



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:50 PM GMT

PDB ID : 3VHN
Title : Y61G mutant of Cellulase 12A from thermotoga maritima
Authors : Cheng, Y.-S.; Ko, T.-P.; Guo, R.-T.; Liu, J.-R.
Deposited on : 2011-08-30
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

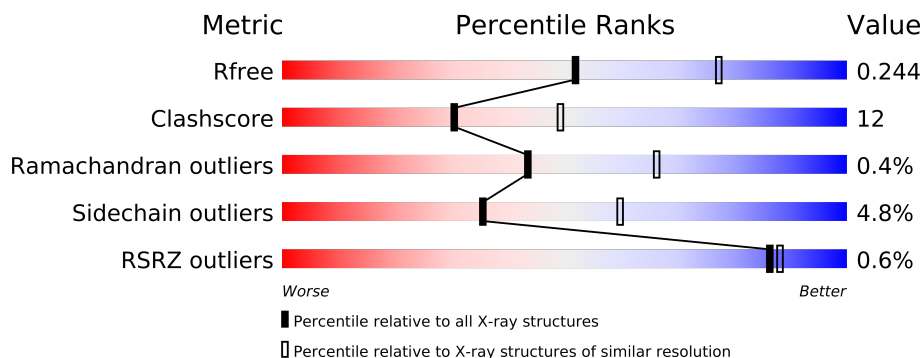
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	265	
1	B	265	
1	C	265	
1	D	265	
1	E	265	
1	F	265	
1	G	265	
1	H	265	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17709 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Endo-1,4-beta-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2079	1359	323	390	7			
1	B	256	Total	C	N	O	S	0	0	0
			2090	1365	327	391	7			
1	C	256	Total	C	N	O	S	0	0	0
			2090	1365	327	391	7			
1	D	255	Total	C	N	O	S	0	0	0
			2079	1359	323	390	7			
1	E	256	Total	C	N	O	S	0	0	0
			2090	1365	327	391	7			
1	F	255	Total	C	N	O	S	0	0	0
			2079	1359	323	390	7			
1	G	256	Total	C	N	O	S	0	0	0
			2090	1365	327	391	7			
1	H	255	Total	C	N	O	S	0	0	0
			2079	1359	323	390	7			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP Q60032
A	-6	GLY	-	EXPRESSION TAG	UNP Q60032
A	-5	HIS	-	EXPRESSION TAG	UNP Q60032
A	-4	HIS	-	EXPRESSION TAG	UNP Q60032
A	-3	HIS	-	EXPRESSION TAG	UNP Q60032
A	-2	HIS	-	EXPRESSION TAG	UNP Q60032
A	-1	HIS	-	EXPRESSION TAG	UNP Q60032
A	0	HIS	-	EXPRESSION TAG	UNP Q60032
A	61	GLY	TYR	ENGINEERED MUTATION	UNP Q60032
B	-7	MET	-	EXPRESSION TAG	UNP Q60032
B	-6	GLY	-	EXPRESSION TAG	UNP Q60032
B	-5	HIS	-	EXPRESSION TAG	UNP Q60032
B	-4	HIS	-	EXPRESSION TAG	UNP Q60032

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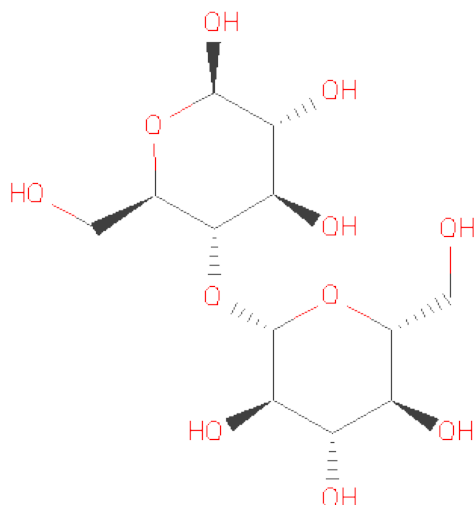
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	EXPRESSION TAG	UNP Q60032
B	-2	HIS	-	EXPRESSION TAG	UNP Q60032
B	-1	HIS	-	EXPRESSION TAG	UNP Q60032
B	0	HIS	-	EXPRESSION TAG	UNP Q60032
B	61	GLY	TYR	ENGINEERED MUTATION	UNP Q60032
C	-7	MET	-	EXPRESSION TAG	UNP Q60032
C	-6	GLY	-	EXPRESSION TAG	UNP Q60032
C	-5	HIS	-	EXPRESSION TAG	UNP Q60032
C	-4	HIS	-	EXPRESSION TAG	UNP Q60032
C	-3	HIS	-	EXPRESSION TAG	UNP Q60032
C	-2	HIS	-	EXPRESSION TAG	UNP Q60032
C	-1	HIS	-	EXPRESSION TAG	UNP Q60032
C	0	HIS	-	EXPRESSION TAG	UNP Q60032
C	61	GLY	TYR	ENGINEERED MUTATION	UNP Q60032
D	-7	MET	-	EXPRESSION TAG	UNP Q60032
D	-6	GLY	-	EXPRESSION TAG	UNP Q60032
D	-5	HIS	-	EXPRESSION TAG	UNP Q60032
D	-4	HIS	-	EXPRESSION TAG	UNP Q60032
D	-3	HIS	-	EXPRESSION TAG	UNP Q60032
D	-2	HIS	-	EXPRESSION TAG	UNP Q60032
D	-1	HIS	-	EXPRESSION TAG	UNP Q60032
D	0	HIS	-	EXPRESSION TAG	UNP Q60032
D	61	GLY	TYR	ENGINEERED MUTATION	UNP Q60032
E	-7	MET	-	EXPRESSION TAG	UNP Q60032
E	-6	GLY	-	EXPRESSION TAG	UNP Q60032
E	-5	HIS	-	EXPRESSION TAG	UNP Q60032
E	-4	HIS	-	EXPRESSION TAG	UNP Q60032
E	-3	HIS	-	EXPRESSION TAG	UNP Q60032
E	-2	HIS	-	EXPRESSION TAG	UNP Q60032
E	-1	HIS	-	EXPRESSION TAG	UNP Q60032
E	0	HIS	-	EXPRESSION TAG	UNP Q60032
E	61	GLY	TYR	ENGINEERED MUTATION	UNP Q60032
F	-7	MET	-	EXPRESSION TAG	UNP Q60032
F	-6	GLY	-	EXPRESSION TAG	UNP Q60032
F	-5	HIS	-	EXPRESSION TAG	UNP Q60032
F	-4	HIS	-	EXPRESSION TAG	UNP Q60032
F	-3	HIS	-	EXPRESSION TAG	UNP Q60032
F	-2	HIS	-	EXPRESSION TAG	UNP Q60032
F	-1	HIS	-	EXPRESSION TAG	UNP Q60032
F	0	HIS	-	EXPRESSION TAG	UNP Q60032
F	61	GLY	TYR	ENGINEERED MUTATION	UNP Q60032
G	-7	MET	-	EXPRESSION TAG	UNP Q60032

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	GLY	-	EXPRESSION TAG	UNP Q60032
G	-5	HIS	-	EXPRESSION TAG	UNP Q60032
G	-4	HIS	-	EXPRESSION TAG	UNP Q60032
G	-3	HIS	-	EXPRESSION TAG	UNP Q60032
G	-2	HIS	-	EXPRESSION TAG	UNP Q60032
G	-1	HIS	-	EXPRESSION TAG	UNP Q60032
G	0	HIS	-	EXPRESSION TAG	UNP Q60032
G	61	GLY	TYR	ENGINEERED MUTATION	UNP Q60032
H	-7	MET	-	EXPRESSION TAG	UNP Q60032
H	-6	GLY	-	EXPRESSION TAG	UNP Q60032
H	-5	HIS	-	EXPRESSION TAG	UNP Q60032
H	-4	HIS	-	EXPRESSION TAG	UNP Q60032
H	-3	HIS	-	EXPRESSION TAG	UNP Q60032
H	-2	HIS	-	EXPRESSION TAG	UNP Q60032
H	-1	HIS	-	EXPRESSION TAG	UNP Q60032
H	0	HIS	-	EXPRESSION TAG	UNP Q60032
H	61	GLY	TYR	ENGINEERED MUTATION	UNP Q60032

- Molecule 2 is SUGAR (CELLOBIOSE) (three-letter code: CBI) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			23	12	11		
2	E	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		
2	G	1	Total	C	O	0	0
			23	12	11		
2	H	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is water.

