



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2017 – 02:52 AM EDT

PDB ID : 3TPC  
Title : Crystal structure of a hypothetical protein SMa1452 from Sinorhizobium meliloti 1021  
Authors : Agarwal, R.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRC)  
Deposited on : unknown  
Resolution : 2.34 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](mailto: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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

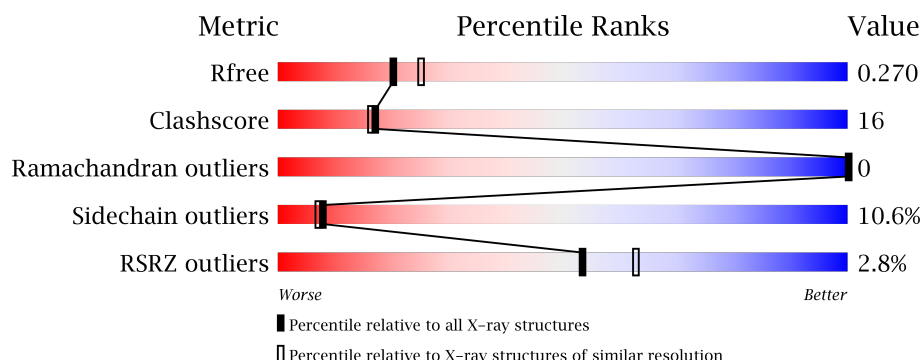
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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))
$R_{free}$	100719	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	257	
1	B	257	
1	C	257	
1	D	257	
1	E	257	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	257	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%64%19%••13%</div></div>
1	G	257	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%66%17%•14%</div></div>
1	H	257	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%69%15%•14%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13015 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 Short chain alcohol dehydrogenase-related dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	Se	0	0	0
			1627	1022	295	303	2	5			
1	B	221	Total	C	N	O	S	Se	0	0	0
			1573	989	280	297	2	5			
1	C	224	Total	C	N	O	S	Se	0	0	0
			1604	1007	288	302	2	5			
1	D	226	Total	C	N	O	S	Se	0	0	0
			1597	1007	282	301	2	5			
1	E	225	Total	C	N	O	S	Se	0	0	0
			1624	1021	295	301	2	5			
1	F	223	Total	C	N	O	S	Se	0	0	0
			1593	1000	289	297	2	5			
1	G	222	Total	C	N	O	S	Se	0	0	0
			1542	968	275	292	2	5			
1	H	222	Total	C	N	O	S	Se	0	0	0
			1592	997	290	298	2	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP Q92YS1
A	2	VAL	-	EXPRESSION TAG	UNP Q92YS1
B	1	MSE	-	EXPRESSION TAG	UNP Q92YS1
B	2	VAL	-	EXPRESSION TAG	UNP Q92YS1
C	1	MSE	-	EXPRESSION TAG	UNP Q92YS1
C	2	VAL	-	EXPRESSION TAG	UNP Q92YS1
D	1	MSE	-	EXPRESSION TAG	UNP Q92YS1
D	2	VAL	-	EXPRESSION TAG	UNP Q92YS1
E	1	MSE	-	EXPRESSION TAG	UNP Q92YS1
E	2	VAL	-	EXPRESSION TAG	UNP Q92YS1
F	1	MSE	-	EXPRESSION TAG	UNP Q92YS1
F	2	VAL	-	EXPRESSION TAG	UNP Q92YS1
G	1	MSE	-	EXPRESSION TAG	UNP Q92YS1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	2	VAL	-	EXPRESSION TAG	UNP Q92YS1
H	1	MSE	-	EXPRESSION TAG	UNP Q92YS1
H	2	VAL	-	EXPRESSION TAG	UNP Q92YS1

- Molecule 2 is water.

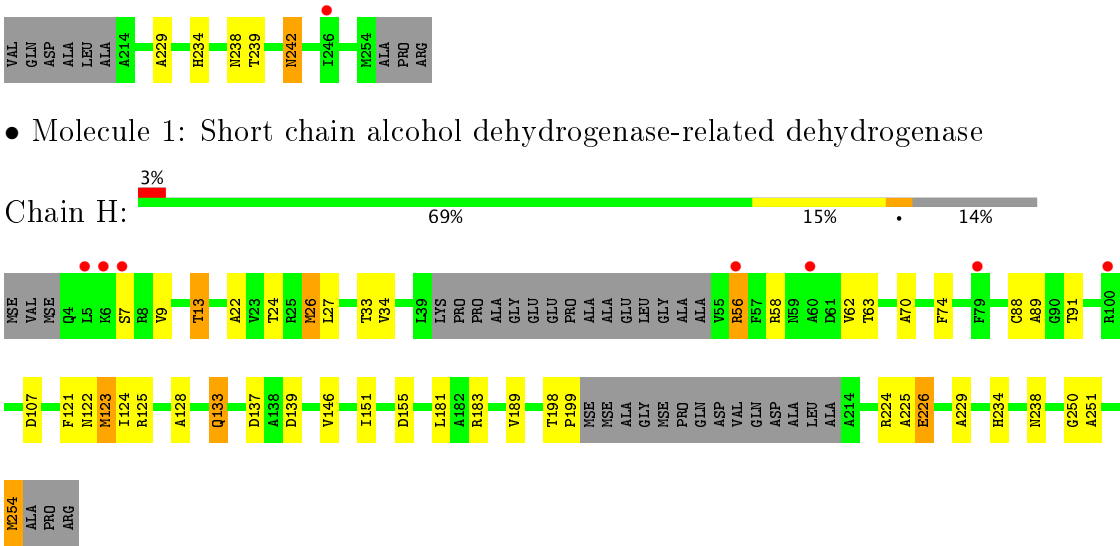
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total	O	0	0
			32	32		
2	B	36	Total	O	0	0
			36	36		
2	C	42	Total	O	0	0
			42	42		
2	D	39	Total	O	0	0
			39	39		
2	E	41	Total	O	0	0
			41	41		
2	F	30	Total	O	0	0
			30	30		
2	G	24	Total	O	0	0
			24	24		
2	H	19	Total	O	0	0
			19	19		



- Molecule 1: Short chain alcohol dehydrogenase-related dehydrogenase



- [illegible]





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.15Å 69.38Å 121.85Å 98.36° 92.72° 113.01°	Depositor
Resolution (Å)	46.20 – 2.34 46.20 – 2.34	Depositor EDS
% Data completeness (in resolution range)	97.4 (46.20-2.34) 91.4 (46.20-2.34)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.212 , 0.270 0.212 , 0.270	Depositor DCC
$R_{free}$ test set	4193 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	1.02	2/1646 (0.1%)	0.94	2/2223 (0.1%)
1	B	0.95	1/1589 (0.1%)	0.95	2/2149 (0.1%)
