CG	1:B:276:HIS:HD2	2.38	0.42
1:F:140:GLN:O	1:F:141:ASN:HB2	2.18	0.42
1:B:68:HIS:HB2	1:B:241:ARG:HB3	2.02	0.42
1:B:231:GLY:HA3	1:B:264:ASN:OD1	2.19	0.42
1:C:165:THR:HG21	1:C:170:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:LYS:HB2	1:F:191:TYR:CD1	2.55	0.42
1:C:44:ASP:HB2	1:C:216:HIS:HB3	2.02	0.41
1:G:37:LYS:HE2	1:G:276:HIS:NE2	2.35	0.41
1:E:91:LEU:HD12	1:E:213:THR:O	2.19	0.41
1:F:51:GLN:HA	1:F:208:PRO:O	2.20	0.41
1:F:270:GLU:OE1	1:F:281:LYS:HE3	2.21	0.41
1:E:70:LYS:CD	1:E:188:PRO:HA	2.50	0.41
1:E:118:ASN:C	1:E:118:ASN:ND2	2.72	0.41
1:A:36:VAL:HB	1:A:45:ALA:HB3	2.03	0.41
1:C:268:LYS:NZ	2:C:361:HOH:O	2.53	0.41
1:F:180:GLY:N	1:F:192:PHE:HA	2.35	0.41
1:H:200:PRO:HA	1:H:203:HIS:CE1	2.56	0.41
1:A:200:PRO:HA	1:A:203:HIS:CE1	2.55	0.41
1:B:35:PHE:CZ	1:B:271:VAL:CG2	3.04	0.41
1:E:16:ARG:HB2	1:E:278:ILE:HD11	2.02	0.41
1:E:33:PHE:CG	1:E:278:ILE:HD13	2.55	0.41
1:E:140:GLN:O	1:E:141:ASN:HB2	2.21	0.41
1:F:64:LYS:HE3	1:F:65:ASN:ND2	2.35	0.41
1:F:244:THR:OG1	1:F:248:ASN:ND2	2.53	0.41
1:G:51:GLN:HA	1:G:208:PRO:O	2.20	0.41
1:G:96:PRO:HD2	1:G:210:PHE:CD1	2.56	0.41
1:D:201:LEU:HG	2:D:289:HOH:O	2.21	0.41
1:E:187:ASN:HB3	1:E:190:ASP:OD2	2.20	0.41
1:A:109:LEU:HD13	1:A:109:LEU:C	2.41	0.41
1:D:91:LEU:HA	1:D:214:VAL:HG12	2.03	0.41
1:E:16:ARG:HB3	1:E:278:ILE:HD12	2.02	0.41
1:E:89:VAL:HG13	1:E:215:SER:O	2.20	0.41
1:H:104:ASN:HD21	1:H:106:SER:HB2	1.86	0.41
1:D:141:ASN:OD1	1:D:199:PRO:HB3	2.21	0.41
1:E:50:MET:HB3	1:E:230:TYR:OH	2.20	0.41
1:E:82:LEU:HD13	1:E:228:ILE:HG12	2.03	0.41
1:B:71:ALA:HB2	1:B:238:HIS:HD2	1.87	0.40
1:E:26:GLY:HA3	1:E:55:ASN:HD22	1.86	0.40
1:H:49:LYS:HE2	1:H:51:GLN:NE2	2.36	0.40
1:H:264:ASN:O	1:H:284:ASN:ND2	2.54	0.40
1:D:32:GLN:HB2	1:D:49:LYS:HB3	2.03	0.40
1:E:71:ALA:HB2	1:E:238:HIS:CD2	2.56	0.40
1:G:82:LEU:HD13	1:G:82:LEU:C	2.41	0.40
1:G:272:ASN:C	1:G:272:ASN:HD22	2.23	0.40
1:A:255:ARG:HG3	1:A:256:ILE:N	2.36	0.40
1:E:203:HIS:HD2	1:E:204:SER:OG	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:LYS:HG2	1:F:65:ASN:ND2	2.36	0.40
1:F:74:TRP:HB2	1:F:75:PRO:HD2	2.04	0.40
1:A:105:VAL:O	1:A:136:SER:HA	2.21	0.40
1:A:174:ASP:HA	1:A:175:PRO:HD3	1.95	0.40
1:H:142:TYR:CG	1:H:201:LEU:HD12	2.57	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	255/284 (90%)	243 (95%)	12 (5%)	0	100	100
1	B	263/284 (93%)	253 (96%)	9 (3%)	1 (0%)	34	30
1	C	261/284 (92%)	250 (96%)	11 (4%)	0	100	100
1	D	257/284 (90%)	248 (96%)	9 (4%)	0	100	100
1	E	265/284 (93%)	252 (95%)	12 (4%)	1 (0%)	34	30
1	F	259/284 (91%)	251 (97%)	7 (3%)	1 (0%)	34	30
1	G	263/284 (93%)	251 (95%)	11 (4%)	1 (0%)	34	30
1	H	262/284 (92%)	248 (95%)	13 (5%)	1 (0%)	34	30
All	All	2085/2272 (92%)	1996 (96%)	84 (4%)	5 (0%)	47	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	9	ASP
1	F	9	ASP
1	E	246	TYR
1	G	246	TYR
1	B	42	ASN