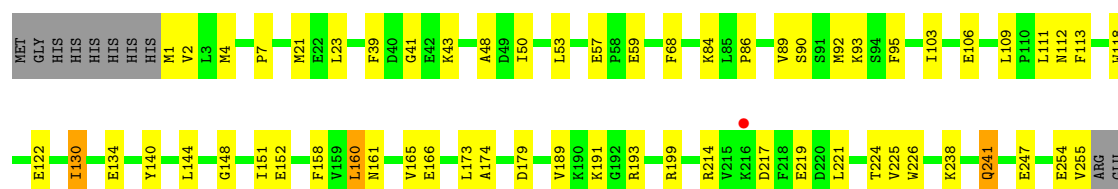
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	141	Total	O	0	0
			141	141		
3	B	119	Total	O	0	0
			119	119		
3	C	111	Total	O	0	0
			111	111		
3	D	122	Total	O	0	0
			122	122		
3	E	116	Total	O	0	0
			116	116		
3	F	77	Total	O	0	0
			77	77		
3	G	90	Total	O	0	0
			90	90		
3	H	73	Total	O	0	0
			73	73		

3 Residue-property plots

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.

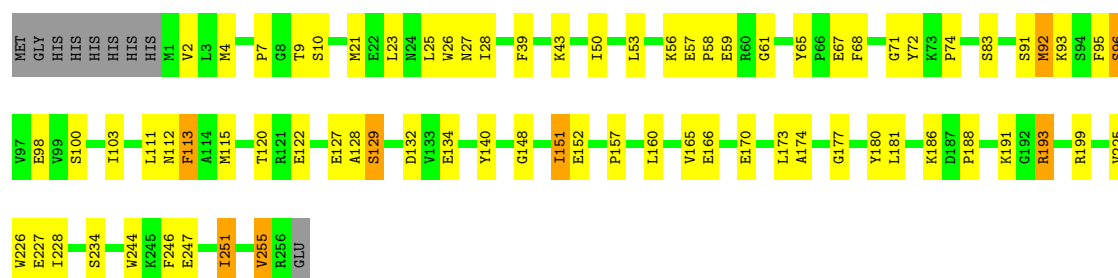
- Molecule 1: Endo-1,4-beta-glucanase

Chain A:



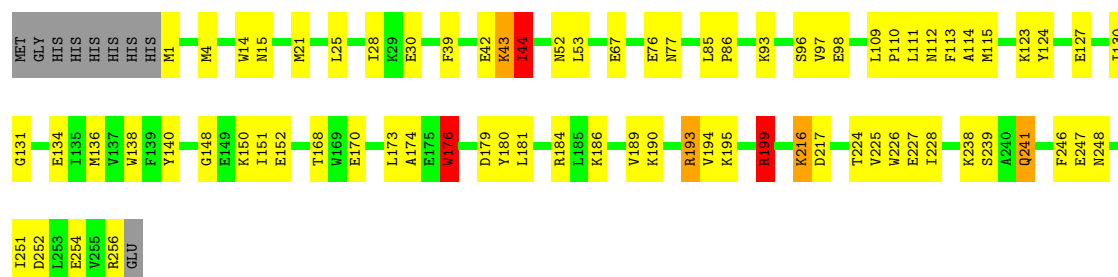
- Molecule 1: Endo-1,4-beta-glucanase

Chain B:



- Molecule 1: Endo-1,4-beta-glucanase

Chain C:



- Molecule 1: Endo-1,4-beta-glucanase

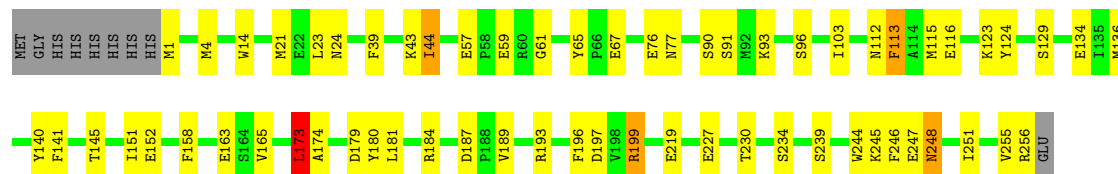
Chain D:





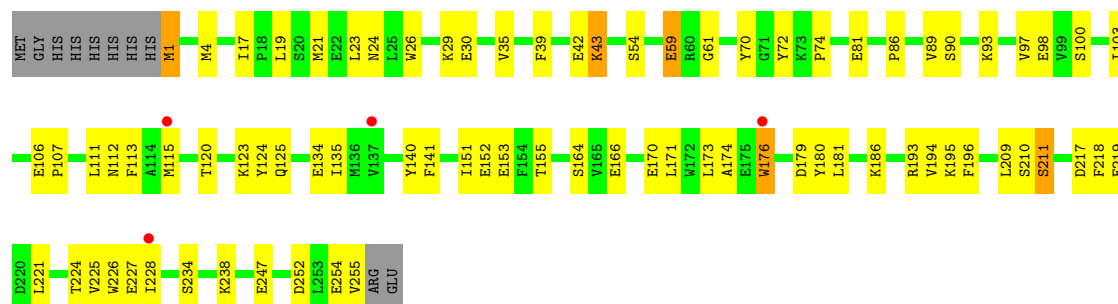
• Molecule 1: Endo-1,4-beta-glucanase

Chain E:



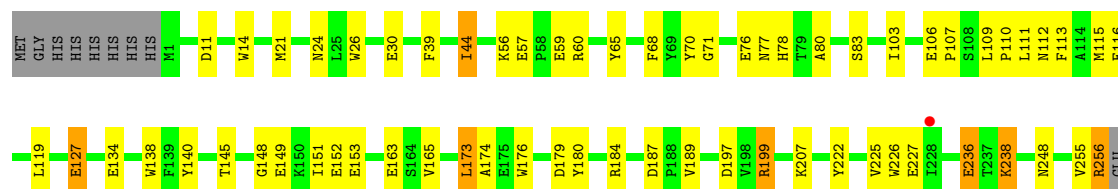
• Molecule 1: Endo-1,4-beta-glucanase

Chain F:



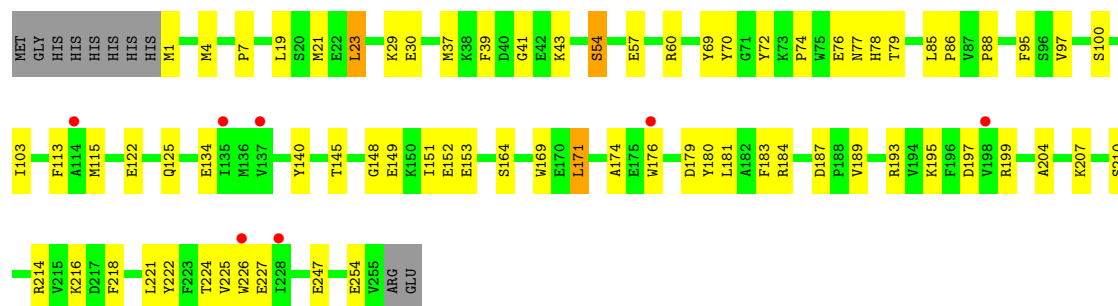
• Molecule 1: Endo-1,4-beta-glucanase

Chain G:



• Molecule 1: Endo-1,4-beta-glucanase

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.91Å 124.04Å 127.56Å 90.00° 107.06° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 25.12 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.5 (25.00-2.50) 90.8 (25.12-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.185 , 0.245 0.186 , 0.244	Depositor DCC
R_{free} test set	4340 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.848	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 85492 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17709	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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 38.46 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6758e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.84	0/2147	0.90	0/2915
1	B	0.84	0/2158	0.89	2/2929 (0.1%)
1	C	0.84	1/2158 (0.0%)	0.89	2/2929 (0.1%)
1	D	0.82	1/2147 (0.0%)	0.89	3/2915 (0.1%)
1	E	0.81	0/2158	0.89	3/2929 (0.1%)
1	F	0.72	0/2147	0.83	1/2915 (0.0%)
1	G	0.75	0/2158	0.87	0/2929
1	H	0.73	0/2147	0.84	1/2915 (0.0%)
All	All	0.80	2/17220 (0.0%)	0.87	12/23376 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	42	GLU	CG-CD	6.84	1.62	1.51
1	D	93	LYS	CD-CE	5.03	1.63	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	173	LEU	CA-CB-CG	8.26	134.31	115.30
1	C	199	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	E	23	LEU	N-CA-C	-5.76	95.44	111.00
1	D	23	LEU	N-CA-C	-5.73	95.53	111.00
1	E	113	PHE	N-CA-C	-5.40	96.42	111.00
1	B	113	PHE	N-CA-C	-5.26	96.80	111.00
1	D	113	PHE	N-CA-C	-5.17	97.06	111.00
1	C	44	ILE	CB-CA-C	-5.12	101.36	111.60
1	D	155	THR	N-CA-C	-5.06	97.33	111.00
1	H	23	LEU	N-CA-C	-5.06	97.34	111.00
1	F	23	LEU	N-CA-C	-5.01	97.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	LEU	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2079	0	1983	52	0
1	B	2090	0	1996	57	0
1	C	2090	0	1996	55	0
1	D	2079	0	1983	37	0
1	E	2090	0	1996	47	0
1	F	2079	0	1983	55	0
1	G	2090	0	1996	45	0
1	H	2079	0	1983	46	0
2	A	23	0	22	1	0
2	B	23	0	22	1	0
2	C	23	0	22	1	0
2	D	23	0	22	1	0
2	E	23	0	22	1	0
2	F	23	0	22	2	0
2	G	23	0	22	0	0
2	H	23	0	22	1	0
3	A	141	0	0	2	0
3	B	119	0	0	0	0
3	C	111	0	0	5	0
3	D	122	0	0	2	0
3	E	116	0	0	0	0
3	F	77	0	0	1	0
3	G	90	0	0	4	0
3	H	73	0	0	2	0
All	All	17709	0	16092	393	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (393) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:86:PRO:HB3	1:H:224:THR:HA	1.31	1.12
1:C:44:ILE:HD12	1:C:246:PHE:HB2	1.41	1.02
1:G:256:ARG:HA	3:G:640:HOH:O	1.66	0.94
1:B:151:ILE:HG12	1:B:152:GLU:HG3	1.55	0.86
1:F:180:TYR:O	1:F:181:LEU:HD12	1.78	0.83
1:G:21:MET:HE1	1:G:39:PHE:HB2	1.60	0.82
1:H:151:ILE:HG13	1:H:152:GLU:HG2	1.61	0.82
1:E:151:ILE:CD1	1:E:173:LEU:HD23	2.09	0.81
1:C:44:ILE:CD1	1:C:246:PHE:HB2	2.10	0.81
1:E:151:ILE:HG13	1:E:152:GLU:HG2	1.63	0.81
1:D:180:TYR:C	1:D:181:LEU:HD12	2.00	0.81
1:D:176:TRP:HB2	3:D:368:HOH:O	1.80	0.80
1:A:21:MET:HE1	1:A:39:PHE:CB	2.13	0.79
1:A:21:MET:CE	1:A:39:PHE:HB2	2.13	0.79
1:F:43:LYS:HB3	1:F:247:GLU:HG2	1.63	0.79
1:A:21:MET:HE1	1:A:39:PHE:HB2	1.63	0.79
1:F:4:MET:HE1	1:F:21:MET:HG3	1.67	0.77
1:E:93:LYS:HE3	1:E:256:ARG:HG3	1.64	0.77
1:G:30:GLU:HB3	3:G:838:HOH:O	1.84	0.76
1:F:151:ILE:HD12	1:F:173:LEU:HB3	1.66	0.76
1:F:42:GLU:OE1	1:F:43:LYS:HG2	1.87	0.75
1:B:100:SER:HB3	1:B:193:ARG:HG3	1.67	0.75
1:D:173:LEU:HD12	1:D:174:ALA:N	2.02	0.74
1:G:207:LYS:HD3	3:G:446:HOH:O	1.88	0.74
1:G:255:VAL:O	1:G:256:ARG:HB2	1.87	0.74
1:G:148:GLY:HA3	1:G:174:ALA:HB2	1.69	0.73
1:G:21:MET:CE	1:G:39:PHE:HB2	2.20	0.72
1:F:93:LYS:HB3	1:F:93:LYS:NZ	2.05	0.72
1:G:57:GLU:OE2	1:G:59:GLU:HB3	1.90	0.72
1:B:225:VAL:HG22	1:B:226:TRP:N	2.05	0.72
1:D:173:LEU:HD12	1:D:174:ALA:H	1.55	0.71
1:G:256:ARG:HB3	1:G:256:ARG:CZ	2.20	0.71
1:H:145:THR:HG22	1:H:184:ARG:HH12	1.54	0.71
1:E:163:GLU:O	1:E:165:VAL:HG13	1.92	0.70
1:F:4:MET:CE	1:F:21:MET:HG3	2.21	0.69
1:A:151:ILE:HG13	1:A:152:GLU:HG2	1.75	0.69
1:F:151:ILE:CD1	1:F:173:LEU:HD23	2.24	0.68