1	C	1.04	1/1622 (0.1%)	0.94	2/2193 (0.1%)
1	D	0.93	0/1616	0.92	2/2189 (0.1%)
1	E	0.95	0/1643	0.89	0/2219
1	F	0.94	1/1610 (0.1%)	0.92	3/2174 (0.1%)
1	G	0.86	0/1558	0.88	1/2112 (0.0%)
1	H	0.92	0/1609	0.87	0/2173
All	All	0.95	5/12893 (0.0%)	0.91	12/17432 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	107	ASP	CB-CG	5.79	1.64	1.51
1	A	226	GLU	CG-CD	5.72	1.60	1.51
1	F	244	GLU	CG-CD	5.67	1.60	1.51
1	B	9	VAL	N-CA	5.20	1.56	1.46
1	A	130	VAL	CB-CG1	-5.02	1.42	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ASP	CB-CG-OD1	5.93	123.64	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	GLY	N-CA-C	5.87	127.77	113.10
1	C	107	ASP	CB-CG-OD2	5.70	123.43	118.30
1	F	125	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	132	SER	N-CA-CB	-5.28	102.58	110.50
1	G	199	PRO	CA-C-O	-5.22	107.66	120.20
1	D	195	ILE	CB-CA-C	-5.19	101.22	111.60
1	D	144	VAL	CB-CA-C	-5.15	101.62	111.40
1	F	26	MSE	CB-CG-SE	5.10	128.00	112.70
1	F	26	MSE	CA-CB-CG	5.03	121.85	113.30
1	B	137	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	215	SER	N-CA-CB	-5.02	102.97	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	211	ALA	Peptide
1	C	198	THR	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	1627	0	1636	43	0
1	B	1573	0	1566	82	0
1	C	1604	0	1598	41	0
1	D	1597	0	1578	65	0
1	E	1624	0	1634	45	0
1	F	1593	0	1586	47	0
1	G	1542	0	1498	47	0
1	H	1592	0	1581	47	0
2	A	32	0	0	4	0
2	B	36	0	0	3	0
2	C	42	0	0	2	0
2	D	39	0	0	1	0
2	E	41	0	0	2	0
2	F	30	0	0	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	24	0	0	0	0
2	H	19	0	0	0	0
All	All	13015	0	12677	397	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (397) 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:B:234:HIS:ND1	1:D:234:HIS:HB3	1.37	1.37
1:B:234:HIS:CE1	1:D:234:HIS:HB3	1.74	1.20
1:G:68:ALA:CB	1:G:123:MSE:HE1	1.74	1.18
1:A:123:MSE:CE	1:A:123:MSE:HA	1.74	1.17
1:G:68:ALA:HB1	1:G:123:MSE:HE1	1.28	1.14
1:H:9:VAL:HG22	1:H:33:THR:HB	1.24	1.12
1:A:123:MSE:HE2	1:A:123:MSE:HA	1.19	1.12
1:H:123:MSE:CE	1:H:123:MSE:HA	1.79	1.11
1:C:68:ALA:CB	1:C:123:MSE:HE1	1.83	1.08
1:C:68:ALA:HB1	1:C:123:MSE:HE1	1.32	1.05
1:B:26:MSE:HE3	1:B:27:LEU:CD2	1.87	1.02
1:B:234:HIS:ND1	1:D:234:HIS:CB	2.24	1.01
1:E:199:PRO:HA	2:E:339:HOH:O	1.63	0.97
1:E:13:THR:HG22	1:E:88:CYS:H	1.30	0.97
1:F:91:THR:HG22	1:F:93:PRO:HD3	1.49	0.92
1:F:116:ASN:O	1:F:120:THR:HG23	1.71	0.91
1:B:234:HIS:HB3	1:D:234:HIS:CE1	2.06	0.91
1:H:123:MSE:HA	1:H:123:MSE:HE2	1.51	0.90
1:H:9:VAL:HG22	1:H:33:THR:CB	2.02	0.90
1:H:13:THR:HG22	1:H:89:ALA:H	1.38	0.88
1:E:26:MSE:HE3	1:E:27:LEU:HG	1.55	0.88
1:B:122:ASN:HD22	1:B:125:ARG:HE	1.20	0.87
1:H:56:ARG:HH11	1:H:56:ARG:HB3	1.36	0.87
1:D:129:GLU:O	1:D:132:SER:HB3	1.74	0.86
1:B:129:GLU:O	1:B:132:SER:HB2	1.77	0.85
1:A:41:PRO:HD3	1:A:59:ASN:OD1	1.75	0.85
1:H:123:MSE:HA	1:H:123:MSE:HE3	1.58	0.84
1:G:68:ALA:HB2	1:G:123:MSE:HE1	1.58	0.84
1:D:151:ILE:HG22	1:D:254:MSE:HE2	1.58	0.84
1:B:26:MSE:HE3	1:B:27:LEU:HD23	1.58	0.84
1:B:128:ALA:HA	1:B:131:MSE:HE2	1.60	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:ASN:ND2	1:G:125:ARG:HH11	1.76	0.83
1:C:13:THR:CG2	1:C:89:ALA:H	1.90	0.83
1:C:13:THR:HG22	1:C:89:ALA:H	1.43	0.83
1:C:13:THR:HG21	2:C:286:HOH:O	1.79	0.82
1:C:65:GLU:HG3	1:C:125:ARG:NH2	1.95	0.82
1:E:13:THR:HG22	1:E:88:CYS:N	1.95	0.82
1:E:198:THR:HB	1:E:199:PRO:HD2	1.61	0.81
