Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:54 PM GMT

PDB ID	:	4Q79
Title	:	Structure of a HG-derivative CsgG
Authors	:	Huang, Y.; Zhang, C.X.; Cao, B.; Zhao, Y.; Kou, Y.; Ni, D.
Deposited on	:	2014-04-24
Resolution	:	3.10 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 ⓘ symbol.

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

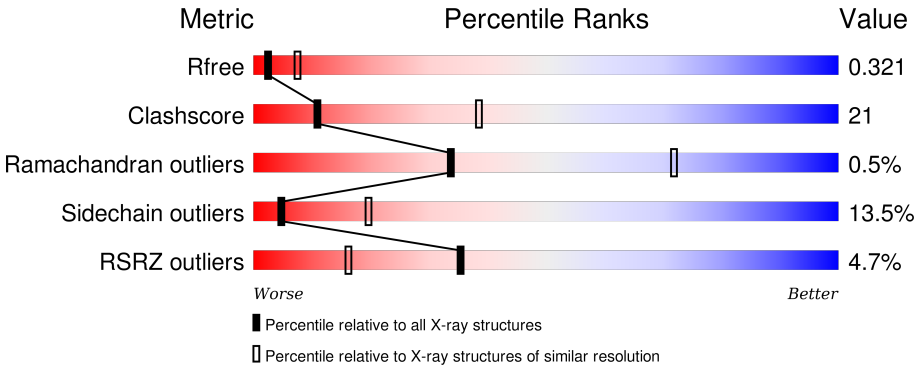
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 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.



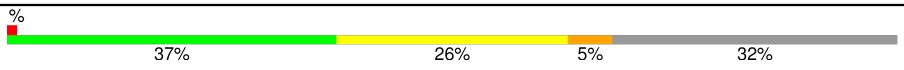
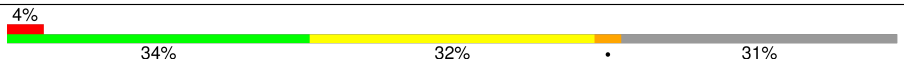
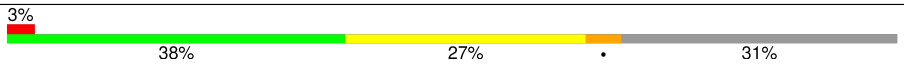
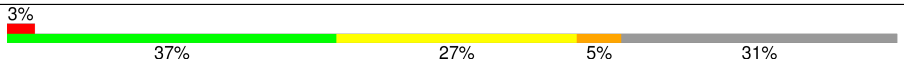
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	277	5% 36% 31% • 29%
1	B	277	4% 38% 26% 5% 31%
1	C	277	2% 37% 29% 6% 29%
1	D	277	4% 40% 25% • 32%
1	E	277	3% 40% 26% 5% 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	277	
1	G	277	
1	H	277	
1	I	277	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13035 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 CsgG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	189	Total	C	N	O	S	0	0	0
			1424	904	236	279	5			
1	A	196	Total	C	N	O	S	0	0	0
			1467	932	243	287	5			
1	B	190	Total	C	N	O	S	0	0	0
			1423	902	236	280	5			
1	C	198	Total	C	N	O	S	0	0	0
			1494	952	248	289	5			
1	E	198	Total	C	N	O	S	0	0	0
			1494	952	248	289	5			
1	F	189	Total	C	N	O	S	0	0	0
			1424	904	236	279	5			
1	G	190	Total	C	N	O	S	0	0	0
			1440	918	237	280	5			
1	H	191	Total	C	N	O	S	0	0	0
			1437	913	238	281	5			
1	I	190	Total	C	N	O	S	0	0	0
			1423	902	236	280	5			

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Hg	0	0
			1	1		
2	D	1	Total	Hg	0	0
			1	1		
2	E	1	Total	Hg	0	0
			1	1		
2	H	1	Total	Hg	0	0
			1	1		
2	B	1	Total	Hg	0	0
			1	1		

Continued on next page...

Continued from previous page...

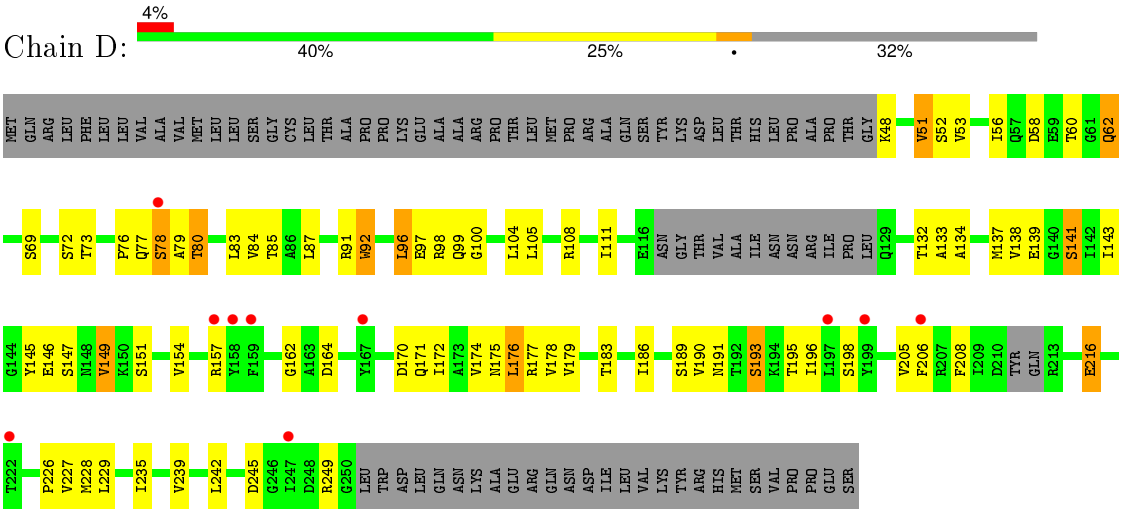
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total Hg 1 1	0	0
2	C	1	Total Hg 1 1	0	0
2	A	1	Total Hg 1 1	0	0
2	F	1	Total Hg 1 1	0	0

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.

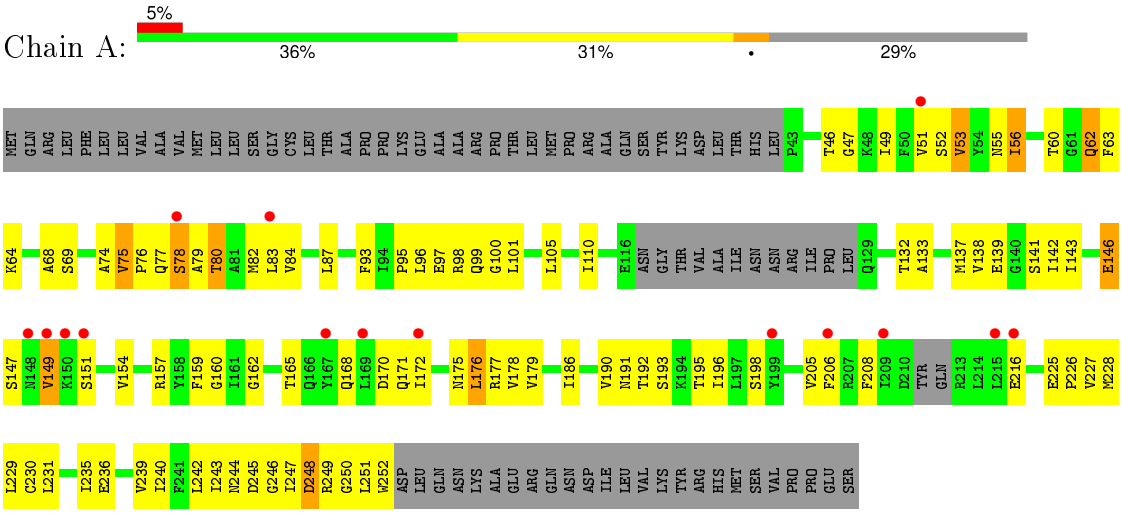
- Molecule 1: CsgG

Chain D:



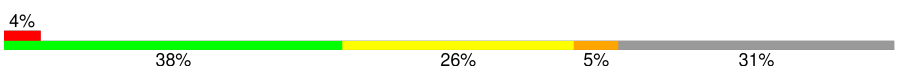
- Molecule 1: CsgG

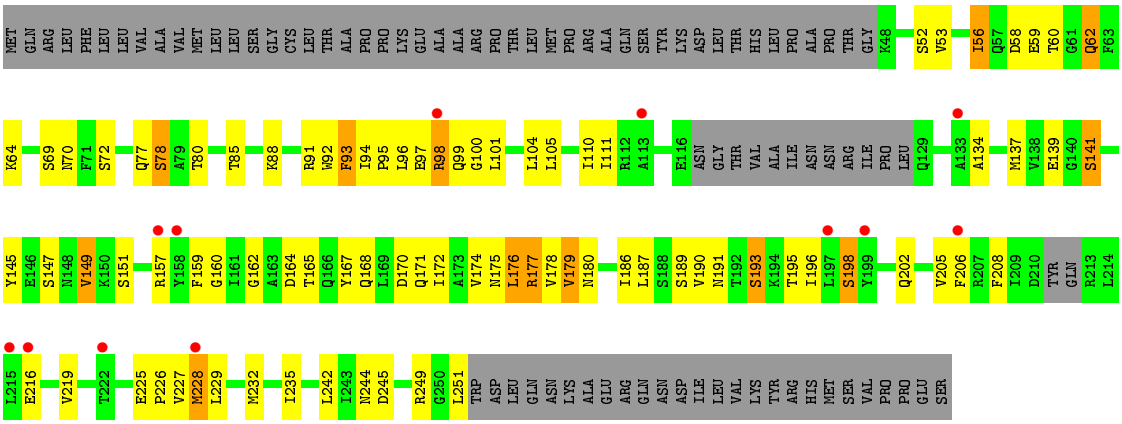
Chain A:



- Molecule 1: CsgG

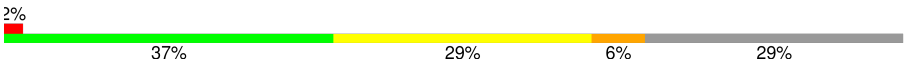
Chain B:

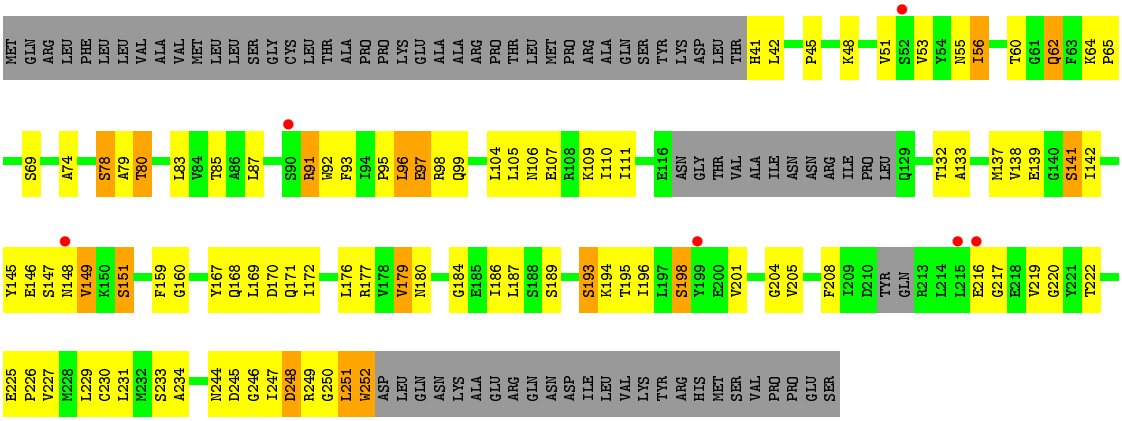




• Molecule 1: CsgG

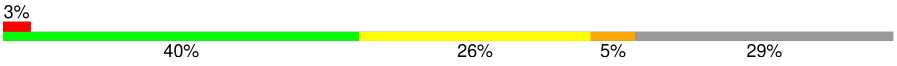
Chain C:

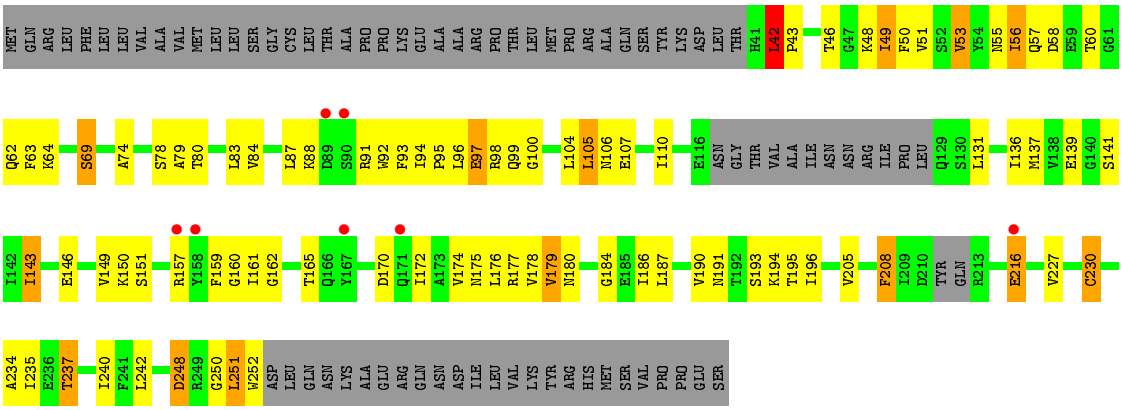




• Molecule 1: CsgG

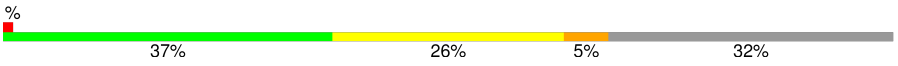
Chain E:

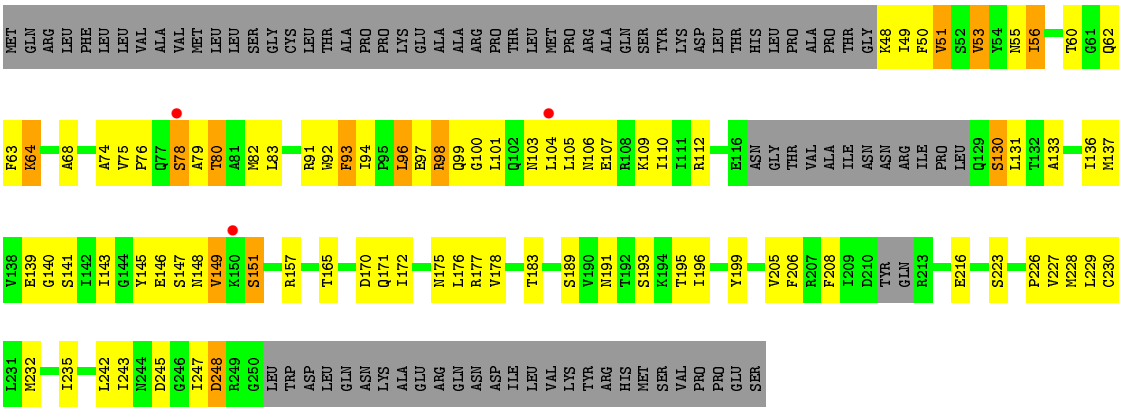




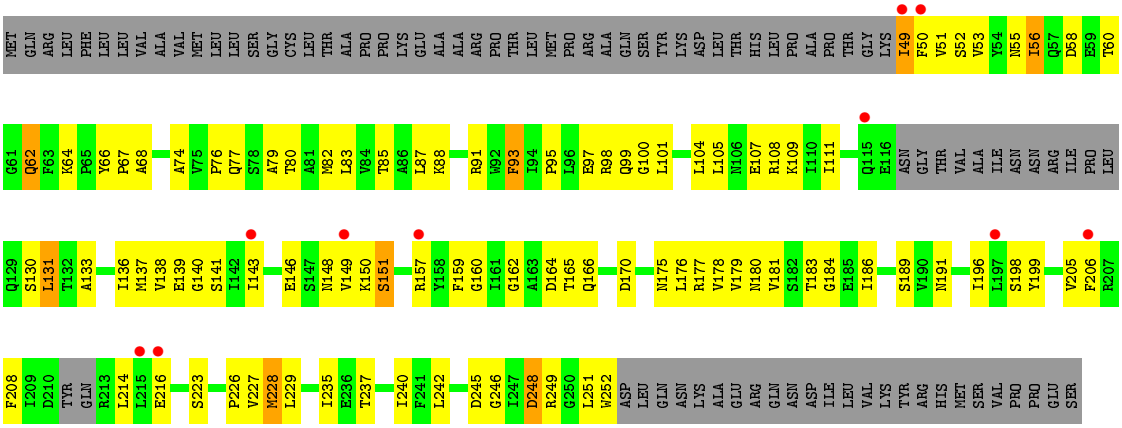
• Molecule 1: CsgG

Chain F:

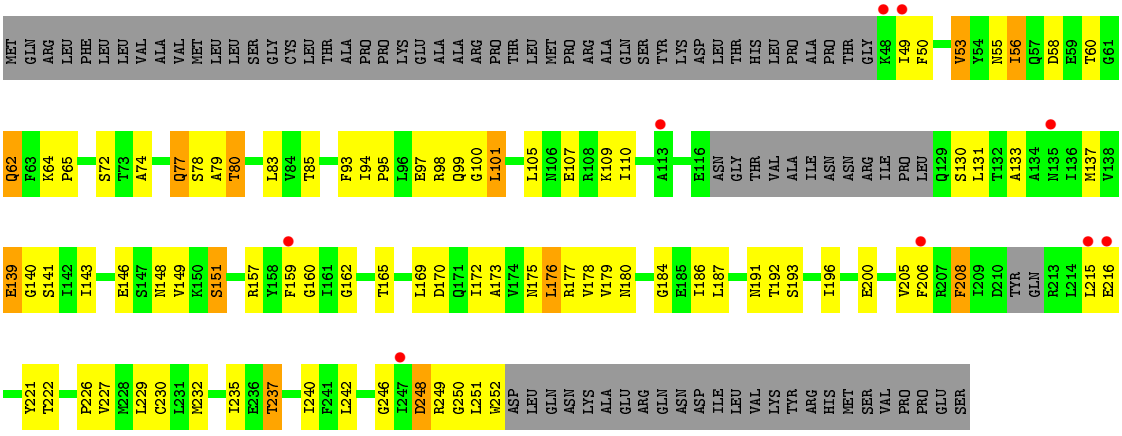




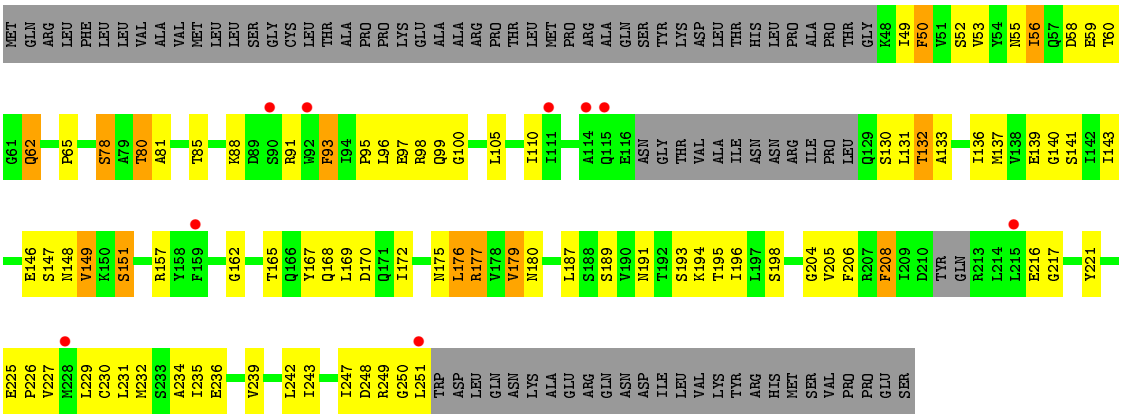
• Molecule 1: CsgG



• Molecule 1: CsgG



• Molecule 1: CsgG


MET GLN ARG LEU PHE LEU LEU VAL ALA VAL MET LEU LEU SER GLY CYS LEU THR ALA PRO PRO LYS GLU ALA ALA ARG PRO THR LEU MET PRO ARG ALA GLN SER TYR LYS ASP LEU THR HIS LEU PRO ALA PRO THR GLY K48 I49 F50 V51 S52 V53 Y54 N55 I56 Q57 D58 E59 T60
G61 Q62 P65 S78 A79 T80 A81 T85 K88 D89 S90 R91 W92 F93 I94 P95 L96 E97 R98 Q99 G100 L105 I110 I111 A114 Q115 E116 ASN GLY THR VAL ALA ILE ASN ASN ARG ILE PRO LEU Q129 S130 L131 T132 A133 I136 M137 V138 E139 G140 S141 I142 I143
E146 S147 N148 V149 K150 S151 R157 Y158 F159 G162 T165 Q166 Y167 Q168 L169 D170 Q171 I172 N175 L176 R177 V178 V179 N180 L187 S188 S189 V190 N191 T192 S193 K194 T195 I196 L197 S198 G204 V205 F206 R207 F208 I209 D210 TYR GLN R213 L214 L215 E216 G217 Y221
E225 P226 V227 M228 L229 C230 L231 M232 S233 A234 I235 E236 V239 L242 I243 I247 D248 R249 G250 L251 TRP ASP LEU GLN ASN LYS ALA GLU ARG GLN ASN ASP ILE LEU VAL LYS TYR ARG HIS MET SER VAL PRO PRO GLU SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	171.64Å 176.88Å 104.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 3.10 49.25 – 3.09	Depositor EDS
% Data completeness (in resolution range)	58.3 (49.25-3.10) 59.0 (49.25-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.236 , 0.278 0.300 , 0.321	Depositor DCC
R_{free} test set	1752 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	82.4	Xtriage
Anisotropy	1.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 64.5	EDS
Estimated twinning fraction	0.045 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	4 of 35096 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13035	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG

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	0.32	0/1488	0.60	0/2019
1	B	0.32	0/1440	0.59	0/1951
1	C	0.35	0/1518	0.65	1/2062 (0.0%)
1	D	0.32	0/1443	0.57	0/1956
1	E	0.33	0/1518	0.64	2/2062 (0.1%)
1	F	0.31	0/1443	0.56	0/1956
1	G	0.31	0/1461	0.59	0/1983
1	H	0.30	0/1456	0.58	0/1974
1	I	0.30	0/1440	0.57	0/1951
All	All	0.32	0/13207	0.60	3/17914 (0.0%)

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	C	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	251	LEU	CA-CB-CG	5.87	128.80	115.30
1	C	251	LEU	CA-CB-CG	5.82	128.68	115.30
1	E	42	LEU	CA-CB-CG	5.15	127.15	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	91	ARG	Peptide

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	1467	0	1450	77	0
1	B	1423	0	1410	63	0
1	C	1494	0	1475	82	0
1	D	1424	0	1407	69	0
1	E	1494	0	1475	73	0
1	F	1424	0	1407	76	0
1	G	1440	0	1424	69	0
1	H	1437	0	1420	70	0
1	I	1423	0	1410	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
All	All	13035	0	12878	544	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 21.