1:H:23:LEU:HA	1:H:37:MET:HE3	1.75	0.68
1:A:255:VAL:HG23	1:A:255:VAL:O	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:7:PRO:HG3	1:B:25:LEU:HD12	1.75	0.68
1:E:57:GLU:HG3	1:E:59:GLU:HG2	1.75	0.68
1:H:225:VAL:HG22	1:H:226:TRP:N	2.08	0.68
1:E:197:ASP:OD1	1:E:199:ARG:HB2	1.95	0.67
1:D:181:LEU:N	1:D:181:LEU:HD12	2.10	0.66
1:G:197:ASP:OD1	1:G:199:ARG:HB2	1.95	0.66
1:F:225:VAL:HG22	1:F:226:TRP:N	2.10	0.66
1:D:111:LEU:HD23	1:D:112:ASN:N	2.10	0.66
1:E:43:LYS:HD2	1:E:245:LYS:HD2	1.77	0.66
1:F:100:SER:HB3	1:F:193:ARG:HG3	1.77	0.66
1:D:43:LYS:HB3	1:D:247:GLU:HG2	1.78	0.65
1:E:14:TRP:CZ3	1:E:44:ILE:HD11	2.31	0.65
1:E:193:ARG:NH1	1:E:248:ASN:HB3	2.12	0.65
1:A:103:ILE:CD1	1:A:113:PHE:HB2	2.27	0.64
1:B:4:MET:CE	1:B:21:MET:HG3	2.28	0.64
1:D:57:GLU:OE1	1:D:59:GLU:HB2	1.98	0.64
1:B:148:GLY:HA3	1:B:174:ALA:HB2	1.79	0.64
1:A:134:GLU:OE2	2:A:300:CBI:H1'	1.97	0.64
1:A:111:LEU:HD23	1:A:112:ASN:N	2.12	0.64
1:G:14:TRP:CZ3	1:G:44:ILE:HD11	2.32	0.63
1:H:134:GLU:OE2	2:H:300:CBI:H1'	1.97	0.63
1:H:214:ARG:HD2	3:H:465:HOH:O	1.98	0.62
1:C:151:ILE:HG13	1:C:152:GLU:HG2	1.81	0.62
1:F:123:LYS:HG2	1:F:124:TYR:CD2	2.35	0.62
1:B:173:LEU:HD12	1:B:174:ALA:N	2.15	0.62
1:C:173:LEU:HD12	1:C:181:LEU:HG	1.82	0.61
1:C:241:GLN:O	1:C:241:GLN:HG3	1.98	0.61
1:G:148:GLY:CA	1:G:174:ALA:HB2	2.30	0.61
1:F:70:TYR:O	1:F:225:VAL:HG23	2.00	0.61
1:B:103:ILE:CD1	1:B:113:PHE:HB2	2.30	0.61
1:D:22:GLU:OE1	1:D:73:LYS:NZ	2.34	0.61
1:G:238:LYS:HG2	3:G:842:HOH:O	2.00	0.61
1:G:151:ILE:HD13	1:G:173:LEU:HB3	1.82	0.61
1:D:140:TYR:HB2	1:D:189:VAL:O	2.00	0.60
1:C:150:LYS:HE3	1:C:170:GLU:HG2	1.83	0.60
1:H:174:ALA:HB1	1:H:176:TRP:CZ2	2.36	0.59
1:G:256:ARG:HB3	1:G:256:ARG:NH1	2.17	0.59
1:A:112:ASN:HB3	1:A:144:LEU:HD23	1.84	0.59
1:B:115:MET:HG2	1:B:228:ILE:HG12	1.84	0.59
1:F:123:LYS:HG2	1:F:124:TYR:CE2	2.37	0.59
1:B:157:PRO:HB3	1:B:166:GLU:OE2	2.02	0.59
1:B:91:SER:O	1:B:255:VAL:HA	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:4:MET:HE2	1:C:21:MET:HG3	1.85	0.59
1:E:173:LEU:HD13	1:E:181:LEU:CD1	2.33	0.59
1:B:21:MET:HE1	1:B:39:PHE:HB2	1.84	0.59
1:C:134:GLU:OE2	2:C:300:CBI:H1'	2.02	0.58
1:B:2:VAL:HG11	1:B:21:MET:SD	2.44	0.58
1:D:148:GLY:HA3	1:D:174:ALA:HB2	1.85	0.58
1:E:134:GLU:OE2	2:E:300:CBI:H1'	2.03	0.58
1:F:103:ILE:CD1	1:F:113:PHE:HB2	2.34	0.58
1:B:129:SER:HA	1:B:177:GLY:O	2.04	0.58
1:C:176:TRP:HB2	3:C:323:HOH:O	2.03	0.58
1:A:4:MET:CE	1:A:21:MET:HG3	2.33	0.57
1:A:1:MET:HG2	3:A:260:HOH:O	2.04	0.57
1:A:21:MET:HE1	1:A:39:PHE:HB3	1.86	0.57
1:C:1:MET:HE3	3:C:276:HOH:O	2.04	0.57
1:E:173:LEU:HD13	1:E:181:LEU:HD12	1.85	0.57
1:E:103:ILE:CD1	1:E:113:PHE:HB2	2.35	0.57
1:F:21:MET:HE1	1:F:39:PHE:HB2	1.87	0.57
1:C:43:LYS:HB3	1:C:247:GLU:HG2	1.87	0.57
1:C:25:LEU:HB3	1:C:28:ILE:HD12	1.87	0.57
1:H:4:MET:HE1	1:H:21:MET:HG3	1.87	0.57
1:H:88:PRO:HG3	1:H:222:TYR:CE1	2.41	0.56
1:A:103:ILE:HD13	1:A:113:PHE:HB2	1.87	0.56
1:C:140:TYR:HB2	1:C:189:VAL:O	2.06	0.56
1:H:100:SER:HB3	1:H:193:ARG:HG3	1.88	0.56
1:A:50:ILE:HD12	1:A:53:LEU:HD21	1.87	0.56
1:C:148:GLY:HA3	1:C:174:ALA:HB2	1.89	0.55
1:B:225:VAL:CG2	1:B:226:TRP:N	2.70	0.55
1:E:193:ARG:HH12	1:E:248:ASN:HB3	1.70	0.55
1:H:174:ALA:HB1	1:H:176:TRP:CE2	2.42	0.55
1:C:176:TRP:HE3	3:C:323:HOH:O	1.89	0.55
1:C:111:LEU:HD23	1:C:111:LEU:C	2.27	0.55
1:B:103:ILE:HD13	1:B:113:PHE:HB2	1.89	0.55
1:B:134:GLU:OE2	2:B:300:CBI:H1'	2.07	0.55
1:B:151:ILE:HG12	1:B:152:GLU:N	2.19	0.54
1:H:148:GLY:HA3	1:H:174:ALA:HB2	1.88	0.54
1:E:43:LYS:HB3	1:E:247:GLU:HG2	1.89	0.54
1:C:252:ASP:OD1	1:C:254:GLU:OE2	2.25	0.54
1:A:43:LYS:HB3	1:A:247:GLU:HG2	1.90	0.54
1:H:23:LEU:CA	1:H:37:MET:HE3	2.38	0.54
1:E:57:GLU:CG	1:E:59:GLU:HG2	2.38	0.53
1:G:151:ILE:HG13	1:G:152:GLU:HG2	1.90	0.53
1:C:123:LYS:HG2	1:C:124:TYR:CE2	2.42	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:180:TYR:C	1:F:181:LEU:HD12	2.29	0.53
1:F:97:VAL:O	1:F:195:LYS:HA	2.08	0.53
1:A:21:MET:HE2	1:A:39:PHE:HB2	1.89	0.53
1:E:113:PHE:HB3	1:E:140:TYR:HB3	1.90	0.53
1:F:176:TRP:CD1	3:F:422:HOH:O	2.54	0.53