1:H:13:THR:CG2	1:H:89:ALA:H	1.94	0.80
1:F:111:ARG:HD2	2:F:278:HOH:O	1.81	0.79
1:D:13:THR:HG22	1:D:89:ALA:H	1.47	0.79
1:B:234:HIS:CG	1:D:234:HIS:CD2	2.70	0.79
1:C:13:THR:HG23	1:C:89:ALA:HB2	1.65	0.79
1:G:122:ASN:ND2	1:G:125:ARG:NH1	2.32	0.78
1:B:234:HIS:HB3	1:D:234:HIS:CD2	2.18	0.78
1:B:234:HIS:CE1	1:D:234:HIS:CB	2.62	0.78
1:D:13:THR:CG2	1:D:89:ALA:H	1.97	0.77
1:E:6:LYS:HG3	1:E:31:GLY:HA3	1.66	0.77
1:E:13:THR:CG2	1:E:89:ALA:H	1.98	0.77
1:E:123:MSE:HE2	1:E:123:MSE:HA	1.66	0.76
1:C:122:ASN:HD22	1:C:125:ARG:HE	1.32	0.76
1:B:26:MSE:CE	1:B:27:LEU:CD2	2.62	0.76
1:D:68:ALA:CB	1:D:123:MSE:HE1	2.16	0.76
1:F:61:ASP:OD1	1:F:63:THR:HB	1.86	0.76
1:B:234:HIS:CB	1:D:234:HIS:CD2	2.69	0.75
1:E:173:LEU:HD13	1:G:165:ALA:HB2	1.68	0.75
1:C:68:ALA:HB2	1:C:123:MSE:HE1	1.69	0.75
1:G:80:GLY:C	1:G:81:HIS:CD2	2.60	0.75
1:G:13:THR:HG22	1:G:89:ALA:H	1.51	0.75
1:B:234:HIS:HB3	1:D:234:HIS:NE2	2.01	0.75
1:G:13:THR:CG2	1:G:89:ALA:H	1.99	0.75
1:B:26:MSE:CE	1:B:27:LEU:HD23	2.17	0.74
1:B:68:ALA:HB2	1:B:123:MSE:HE1	1.68	0.74
1:D:13:THR:HG22	1:D:88:CYS:H	1.51	0.74
1:E:123:MSE:CA	1:E:123:MSE:HE2	2.18	0.74
1:F:13:THR:HG22	1:F:88:CYS:H	1.52	0.74
1:G:116:ASN:O	1:G:120:THR:HG23	1.88	0.73
1:B:68:ALA:CB	1:B:123:MSE:HE1	2.19	0.73
1:H:133:GLN:HA	1:H:133:GLN:HE21	1.52	0.72
1:G:80:GLY:C	1:G:81:HIS:HD2	1.92	0.72
1:F:171:ALA:O	1:F:174:THR:HG23	1.88	0.72
1:B:26:MSE:HE3	1:B:27:LEU:CG	2.19	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:THR:HG23	1:D:34:VAL:HG11	1.70	0.72
1:C:13:THR:HG22	1:C:88:CYS:H	1.53	0.71
1:F:122:ASN:ND2	1:F:125:ARG:HH11	1.88	0.71
1:C:65:GLU:HG3	1:C:125:ARG:HH22	1.55	0.71
1:G:122:ASN:HD21	1:G:125:ARG:NH1	1.88	0.71
1:B:131:MSE:HE1	1:B:186:ILE:HG21	1.73	0.71
1:H:26:MSE:HG2	1:H:229:ALA:HB1	1.73	0.71
1:B:120:THR:HG22	2:B:277:HOH:O	1.89	0.70
1:D:151:ILE:CG2	1:D:254:MSE:HE2	2.21	0.70
1:E:40:LYS:HE3	1:E:41:PRO:HD2	1.71	0.70
1:C:135:GLU:HG2	1:C:136:PRO:HD2	1.74	0.70
1:A:123:MSE:CA	1:A:123:MSE:CE	2.65	0.70
1:B:234:HIS:CG	1:D:234:HIS:CG	2.80	0.70
1:F:116:ASN:O	1:F:120:THR:CG2	2.39	0.69
1:G:199:PRO:HD2	1:G:199:PRO:O	1.93	0.69
1:D:116:ASN:O	1:D:120:THR:HG23	1.93	0.69
1:E:226:GLU:H	1:E:226:GLU:CD	1.96	0.68
1:A:26:MSE:HE3	1:A:27:LEU:HG	1.76	0.68
1:D:26:MSE:HE3	1:D:27:LEU:HG	1.75	0.68
1:G:80:GLY:O	1:G:81:HIS:HD2	1.77	0.68
1:H:24:THR:HG23	1:H:34:VAL:HG11	1.76	0.67
1:G:199:PRO:CD	1:G:199:PRO:O	2.37	0.67
1:C:13:THR:HG23	1:C:89:ALA:CB	2.23	0.67
1:B:129:GLU:O	1:B:132:SER:CB	2.42	0.67
1:G:68:ALA:HB1	1:G:123:MSE:CE	2.17	0.67
1:G:72:LEU:HD11	1:G:127:ALA:HA	1.76	0.67
1:H:9:VAL:CG2	1:H:33:THR:HB	2.15	0.67
1:E:62:VAL:HG22	1:E:123:MSE:SE	2.45	0.66
1:D:122:ASN:HD22	1:D:125:ARG:HE	1.42	0.66
1:A:13:THR:HG22	1:A:88:CYS:H	1.60	0.65
1:H:13:THR:O	1:H:88:CYS:HB2	1.97	0.65
1:E:13:THR:HG23	1:E:89:ALA:H	1.61	0.65
1:B:26:MSE:HE3	1:B:27:LEU:HG	1.78	0.65
1:B:82:VAL:HG23	1:B:130:VAL:HG11	1.78	0.65
1:C:13:THR:HG22	1:C:89:ALA:N	2.11	0.65
1:B:234:HIS:ND1	1:D:234:HIS:CG	2.65	0.64
1:E:68:ALA:CB	1:E:123:MSE:HE1	2.27	0.64
1:B:13:THR:CG2	1:B:89:ALA:H	2.10	0.64
1:D:68:ALA:HB2	1:D:123:MSE:HE1	1.77	0.64
1:E:116:ASN:HB2	1:E:166:SER:OG	1.97	0.64
1:B:9:VAL:HG22	1:B:33:THR:HB	1.79	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:THR:HG23	1:B:89:ALA:HB2	1.78	0.64
1:B:234:HIS:HB3	1:D:234:HIS:CG	2.33	0.63
1:F:22:ALA:HA	1:F:25:ARG:NH1	2.13	0.63
1:F:122:ASN:HA	1:F:125:ARG:HD3	1.80	0.63
