Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:49 PM GMT

PDB ID	:	3S6J
Title	:	The crystal structure of a hydrolase from Pseudomonas syringae
Authors	:	Zhang, Z.; Syed Ibrahim, B.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2011-05-25
Resolution	:	2.20 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:

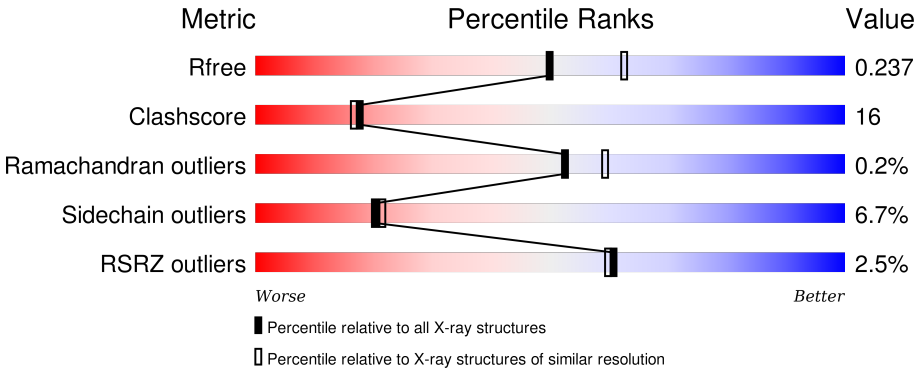
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	233	3% 68% 22% • 7%
1	B	233	2% 65% 22% • 10%
1	C	233	3% 64% 24% • 9%
1	D	233	3% 70% 20% • 7%
1	E	233	3% 68% 22% • 6%