1:H:225:VAL:CG2	1:H:226:TRP:N	2.71	0.53
1:H:78:HIS:CD2	1:H:78:HIS:C	2.81	0.53
1:F:111:LEU:HD23	1:F:112:ASN:N	2.24	0.53
1:B:151:ILE:CG1	1:B:152:GLU:HG3	2.34	0.53
1:E:151:ILE:HD13	1:E:173:LEU:HD23	1.90	0.53
1:D:111:LEU:HD23	1:D:111:LEU:C	2.29	0.53
1:B:27:ASN:OD1	1:B:56:LYS:HB2	2.09	0.53
1:F:93:LYS:HB3	1:F:93:LYS:HZ3	1.71	0.52
1:C:4:MET:CE	1:C:21:MET:HG3	2.39	0.52
1:B:111:LEU:HD23	1:B:112:ASN:N	2.25	0.52
1:F:115:MET:HA	1:F:227:GLU:O	2.09	0.52
1:E:112:ASN:OD1	1:E:112:ASN:C	2.47	0.52
1:E:14:TRP:HZ3	1:E:44:ILE:HD11	1.74	0.52
1:B:173:LEU:HD12	1:B:174:ALA:H	1.73	0.52
1:D:134:GLU:OE2	2:D:300:CBI:H3'	2.10	0.51
1:A:158:PHE:HE1	1:A:160:LEU:HD22	1.74	0.51
1:C:115:MET:HG2	1:C:228:ILE:HG12	1.91	0.51
1:B:115:MET:HA	1:B:227:GLU:O	2.09	0.51
1:D:77:ASN:HB2	1:D:126:THR:HG22	1.93	0.51
1:C:93:LYS:O	1:C:199:ARG:HG3	2.09	0.51
1:G:113:PHE:HB3	1:G:140:TYR:HB3	1.92	0.51
1:H:174:ALA:HB3	1:H:180:TYR:HB3	1.93	0.51
1:H:39:PHE:CZ	1:H:41:GLY:HA2	2.45	0.51
1:G:225:VAL:HG22	1:G:226:TRP:N	2.26	0.51
1:A:151:ILE:HG13	1:A:152:GLU:N	2.25	0.51
1:H:180:TYR:O	1:H:181:LEU:HD12	2.10	0.51
1:F:113:PHE:HB3	1:F:140:TYR:HB3	1.93	0.51
1:E:123:LYS:HG2	1:E:124:TYR:CE2	2.45	0.51
1:C:180:TYR:C	1:C:181:LEU:HD12	2.31	0.51
1:G:238:LYS:HB3	1:G:238:LYS:NZ	2.26	0.51
1:A:90:SER:HB3	1:A:219:GLU:HB3	1.93	0.51
1:E:44:ILE:HD12	1:E:246:PHE:HB2	1.92	0.51
1:B:4:MET:HE2	1:B:21:MET:HG3	1.92	0.51
1:B:21:MET:CE	1:B:39:PHE:HB2	2.40	0.51
1:D:67:GLU:OE1	1:D:227:GLU:OE1	2.29	0.51
1:G:138:TRP:CD1	1:G:138:TRP:N	2.78	0.51
1:F:120:THR:HB	1:F:125:GLN:CD	2.31	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:180:TYR:C	1:B:181:LEU:HD12	2.32	0.50
1:F:115:MET:HG2	1:F:228:ILE:HG12	1.94	0.50
1:E:21:MET:CE	1:E:39:PHE:HB2	2.41	0.50
1:B:151:ILE:HG12	1:B:152:GLU:CG	2.35	0.50
1:F:111:LEU:HD23	1:F:111:LEU:C	2.32	0.50
1:F:225:VAL:CG2	1:F:226:TRP:N	2.74	0.50
1:H:57:GLU:CG	1:H:60:ARG:HG2	2.42	0.50
1:H:140:TYR:HB2	1:H:189:VAL:O	2.11	0.50
1:H:72:TYR:O	1:H:74:PRO:HD3	2.11	0.50
1:H:43:LYS:HB3	1:H:247:GLU:HG2	1.94	0.50
1:A:122:GLU:OE1	1:A:122:GLU:HA	2.11	0.50
1:D:88:PRO:HD2	1:D:91:SER:OG	2.12	0.50
1:A:86:PRO:HB3	1:A:224:THR:HA	1.93	0.49
1:A:4:MET:HE1	1:A:21:MET:HG3	1.93	0.49
1:H:153:GLU:HA	1:H:169:TRP:O	2.13	0.49
1:E:91:SER:O	1:E:255:VAL:HA	2.12	0.49
1:C:15:ASN:ND2	3:C:701:HOH:O	2.38	0.49
1:D:255:VAL:C	3:D:267:HOH:O	2.49	0.49
1:B:61:GLY:O	1:B:234:SER:HA	2.12	0.49
1:E:145:THR:HG22	1:E:184:ARG:HH12	1.78	0.49
1:A:130:ILE:HG13	3:A:275:HOH:O	2.12	0.49
1:E:76:GLU:O	1:E:77:ASN:C	2.51	0.49
1:G:116:GLU:OE2	1:G:134:GLU:OE2	2.31	0.49
1:C:168:THR:CG2	1:C:186:LYS:HD3	2.42	0.49
1:F:171:LEU:HD11	1:F:181:LEU:HG	1.95	0.49
1:H:78:HIS:CD2	1:H:79:THR:N	2.81	0.49
1:E:4:MET:HE1	1:E:21:MET:HG3	1.93	0.49
1:F:151:ILE:O	1:F:152:GLU:HB2	2.12	0.48
1:H:23:LEU:HA	1:H:37:MET:CE	2.42	0.48
1:H:57:GLU:HG3	1:H:60:ARG:HG2	1.95	0.48
1:G:145:THR:HG22	1:G:184:ARG:HH12	1.78	0.48
1:E:24:ASN:HB3	1:E:65:TYR:O	2.13	0.48
1:D:25:LEU:HB3	1:D:28:ILE:HD12	1.96	0.48
1:G:21:MET:HA	1:G:68:PHE:HA	1.96	0.48
1:G:70:TYR:O	1:G:225:VAL:HG23	2.13	0.48
1:B:71:GLY:HA2	1:B:83:SER:OG	2.13	0.48
1:A:2:VAL:HB	1:A:39:PHE:HB3	1.96	0.48
1:B:251:ILE:HG12	1:B:251:ILE:O	2.14	0.48
1:C:97:VAL:O	1:C:195:LYS:HA	2.13	0.47
1:D:57:GLU:HG3	1:D:60:ARG:HG2	1.95	0.47
1:G:112:ASN:OD1	1:G:112:ASN:C	2.53	0.47
1:B:92:MET:HE3	1:B:95:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:165:VAL:HG12	1:A:166:GLU:N	2.28	0.47
1:A:4:MET:HE2	1:A:21:MET:HG3	1.95	0.47
1:A:48:ALA:O	1:A:241:GLN:HA	2.14	0.47
1:E:140:TYR:HB2	1:E:189:VAL:O	2.14	0.47
1:F:134:GLU:OE2	2:F:300:CBI:H1'	2.14	0.47
1:A:92:MET:CE	1:A:95:PHE:HB2	2.45	0.47
1:D:138:TRP:HB2	1:D:184:ARG:HA	1.96	0.47
1:G:163:GLU:O	1:G:165:VAL:HG13	2.15	0.47
1:C:241:GLN:HE21	1:C:241:GLN:HB2	1.40	0.47
1:G:76:GLU:O	1:G:77:ASN:C	2.51	0.46
1:H:76:GLU:O	1:H:77:ASN:C	2.54	0.46
1:E:151:ILE:HD12	1:E:173:LEU:HD23	1.94	0.46
1:H:30:GLU:HG2	1:H:54:SER:OG	2.15	0.46
1:C:113:PHE:HB3	1:C:140:TYR:HB3	1.97	0.46
1:A:130:ILE:HD13	1:A:214:ARG:NH1	2.29	0.46