1:H:198:THR:HB	1:H:199:PRO:CD	2.29	0.63
1:B:116:ASN:O	1:B:120:THR:HG23	1.99	0.63
1:B:122:ASN:ND2	1:B:125:ARG:HE	1.94	0.63
1:H:13:THR:HG23	1:H:89:ALA:HB2	1.80	0.62
1:E:224:ARG:HB3	1:E:226:GLU:OE1	1.99	0.62
1:B:188:VAL:H	1:B:242:ASN:ND2	1.97	0.62
1:C:58:ARG:HG3	2:C:362:HOH:O	1.98	0.62
1:D:171:ALA:O	1:D:174:THR:HG23	2.00	0.62
1:G:13:THR:HG23	1:G:89:ALA:HB2	1.82	0.62
1:A:13:THR:CG2	1:A:89:ALA:H	2.11	0.62
1:A:13:THR:HG22	1:A:89:ALA:H	1.64	0.62
1:D:13:THR:HG22	1:D:88:CYS:N	2.15	0.62
1:E:123:MSE:HE2	1:E:123:MSE:N	2.15	0.61
1:G:72:LEU:HD12	1:G:130:VAL:HG21	1.82	0.61
1:D:188:VAL:H	1:D:242:ASN:ND2	1.98	0.61
1:B:13:THR:HG22	1:B:89:ALA:H	1.63	0.61
1:B:62:VAL:CG1	1:B:119:GLY:HA3	2.30	0.61
1:D:116:ASN:O	1:D:120:THR:CG2	2.48	0.61
1:D:129:GLU:O	1:D:132:SER:CB	2.48	0.61
1:D:122:ASN:ND2	1:D:125:ARG:HH21	1.99	0.61
1:F:5:LEU:O	1:F:8:ARG:HG2	2.01	0.60
1:B:61:ASP:OD1	1:B:63:THR:HB	2.01	0.60
1:H:13:THR:HG23	1:H:89:ALA:CB	2.31	0.60
1:D:219:PRO:HB2	1:D:221:ARG:HG2	1.83	0.60
1:A:123:MSE:CA	1:A:123:MSE:HE2	2.12	0.60
1:H:226:GLU:H	1:H:226:GLU:CD	2.05	0.60
1:A:13:THR:HG23	1:A:89:ALA:HB2	1.84	0.60
1:B:131:MSE:CE	1:B:186:ILE:HD13	2.32	0.59
1:C:13:THR:CG2	1:C:89:ALA:N	2.64	0.59
1:H:13:THR:HG22	1:H:88:CYS:H	1.68	0.59
1:B:234:HIS:HB3	1:D:234:HIS:ND1	2.17	0.59
1:E:90:GLY:HA2	1:E:116:ASN:OD1	2.03	0.59
1:D:195:ILE:CG2	1:D:222:LEU:HD22	2.33	0.59
1:F:13:THR:HG21	2:F:269:HOH:O	2.01	0.59
1:A:180:GLU:HG3	1:D:158:ILE:HG23	1.84	0.59
1:A:123:MSE:HE3	1:A:123:MSE:HA	1.78	0.58
1:F:151:ILE:HG13	1:F:247:ARG:NH2	2.18	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:ASP:OD1	1:G:63:THR:HB	2.03	0.58
1:H:224:ARG:HB3	1:H:226:GLU:OE1	2.03	0.58
1:D:122:ASN:HD21	1:D:125:ARG:HH21	1.51	0.58
1:H:198:THR:HB	1:H:199:PRO:HD2	1.85	0.58
1:H:56:ARG:HH11	1:H:56:ARG:CB	2.14	0.58
1:D:35:LEU:HD22	1:D:75:ALA:HB2	1.85	0.58
1:C:61:ASP:OD1	1:C:63:THR:HB	2.04	0.57
1:F:128:ALA:O	1:F:132:SER:HB2	2.05	0.57
1:H:26:MSE:HE3	1:H:27:LEU:HG	1.87	0.57
1:B:173:LEU:HD13	1:C:165:ALA:HB2	1.87	0.57
1:E:198:THR:HB	1:E:199:PRO:CD	2.34	0.57
1:D:171:ALA:O	1:D:174:THR:CG2	2.53	0.56
1:F:13:THR:CG2	1:F:89:ALA:H	2.18	0.56
1:F:151:ILE:HG22	1:F:254:MSE:HE2	1.86	0.56
1:F:13:THR:HG23	1:F:89:ALA:HB2	1.87	0.56
1:C:116:ASN:HB2	1:C:166:SER:OG	2.04	0.56
1:C:151:ILE:HG12	1:C:247:ARG:NH2	2.20	0.56
1:A:13:THR:HG22	1:A:88:CYS:N	2.19	0.56
1:B:188:VAL:H	1:B:242:ASN:HD21	1.52	0.56
1:E:68:ALA:HB2	1:E:123:MSE:HE1	1.87	0.56
1:C:122:ASN:HD21	1:C:125:ARG:HH21	1.52	0.56
1:A:151:ILE:HD13	1:A:249:ASP:HB3	1.86	0.55
1:C:13:THR:HG22	1:C:88:CYS:N	2.19	0.55
1:F:122:ASN:O	1:F:125:ARG:HG2	2.06	0.55
1:D:142:ARG:NH1	2:D:265:HOH:O	2.39	0.55
1:F:13:THR:HG22	1:F:89:ALA:H	1.72	0.55
1:A:122:ASN:ND2	1:A:125:ARG:HH11	2.04	0.55
1:H:13:THR:HG22	1:H:88:CYS:N	2.22	0.55
1:B:180:GLU:HG2	1:B:181:LEU:HD13	1.88	0.55
1:E:114:ALA:HA	1:E:118:ILE:HG13	1.90	0.54
1:B:13:THR:HG22	1:B:88:CYS:H	1.72	0.54
1:C:151:ILE:HD13	1:C:249:ASP:HB3	1.89	0.54
1:B:62:VAL:HG12	1:B:119:GLY:HA3	1.90	0.54
1:G:13:THR:HG22	1:G:88:CYS:H	1.73	0.54
1:B:250:GLY:O	1:B:251:ALA:HB3	2.08	0.53
1:H:122:ASN:ND2	1:H:125:ARG:HH21	2.05	0.53
1:H:13:THR:HG22	1:H:89:ALA:N	2.17	0.53
1:A:120:THR:HG23	2:A:354:HOH:O	2.09	0.53
1:B:101:SER:HB2	2:B:263:HOH:O	2.09	0.53
1:E:5:LEU:HD13	1:E:27:LEU:HD23	1.90	0.53
1:C:124:ILE:HG12	1:C:145:ILE:HG21	1.91	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASP:OD1	1:A:63:THR:HB	2.10	0.52