All (544) 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:177:ARG:NH1	1:I:97:GLU:OE2	2.04	0.90
1:G:98:ARG:HG3	1:G:101:LEU:HD12	1.55	0.85
1:F:97:GLU:OE2	1:H:177:ARG:NH1	2.10	0.84
1:H:56:ILE:HG13	1:H:141:SER:HA	1.59	0.83
1:G:170:ASP:HB2	1:G:196:ILE:HB	1.61	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:ASP:HB2	1:F:196:ILE:HB	1.62	0.81
1:F:205:VAL:O	1:F:216:GLU:HA	1.81	0.80
1:C:56:ILE:HG13	1:C:141:SER:HA	1.63	0.80
1:E:60:THR:HG23	1:E:62:GLN:H	1.47	0.79
1:A:196:ILE:HD13	1:A:227:VAL:HG22	1.65	0.79
1:E:175:ASN:ND2	1:E:191:ASN:OD1	2.15	0.79
1:E:177:ARG:NH1	1:H:97:GLU:OE2	2.17	0.78
1:C:205:VAL:O	1:C:216:GLU:HA	1.83	0.77
1:I:60:THR:HG23	1:I:62:GLN:H	1.48	0.77
1:I:205:VAL:O	1:I:216:GLU:HA	1.84	0.77
1:A:186:ILE:HD12	1:B:95:PRO:HB2	1.67	0.77
1:F:196:ILE:HD13	1:F:227:VAL:HG22	1.67	0.76
1:C:194:LYS:HE3	1:C:234:ALA:HA	1.68	0.75
1:A:56:ILE:HG22	1:A:80:THR:HG23	1.68	0.75
1:G:56:ILE:HG13	1:G:141:SER:HA	1.69	0.74
1:D:56:ILE:HG13	1:D:141:SER:HA	1.70	0.74
1:D:56:ILE:HG22	1:D:80:THR:HG23	1.70	0.74
1:B:196:ILE:HD13	1:B:227:VAL:HG22	1.68	0.74
1:I:143:ILE:HD11	1:I:175:ASN:HB2	1.70	0.73
1:E:56:ILE:HG13	1:E:141:SER:HA	1.70	0.73
1:D:186:ILE:HD12	1:C:95:PRO:HB2	1.70	0.73
1:H:205:VAL:O	1:H:216:GLU:HA	1.89	0.73
1:D:170:ASP:HB2	1:D:196:ILE:HB	1.72	0.72
1:G:237:THR:HA	1:G:240:ILE:HD12	1.72	0.72
1:B:205:VAL:O	1:B:216:GLU:HA	1.91	0.71
1:A:205:VAL:O	1:A:216:GLU:HA	1.91	0.71
1:H:175:ASN:ND2	1:H:191:ASN:OD1	2.23	0.70
1:C:137:MET:HB3	1:C:179:VAL:HG13	1.72	0.70
1:A:53:VAL:HG21	1:A:83:LEU:HD12	1.74	0.70
1:A:62:GLN:OE1	1:B:64:LYS:NZ	2.25	0.70
1:H:148:ASN:HB3	1:H:151:SER:HB3	1.74	0.70
1:G:56:ILE:HG22	1:G:80:THR:HG23	1.74	0.69
1:F:103:ASN:ND2	1:H:139:GLU:OE2	2.26	0.69
1:D:196:ILE:HD13	1:D:227:VAL:HG22	1.74	0.69
1:D:48:LYS:HA	1:D:92:TRP:HB3	1.73	0.69
1:A:170:ASP:HB2	1:A:196:ILE:HB	1.74	0.69
1:I:170:ASP:HB2	1:I:196:ILE:HB	1.74	0.69
1:C:170:ASP:O	1:C:195:THR:HA	1.93	0.68
1:G:175:ASN:ND2	1:G:191:ASN:OD1	2.26	0.68
1:A:56:ILE:HG13	1:A:141:SER:HA	1.75	0.68
1:E:175:ASN:HD21	1:H:85:THR:HG21	1.58	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:53:VAL:HG21	1:H:83:LEU:HD12	1.76	0.67
1:D:97:GLU:OE2	1:F:177:ARG:NH1	2.28	0.67
1:I:176:LEU:HB3	1:I:242:LEU:HD11	1.76	0.67
1:G:76:PRO:HG2	1:G:228:MET:HB2	1.77	0.67
1:A:172:ILE:HD11	1:A:227:VAL:HG13	1.78	0.66
1:D:78:SER:OG	1:F:143:ILE:O	2.13	0.66
1:G:196:ILE:HD13	1:G:227:VAL:HG22	1.77	0.66
1:F:56:ILE:HG13	1:F:141:SER:HA	1.76	0.66
1:C:245:ASP:HB3	1:C:249:ARG:HH21	1.60	0.66
1:F:110:ILE:HG22	1:H:133:ALA:HB2	1.78	0.66
1:I:157:ARG:HH22	1:I:206:PHE:HB2	1.61	0.65
1:I:172:ILE:HD11	1:I:227:VAL:HG13	1.77	0.65
1:H:170:ASP:HB2	1:H:196:ILE:HB	1.78	0.65
1:F:226:PRO:HB2	1:F:229:LEU:HB2	1.78	0.65
1:H:176:LEU:HB3	1:H:242:LEU:HD11	1.79	0.65
1:G:140:GLY:HA3	1:G:175:ASN:O	1.96	0.65
1:B:177:ARG:NH1	1:E:97:GLU:OE2	2.30	0.65
1:E:205:VAL:O	1:E:216:GLU:HA	1.97	0.64
1:I:175:ASN:ND2	1:I:191:ASN:OD1	2.27	0.64
1:G:55:ASN:HA	1:G:80:THR:HG21	1.79	0.64
1:C:169:LEU:HA	1:C:196:ILE:O	1.96	0.64
1:G:205:VAL:O	1:G:216:GLU:HA	1.97	0.64
1:A:97:GLU:OE2	1:I:177:ARG:NH1	2.30	0.64
1:H:157:ARG:HH22	1:H:206:PHE:HB2	1.62	0.64
1:D:172:ILE:HG13	1:D:196:ILE:HD11	1.80	0.64
1:C:171:GLN:HG2	1:C:195:THR:HG22	1.80	0.63
1:D:245:ASP:HB3	1:D:249:ARG:HH21	1.64	0.63
1:H:237:THR:HA	1:H:240:ILE:HD12	1.81	0.63
1:E:98:ARG:NH1	1:H:107:GLU:OE1	2.32	0.62
1:B:137:MET:HB3	1:B:179:VAL:HG13	1.80	0.62
1:G:164:ASP:OD2	1:G:166:GLN:NE2	2.33	0.62
1:G:176:LEU:HB3	1:G:242:LEU:HD11	1.81	0.62
1:D:205:VAL:O	1:D:216:GLU:HA	1.99	0.62
1:D:147:SER:HA	1:D:149:VAL:HG23	1.81	0.62
1:E:48:LYS:HG2	1:E:92:TRP:HB2	1.80	0.62
1:C:194:LYS:NZ	1:C:233:SER:OG	2.32	0.62
1:B:56:ILE:HG13	1:B:141:SER:HA	1.82	0.61
1:A:172:ILE:HG13	1:A:196:ILE:HD11	1.83	0.61
1:F:143:ILE:HD11	1:F:175:ASN:HB2	1.81	0.61
1:I:180:ASN:HB2	1:I:187:LEU:HD11	1.83	0.61
1:D:137:MET:HB3	1:D:179:VAL:HG13	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:ILE:HD11	1:D:227:VAL:HG13	1.83	0.61
1:E:55:ASN:HB3	1:E:57:GLN:HE21	1.63	0.61
1:D:99:GLN:HG2	1:F:177:ARG:HH22	1.66	0.61
1:A:157:ARG:HH22	1:A:206:PHE:HB2	1.65	0.60
1:C:56:ILE:HG22	1:C:80:THR:HG23	1.82	0.60
1:E:92:TRP:HE3	1:E:92:TRP:H	1.48	0.60
1:C:53:VAL:HG21	1:C:83:LEU:HD12	1.82	0.60
1:B:178:VAL:HG23	1:B:242:LEU:HD22	1.82	0.60
1:H:60:THR:HG23	1:H:62:GLN:H	1.65	0.60
1:C:64:LYS:HG2	1:C:74:ALA:HA	1.83	0.60
1:G:49:ILE:HB	1:G:252:TRP:HZ3	1.65	0.60
1:E:56:ILE:HG22	1:E:80:THR:HG23	1.84	0.59
1:G:98:ARG:NH2	1:I:110:ILE:HD13	2.17	0.59
1:A:64:LYS:NZ	1:I:62:GLN:OE1	2.34	0.59
1:D:149:VAL:HG13	1:C:226:PRO:HG3	1.83	0.59
1:B:176:LEU:HB3	1:B:242:LEU:HD11	1.84	0.59
1:F:226:PRO:HG2	1:F:229:LEU:HD12	1.84	0.59
1:E:248:ASP:OD1	1:E:248:ASP:N	2.36	0.59
1:B:172:ILE:HD11	1:B:227:VAL:HG13	1.83	0.59
1:A:249:ARG:H	1:A:250:GLY:HA2	1.67	0.59
1:D:172:ILE:O	1:D:193:SER:HA	2.02	0.59
1:G:79:ALA:O	1:G:80:THR:OG1	2.18	0.59
1:E:79:ALA:O	1:E:80:THR:OG1	2.19	0.59
1:C:51:VAL:HG11	1:C:87:LEU:HD13	1.85	0.58
1:D:62:GLN:OE1	1:C:64:LYS:NZ	2.32	0.58
1:H:79:ALA:O	1:H:80:THR:OG1	2.18	0.58
1:C:48:LYS:HG2	1:C:92:TRP:HB2	1.84	0.58
1:D:137:MET:HE1	1:C:104:LEU:HA	1.84	0.58
1:C:147:SER:HB2	1:C:148:ASN:HA	1.85	0.58
1:C:177:ARG:NH1	1:G:97:GLU:OE2	2.37	0.58
1:F:172:ILE:HD11	1:F:227:VAL:HG13	1.86	0.58
1:D:60:THR:HG23	1:D:62:GLN:HB2	1.85	0.58
1:D:177:ARG:HH22	1:C:99:GLN:HG2	1.67	0.58
1:D:53:VAL:HG21	1:D:83:LEU:HD12	1.86	0.58
1:G:64:LYS:HG2	1:G:74:ALA:HA	1.85	0.58
1:H:173:ALA:HA	1:H:192:THR:O	2.04	0.57
1:F:48:LYS:HD3	1:F:94:ILE:HD11	1.86	0.57
1:F:178:VAL:HG23	1:F:242:LEU:HD22	1.86	0.57
1:A:248:ASP:OD1	1:A:248:ASP:N	2.37	0.57
1:E:170:ASP:O	1:E:195:THR:HA	2.04	0.57
1:G:248:ASP:OD1	1:G:248:ASP:N	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:VAL:HG11	1:C:171:GLN:HG3	1.85	0.57
1:F:149:VAL:HG21	1:F:171:GLN:HG3	1.87	0.57
1:B:170:ASP:HB2	1:B:196:ILE:HB	1.87	0.56
1:A:68:ALA:HA	1:I:65:PRO:HB3	1.88	0.56
1:H:143:ILE:HD11	1:H:175:ASN:HB2	1.86	0.56
1:C:170:ASP:HB2	1:C:196:ILE:HB	1.86	0.56
1:A:99:GLN:HG2	1:I:177:ARG:HH22	1.71	0.56
1:E:143:ILE:HG12	1:H:78:SER:HB2	1.87	0.56
1:E:161:ILE:HG13	1:E:205:VAL:HG22	1.88	0.56