1:F:24:ASN:OD1	1:F:26:TRP:HB3	2.15	0.46
1:F:1:MET:HB3	1:F:1:MET:HE2	1.65	0.46
1:E:93:LYS:O	1:E:199:ARG:HG3	2.15	0.46
1:H:72:TYR:O	1:H:225:VAL:HB	2.16	0.46
1:F:153:GLU:OE2	1:F:186:LYS:HE3	2.16	0.46
1:E:21:MET:HE2	1:E:39:PHE:HB2	1.98	0.46
1:B:191:LYS:O	1:B:191:LYS:HG2	2.16	0.46
1:B:72:TYR:O	1:B:74:PRO:HD3	2.16	0.46
1:F:196:PHE:CD2	1:F:196:PHE:N	2.84	0.46
1:C:76:GLU:O	1:C:77:ASN:C	2.54	0.46
1:C:67:GLU:OE1	1:C:227:GLU:OE1	2.33	0.46
1:G:119:LEU:HA	1:G:222:TYR:O	2.14	0.46
1:F:174:ALA:HB3	1:F:180:TYR:HB3	1.97	0.46
1:F:86:PRO:HB3	1:F:224:THR:HA	1.97	0.46
1:C:193:ARG:HH21	1:C:248:ASN:HB3	1.81	0.46
1:D:236:GLU:OE2	1:D:236:GLU:N	2.49	0.46
1:A:122:GLU:OE1	1:D:93:LYS:HE2	2.16	0.45
1:E:61:GLY:O	1:E:234:SER:HA	2.16	0.45
1:D:148:GLY:CA	1:D:174:ALA:HB2	2.47	0.45
1:G:140:TYR:HB2	1:G:189:VAL:O	2.16	0.45
1:B:43:LYS:HB3	1:B:247:GLU:HG2	1.97	0.45
1:C:96:SER:O	1:C:251:ILE:HA	2.16	0.45
1:D:113:PHE:HB3	1:D:140:TYR:HB3	1.98	0.45
1:F:252:ASP:OD1	1:F:254:GLU:OE2	2.35	0.45
1:D:140:TYR:CE1	1:D:190:LYS:HB2	2.51	0.45
1:B:96:SER:O	1:B:251:ILE:HA	2.17	0.45
1:D:92:MET:HE1	1:D:95:PHE:HD2	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:89:VAL:HG23	1:F:221:LEU:O	2.17	0.45
1:A:57:GLU:OE2	1:A:59:GLU:HB2	2.15	0.45
1:H:97:VAL:O	1:H:195:LYS:HA	2.17	0.45
1:A:106:GLU:HG3	1:A:109:LEU:HB2	1.99	0.45
1:A:225:VAL:HG22	1:A:226:TRP:N	2.32	0.45
1:C:109:LEU:HA	1:C:110:PRO:HD3	1.87	0.45
1:B:127:GLU:HG3	1:B:128:ALA:N	2.31	0.45
1:A:112:ASN:OD1	1:A:112:ASN:C	2.54	0.45
1:G:24:ASN:HB3	1:G:65:TYR:O	2.17	0.45
1:E:173:LEU:HA	1:E:180:TYR:O	2.17	0.45
1:A:113:PHE:HB3	1:A:140:TYR:HB3	1.99	0.45
1:B:173:LEU:HA	1:B:180:TYR:O	2.17	0.45
1:G:145:THR:HG22	1:G:184:ARG:NH1	2.32	0.45
1:E:230:THR:HG21	1:E:244:TRP:CD1	2.51	0.44
1:F:238:LYS:HA	1:F:238:LYS:HD3	1.79	0.44
1:E:174:ALA:HB3	1:E:180:TYR:HB3	1.99	0.44
1:G:115:MET:HA	1:G:227:GLU:O	2.17	0.44
1:B:21:MET:HA	1:B:68:PHE:HA	1.99	0.44
1:D:57:GLU:OE2	1:D:58:PRO:HD2	2.17	0.44
1:G:103:ILE:HD13	1:G:113:PHE:HB2	2.00	0.44
1:H:57:GLU:HG3	1:H:57:GLU:O	2.17	0.44
1:F:61:GLY:O	1:F:234:SER:HA	2.17	0.44
1:C:53:LEU:HG	1:C:238:LYS:O	2.18	0.44
1:E:115:MET:HA	1:E:227:GLU:O	2.17	0.44
1:B:25:LEU:HD22	1:B:28:ILE:HD12	1.98	0.44
1:B:140:TYR:HD1	1:B:188:PRO:HB2	1.82	0.44
1:F:29:LYS:HD3	1:F:30:GLU:OE2	2.17	0.44
1:D:76:GLU:O	1:D:77:ASN:C	2.56	0.44
1:E:123:LYS:HG2	1:E:124:TYR:CD2	2.53	0.44
1:B:244:TRP:CZ3	1:B:246:PHE:CD2	3.05	0.44
1:A:39:PHE:CZ	1:A:41:GLY:HA2	2.52	0.44
1:F:59:GLU:HG2	1:F:59:GLU:O	2.18	0.44
1:H:218:PHE:HA	1:H:221:LEU:HD12	2.00	0.44
1:D:115:MET:HA	1:D:227:GLU:O	2.18	0.44
1:C:98:GLU:HG2	1:C:195:LYS:CG	2.47	0.44
1:F:155:THR:HG22	1:F:166:GLU:OE1	2.17	0.44
1:D:181:LEU:CD1	1:D:181:LEU:N	2.78	0.44
1:H:180:TYR:C	1:H:181:LEU:HD12	2.39	0.44
1:B:165:VAL:HG12	1:B:166:GLU:N	2.32	0.43
1:E:145:THR:HG22	1:E:184:ARG:NH1	2.32	0.43
1:A:7:PRO:HA	1:A:23:LEU:O	2.18	0.43
1:H:95:PHE:N	1:H:197:ASP:OD1	2.46	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:138:TRP:HB2	1:C:184:ARG:HA	2.00	0.43
1:H:103:ILE:CD1	1:H:113:PHE:HB2	2.48	0.43
1:H:122:GLU:HB2	1:H:125:GLN:HG2	2.00	0.43
1:A:255:VAL:CG2	1:A:255:VAL:O	2.65	0.43
1:C:98:GLU:HA	1:C:194:VAL:O	2.18	0.43
1:E:67:GLU:OE1	1:E:227:GLU:OE1	2.36	0.43
1:B:50:ILE:HD12	1:B:53:LEU:HD21	2.01	0.43
1:A:238:LYS:HB3	1:A:238:LYS:HE3	1.67	0.43
1:H:1:MET:HB3	1:H:1:MET:HE2	1.81	0.43
1:H:7:PRO:HA	1:H:23:LEU:O	2.18	0.43
1:C:4:MET:HE2	1:C:21:MET:SD	2.58	0.43
1:F:90:SER:HB3	1:F:219:GLU:O	2.17	0.43
1:C:131:GLY:O	1:C:216:LYS:NZ	2.52	0.43
1:C:98:GLU:HG3	3:C:261:HOH:O	2.19	0.43
1:F:98:GLU:HA	1:F:194:VAL:O	2.18	0.43
1:A:2:VAL:HB	1:A:21:MET:HE1	2.00	0.43
1:A:140:TYR:HB2	1:A:189:VAL:O	2.18	0.43
1:E:21:MET:HE1	1:E:39:PHE:CB	2.49	0.43
1:F:26:TRP:CZ2	2:F:300:CBI:H4'	2.53	0.43
1:A:89:VAL:HG23	1:A:221:LEU:O	2.19	0.43
1:F:100:SER:HA	1:F:193:ARG:HA	1.99	0.42
1:C:4:MET:HE2	1:C:21:MET:CG	2.49	0.42
1:A:21:MET:HA	1:A:68:PHE:HA	2.01	0.42
1:A:151:ILE:HG13	1:A:152:GLU:H	1.82	0.42
1:D:103:ILE:CD1	1:D:113:PHE:HB2	2.49	0.42