1:D:72:LEU:HD11	1:D:127:ALA:HA	1.90	0.52
1:H:122:ASN:HD21	1:H:125:ARG:HH21	1.56	0.52
1:D:13:THR:HG23	1:D:89:ALA:HB2	1.91	0.52
1:E:188:VAL:H	1:E:242:ASN:ND2	2.07	0.52
1:A:120:THR:CG2	2:A:354:HOH:O	2.58	0.52
1:E:189:VAL:HG11	1:E:235:ILE:HD13	1.91	0.52
1:A:62:VAL:HG12	1:A:119:GLY:HA3	1.91	0.52
1:B:142:ARG:HB2	1:B:184:PHE:O	2.08	0.52
1:B:136:PRO:HD3	1:B:142:ARG:NH1	2.25	0.52
1:G:188:VAL:H	1:G:242:ASN:ND2	2.08	0.52
1:C:151:ILE:HD12	1:C:192:ALA:O	2.10	0.52
1:E:68:ALA:HB1	1:E:123:MSE:HE1	1.90	0.52
1:G:19:LEU:O	1:G:23:VAL:HG23	2.10	0.52
1:F:122:ASN:HD22	1:F:125:ARG:HD3	1.74	0.52
1:H:9:VAL:HG22	1:H:33:THR:CG2	2.39	0.51
1:G:72:LEU:HD12	1:G:130:VAL:CG2	2.41	0.51
1:H:22:ALA:CB	1:H:225:ALA:HB1	2.40	0.51
1:B:13:THR:HG22	1:B:88:CYS:N	2.25	0.51
1:H:26:MSE:HE3	1:H:27:LEU:CD2	2.40	0.51
1:D:195:ILE:HG21	1:D:222:LEU:HD22	1.92	0.51
1:G:83:HIS:O	1:G:143:GLY:HA2	2.11	0.51
1:F:129:GLU:O	1:F:132:SER:HB3	2.10	0.51
1:G:122:ASN:HA	1:G:125:ARG:HD3	1.93	0.51
1:A:122:ASN:HD22	1:A:125:ARG:HH11	1.58	0.50
1:B:234:HIS:CB	1:D:234:HIS:NE2	2.71	0.50
1:D:6:LYS:O	1:D:7:SER:HB2	2.10	0.50
1:D:5:LEU:O	1:D:8:ARG:HG2	2.11	0.50
1:F:188:VAL:H	1:F:242:ASN:ND2	2.08	0.50
1:D:33:THR:HG21	1:D:79:PHE:CD1	2.46	0.50
1:G:13:THR:HG22	1:G:88:CYS:N	2.25	0.50
1:F:13:THR:HG22	1:F:88:CYS:N	2.23	0.50
1:D:62:VAL:HG22	1:D:123:MSE:HG2	1.94	0.50
1:H:26:MSE:HE3	1:H:27:LEU:HD23	1.93	0.49
1:C:162:ALA:O	1:C:166:SER:HB2	2.12	0.49
1:C:157:GLN:HG3	1:C:160:GLN:OE1	2.12	0.49
1:E:123:MSE:CA	1:E:123:MSE:CE	2.90	0.49
1:G:13:THR:HG23	1:G:89:ALA:CB	2.41	0.49
1:A:128:ALA:O	1:A:132:SER:HB2	2.11	0.49
1:A:8:ARG:NH1	1:A:83:HIS:CD2	2.80	0.49
1:A:13:THR:HG22	1:A:89:ALA:N	2.28	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:THR:HG23	1:D:89:ALA:CB	2.43	0.49
1:H:151:ILE:HG13	1:H:254:MSE:HE2	1.94	0.49
1:A:160:GLN:HG2	2:A:282:HOH:O	2.13	0.48
1:C:90:GLY:HA2	1:C:116:ASN:OD1	2.13	0.48
1:B:131:MSE:HE3	1:B:186:ILE:HD13	1.94	0.48
1:B:226:GLU:HG2	2:B:344:HOH:O	2.13	0.48
1:C:123:MSE:HA	1:C:123:MSE:HE2	1.95	0.48
1:A:55:VAL:N	2:A:371:HOH:O	2.46	0.48
1:H:226:GLU:N	1:H:226:GLU:CD	2.67	0.48
1:C:122:ASN:ND2	1:C:125:ARG:HE	2.07	0.48
1:E:13:THR:HG23	1:E:89:ALA:N	2.28	0.48
1:B:26:MSE:HE3	1:B:27:LEU:HD21	1.89	0.48
1:E:123:MSE:HA	1:E:123:MSE:CE	2.40	0.48
1:F:141:GLU:OE1	1:F:144:VAL:CG2	2.61	0.48
1:B:132:SER:HB3	1:B:133:GLN:HG3	1.95	0.47
1:C:153:ALA:HB1	1:C:168:GLY:HA2	1.96	0.47
1:A:26:MSE:CE	1:A:27:LEU:HG	2.43	0.47
1:D:128:ALA:O	1:D:132:SER:HB2	2.13	0.47
1:F:26:MSE:C	1:F:26:MSE:SE	3.03	0.47
1:B:72:LEU:HD11	1:B:127:ALA:HA	1.97	0.47
1:D:195:ILE:HG21	1:D:222:LEU:CD2	2.44	0.47
1:F:127:ALA:O	1:F:131:MSE:HG3	2.13	0.47
1:B:10:PHE:CD1	1:B:84:GLY:HA3	2.50	0.47
1:B:13:THR:HG23	1:B:89:ALA:CB	2.44	0.47
1:E:157:GLN:O	1:E:160:GLN:HB2	2.14	0.47
1:F:122:ASN:HD22	1:F:125:ARG:HH11	1.60	0.47
1:H:26:MSE:HE3	1:H:27:LEU:CG	2.45	0.47
1:A:35:LEU:HD11	1:A:58:ARG:HG3	1.97	0.47
1:B:68:ALA:HB1	1:B:123:MSE:HE1	1.96	0.47
1:B:122:ASN:HD21	1:B:125:ARG:HH21	1.61	0.47
1:C:250:GLY:O	1:C:251:ALA:HB3	2.15	0.47
1:E:40:LYS:HA	1:E:40:LYS:HD2	1.73	0.47
1:G:122:ASN:HD22	1:G:125:ARG:HH11	1.55	0.47
1:G:188:VAL:H	1:G:242:ASN:HD21	1.62	0.47
1:A:127:ALA:O	1:A:131:MSE:HG3	2.15	0.47
1:B:131:MSE:HE3	1:B:186:ILE:CD1	2.45	0.47
1:G:81:HIS:N	1:G:81:HIS:CD2	2.83	0.47
1:D:188:VAL:H	1:D:242:ASN:HD21	1.61	0.46