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Mol	Chain	Length	Quality of chain
1	F	233	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10211 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 Hydrolase, haloacid dehalogenase-like family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	Se	0	0	0
			1666	1053	284	322	3	4			
1	B	209	Total	C	N	O	S	Se	0	0	0
			1610	1019	273	311	3	4			
1	C	212	Total	C	N	O	S	Se	0	0	0
			1627	1027	276	316	3	5			
1	D	216	Total	C	N	O	S	Se	0	0	0
			1666	1052	284	323	3	4			
1	E	220	Total	C	N	O	S	Se	0	0	0
			1691	1067	288	328	3	5			
1	F	219	Total	C	N	O	S	Se	0	0	0
			1684	1062	287	327	3	5			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	MSE	-	EXPRESSION TAG	UNP Q88AV7
A	103	SER	-	EXPRESSION TAG	UNP Q88AV7
A	104	LEU	-	EXPRESSION TAG	UNP Q88AV7
A	327	GLU	-	EXPRESSION TAG	UNP Q88AV7
A	328	GLY	-	EXPRESSION TAG	UNP Q88AV7
A	329	HIS	-	EXPRESSION TAG	UNP Q88AV7
A	330	HIS	-	EXPRESSION TAG	UNP Q88AV7
A	331	HIS	-	EXPRESSION TAG	UNP Q88AV7
A	332	HIS	-	EXPRESSION TAG	UNP Q88AV7
A	333	HIS	-	EXPRESSION TAG	UNP Q88AV7
A	334	HIS	-	EXPRESSION TAG	UNP Q88AV7
B	102	MSE	-	EXPRESSION TAG	UNP Q88AV7
B	103	SER	-	EXPRESSION TAG	UNP Q88AV7
B	104	LEU	-	EXPRESSION TAG	UNP Q88AV7
B	327	GLU	-	EXPRESSION TAG	UNP Q88AV7
B	328	GLY	-	EXPRESSION TAG	UNP Q88AV7
B	329	HIS	-	EXPRESSION TAG	UNP Q88AV7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	330	HIS	-	EXPRESSION TAG	UNP Q88AV7
B	331	HIS	-	EXPRESSION TAG	UNP Q88AV7
B	332	HIS	-	EXPRESSION TAG	UNP Q88AV7
B	333	HIS	-	EXPRESSION TAG	UNP Q88AV7
B	334	HIS	-	EXPRESSION TAG	UNP Q88AV7
C	102	MSE	-	EXPRESSION TAG	UNP Q88AV7
C	103	SER	-	EXPRESSION TAG	UNP Q88AV7
C	104	LEU	-	EXPRESSION TAG	UNP Q88AV7
C	327	GLU	-	EXPRESSION TAG	UNP Q88AV7
C	328	GLY	-	EXPRESSION TAG	UNP Q88AV7
C	329	HIS	-	EXPRESSION TAG	UNP Q88AV7
C	330	HIS	-	EXPRESSION TAG	UNP Q88AV7
C	331	HIS	-	EXPRESSION TAG	UNP Q88AV7
C	332	HIS	-	EXPRESSION TAG	UNP Q88AV7
C	333	HIS	-	EXPRESSION TAG	UNP Q88AV7
C	334	HIS	-	EXPRESSION TAG	UNP Q88AV7
D	102	MSE	-	EXPRESSION TAG	UNP Q88AV7
D	103	SER	-	EXPRESSION TAG	UNP Q88AV7
D	104	LEU	-	EXPRESSION TAG	UNP Q88AV7
D	327	GLU	-	EXPRESSION TAG	UNP Q88AV7
D	328	GLY	-	EXPRESSION TAG	UNP Q88AV7
D	329	HIS	-	EXPRESSION TAG	UNP Q88AV7
D	330	HIS	-	EXPRESSION TAG	UNP Q88AV7
D	331	HIS	-	EXPRESSION TAG	UNP Q88AV7
D	332	HIS	-	EXPRESSION TAG	UNP Q88AV7
D	333	HIS	-	EXPRESSION TAG	UNP Q88AV7
D	334	HIS	-	EXPRESSION TAG	UNP Q88AV7
E	102	MSE	-	EXPRESSION TAG	UNP Q88AV7
E	103	SER	-	EXPRESSION TAG	UNP Q88AV7
E	104	LEU	-	EXPRESSION TAG	UNP Q88AV7
E	327	GLU	-	EXPRESSION TAG	UNP Q88AV7
E	328	GLY	-	EXPRESSION TAG	UNP Q88AV7
E	329	HIS	-	EXPRESSION TAG	UNP Q88AV7
E	330	HIS	-	EXPRESSION TAG	UNP Q88AV7
E	331	HIS	-	EXPRESSION TAG	UNP Q88AV7
E	332	HIS	-	EXPRESSION TAG	UNP Q88AV7
E	333	HIS	-	EXPRESSION TAG	UNP Q88AV7
E	334	HIS	-	EXPRESSION TAG	UNP Q88AV7
F	102	MSE	-	EXPRESSION TAG	UNP Q88AV7
F	103	SER	-	EXPRESSION TAG	UNP Q88AV7
F	104	LEU	-	EXPRESSION TAG	UNP Q88AV7
F	327	GLU	-	EXPRESSION TAG	UNP Q88AV7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	328	GLY	-	EXPRESSION TAG	UNP Q88AV7
F	329	HIS	-	EXPRESSION TAG	UNP Q88AV7
F	330	HIS	-	EXPRESSION TAG	UNP Q88AV7
F	331	HIS	-	EXPRESSION TAG	UNP Q88AV7
F	332	HIS	-	EXPRESSION TAG	UNP Q88AV7
F	333	HIS	-	EXPRESSION TAG	UNP Q88AV7
F	334	HIS	-	EXPRESSION TAG	UNP Q88AV7

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Ca 1 1	0	0
2	E	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is water.

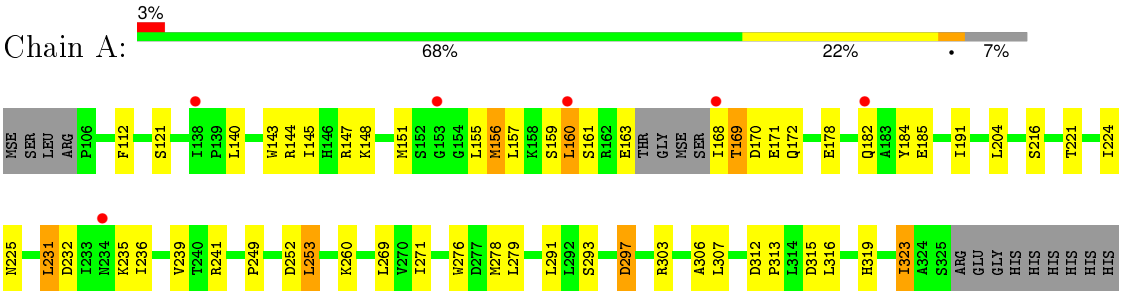
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	46	Total O 46 46	0	0
3	B	40	Total O 40 40	0	0
3	C	45	Total O 45 45	0	0
3	D	34	Total O 34 34	0	0
3	E	49	Total O 49 49	0	0
3	F	44	Total O 44 44	0	0

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.