1:D:101:PHE:N	1:D:101:PHE:CD2	2.87	0.42
1:C:14:TRP:CZ3	1:C:44:ILE:HD11	2.55	0.42
1:E:116:GLU:OE2	1:E:134:GLU:OE2	2.37	0.42
1:H:171:LEU:HD12	1:H:183:PHE:CE1	2.54	0.42
1:A:160:LEU:HD12	1:A:161:ASN:ND2	2.34	0.42
1:F:170:GLU:OE2	1:F:186:LYS:HE2	2.19	0.42
1:F:17:ILE:HG22	1:F:19:LEU:HG	2.00	0.42
1:B:98:GLU:OE2	1:B:193:ARG:NH1	2.40	0.42
1:B:120:THR:HA	1:B:132:ASP:OD1	2.20	0.42
1:G:11:ASP:OD1	1:G:78:HIS:NE2	2.48	0.42
1:B:148:GLY:CA	1:B:174:ALA:HB2	2.47	0.42
1:C:52:ASN:HA	1:C:238:LYS:HZ2	1.85	0.42
1:B:21:MET:HE2	1:B:21:MET:HB3	1.77	0.42
1:B:4:MET:HE1	1:B:21:MET:HG3	2.01	0.42
1:C:21:MET:CE	1:C:39:PHE:HB2	2.49	0.42
1:C:111:LEU:HD23	1:C:112:ASN:N	2.35	0.42
1:B:26:TRP:CE3	1:B:27:ASN:HB2	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:9:THR:HG22	1:B:10:SER:N	2.34	0.42
1:F:93:LYS:HB3	1:F:93:LYS:HZ2	1.83	0.42
1:E:140:TYR:CG	1:E:141:PHE:N	2.88	0.42
1:C:168:THR:HG22	1:C:186:LYS:HD3	2.02	0.42
1:B:92:MET:HE3	1:B:92:MET:HB3	1.90	0.42
1:D:109:LEU:HD12	1:D:110:PRO:HD2	2.01	0.42
1:C:114:ALA:HB1	1:C:136:MET:HE2	2.02	0.42
1:C:86:PRO:HB3	1:C:224:THR:HA	2.02	0.42
1:B:65:TYR:O	1:B:67:GLU:HG2	2.20	0.41
1:H:69:TYR:HB3	1:H:227:GLU:HA	2.02	0.41
1:A:103:ILE:HD11	1:A:113:PHE:HB2	2.01	0.41
1:C:52:ASN:HA	1:C:238:LYS:NZ	2.35	0.41
1:G:71:GLY:HA2	1:G:83:SER:OG	2.21	0.41
1:C:181:LEU:N	1:C:181:LEU:HD12	2.35	0.41
1:E:158:PHE:HB2	1:E:196:PHE:HB3	2.01	0.41
1:G:26:TRP:O	1:G:56:LYS:HE3	2.19	0.41
1:B:57:GLU:HA	1:B:58:PRO:HD2	1.91	0.41
1:C:85:LEU:HD23	1:C:85:LEU:HA	1.90	0.41
1:F:72:TYR:O	1:F:74:PRO:HD3	2.21	0.41
1:A:160:LEU:HD12	1:A:161:ASN:N	2.35	0.41
1:G:106:GLU:HA	1:G:107:PRO:HD3	1.84	0.41
1:C:225:VAL:HG22	1:C:226:TRP:N	2.35	0.41
1:B:111:LEU:HD23	1:B:111:LEU:C	2.41	0.41
1:H:254:GLU:HA	3:H:852:HOH:O	2.20	0.41
1:B:170:GLU:OE2	1:B:186:LYS:NZ	2.51	0.41
1:H:204:ALA:HA	1:H:207:LYS:HE2	2.03	0.41
1:G:173:LEU:HA	1:G:180:TYR:O	2.21	0.41
1:H:19:LEU:HD23	1:H:70:TYR:HA	2.02	0.41
1:E:90:SER:HA	1:E:219:GLU:HG3	2.02	0.41
1:H:85:LEU:HB3	1:H:86:PRO:HA	2.01	0.41
1:D:57:GLU:CD	1:D:59:GLU:HB2	2.40	0.41
1:G:236:GLU:O	1:G:238:LYS:HD3	2.21	0.41
1:C:140:TYR:CE1	1:C:190:LYS:HB2	2.55	0.41
1:F:209:LEU:O	1:F:211:SER:N	2.54	0.41
1:A:93:LYS:HB3	1:A:254:GLU:O	2.21	0.41
1:G:149:GLU:O	1:G:151:ILE:HG23	2.20	0.41
1:E:103:ILE:HD13	1:E:113:PHE:HB2	2.02	0.41
1:G:11:ASP:OD2	1:G:80:ALA:HA	2.21	0.41
1:A:148:GLY:HA3	1:A:174:ALA:HB2	2.02	0.41
1:F:135:ILE:HA	1:F:181:LEU:O	2.21	0.41
1:B:225:VAL:HG22	1:B:226:TRP:H	1.85	0.41
1:B:2:VAL:CG1	1:B:21:MET:SD	3.09	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:118:TRP:CZ3	1:A:134:GLU:HB2	2.55	0.41
1:F:140:TYR:CG	1:F:141:PHE:N	2.88	0.41
1:H:115:MET:HA	1:H:227:GLU:O	2.21	0.41
1:A:84:LYS:HD3	1:A:84:LYS:HA	1.90	0.41
1:A:92:MET:HE3	1:A:95:PHE:HB2	2.02	0.40
1:C:115:MET:HA	1:C:227:GLU:O	2.22	0.40
1:D:66:PRO:HD2	1:D:230:THR:O	2.21	0.40
1:F:112:ASN:C	1:F:112:ASN:OD1	2.60	0.40
1:G:111:LEU:C	1:G:111:LEU:HD23	2.42	0.40
1:D:151:ILE:HD13	1:D:173:LEU:CB	2.52	0.40
1:G:57:GLU:CG	1:G:60:ARG:HG2	2.52	0.40
1:G:236:GLU:O	1:G:238:LYS:CD	2.70	0.40
1:E:96:SER:O	1:E:251:ILE:HA	2.22	0.40
1:C:148:GLY:CA	1:C:174:ALA:HB2	2.51	0.40
1:C:123:LYS:HG2	1:C:124:TYR:CD2	2.57	0.40
1:F:106:GLU:HA	1:F:107:PRO:HD3	1.85	0.40
1:D:97:VAL:O	1:D:195:LYS:HA	2.20	0.40
1:G:109:LEU:HA	1:G:110:PRO:HD3	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	253/265 (96%)	243 (96%)	10 (4%)	0	100	100
1	B	254/265 (96%)	241 (95%)	13 (5%)	0	100	100
1	C	254/265 (96%)	242 (95%)	11 (4%)	1 (0%)	43	66
1	D	253/265 (96%)	241 (95%)	10 (4%)	2 (1%)	27	46
1	E	254/265 (96%)	237 (93%)	17 (7%)	0	100	100
1	F	253/265 (96%)	237 (94%)	14 (6%)	2 (1%)	27	46
1	G	254/265 (96%)	235 (92%)	17 (7%)	2 (1%)	27	46
1	H	253/265 (96%)	237 (94%)	15 (6%)	1 (0%)	43	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2028/2120 (96%)	1913 (94%)	107 (5%)	8 (0%)	43 66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	176	TRP
1	D	218	PHE
1	F	210	SER
1	H	210	SER
1	D	176	TRP
1	G	176	TRP
1	F	218	PHE
1	G	127	GLU