1:F:151:ILE:HD13	1:F:192:ALA:O	2.15	0.46
1:F:188:VAL:H	1:F:242:ASN:HD21	1.62	0.46
1:H:198:THR:CB	1:H:199:PRO:CD	2.90	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:GLY:HA2	1:D:116:ASN:OD1	2.14	0.46
1:G:90:GLY:HA2	1:G:116:ASN:OD1	2.14	0.46
1:F:174:THR:HG21	1:F:190:THR:OG1	2.16	0.46
1:G:80:GLY:O	1:G:81:HIS:CD2	2.62	0.46
1:C:97:ILE:HA	1:C:104:HIS:HB2	1.96	0.46
1:H:234:HIS:CE1	1:H:238:ASN:HD22	2.32	0.46
1:B:82:VAL:HG23	1:B:130:VAL:CG1	2.43	0.46
1:G:26:MSE:CG	1:G:229:ALA:HB1	2.45	0.46
1:H:58:ARG:HH21	1:H:70:ALA:HB1	1.81	0.46
1:A:26:MSE:SE	1:A:233:LYS:HB2	2.65	0.46
1:B:10:PHE:CE1	1:B:84:GLY:HA3	2.50	0.46
1:F:24:THR:HG23	1:F:34:VAL:HG11	1.98	0.46
1:E:162:ALA:O	1:E:166:SER:HB2	2.16	0.46
1:G:26:MSE:HE3	1:G:27:LEU:HG	1.98	0.46
1:D:114:ALA:HA	1:D:118:ILE:HG12	1.97	0.46
1:F:26:MSE:O	1:F:30:GLU:HG2	2.16	0.46
1:A:156:GLY:HA3	1:D:176:PRO:HD3	1.98	0.46
1:G:234:HIS:CE1	1:G:238:ASN:HD22	2.34	0.46
1:E:199:PRO:CA	2:E:339:HOH:O	2.40	0.45
1:F:174:THR:CG2	1:F:190:THR:OG1	2.64	0.45
1:H:122:ASN:HD21	1:H:125:ARG:NH2	2.15	0.45
1:H:146:VAL:HA	1:H:189:VAL:O	2.16	0.45
1:A:151:ILE:HG12	1:A:247:ARG:NH2	2.30	0.45
1:C:107:ASP:O	1:C:111:ARG:HG3	2.16	0.45
1:B:131:MSE:CE	1:B:186:ILE:HG21	2.45	0.45
1:C:122:ASN:ND2	1:C:125:ARG:HH21	2.14	0.45
1:G:116:ASN:O	1:G:120:THR:CG2	2.62	0.45
1:B:114:ALA:HA	1:B:118:ILE:CG1	2.46	0.45
1:E:40:LYS:CE	1:E:41:PRO:HD2	2.45	0.45
1:F:122:ASN:ND2	1:F:125:ARG:NH1	2.62	0.45
1:H:56:ARG:HD2	1:H:74:PHE:HE1	1.82	0.45
1:B:19:LEU:O	1:B:23:VAL:HG23	2.17	0.45
1:G:39:LEU:HD21	1:G:61:ASP:HB2	1.99	0.45
1:B:26:MSE:CE	1:B:27:LEU:HD21	2.44	0.44
1:C:198:THR:HB	1:C:199:PRO:HD3	1.98	0.44
1:H:122:ASN:ND2	1:H:125:ARG:NH2	2.65	0.44
1:E:56:ARG:HB2	1:E:56:ARG:CZ	2.48	0.44
1:E:146:VAL:HA	1:E:189:VAL:O	2.18	0.44
1:D:62:VAL:HA	1:D:123:MSE:HE3	2.00	0.44
1:D:163:TYR:O	1:D:166:SER:HB2	2.16	0.44
1:G:146:VAL:HA	1:G:189:VAL:O	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:HG23	1:A:89:ALA:CB	2.48	0.44
1:B:116:ASN:O	1:B:120:THR:CG2	2.64	0.44
1:G:10:PHE:CE1	1:G:84:GLY:HA3	2.53	0.44
1:A:188:VAL:H	1:A:242:ASN:ND2	2.16	0.44
1:E:72:LEU:HD12	1:E:130:VAL:HG21	2.00	0.44
1:G:129:GLU:O	1:G:132:SER:HB3	2.17	0.44
1:D:41:PRO:HD3	1:D:59:ASN:OD1	2.18	0.43
1:F:72:LEU:HD13	1:F:72:LEU:HA	1.87	0.43
1:A:5:LEU:HD13	1:A:27:LEU:HD23	2.01	0.43
1:H:22:ALA:HB2	1:H:225:ALA:HB1	2.00	0.43
1:D:106:LEU:HD12	1:D:106:LEU:HA	1.82	0.43
1:B:187:ARG:HD2	1:B:187:ARG:HH11	1.64	0.43
1:F:125:ARG:HG2	1:F:126:LEU:H	1.83	0.43
1:B:75:ALA:O	1:B:79:PHE:HB2	2.18	0.43
1:E:26:MSE:HE3	1:E:27:LEU:CG	2.36	0.43
1:B:106:LEU:HD12	1:B:106:LEU:HA	1.92	0.43
1:C:85:LEU:HD21	1:C:123:MSE:HB3	2.01	0.43
1:F:114:ALA:HA	1:F:118:ILE:HG12	2.01	0.43
1:F:181:LEU:HB3	1:F:186:ILE:HB	2.00	0.43
1:B:62:VAL:HG13	1:B:119:GLY:CA	2.49	0.43
1:B:234:HIS:CB	1:D:234:HIS:CG	2.99	0.43
1:E:187:ARG:HD2	1:E:241:LEU:O	2.18	0.43
1:E:97:ILE:HA	1:E:104:HIS:HB2	2.01	0.43
1:F:62:VAL:HG12	1:F:119:GLY:CA	2.49	0.43
1:F:125:ARG:HG2	1:F:126:LEU:N	2.34	0.43
1:C:10:PHE:CD1	1:C:84:GLY:HA3	2.54	0.42
1:D:151:ILE:HG13	1:D:247:ARG:NH2	2.34	0.42
1:A:68:ALA:HB1	1:A:123:MSE:CE	2.49	0.42
1:H:124:ILE:O	1:H:128:ALA:HB2	2.19	0.42
1:H:137:ASP:OD1	1:H:137:ASP:C	2.57	0.42
1:H:26:MSE:CE	1:H:27:LEU:HD23	2.49	0.42
1:C:39:LEU:HA	1:C:39:LEU:HD23	1.74	0.42
1:A:240:MSE:HB3	1:A:240:MSE:HE3	1.94	0.42
1:E:125:ARG:NH1	1:G:104:HIS:O	2.52	0.42
1:F:151:ILE:CD1	1:F:192:ALA:O	2.67	0.42