1:A:143:ILE:HD11	1:A:175:ASN:HB2	1.87	0.56
1:G:148:ASN:HB3	1:G:151:SER:HB3	1.88	0.56
1:I:140:GLY:HA3	1:I:175:ASN:O	2.06	0.56
1:B:98:ARG:NH2	1:E:110:ILE:HD13	2.21	0.55
1:C:167:TYR:HA	1:C:198:SER:O	2.07	0.55
1:D:53:VAL:HG22	1:D:80:THR:HG22	1.87	0.55
1:F:60:THR:HG23	1:F:62:GLN:H	1.72	0.55
1:H:55:ASN:HA	1:H:80:THR:HG21	1.89	0.55
1:E:179:VAL:HB	1:E:186:ILE:HG12	1.88	0.55
1:A:46:THR:HB	1:A:47:GLY:HA3	1.87	0.55
1:B:180:ASN:HB2	1:B:187:LEU:HD11	1.87	0.55
1:A:55:ASN:HA	1:A:80:THR:HG21	1.89	0.55
1:A:147:SER:HA	1:A:149:VAL:HG23	1.88	0.55
1:C:133:ALA:HB1	1:G:111:ILE:HG12	1.87	0.55
1:B:70:ASN:HA	1:E:69:SER:HB2	1.89	0.55
1:H:200:GLU:HB3	1:H:222:THR:HG22	1.89	0.55
1:B:157:ARG:HH22	1:B:206:PHE:HB2	1.72	0.54
1:D:175:ASN:ND2	1:D:191:ASN:OD1	2.30	0.54
1:C:179:VAL:HG21	1:G:97:GLU:HG3	1.89	0.54
1:D:99:GLN:HB3	1:D:100:GLY:HA3	1.88	0.54
1:A:249:ARG:N	1:A:250:GLY:HA2	2.22	0.54
1:D:151:SER:OG	1:C:222:THR:OG1	2.24	0.54
1:D:176:LEU:HB3	1:D:242:LEU:HD11	1.88	0.54
1:G:157:ARG:HH22	1:G:206:PHE:HB2	1.72	0.54
1:B:98:ARG:HG3	1:B:101:LEU:HD12	1.89	0.54
1:D:73:THR:HG21	1:D:77:GLN:HE22	1.72	0.54
1:F:48:LYS:HA	1:F:92:TRP:HB2	1.89	0.54
1:I:226:PRO:HB2	1:I:229:LEU:HG	1.89	0.54
1:G:82:MET:HB3	1:G:235:ILE:HG21	1.89	0.54
1:D:79:ALA:O	1:D:80:THR:OG1	2.21	0.54
1:E:170:ASP:HB2	1:E:196:ILE:HB	1.90	0.54
1:E:150:LYS:HG3	1:H:221:TYR:HE1	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:VAL:HG12	1:C:219:VAL:HG12	1.89	0.54
1:F:110:ILE:HD13	1:H:98:ARG:NH2	2.23	0.53
1:E:237:THR:HA	1:E:240:ILE:HD12	1.90	0.53
1:A:137:MET:HE1	1:B:104:LEU:HA	1.90	0.53
1:B:172:ILE:HG13	1:B:196:ILE:HD11	1.90	0.53
1:H:226:PRO:HB2	1:H:229:LEU:HB2	1.91	0.53
1:A:226:PRO:O	1:A:229:LEU:N	2.39	0.53
1:E:175:ASN:ND2	1:H:85:THR:HG21	2.23	0.53
1:D:111:ILE:HG12	1:F:133:ALA:HB1	1.89	0.53
1:H:248:ASP:OD1	1:H:248:ASP:N	2.42	0.53
1:E:64:LYS:HD3	1:E:74:ALA:HA	1.91	0.53
1:G:150:LYS:HG3	1:I:221:TYR:HE1	1.74	0.53
1:B:60:THR:OG1	1:B:145:TYR:N	2.42	0.53
1:F:97:GLU:HG2	1:H:186:ILE:HG12	1.91	0.52
1:H:196:ILE:HD13	1:H:227:VAL:HG22	1.90	0.52
1:B:174:VAL:O	1:B:191:ASN:HA	2.08	0.52
1:H:56:ILE:HG22	1:H:80:THR:HG23	1.92	0.52
1:C:92:TRP:H	1:C:92:TRP:HE3	1.56	0.52
1:I:98:ARG:NH2	1:I:132:THR:O	2.42	0.52
1:E:196:ILE:HG12	1:E:230:CYS:SG	2.49	0.52
1:E:180:ASN:HB2	1:E:187:LEU:HD11	1.91	0.52
1:D:53:VAL:HG11	1:D:84:VAL:HG22	1.92	0.52
1:B:186:ILE:HD11	1:E:97:GLU:HA	1.90	0.52
1:C:45:PRO:HG3	1:C:92:TRP:CZ2	2.44	0.52
1:F:110:ILE:HG21	1:H:98:ARG:NH2	2.24	0.52
1:F:175:ASN:ND2	1:F:191:ASN:OD1	2.43	0.52
1:H:60:THR:O	1:H:62:GLN:NE2	2.42	0.52
1:I:88:LYS:HB2	1:I:95:PRO:HG2	1.90	0.52
1:G:60:THR:HG23	1:G:62:GLN:H	1.75	0.52
1:C:145:TYR:OH	1:C:170:ASP:OD2	2.15	0.51
1:I:151:SER:HB2	1:I:168:GLN:HA	1.91	0.51
1:F:104:LEU:HD11	1:H:184:GLY:HA2	1.92	0.51
1:C:177:ARG:HG2	1:C:189:SER:HB2	1.92	0.51
1:F:226:PRO:O	1:F:229:LEU:N	2.41	0.51
1:C:151:SER:HB2	1:C:168:GLN:HA	1.92	0.51
1:A:133:ALA:HB1	1:B:111:ILE:HG12	1.93	0.51
1:C:189:SER:OG	1:G:85:THR:HG22	2.11	0.51
1:B:58:ASP:OD1	1:B:60:THR:HG22	2.10	0.51
1:G:143:ILE:O	1:I:78:SER:OG	2.23	0.51
1:D:174:VAL:O	1:D:191:ASN:HA	2.11	0.51
1:D:171:GLN:HG2	1:D:195:THR:HG22	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASN:HA	1:A:247:ILE:HB	1.92	0.51
1:A:110:ILE:HG22	1:I:133:ALA:HB2	1.93	0.51
1:I:232:MET:HA	1:I:235:ILE:HG22	1.91	0.51
1:H:226:PRO:O	1:H:229:LEU:N	2.42	0.51
1:D:133:ALA:HB1	1:C:111:ILE:HG12	1.92	0.51
1:E:99:GLN:HB3	1:E:100:GLY:HA3	1.91	0.51
1:C:79:ALA:O	1:C:80:THR:OG1	2.26	0.51
1:E:84:VAL:HG13	1:E:95:PRO:HB3	1.93	0.51
1:G:246:GLY:O	1:G:252:TRP:NE1	2.42	0.50
1:A:63:PHE:H	1:B:72:SER:HB3	1.76	0.50
1:I:88:LYS:HD3	1:I:95:PRO:HD2	1.93	0.50
1:H:140:GLY:HA3	1:H:175:ASN:O	2.11	0.50
1:D:52:SER:HB2	1:D:134:ALA:HB3	1.92	0.50
1:A:177:ARG:NH1	1:B:97:GLU:OE2	2.44	0.50
1:F:56:ILE:HG22	1:F:80:THR:HG23	1.94	0.50
1:A:239:VAL:O	1:A:243:ILE:HG13	2.12	0.50
1:E:83:LEU:HD23	1:E:235:ILE:HD11	1.94	0.50
1:B:98:ARG:NH1	1:E:107:GLU:OE1	2.45	0.50
1:B:149:VAL:HG11	1:B:171:GLN:HG3	1.93	0.50
1:C:248:ASP:OD1	1:C:248:ASP:N	2.43	0.50
1:F:145:TYR:HA	1:F:171:GLN:O	2.12	0.50
1:C:201:VAL:O	1:C:220:GLY:HA2	2.11	0.50
1:F:79:ALA:O	1:F:80:THR:OG1	2.27	0.50
1:B:177:ARG:HB3	1:B:189:SER:HB3	1.93	0.50
1:D:183:THR:HB	1:C:132:THR:HG23	1.92	0.49
1:A:87:LEU:O	1:A:93:PHE:HB2	2.12	0.49
1:C:106:ASN:OD1	1:C:109:LYS:NZ	2.45	0.49
1:C:193:SER:OG	1:C:193:SER:O	2.27	0.49
1:A:149:VAL:HG13	1:B:226:PRO:HG3	1.94	0.49
1:I:52:SER:O	1:I:137:MET:HG3	2.12	0.49
1:F:243:ILE:O	1:F:247:ILE:HG13	2.12	0.49
1:A:142:ILE:HD13	1:A:231:LEU:HD11	1.95	0.49
1:H:172:ILE:O	1:H:193:SER:HA	2.12	0.49
1:B:167:TYR:HA	1:B:198:SER:O	2.13	0.49
1:D:226:PRO:O	1:D:229:LEU:N	2.45	0.49
1:F:232:MET:HA	1:F:235:ILE:HG22	1.95	0.49
1:D:58:ASP:OD1	1:D:60:THR:HG22	2.13	0.49
1:F:97:GLU:HB3	1:F:98:ARG:H	1.53	0.48
1:B:98:ARG:HH22	1:E:110:ILE:HG21	1.78	0.48
1:D:98:ARG:NH2	1:C:110:ILE:HG21	2.28	0.48
1:G:143:ILE:HD11	1:G:175:ASN:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:LEU:HA	1:H:137:MET:HE1	1.94	0.48
1:G:226:PRO:O	1:G:229:LEU:N	2.45	0.48
1:H:50:PHE:HD1	1:H:94:ILE:HB	1.79	0.48
1:F:107:GLU:HA	1:F:110:ILE:HD12	1.94	0.48
1:D:137:MET:HB2	1:D:137:MET:HE2	1.74	0.48
1:A:191:ASN:OD1	1:B:85:THR:HG21	2.13	0.48
1:G:99:GLN:HB3	1:G:100:GLY:HA3	1.95	0.48
1:G:245:ASP:HB3	1:G:249:ARG:HH21	1.78	0.48
1:G:52:SER:O	1:G:137:MET:HG3	2.13	0.48
1:G:133:ALA:HB2	1:I:110:ILE:HG22	1.96	0.48
1:A:60:THR:HG23	1:A:62:GLN:HB2	1.95	0.48
1:C:246:GLY:O	1:C:250:GLY:HA2	2.12	0.48
1:A:99:GLN:HB3	1:A:100:GLY:HA3	1.96	0.48
1:C:225:GLU:HA	1:C:226:PRO:HD3	1.68	0.48
1:A:79:ALA:O	1:A:80:THR:OG1	2.27	0.48
1:F:176:LEU:HB3	1:F:242:LEU:HD11	1.95	0.48
1:B:232:MET:HA	1:B:235:ILE:HG22	1.95	0.48
1:H:107:GLU:HA	1:H:110:ILE:HD12	1.96	0.48
1:C:55:ASN:HA	1:C:80:THR:HG21	1.94	0.48
1:H:226:PRO:HG2	1:H:229:LEU:HD12	1.95	0.48
1:A:196:ILE:HG12	1:A:230:CYS:SG	2.53	0.48
1:F:107:GLU:CD	1:H:98:ARG:HH12	2.16	0.48
1:E:98:ARG:NH2	1:H:110:ILE:HD13	2.29	0.48
1:E:91:ARG:HA	1:E:93:PHE:N	2.29	0.48
1:F:99:GLN:HB3	1:F:100:GLY:HA3	1.96	0.48
1:D:245:ASP:O	1:D:249:ARG:HB2	2.14	0.47
1:D:96:LEU:HD12	1:D:98:ARG:NH1	2.28	0.47