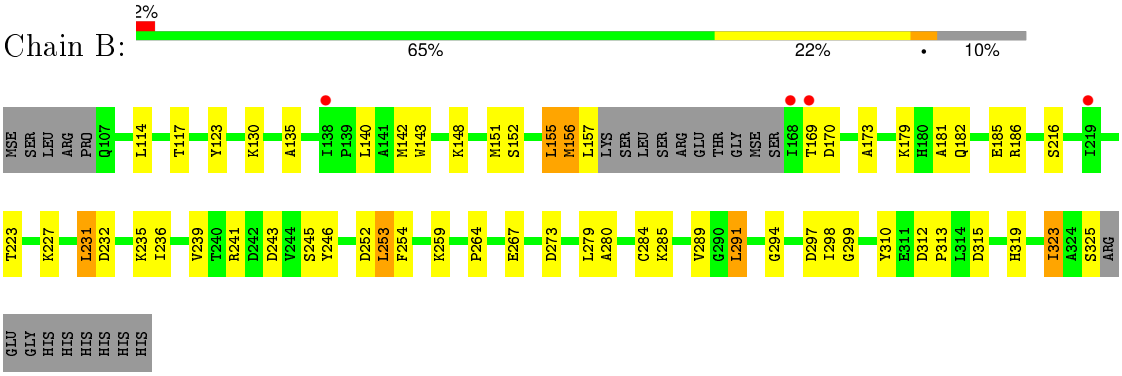
- Molecule 1: Hydrolase, haloacid dehalogenase-like family

Chain A:



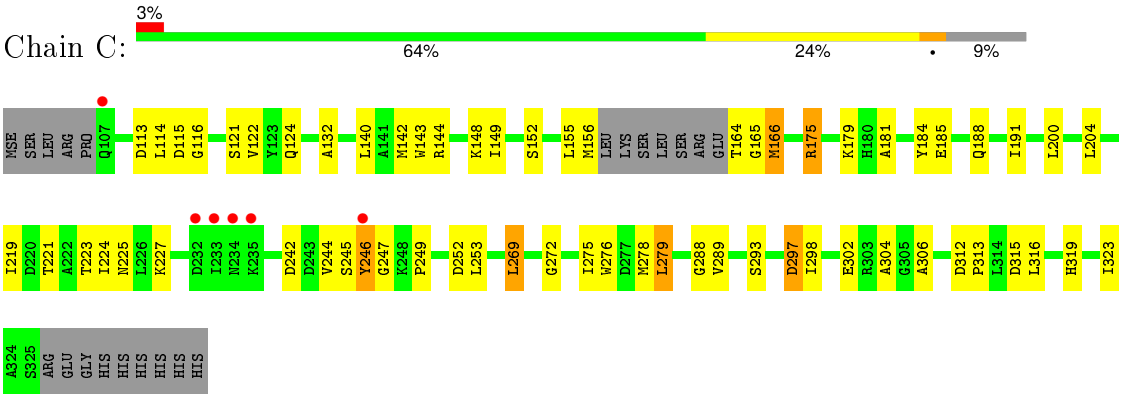
- Molecule 1: Hydrolase, haloacid dehalogenase-like family

Chain B:



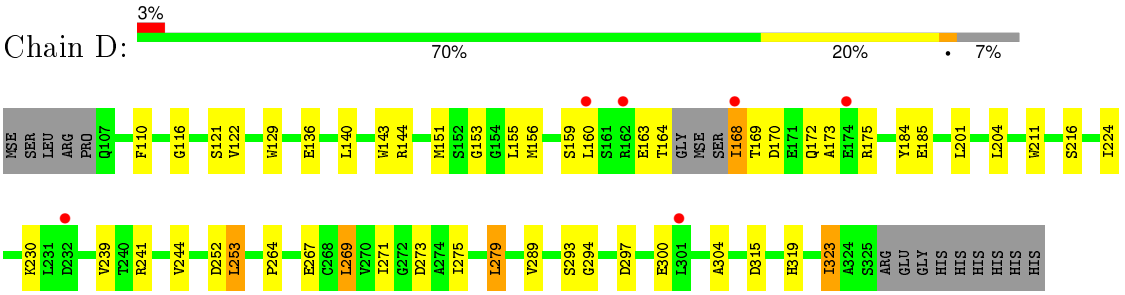
- Molecule 1: Hydrolase, haloacid dehalogenase-like family

Chain C:



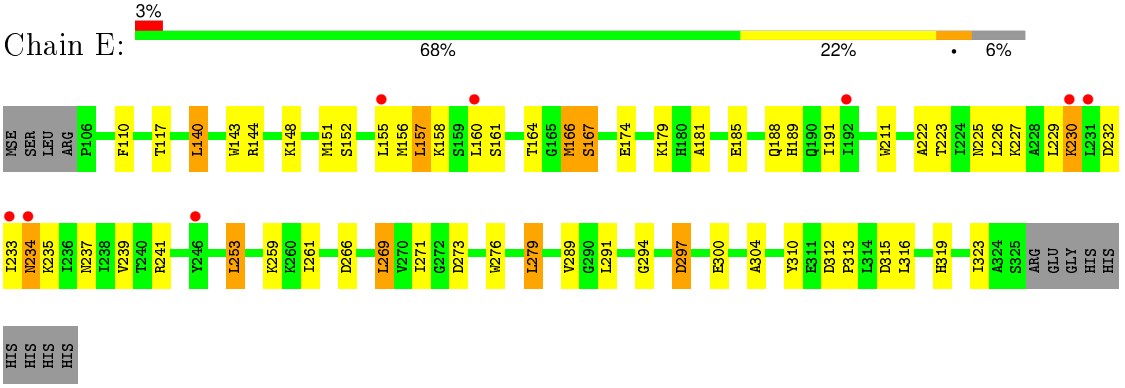
- Molecule 1: Hydrolase, haloacid dehalogenase-like family

Chain D:



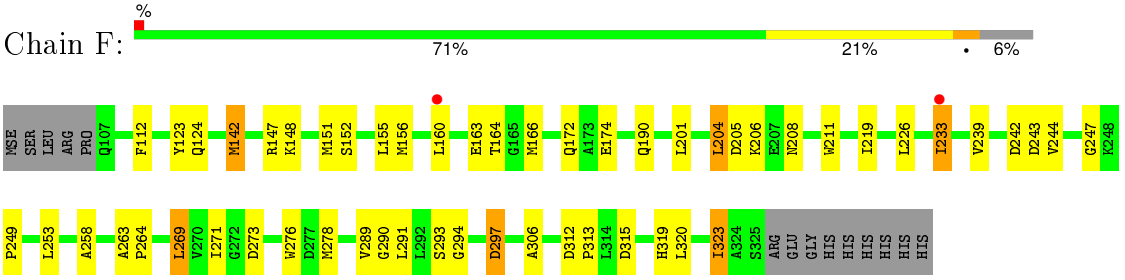
• Molecule 1: Hydrolase, haloacid dehalogenase-like family

Chain E:



• Molecule 1: Hydrolase, haloacid dehalogenase-like family

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.53Å 74.89Å 75.11Å 59.77° 67.49° 88.00°	Depositor
Resolution (Å)	49.89 – 2.20 49.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.3 (49.89-2.20) 76.1 (49.89-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.195 , 0.243 0.187 , 0.237	Depositor DCC
R_{free} test set	2887 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 55.2	EDS
Estimated twinning fraction	0.015 for -h,k,k-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 57194 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10211	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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: CA