1:G:187:ARG:HD3	1:G:239:THR:O	2.19	0.42
1:B:13:THR:HG22	1:B:89:ALA:N	2.32	0.42
1:D:217:PRO:HD2	1:D:250:GLY:O	2.19	0.42
1:H:9:VAL:HA	1:H:33:THR:O	2.19	0.42
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.53	0.42
1:H:250:GLY:O	1:H:251:ALA:HB3	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:TYR:CE1	1:B:167:LYS:HE3	2.55	0.42
1:C:142:ARG:HH11	1:C:142:ARG:HD3	1.70	0.42
1:G:137:ASP:OD1	1:G:137:ASP:C	2.58	0.42
1:A:13:THR:CG2	1:A:89:ALA:N	2.82	0.41
1:D:250:GLY:O	1:D:251:ALA:HB3	2.20	0.41
1:B:124:ILE:HD11	1:B:147:ASN:HD21	1.85	0.41
1:B:16:SER:HB2	1:B:38:ASP:OD2	2.20	0.41
1:D:26:MSE:SE	1:D:26:MSE:C	3.09	0.41
1:G:87:ASN:HD21	1:G:123:MSE:HB2	1.85	0.41
1:A:68:ALA:HB1	1:A:123:MSE:HE1	2.01	0.41
1:F:23:VAL:HG11	1:F:86:VAL:HG11	2.02	0.41
1:B:72:LEU:HD12	1:B:130:VAL:HG21	2.03	0.41
1:C:188:VAL:H	1:C:242:ASN:ND2	2.17	0.41
1:B:90:GLY:HA2	1:B:116:ASN:OD1	2.21	0.41
1:F:6:LYS:HE3	1:F:31:GLY:HA3	2.03	0.41
1:B:131:MSE:HE1	1:B:186:ILE:CG2	2.48	0.41
1:F:72:LEU:CD2	1:F:123:MSE:HE1	2.50	0.41
1:F:87:ASN:HB2	1:F:147:ASN:HD22	1.85	0.41
1:B:26:MSE:C	1:B:26:MSE:SE	3.10	0.41
1:D:68:ALA:HB1	1:D:123:MSE:HE1	1.99	0.41
1:B:163:TYR:HE1	1:B:167:LYS:HE3	1.86	0.41
1:G:35:LEU:HD12	1:G:56:ARG:O	2.20	0.41
1:A:122:ASN:HA	1:A:125:ARG:HD3	2.03	0.41
1:E:122:ASN:C	1:E:123:MSE:HE2	2.41	0.41
1:A:122:ASN:O	1:A:125:ARG:HG2	2.21	0.40
1:A:247:ARG:NH2	1:A:253:ARG:HD3	2.36	0.40
1:E:180:GLU:O	1:E:183:ARG:HB2	2.21	0.40
1:H:121:PHE:O	1:H:125:ARG:HG2	2.22	0.40
1:A:142:ARG:HH11	1:A:142:ARG:HD3	1.73	0.40
1:D:195:ILE:HG22	1:D:222:LEU:HD22	2.04	0.40
1:A:5:LEU:HD21	1:A:236:CYS:HB3	2.03	0.40
1:B:58:ARG:HH11	1:B:60:ALA:HB2	1.87	0.40
1:D:68:ALA:CB	1:D:123:MSE:CE	2.94	0.40
1:E:87:ASN:HD21	1:E:123:MSE:HB3	1.86	0.40
1:E:34:VAL:HB	1:E:55:VAL:HB	2.02	0.40
1:B:180:GLU:O	1:B:183:ARG:HB2	2.21	0.40
1:F:125:ARG:CG	1:F:126:LEU:N	2.85	0.40
1:F:191:ILE:HG21	1:F:228:TYR:CE2	2.57	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	219/257 (85%)	213 (97%)	6 (3%)	0	100	100
1	B	215/257 (84%)	206 (96%)	9 (4%)	0	100	100
1	C	218/257 (85%)	208 (95%)	10 (5%)	0	100	100
1	D	220/257 (86%)	211 (96%)	9 (4%)	0	100	100
1	E	219/257 (85%)	206 (94%)	13 (6%)	0	100	100
1	F	217/257 (84%)	204 (94%)	13 (6%)	0	100	100
1	G	216/257 (84%)	202 (94%)	14 (6%)	0	100	100
1	H	216/257 (84%)	204 (94%)	12 (6%)	0	100	100
All	All	1740/2056 (85%)	1654 (95%)	86 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	160/173 (92%)	144 (90%)	16 (10%)	9	8
1	B	151/173 (87%)	135 (89%)	16 (11%)	8	7
1	C	156/173 (90%)	139 (89%)	17 (11%)	7	7
1	D	153/173 (88%)	136 (89%)	17 (11%)	7	6
1	E	159/173 (92%)	143 (90%)	16 (10%)	9	8
1	F	153/173 (88%)	137 (90%)	16 (10%)	8	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	143/173 (83%)	127 (89%)	16 (11%)	7	6
1	H	153/173 (88%)	137 (90%)	16 (10%)	8	7
All	All	1228/1384 (89%)	1098 (89%)	130 (11%)	8	7

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	13	THR
1	A	55	VAL
1	A	62	VAL
1	A	63	THR
1	A	76	LYS
1	A	91	THR
1	A	101	SER
1	A	108	SER
1	A	123	MSE
1	A	142	ARG
1	A	151	ILE
1	A	166	SER
1	A	183	ARG
1	A	215	SER
1	A	242	ASN
1	B	13	THR
1	B	26	MSE
1	B	56	ARG
1	B	62	VAL
1	B	69	THR
1	B	91	THR
1	B	101	SER
1	B	120	THR
1	B	132	SER
1	B	139	ASP
1	B	181	LEU
1	B	183	ARG
1	B	195	ILE
1	B	210	ASP
1	B	215	SER
1	B	242	ASN
1	C	13	THR
1	C	40	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	63	THR