1:D:177:ARG:NH1	1:C:97:GLU:OE2	2.47	0.47
1:F:60:THR:HG23	1:F:62:GLN:N	2.30	0.47
1:G:83:LEU:HB2	1:G:235:ILE:HD11	1.96	0.47
1:C:244:ASN:O	1:C:247:ILE:HB	2.14	0.47
1:F:64:LYS:HD3	1:F:74:ALA:HA	1.94	0.47
1:I:147:SER:HA	1:I:149:VAL:HG23	1.96	0.47
1:D:143:ILE:O	1:C:78:SER:OG	2.20	0.47
1:A:243:ILE:O	1:A:247:ILE:N	2.46	0.47
1:A:151:SER:HB2	1:A:168:GLN:HG2	1.97	0.47
1:F:98:ARG:HG3	1:F:101:LEU:HD12	1.95	0.47
1:C:60:THR:OG1	1:C:145:TYR:N	2.47	0.47
1:A:178:VAL:HG23	1:A:242:LEU:HD13	1.96	0.47
1:E:55:ASN:HA	1:E:80:THR:HG21	1.96	0.47
1:F:78:SER:HB2	1:F:82:MET:SD	2.55	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:VAL:HA	1:C:186:ILE:HA	1.97	0.47
1:C:51:VAL:HG13	1:C:95:PRO:HA	1.97	0.47
1:C:91:ARG:HA	1:C:93:PHE:N	2.29	0.47
1:F:53:VAL:HG21	1:F:83:LEU:HD12	1.97	0.47
1:E:175:ASN:HA	1:E:190:VAL:O	2.15	0.47
1:I:235:ILE:O	1:I:239:VAL:HG23	2.15	0.47
1:I:99:GLN:HB3	1:I:100:GLY:HA3	1.97	0.47
1:A:64:LYS:HD3	1:A:74:ALA:HA	1.97	0.46
1:G:138:VAL:HG22	1:G:178:VAL:HG22	1.97	0.46
1:E:97:GLU:HB3	1:E:98:ARG:H	1.53	0.46
1:G:60:THR:HG23	1:G:62:GLN:N	2.29	0.46
1:B:245:ASP:HB3	1:B:249:ARG:HH21	1.80	0.46
1:C:172:ILE:HD11	1:C:196:ILE:HD11	1.97	0.46
1:B:147:SER:HA	1:B:149:VAL:HG23	1.96	0.46
1:F:55:ASN:HA	1:F:80:THR:HG21	1.97	0.46
1:C:97:GLU:HB3	1:C:98:ARG:H	1.53	0.46
1:F:149:VAL:HG11	1:F:171:GLN:HG3	1.97	0.46
1:A:143:ILE:O	1:B:78:SER:OG	2.15	0.46
1:D:138:VAL:HG22	1:D:178:VAL:HG22	1.98	0.46
1:G:177:ARG:HG2	1:G:189:SER:HB2	1.97	0.46
1:B:97:GLU:HB3	1:B:98:ARG:H	1.53	0.46
1:A:51:VAL:HG21	1:A:87:LEU:HD13	1.98	0.46
1:H:159:PHE:HA	1:H:160:GLY:HA2	1.51	0.46
1:G:199:TYR:CZ	1:G:223:SER:HB3	2.50	0.46
1:D:235:ILE:O	1:D:239:VAL:HG23	2.15	0.46
1:A:84:VAL:HG13	1:A:95:PRO:HB3	1.97	0.46
1:B:91:ARG:HA	1:B:93:PHE:N	2.30	0.46
1:I:55:ASN:HA	1:I:80:THR:HG21	1.98	0.46
1:B:60:THR:HG23	1:B:62:GLN:HB2	1.96	0.46
1:B:171:GLN:HG2	1:B:195:THR:HG22	1.98	0.46
1:B:164:ASP:OD1	1:B:202:GLN:HB2	2.16	0.46
1:G:91:ARG:HA	1:G:93:PHE:N	2.31	0.46
1:H:99:GLN:HB3	1:H:100:GLY:HA3	1.98	0.46
1:A:226:PRO:HG2	1:A:229:LEU:HD12	1.98	0.46
1:C:204:GLY:HA2	1:C:217:GLY:O	2.16	0.46
1:E:159:PHE:HA	1:E:160:GLY:HA2	1.43	0.46
1:C:65:PRO:HB3	1:G:68:ALA:HA	1.97	0.46
1:I:194:LYS:HG3	1:I:234:ALA:HB2	1.98	0.46
1:D:104:LEU:O	1:D:108:ARG:HG3	2.16	0.46
1:A:97:GLU:HG3	1:I:179:VAL:HG21	1.97	0.45
1:I:91:ARG:HA	1:I:93:PHE:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:GLU:HA	1:E:110:ILE:HD12	1.98	0.45
1:D:72:SER:HB3	1:F:63:PHE:HB2	1.97	0.45
1:B:52:SER:HB2	1:B:134:ALA:HB3	1.98	0.45
1:G:186:ILE:CG1	1:I:97:GLU:HG2	2.46	0.45
1:D:226:PRO:HB2	1:D:229:LEU:HB2	1.98	0.45
1:D:60:THR:OG1	1:D:145:TYR:N	2.48	0.45
1:C:83:LEU:HD11	1:C:138:VAL:HG11	1.98	0.45
1:C:249:ARG:HB3	1:C:250:GLY:C	2.37	0.45
1:F:96:LEU:HD22	1:F:96:LEU:HA	1.65	0.45
1:B:226:PRO:O	1:B:229:LEU:N	2.49	0.45
1:I:148:ASN:HB3	1:I:151:SER:HB3	1.99	0.45
1:E:50:PHE:HD1	1:E:94:ILE:HB	1.82	0.45
1:I:208:PHE:HD1	1:I:208:PHE:HA	1.67	0.45
1:G:101:LEU:O	1:G:101:LEU:HD23	2.17	0.45
1:I:232:MET:O	1:I:236:GLU:N	2.49	0.45
1:I:167:TYR:HA	1:I:198:SER:O	2.17	0.45
1:E:53:VAL:HG22	1:E:80:THR:HG22	1.98	0.45
1:A:46:THR:CB	1:A:47:GLY:HA3	2.46	0.45
1:E:51:VAL:HG11	1:E:87:LEU:HD13	1.99	0.45
1:F:82:MET:HE2	1:F:232:MET:HB2	1.99	0.45
1:I:177:ARG:HB3	1:I:189:SER:HB3	1.99	0.45
1:F:94:ILE:O	1:F:96:LEU:HD23	2.17	0.45
1:B:225:GLU:HA	1:B:226:PRO:HD3	1.78	0.45
1:D:76:PRO:HG2	1:D:228:MET:HA	1.98	0.45
1:A:159:PHE:HA	1:A:160:GLY:HA2	1.56	0.45
1:A:225:GLU:HA	1:A:226:PRO:HD3	1.64	0.44
1:H:97:GLU:HB3	1:H:98:ARG:H	1.48	0.44
1:F:107:GLU:OE1	1:H:98:ARG:NH1	2.51	0.44
1:B:59:GLU:OE1	1:E:78:SER:HA	2.18	0.44
1:B:88:LYS:HA	1:B:88:LYS:HD2	1.85	0.44
1:D:157:ARG:HA	1:D:162:GLY:HA2	1.99	0.44
1:B:172:ILE:O	1:B:193:SER:HA	2.18	0.44
1:E:172:ILE:HG13	1:E:196:ILE:HD11	1.99	0.44
1:C:184:GLY:HA3	1:G:131:LEU:HD11	1.99	0.44
1:A:236:GLU:O	1:A:240:ILE:HG13	2.18	0.44
1:D:72:SER:HB3	1:F:63:PHE:N	2.33	0.44
1:H:64:LYS:HG2	1:H:74:ALA:HA	2.00	0.44
1:I:170:ASP:O	1:I:195:THR:HA	2.17	0.44
1:C:147:SER:HA	1:C:149:VAL:HG23	1.99	0.44
1:E:208:PHE:HA	1:E:208:PHE:HD1	1.69	0.44
1:A:246:GLY:HA3	1:A:252:TRP:CZ3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ILE:HD11	1:C:231:LEU:HD11	1.99	0.44
1:F:109:LYS:HA	1:F:112:ARG:NH1	2.33	0.44
1:F:196:ILE:HG12	1:F:230:CYS:SG	2.57	0.44
1:E:137:MET:HB3	1:E:179:VAL:HG13	2.00	0.44
1:D:91:ARG:HA	1:D:92:TRP:C	2.37	0.44
1:G:66:TYR:CG	1:G:67:PRO:HA	2.53	0.44
1:B:145:TYR:HD1	1:B:172:ILE:HG12	1.82	0.43
1:G:178:VAL:HG23	1:G:242:LEU:HD13	1.99	0.43
1:G:104:LEU:O	1:G:108:ARG:HG3	2.18	0.43
1:A:76:PRO:HG2	1:A:228:MET:HA	2.00	0.43
1:G:159:PHE:HA	1:G:160:GLY:HA2	1.50	0.43
1:C:45:PRO:HG3	1:C:92:TRP:HZ2	1.83	0.43
1:C:133:ALA:CB	1:G:111:ILE:HG12	2.48	0.43
1:G:58:ASP:OD1	1:G:60:THR:HG22	2.18	0.43
1:E:250:GLY:O	1:E:252:TRP:CD1	2.71	0.43
1:F:56:ILE:CG2	1:F:80:THR:HG23	2.48	0.43
1:A:98:ARG:NH2	1:B:110:ILE:HG21	2.34	0.43
1:F:106:ASN:HA	1:F:109:LYS:NZ	2.33	0.43
1:E:194:LYS:HE3	1:E:234:ALA:HA	2.00	0.43
1:E:88:LYS:HA	1:E:88:LYS:HD2	1.69	0.43
1:G:157:ARG:HA	1:G:162:GLY:HA2	1.99	0.43
1:E:60:THR:HG23	1:E:62:GLN:N	2.24	0.43
1:D:157:ARG:HD3	1:C:216:GLU:OE1	2.19	0.43
1:F:97:GLU:HG2	1:H:186:ILE:CG1	2.49	0.43
1:H:157:ARG:HA	1:H:162:GLY:HA2	2.01	0.43
1:E:196:ILE:HD13	1:E:227:VAL:HG22	2.00	0.43
1:E:105:LEU:HA	1:E:105:LEU:HD23	1.76	0.43
1:F:137:MET:HE2	1:F:137:MET:HB2	1.87	0.43
1:E:63:PHE:HB2	1:H:72:SER:HB3	2.00	0.43
1:F:170:ASP:O	1:F:195:THR:HA	2.18	0.43
1:F:68:ALA:HA	1:H:65:PRO:HB3	2.01	0.43
1:G:175:ASN:HD21	1:I:85:THR:HG21	1.84	0.43
1:D:96:LEU:HD12	1:D:98:ARG:CZ	2.49	0.43
1:I:157:ARG:HA	1:I:162:GLY:HA2	1.99	0.43
1:B:151:SER:HB2	1:B:168:GLN:HA	2.01	0.43
1:G:105:LEU:HD23	1:G:105:LEU:HA	1.76	0.43
1:B:60:THR:O	1:B:62:GLN:NE2	2.51	0.43
1:C:196:ILE:HD13	1:C:227:VAL:HA	2.01	0.43
1:E:98:ARG:HH12	1:H:107:GLU:CD	2.21	0.43
1:C:244:ASN:HA	1:C:247:ILE:HG13	2.00	0.43
1:E:49:ILE:HD13	1:E:252:TRP:CE3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:LEU:HA	1:H:105:LEU:HD23	1.77	0.43
1:I:231:LEU:O	1:I:235:ILE:N	2.43	0.42
1:A:176:LEU:HD12	1:A:176:LEU:HA	1.77	0.42
1:E:50:PHE:CD1	1:E:94:ILE:HB	2.54	0.42
1:F:245:ASP:N	1:F:245:ASP:OD1	2.52	0.42