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	225/254 (89%)	221 (98%)	4 (2%)	59	63
1	B	230/254 (91%)	223 (97%)	7 (3%)	41	41
1	C	231/254 (91%)	228 (99%)	3 (1%)	69	74
1	D	229/254 (90%)	223 (97%)	6 (3%)	46	48
1	E	227/254 (89%)	221 (97%)	6 (3%)	46	48
1	F	231/254 (91%)	226 (98%)	5 (2%)	52	55
1	G	231/254 (91%)	225 (97%)	6 (3%)	46	48
1	H	225/254 (89%)	220 (98%)	5 (2%)	52	55
All	All	1829/2032 (90%)	1787 (98%)	42 (2%)	50	53

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	42	ASN
1	A	149	GLN
1	A	189	ARG
1	B	85	ASN
1	B	91	LEU
1	B	149	GLN
1	B	182	LYS
1	B	232	ARG
1	B	235	ASP
1	B	242	ARG
1	C	93	ASN
1	C	149	GLN
1	C	263	ARG
1	D	46	LEU
1	D	93	ASN
1	D	149	GLN
1	D	198	LEU
1	D	201	LEU

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Mol	Chain	Res	Type
1	D	255	ARG
1	E	41	TYR
1	E	109	LEU
1	E	118	ASN
1	E	149	GLN
1	E	181	TYR
1	E	235	ASP
1	F	85	ASN
1	F	91	LEU
1	F	149	GLN
1	F	181	TYR
1	F	248	ASN
1	G	6	ASN
1	G	27	VAL
1	G	109	LEU
1	G	181	TYR
1	G	235	ASP
1	G	272	ASN
1	H	93	ASN
1	H	130	ASN
1	H	138	ASN
1	H	181	TYR
1	H	255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	30	ASN
1	A	42	ASN
1	A	112	ASN
1	A	149	GLN
1	A	257	HIS
1	A	258	ASN
1	B	30	ASN
1	B	65	ASN
1	B	85	ASN
1	B	203	HIS
1	B	248	ASN
1	B	257	HIS
1	B	258	ASN
1	B	276	HIS

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Mol	Chain	Res	Type
1	C	30	ASN
1	C	93	ASN
1	C	149	GLN
1	C	258	ASN
1	C	264	ASN
1	D	30	ASN
1	D	51	GLN
1	D	93	ASN
1	D	112	ASN
1	D	130	ASN
1	D	149	GLN
1	D	203	HIS
1	D	258	ASN
1	E	30	ASN
1	E	32	GLN
1	E	55	ASN
1	E	104	ASN
1	E	138	ASN
1	E	141	ASN
1	E	149	GLN
1	E	203	HIS
1	E	248	ASN
1	F	30	ASN
1	F	65	ASN
1	F	85	ASN
1	F	104	ASN
1	F	138	ASN
1	F	149	GLN
1	F	155	GLN
1	F	248	ASN
1	G	6	ASN
1	G	30	ASN
1	G	32	GLN
1	G	55	ASN
1	G	65	ASN
1	G	140	GLN
1	G	173	HIS
1	G	186	GLN
1	G	203	HIS
1	G	272	ASN
1	H	93	ASN
1	H	104	ASN

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Mol	Chain	Res	Type
1	H	138	ASN
1	H	257	HIS
1	H	258	ASN
1	H	264	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

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	265/284 (93%)	-0.31	0 100 100	22, 32, 48, 60	0
1	B	271/284 (95%)	-0.32	1 (0%) 92 92	22, 34, 51, 59	5 (1%)
1	C	269/284 (94%)	-0.27	3 (1%) 80 79	23, 34, 54, 71	2 (0%)
1	D	267/284 (94%)	-0.27	0 100 100	21, 33, 50, 58	0
1	E	271/284 (95%)	-0.09	3 (1%) 80 79	23, 39, 60, 66	0
1	F	269/284 (94%)	-0.28	0 100 100	23, 33, 49, 59	2 (0%)
1	G	269/284 (94%)	-0.09	5 (1%) 66 65	23, 39, 58, 67	4 (1%)
1	H	270/284 (95%)	-0.24	0 100 100	24, 34, 54, 69	1 (0%)
All	All	2151/2272 (94%)	-0.23	12 (0%) 89 88	21, 35, 54, 71	14 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	246	TYR	3.2
1	G	4	ILE	3.1
1	G	247	GLY	3.0
1	G	13	VAL	3.0
1	G	131	TYR	3.0
1	G	245	HIS	2.8
1	C	246	TYR	2.8
1	E	131	TYR	2.6
1	B	247	GLY	2.5
1	E	247	GLY	2.4
1	C	247	GLY	2.4
1	C	4	ILE	2.2

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.