1	C	72	LEU
1	C	91	THR
1	C	101	SER
1	C	107	ASP
1	C	132	SER
1	C	135	GLU
1	C	151	ILE
1	C	157	GLN
1	C	160	GLN
1	C	181	LEU
1	C	183	ARG
1	C	195	ILE
1	C	217	PRO
1	C	242	ASN
1	D	13	THR
1	D	26	MSE
1	D	55	VAL
1	D	62	VAL
1	D	63	THR
1	D	76	LYS
1	D	91	THR
1	D	107	ASP
1	D	120	THR
1	D	150	SER
1	D	151	ILE
1	D	166	SER
1	D	174	THR
1	D	181	LEU
1	D	183	ARG
1	D	215	SER
1	D	226	GLU
1	E	13	THR
1	E	26	MSE
1	E	55	VAL
1	E	56	ARG
1	E	62	VAL
1	E	63	THR
1	E	91	THR
1	E	123	MSE
1	E	139	ASP
1	E	155	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	166	SER
1	E	181	LEU
1	E	183	ARG
1	E	195	ILE
1	E	217	PRO
1	E	226	GLU
1	F	6	LYS
1	F	13	THR
1	F	26	MSE
1	F	63	THR
1	F	65	GLU
1	F	111	ARG
1	F	120	THR
1	F	125	ARG
1	F	139	ASP
1	F	151	ILE
1	F	155	ASP
1	F	174	THR
1	F	181	LEU
1	F	183	ARG
1	F	215	SER
1	F	242	ASN
1	G	13	THR
1	G	26	MSE
1	G	33	THR
1	G	62	VAL
1	G	63	THR
1	G	65	GLU
1	G	81	HIS
1	G	88	CYS
1	G	91	THR
1	G	120	THR
1	G	125	ARG
1	G	155	ASP
1	G	181	LEU
1	G	183	ARG
1	G	195	ILE
1	G	242	ASN
1	H	7	SER
1	H	13	THR
1	H	26	MSE
1	H	56	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	62	VAL
1	H	63	THR
1	H	91	THR
1	H	107	ASP
1	H	123	MSE
1	H	133	GLN
1	H	139	ASP
1	H	155	ASP
1	H	181	LEU
1	H	183	ARG
1	H	226	GLU
1	H	254	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	122	ASN
1	A	147	ASN
1	A	242	ASN
1	B	87	ASN
1	B	122	ASN
1	B	147	ASN
1	B	242	ASN
1	C	87	ASN
1	C	122	ASN
1	C	147	ASN
1	C	242	ASN
1	D	87	ASN
1	D	122	ASN
1	D	133	GLN
1	D	147	ASN
1	D	242	ASN
1	E	87	ASN
1	E	147	ASN
1	E	242	ASN
1	F	87	ASN
1	F	122	ASN
1	F	133	GLN
1	F	147	ASN
1	F	242	ASN
1	G	81	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	87	ASN
1	G	122	ASN
1	G	147	ASN
1	G	234	HIS
1	G	242	ASN
1	H	87	ASN
1	H	122	ASN
1	H	133	GLN
1	H	147	ASN
1	H	234	HIS
1	H	242	ASN

### 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 [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	220/257 (85%)	-0.22	0 100 100	17, 29, 45, 58	0
1	B	216/257 (84%)	0.13	8 (3%) 42 53	18, 32, 50, 58	0
1	C	219/257 (85%)	0.09	4 (1%) 69 77	17, 30, 49, 60	0
1	D	221/257 (85%)	0.03	6 (2%) 55 64	19, 32, 52, 61	0
1	E	220/257 (85%)	0.12	7 (3%) 48 59	22, 35, 59, 69	0
1	F	218/257 (84%)	0.01	5 (2%) 61 70	21, 33, 48, 64	0
1	G	217/257 (84%)	0.28	12 (5%) 26 36	21, 38, 55, 61	0
1	H	217/257 (84%)	0.21	7 (3%) 48 59	23, 39, 63, 68	0
All	All	1748/2056 (85%)	0.08	49 (2%) 53 63	17, 33, 55, 69	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	80	GLY	4.8
1	C	100	ARG	3.9
1	B	79	PHE	3.9
1	G	199	PRO	3.8
1	F	100	ARG	3.7
1	F	101	SER	3.5
1	G	80	GLY	3.5
1	G	81	HIS	3.5
1	E	100	ARG	3.2
1	H	79	PHE	3.0
1	C	80	GLY	3.0
1	B	80	GLY	2.9
1	E	101	SER	2.9
1	D	41	PRO	2.9
1	G	246	ILE	2.8
1	C	171	ALA	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	170	VAL	2.7
1	B	234	HIS	2.6
1	D	39	LEU	2.6
1	E	79	PHE	2.6
1	E	81	HIS	2.5
1	F	199	PRO	2.5
1	G	197	ASP	2.4
1	G	74	PHE	2.4
1	C	101	SER	2.4
1	B	245	VAL	2.4
1	H	7	SER	2.4
1	G	183	ARG	2.4
1	B	83	HIS	2.3
1	H	60	ALA	2.3
1	F	107	ASP	2.3
1	D	59	ASN	2.3
1	D	57	PHE	2.3
1	G	92	ALA	2.3
1	H	56	ARG	2.2
1	G	79	PHE	2.2
1	H	100	ARG	2.2
1	F	245	VAL	2.2
1	G	57	PHE	2.1
1	B	246	ILE	2.1
1	E	77	GLN	2.1
1	B	28	ALA	2.1
1	H	5	LEU	2.1
1	E	226	GLU	2.1
1	D	101	SER	2.1
1	D	234	HIS	2.1
1	B	99	GLY	2.1
1	H	6	LYS	2.1
1	G	16	SER	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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.