1:C:53:VAL:HG22	1:C:80:THR:HG22	2.00	0.42
1:G:51:VAL:HG11	1:G:87:LEU:HD13	2.01	0.42
1:B:99:GLN:HB3	1:B:100:GLY:HA3	2.01	0.42
1:D:189:SER:OG	1:C:85:THR:HG22	2.19	0.42
1:E:178:VAL:HG23	1:E:242:LEU:HD13	2.00	0.42
1:G:177:ARG:HG2	1:G:189:SER:CB	2.49	0.42
1:H:169:LEU:HA	1:H:196:ILE:O	2.19	0.42
1:B:137:MET:HE1	1:E:104:LEU:HA	2.00	0.42
1:C:226:PRO:O	1:C:229:LEU:N	2.44	0.42
1:B:159:PHE:HA	1:B:160:GLY:HA2	1.48	0.42
1:F:148:ASN:HB3	1:F:151:SER:HB3	2.01	0.42
1:A:97:GLU:HB3	1:A:98:ARG:H	1.53	0.42
1:A:157:ARG:HA	1:A:162:GLY:HA2	2.01	0.42
1:D:69:SER:O	1:D:72:SER:OG	2.37	0.42
1:F:130:SER:OG	1:F:131:LEU:N	2.53	0.42
1:E:42:LEU:HA	1:E:43:PRO:HD3	1.83	0.42
1:C:179:VAL:HB	1:C:186:ILE:HG12	2.01	0.42
1:F:140:GLY:HA3	1:F:175:ASN:O	2.19	0.42
1:B:137:MET:HB2	1:B:137:MET:HE2	1.87	0.42
1:A:75:VAL:HA	1:A:76:PRO:HD3	1.97	0.42
1:H:246:GLY:O	1:H:250:GLY:HA2	2.19	0.42
1:G:137:MET:HE3	1:G:181:VAL:HG22	2.00	0.42
1:G:52:SER:OG	1:G:98:ARG:NH1	2.46	0.42
1:A:186:ILE:HG12	1:B:97:GLU:HG2	2.01	0.42
1:E:106:ASN:O	1:E:110:ILE:HG13	2.20	0.42
1:C:172:ILE:O	1:C:193:SER:HA	2.20	0.42
1:C:146:GLU:OE1	1:G:228:MET:HE1	2.19	0.42
1:A:52:SER:HB2	1:A:98:ARG:HH11	1.85	0.42
1:F:91:ARG:HA	1:F:93:PHE:N	2.35	0.42
1:E:172:ILE:O	1:E:193:SER:HA	2.19	0.42
1:I:225:GLU:HA	1:I:226:PRO:HD3	1.58	0.42
1:D:157:ARG:HH22	1:D:206:PHE:HB2	1.85	0.42
1:A:138:VAL:HA	1:A:177:ARG:O	2.20	0.42
1:A:250:GLY:C	1:A:252:TRP:H	2.23	0.42
1:D:73:THR:HG21	1:D:77:GLN:NE2	2.34	0.42
1:I:56:ILE:HG13	1:I:141:SER:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:ASP:HB3	1:H:77:GLN:NE2	2.35	0.42
1:B:157:ARG:HA	1:B:162:GLY:HA2	2.02	0.42
1:G:105:LEU:O	1:G:109:LYS:HG3	2.20	0.42
1:H:250:GLY:C	1:H:252:TRP:H	2.24	0.42
1:B:175:ASN:HA	1:B:190:VAL:O	2.19	0.42
1:C:60:THR:HG23	1:C:62:GLN:H	1.85	0.42
1:F:51:VAL:HG22	1:F:53:VAL:HG12	2.02	0.42
1:E:194:LYS:HG2	1:E:234:ALA:HB2	2.02	0.42
1:F:76:PRO:HG2	1:F:228:MET:HA	2.01	0.42
1:A:52:SER:O	1:A:137:MET:HG3	2.19	0.41
1:E:46:THR:OG1	1:E:252:TRP:O	2.27	0.41
1:H:105:LEU:O	1:H:109:LYS:HG3	2.20	0.41
1:F:248:ASP:OD1	1:F:248:ASP:N	2.52	0.41
1:I:204:GLY:HA2	1:I:217:GLY:O	2.20	0.41
1:H:232:MET:O	1:H:235:ILE:HG22	2.19	0.41
1:C:60:THR:HG23	1:C:62:GLN:N	2.34	0.41
1:D:96:LEU:HA	1:D:96:LEU:HD22	1.67	0.41
1:C:159:PHE:HA	1:C:160:GLY:HA2	1.54	0.41
1:E:157:ARG:HA	1:E:162:GLY:HA2	2.02	0.41
1:A:172:ILE:CG1	1:A:196:ILE:HD11	2.49	0.41
1:I:58:ASP:OD1	1:I:60:THR:HG22	2.21	0.41
1:C:107:GLU:O	1:C:111:ILE:HG13	2.20	0.41
1:E:83:LEU:O	1:E:87:LEU:HG	2.20	0.41
1:A:171:GLN:HG2	1:A:195:THR:HG22	2.02	0.41
1:E:179:VAL:HG21	1:H:97:GLU:HG3	2.02	0.41
1:A:244:ASN:O	1:A:247:ILE:HB	2.21	0.41
1:F:157:ARG:HH22	1:F:206:PHE:HD2	1.67	0.41
1:H:215:LEU:HD23	1:H:216:GLU:N	2.36	0.41
1:D:178:VAL:HG23	1:D:242:LEU:HD22	2.03	0.41
1:H:178:VAL:HG12	1:H:187:LEU:HB2	2.03	0.41
1:E:174:VAL:HG12	1:E:176:LEU:HD13	2.02	0.41
1:H:98:ARG:HG3	1:H:101:LEU:HD12	2.03	0.41
1:D:97:GLU:HB3	1:D:98:ARG:H	1.56	0.41
1:B:178:VAL:HG23	1:B:242:LEU:HD13	2.02	0.41
1:A:176:LEU:HB3	1:A:242:LEU:HD11	2.02	0.41
1:I:243:ILE:O	1:I:247:ILE:HG13	2.20	0.41
1:I:249:ARG:N	1:I:250:GLY:HA2	2.36	0.41
1:B:94:ILE:HD13	1:B:94:ILE:HA	1.89	0.41
1:I:172:ILE:O	1:I:193:SER:HA	2.21	0.41
1:F:91:ARG:HA	1:F:92:TRP:C	2.41	0.41
1:D:175:ASN:HA	1:D:190:VAL:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:VAL:HG12	1:B:219:VAL:HG12	2.01	0.41
1:C:230:CYS:O	1:C:234:ALA:N	2.40	0.41
1:C:249:ARG:HB3	1:C:250:GLY:O	2.20	0.41
1:E:98:ARG:HD2	1:E:98:ARG:N	2.36	0.41
1:A:246:GLY:HA3	1:A:252:TRP:CH2	2.56	0.41
1:D:132:THR:HG23	1:F:183:THR:HB	2.02	0.41
1:C:180:ASN:HB2	1:C:187:LEU:HD11	2.02	0.41
1:I:50:PHE:HD1	1:I:50:PHE:HA	1.74	0.41
1:G:88:LYS:HD3	1:G:95:PRO:HD2	2.03	0.41
1:A:77:GLN:HB2	1:I:59:GLU:O	2.21	0.41
1:G:186:ILE:HG12	1:I:97:GLU:HG2	2.03	0.41
1:E:58:ASP:OD1	1:E:60:THR:HG22	2.20	0.41
1:F:110:ILE:HG21	1:H:98:ARG:HH22	1.85	0.41
1:E:186:ILE:HD12	1:H:95:PRO:HB2	2.02	0.41
1:I:169:LEU:HA	1:I:196:ILE:O	2.20	0.41
1:F:147:SER:HA	1:F:149:VAL:HG23	2.02	0.41
1:G:107:GLU:O	1:G:111:ILE:HG13	2.21	0.41
1:D:111:ILE:HG12	1:F:133:ALA:CB	2.50	0.41
1:H:249:ARG:HB3	1:H:250:GLY:C	2.40	0.41
1:F:199:TYR:CE1	1:F:223:SER:HB3	2.56	0.41
1:E:184:GLY:HA3	1:H:131:LEU:HD11	2.01	0.41
1:H:208:PHE:HD1	1:H:208:PHE:HA	1.68	0.41
1:A:245:ASP:O	1:A:249:ARG:HB2	2.21	0.41
1:I:93:PHE:HD1	1:I:93:PHE:HA	1.80	0.41
1:D:51:VAL:HG11	1:D:87:LEU:HD13	2.01	0.41
1:C:252:TRP:N	1:C:252:TRP:CD1	2.89	0.41
1:G:98:ARG:HA	1:G:101:LEU:HB2	2.02	0.40
1:C:138:VAL:HA	1:C:177:ARG:O	2.21	0.40
1:H:180:ASN:HB2	1:H:187:LEU:HD21	2.03	0.40
1:G:184:GLY:HA3	1:I:131:LEU:HD11	2.03	0.40
1:A:78:SER:HB2	1:A:82:MET:HG3	2.01	0.40
1:H:60:THR:HG23	1:H:62:GLN:N	2.34	0.40
1:C:96:LEU:O	1:C:98:ARG:HD2	2.21	0.40
1:G:226:PRO:HG2	1:G:229:LEU:HD12	2.02	0.40
1:F:75:VAL:HA	1:F:76:PRO:HD3	1.96	0.40
1:A:146:GLU:OE1	1:B:228:MET:HB3	2.21	0.40
1:A:172:ILE:CD1	1:A:196:ILE:HD11	2.51	0.40
1:F:149:VAL:HG11	1:F:171:GLN:HE21	1.86	0.40
1:G:53:VAL:HG21	1:G:83:LEU:HD12	2.03	0.40
1:B:91:ARG:HA	1:B:92:TRP:C	2.41	0.40
1:I:78:SER:O	1:I:81:ALA:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:ARG:HA	1:E:92:TRP:C	2.42	0.40
1:A:235:ILE:O	1:A:239:VAL:HG23	2.21	0.40
1:G:180:ASN:OD1	1:G:183:THR:N	2.44	0.40
1:D:85:THR:HG22	1:F:189:SER:OG	2.21	0.40
1:A:242:LEU:HA	1:A:242:LEU:HD23	1.84	0.40
1:A:190:VAL:HG12	1:A:192:THR:HG23	2.03	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	190/277 (69%)	177 (93%)	12 (6%)	1 (0%)	34	72
1	B	184/277 (66%)	175 (95%)	8 (4%)	1 (0%)	34	72
1	C	192/277 (69%)	176 (92%)	15 (8%)	1 (0%)	34	72
1	D	183/277 (66%)	173 (94%)	9 (5%)	1 (0%)	34	72
1	E	192/277 (69%)	174 (91%)	17 (9%)	1 (0%)	34	72
1	F	183/277 (66%)	174 (95%)	8 (4%)	1 (0%)	34	72
1	G	184/277 (66%)	174 (95%)	9 (5%)	1 (0%)	34	72
1	H	185/277 (67%)	174 (94%)	10 (5%)	1 (0%)	34	72
1	I	184/277 (66%)	176 (96%)	7 (4%)	1 (0%)	34	72
All	All	1677/2493 (67%)	1573 (94%)	95 (6%)	9 (0%)	34	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	149	VAL
1	A	149	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	149	VAL
1	C	149	VAL
1	E	149	VAL
1	F	149	VAL
1	G	149	VAL
1	H	149	VAL
1	I	149	VAL