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	224/233 (96%)	215 (96%)	9 (4%)	42 68
1	B	225/233 (97%)	213 (95%)	12 (5%)	32 54
1	C	225/233 (97%)	211 (94%)	14 (6%)	26 45
1	D	224/233 (96%)	215 (96%)	9 (4%)	42 68
1	E	225/233 (97%)	215 (96%)	10 (4%)	39 64
1	F	224/233 (96%)	212 (95%)	12 (5%)	31 53
1	G	225/233 (97%)	214 (95%)	11 (5%)	35 59
1	H	224/233 (96%)	215 (96%)	9 (4%)	42 68
All	All	1796/1864 (96%)	1710 (95%)	86 (5%)	35 60

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	ILE
1	A	160	LEU
1	A	173	LEU

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Mol	Chain	Res	Type
1	A	179	ASP
1	A	191	LYS
1	A	193	ARG
1	A	199	ARG
1	A	217	ASP
1	A	241	GLN
1	B	59	GLU
1	B	92	MET
1	B	93	LYS
1	B	96	SER
1	B	122	GLU
1	B	129	SER
1	B	151	ILE
1	B	160	LEU
1	B	193	ARG
1	B	199	ARG
1	B	251	ILE
1	B	255	VAL
1	C	30	GLU
1	C	43	LYS
1	C	44	ILE
1	C	127	GLU
1	C	130	ILE
1	C	176	TRP
1	C	179	ASP
1	C	193	ARG
1	C	199	ARG
1	C	216	LYS
1	C	217	ASP
1	C	239	SER
1	C	241	GLN
1	C	256	ARG
1	D	57	GLU
1	D	59	GLU
1	D	91	SER
1	D	95	PHE
1	D	127	GLU
1	D	176	TRP
1	D	179	ASP
1	D	187	ASP
1	D	216	LYS
1	E	1	MET

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Mol	Chain	Res	Type
1	E	44	ILE
1	E	129	SER
1	E	136	MET
1	E	173	LEU
1	E	179	ASP
1	E	187	ASP
1	E	199	ARG
1	E	239	SER
1	E	248	ASN
1	F	1	MET
1	F	35	VAL
1	F	43	LYS
1	F	54	SER
1	F	59	GLU
1	F	81	GLU
1	F	164	SER
1	F	176	TRP
1	F	179	ASP
1	F	211	SER
1	F	217	ASP
1	F	255	VAL
1	G	44	ILE
1	G	127	GLU
1	G	153	GLU
1	G	173	LEU
1	G	179	ASP
1	G	187	ASP
1	G	199	ARG
1	G	236	GLU
1	G	238	LYS
1	G	248	ASN
1	G	256	ARG
1	H	29	LYS
1	H	54	SER
1	H	149	GLU
1	H	164	SER
1	H	171	LEU
1	H	179	ASP
1	H	187	ASP
1	H	199	ARG
1	H	216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	A	200	HIS
1	A	241	GLN
1	A	248	ASN
1	B	161	ASN
1	C	52	ASN
1	C	241	GLN
1	D	52	ASN
1	D	241	GLN
1	D	248	ASN
1	E	77	ASN
1	E	143	ASN
1	E	248	ASN
1	F	77	ASN
1	F	104	HIS
1	F	241	GLN
1	G	52	ASN
1	G	104	HIS
1	G	248	ASN
1	H	15	ASN
1	H	241	GLN
1	H	248	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CBI	A	300	-	24,24,24	0.41	0	35,35,35	0.92	2 (5%)
2	CBI	B	300	-	24,24,24	0.41	0	35,35,35	1.06	3 (8%)
2	CBI	C	300	-	24,24,24	0.40	0	35,35,35	0.87	1 (2%)
2	CBI	D	300	-	24,24,24	0.40	0	35,35,35	0.93	1 (2%)
2	CBI	E	300	-	24,24,24	0.41	0	35,35,35	0.96	1 (2%)
2	CBI	F	300	-	24,24,24	0.42	0	35,35,35	1.04	2 (5%)
2	CBI	G	300	-	24,24,24	0.44	0	35,35,35	0.89	2 (5%)
2	CBI	H	300	-	24,24,24	0.41	0	35,35,35	1.06	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CBI	A	300	-	-	0/8/48/48	0/2/2/2
2	CBI	B	300	-	-	0/8/48/48	0/2/2/2
2	CBI	C	300	-	-	0/8/48/48	0/2/2/2
2	CBI	D	300	-	-	0/8/48/48	0/2/2/2
2	CBI	E	300	-	-	0/8/48/48	0/2/2/2
2	CBI	F	300	-	-	0/8/48/48	0/2/2/2
2	CBI	G	300	-	-	0/8/48/48	0/2/2/2
2	CBI	H	300	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	300	CBI	C6-C5-C4	-3.32	104.99	113.00
2	B	300	CBI	C1-O4'-C4'	-2.75	110.97	117.99
2	B	300	CBI	C1'-O5'-C5'	-2.63	108.69	113.40
2	B	300	CBI	C6-C5-C4	-2.60	106.71	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	300	CBI	C1-O4'-C4'	-2.58	111.40	117.99
2	H	300	CBI	C6-C5-C4	-2.58	106.77	113.00
2	E	300	CBI	C6-C5-C4	-2.43	107.13	113.00
2	D	300	CBI	C1-O4'-C4'	-2.40	111.86	117.99
2	C	300	CBI	C1-O4'-C4'	-2.31	112.09	117.99
2	A	300	CBI	C1-O4'-C4'	-2.20	112.37	117.99
2	F	300	CBI	C1-O4'-C4'	-2.15	112.51	117.99
2	G	300	CBI	C1-O4'-C4'	-2.07	112.70	117.99
2	G	300	CBI	C4-C3-C2	-2.05	107.02	110.82
2	A	300	CBI	C6-C5-C4	-2.02	108.11	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th 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	255/265 (96%)	-0.40	1 (0%) 90 92	12, 26, 44, 59	0
1	B	256/265 (96%)	-0.37	0 100 100	14, 30, 47, 58	0
1	C	256/265 (96%)	-0.35	0 100 100	14, 29, 47, 54	0
1	D	255/265 (96%)	-0.36	0 100 100	15, 29, 46, 57	0
1	E	256/265 (96%)	-0.27	0 100 100	15, 29, 46, 55	0
1	F	255/265 (96%)	-0.13	4 (1%) 68 71	23, 36, 54, 66	0
1	G	256/265 (96%)	-0.14	1 (0%) 90 92	21, 35, 52, 64	0
1	H	255/265 (96%)	-0.00	7 (2%) 52 54	25, 39, 56, 70	0
All	All	2044/2120 (96%)	-0.25	13 (0%) 86 88	12, 32, 51, 70	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	176	TRP	3.9
1	H	176	TRP	3.5
1	H	226	TRP	3.0
1	H	114	ALA	2.5
1	H	135	ILE	2.3
1	F	115	MET	2.3
1	G	228	ILE	2.3
1	H	228	ILE	2.3
1	H	137	VAL	2.3
1	F	228	ILE	2.3
1	H	198	VAL	2.2
1	A	216	LYS	2.2
1	F	137	VAL	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CBI	D	300	23/23	0.14	0.15	26,30,36,41	0
2	CBI	A	300	23/23	0.12	-0.20	16,22,26,27	0
2	CBI	H	300	23/23	0.14	-0.28	33,36,39,40	0
2	CBI	B	300	23/23	0.13	-0.39	22,25,27,31	0
2	CBI	C	300	23/23	0.13	-0.43	28,30,32,36	0
2	CBI	E	300	23/23	0.13	-0.60	23,26,28,30	0
2	CBI	G	300	23/23	0.13	-0.61	36,38,40,42	0
2	CBI	F	300	23/23	0.12	-0.63	27,32,36,38	0

6.5 Other polymers

There are no such residues in this entry.