5.3.2 Protein sidechains

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	157/236 (66%)	135 (86%)	22 (14%)	4	18
1	B	153/236 (65%)	130 (85%)	23 (15%)	3	15
1	C	160/236 (68%)	139 (87%)	21 (13%)	5	21
1	D	153/236 (65%)	137 (90%)	16 (10%)	8	31
1	E	160/236 (68%)	138 (86%)	22 (14%)	4	19
1	F	153/236 (65%)	132 (86%)	21 (14%)	4	19
1	G	155/236 (66%)	135 (87%)	20 (13%)	5	21
1	H	154/236 (65%)	134 (87%)	20 (13%)	5	21
1	I	153/236 (65%)	129 (84%)	24 (16%)	3	13
All	All	1398/2124 (66%)	1209 (86%)	189 (14%)	5	20

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	51	VAL
1	D	62	GLN
1	D	78	SER
1	D	80	THR
1	D	92	TRP
1	D	96	LEU
1	D	105	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	139	GLU
1	D	141	SER
1	D	146	GLU
1	D	164	ASP
1	D	176	LEU
1	D	193	SER
1	D	198	SER
1	D	208	PHE
1	D	216	GLU
1	A	49	ILE
1	A	53	VAL
1	A	56	ILE
1	A	62	GLN
1	A	69	SER
1	A	75	VAL
1	A	78	SER
1	A	80	THR
1	A	96	LEU
1	A	101	LEU
1	A	105	LEU
1	A	132	THR
1	A	139	GLU
1	A	146	GLU
1	A	165	THR
1	A	176	LEU
1	A	179	VAL
1	A	193	SER
1	A	198	SER
1	A	208	PHE
1	A	248	ASP
1	A	251	LEU
1	B	53	VAL
1	B	56	ILE
1	B	62	GLN
1	B	69	SER
1	B	77	GLN
1	B	78	SER
1	B	80	THR
1	B	93	PHE
1	B	96	LEU
1	B	98	ARG
1	B	105	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	139	GLU
1	B	141	SER
1	B	165	THR
1	B	176	LEU
1	B	177	ARG
1	B	179	VAL
1	B	193	SER
1	B	198	SER
1	B	208	PHE
1	B	228	MET
1	B	244	ASN
1	B	251	LEU
1	C	41	HIS
1	C	42	LEU
1	C	56	ILE
1	C	62	GLN
1	C	69	SER
1	C	78	SER
1	C	80	THR
1	C	96	LEU
1	C	97	GLU
1	C	105	LEU
1	C	139	GLU
1	C	141	SER
1	C	151	SER
1	C	176	LEU
1	C	179	VAL
1	C	193	SER
1	C	198	SER
1	C	208	PHE
1	C	248	ASP
1	C	251	LEU
1	C	252	TRP
1	E	42	LEU
1	E	49	ILE
1	E	53	VAL
1	E	56	ILE
1	E	69	SER
1	E	96	LEU
1	E	97	GLU
1	E	105	LEU
1	E	131	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	136	ILE
1	E	139	GLU
1	E	143	ILE
1	E	146	GLU
1	E	151	SER
1	E	165	THR
1	E	179	VAL
1	E	208	PHE
1	E	216	GLU
1	E	230	CYS
1	E	237	THR
1	E	248	ASP
1	E	251	LEU
1	F	49	ILE
1	F	50	PHE
1	F	51	VAL
1	F	53	VAL
1	F	56	ILE
1	F	64	LYS
1	F	78	SER
1	F	80	THR
1	F	93	PHE
1	F	96	LEU
1	F	98	ARG
1	F	105	LEU
1	F	130	SER
1	F	136	ILE
1	F	139	GLU
1	F	146	GLU
1	F	151	SER
1	F	165	THR
1	F	193	SER
1	F	208	PHE
1	F	248	ASP
1	G	49	ILE
1	G	50	PHE
1	G	56	ILE
1	G	62	GLN
1	G	77	GLN
1	G	93	PHE
1	G	130	SER
1	G	131	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	136	ILE
1	G	139	GLU
1	G	146	GLU
1	G	151	SER
1	G	165	THR
1	G	179	VAL
1	G	198	SER
1	G	208	PHE
1	G	214	LEU
1	G	228	MET
1	G	248	ASP
1	G	251	LEU
1	H	49	ILE
1	H	53	VAL
1	H	56	ILE
1	H	62	GLN
1	H	77	GLN
1	H	80	THR
1	H	93	PHE
1	H	101	LEU
1	H	130	SER
1	H	139	GLU
1	H	146	GLU
1	H	151	SER
1	H	165	THR
1	H	176	LEU
1	H	179	VAL
1	H	208	PHE
1	H	230	CYS
1	H	237	THR
1	H	248	ASP
1	H	251	LEU
1	I	49	ILE
1	I	50	PHE
1	I	53	VAL
1	I	56	ILE
1	I	62	GLN
1	I	78	SER
1	I	80	THR
1	I	93	PHE
1	I	96	LEU
1	I	105	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	130	SER
1	I	132	THR
1	I	136	ILE
1	I	139	GLU
1	I	146	GLU
1	I	151	SER
1	I	165	THR
1	I	176	LEU
1	I	177	ARG
1	I	179	VAL
1	I	208	PHE
1	I	230	CYS
1	I	248	ASP
1	I	251	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	102	GLN
1	E	57	GLN
1	F	102	GLN
1	F	135	ASN
1	F	175	ASN
1	F	191	ASN
1	I	102	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	196/277 (70%)	0.42	15 (7%) 16 5	43, 79, 133, 179	0
1	B	190/277 (68%)	0.46	12 (6%) 23 9	42, 82, 145, 179	0
1	C	198/277 (71%)	0.41	6 (3%) 54 29	31, 73, 143, 173	0
1	D	189/277 (68%)	0.38	10 (5%) 30 13	42, 77, 129, 161	0
1	E	198/277 (71%)	0.51	7 (3%) 48 23	31, 78, 142, 161	0
1	F	189/277 (68%)	0.43	3 (1%) 74 55	29, 77, 140, 166	0
1	G	190/277 (68%)	0.52	10 (5%) 30 13	40, 82, 146, 166	0
1	H	191/277 (68%)	0.37	9 (4%) 35 16	38, 80, 144, 164	0
1	I	190/277 (68%)	0.45	9 (4%) 35 16	42, 77, 150, 181	0
All	All	1731/2493 (69%)	0.44	81 (4%) 35 16	29, 78, 144, 181	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	LYS	4.7
1	B	206	PHE	4.0
1	H	247	ILE	3.6
1	E	157	ARG	3.5
1	H	135	ASN	3.5
1	F	78	SER	3.5
1	I	115	GLN	3.5
1	G	215	LEU	3.5
1	A	169	LEU	3.2
1	G	49	ILE	3.1
1	H	215	LEU	3.0
1	E	90	SER	3.0
1	D	158	TYR	3.0
1	G	206	PHE	3.0
1	A	209	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	215	LEU	2.8
1	A	199	TYR	2.8
1	G	216	GLU	2.8
1	H	216	GLU	2.8
1	E	89	ASP	2.8
1	D	157	ARG	2.7
1	I	215	LEU	2.7
1	B	98	ARG	2.7
1	G	157	ARG	2.7
1	D	197	LEU	2.7
1	B	157	ARG	2.7
1	A	148	ASN	2.7
1	A	78	SER	2.6
1	A	216	GLU	2.6
1	D	222	THR	2.6
1	D	247	ILE	2.6
1	I	114	ALA	2.6
1	A	51	VAL	2.6
1	E	158	TYR	2.6
1	H	113	ALA	2.6
1	C	199	TYR	2.6
1	G	143	ILE	2.6
1	D	159	PHE	2.6
1	C	216	GLU	2.6
1	C	52	SER	2.5
1	B	197	LEU	2.5
1	A	151	SER	2.5
1	A	149	VAL	2.5
1	B	216	GLU	2.5
1	B	113	ALA	2.4
1	C	215	LEU	2.4
1	H	206	PHE	2.4
1	B	133	ALA	2.4
1	C	90	SER	2.4
1	B	222	THR	2.4
1	F	150	LYS	2.4
1	G	149	VAL	2.4
1	A	206	PHE	2.4
1	E	216	GLU	2.3
1	I	251	LEU	2.3
1	F	104	LEU	2.3
1	B	228	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	167	TYR	2.3
1	G	115	GLN	2.2
1	B	215	LEU	2.2
1	D	78	SER	2.2
1	C	148	ASN	2.2
1	A	172	ILE	2.2
1	E	171	GLN	2.2
1	A	83	LEU	2.2
1	H	159	PHE	2.2
1	H	49	ILE	2.2
1	I	111	ILE	2.2
1	I	159	PHE	2.2
1	D	167	TYR	2.1
1	D	199	TYR	2.1
1	I	92	TRP	2.1
1	H	48	LYS	2.1
1	I	228	MET	2.1
1	D	206	PHE	2.1
1	B	199	TYR	2.1
1	G	197	LEU	2.1
1	E	167	TYR	2.1
1	I	90	SER	2.1
1	G	50	PHE	2.0
1	B	158	TYR	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	HG	H	501	1/1	0.96	0.09	-	166,166,166,166	1
2	HG	B	501	1/1	0.93	0.08	-	147,147,147,147	1
2	HG	F	501	1/1	0.98	0.12	-	130,130,130,130	1
2	HG	I	501	1/1	0.96	0.13	-	181,181,181,181	0
2	HG	D	501	1/1	0.96	0.11	-	115,115,115,115	1
2	HG	A	501	1/1	0.95	0.04	-	121,121,121,121	1
2	HG	E	501	1/1	0.96	0.12	-	127,127,127,127	0
2	HG	C	501	1/1	0.99	0.11	-	137,137,137,137	0
2	HG	G	501	1/1	0.97	0.09	-	161,161,161,161	0

6.5 Other polymers (i)

There are no such residues in this entry.