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	0.47	0/1687	0.63	0/2276
1	B	0.43	0/1630	0.62	0/2201
1	C	0.45	0/1646	0.63	0/2220
1	D	0.44	0/1686	0.59	0/2275
1	E	0.44	0/1712	0.61	0/2309
1	F	0.45	0/1704	0.62	0/2298
All	All	0.45	0/10065	0.62	0/13579

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1666	0	1682	56	0
1	B	1610	0	1621	39	0
1	C	1627	0	1634	63	0
1	D	1666	0	1681	50	0
1	E	1691	0	1707	61	0
1	F	1684	0	1699	61	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
3	A	46	0	0	0	0
3	B	40	0	0	3	0
3	C	45	0	0	1	0
3	D	34	0	0	1	0
3	E	49	0	0	1	0
3	F	44	0	0	3	0
All	All	10211	0	10024	317	0

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

All (317) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:MSE:HE3	1:F:306:ALA:CB	1.72	1.18
1:C:278:MSE:HE1	1:C:288:GLY:HA3	1.17	1.11
1:F:278:MSE:HE3	1:F:306:ALA:HB2	1.17	1.11
1:C:164:THR:N	1:C:165:GLY:HA2	1.76	0.98
1:A:151:MSE:HE3	1:A:156:MSE:HA	1.45	0.96
1:E:271:ILE:HD13	1:E:316:LEU:HD21	1.44	0.96
1:C:278:MSE:HE1	1:C:288:GLY:CA	1.95	0.95
1:B:142:MSE:HE1	1:F:124:GLN:HE22	1.32	0.94
1:A:148:LYS:HB3	1:A:151:MSE:HE2	1.49	0.93
1:D:163:GLU:HG2	3:D:348:HOH:O	1.69	0.90
1:A:239:VAL:HG12	1:A:253:LEU:HD12	1.54	0.89
1:F:204:LEU:HD21	1:F:211:TRP:CD1	2.07	0.89
1:F:278:MSE:HE1	1:F:289:VAL:C	1.93	0.88
1:C:316:LEU:HD11	1:C:323:ILE:HD11	1.57	0.86
1:F:278:MSE:HE1	1:F:290:GLY:N	1.91	0.85
1:D:289:VAL:HG21	1:D:323:ILE:CD1	2.07	0.84
1:A:151:MSE:CE	1:A:156:MSE:HA	2.08	0.83
1:A:151:MSE:HE3	1:A:156:MSE:HG2	1.61	0.83
1:A:232:ASP:HB3	1:A:235:LYS:HB2	1.61	0.82
1:C:278:MSE:CE	1:C:288:GLY:HA3	2.06	0.82
1:A:269:LEU:HD11	1:A:323:ILE:HD12	1.61	0.82
1:E:232:ASP:HB3	1:E:235:LYS:HD2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ASP:OD2	1:F:297:ASP:HB3	1.80	0.81
1:F:244:VAL:HG21	1:F:253:LEU:HD22	1.64	0.79
1:B:169:THR:HG22	1:B:170:ASP:H	1.49	0.78
1:A:169:THR:HG22	1:A:172:GLN:H	1.49	0.78
1:F:278:MSE:CE	1:F:306:ALA:HB2	2.07	0.77
1:D:269:LEU:HD21	1:D:323:ILE:HD11	1.64	0.77
1:F:152:SER:HB2	1:F:247:GLY:HA3	1.65	0.77
1:E:161:SER:OG	1:E:167:SER:HA	1.85	0.76
1:E:239:VAL:HG12	1:E:253:LEU:HD12	1.67	0.76
1:F:278:MSE:HE2	1:F:290:GLY:CA	2.16	0.75
1:A:148:LYS:CB	1:A:151:MSE:HE2	2.15	0.75
1:D:269:LEU:HD11	1:D:323:ILE:CD1	2.16	0.75
1:E:232:ASP:CB	1:E:235:LYS:HD2	2.16	0.75
1:C:115:ASP:HB2	1:C:121:SER:OG	1.86	0.75
1:D:151:MSE:CE	1:D:155:LEU:HG	2.18	0.73
1:F:278:MSE:CE	1:F:290:GLY:N	2.52	0.71
1:A:271:ILE:HD13	1:A:316:LEU:HD21	1.72	0.71
1:E:160:LEU:O	1:E:164:THR:HG23	1.90	0.71
1:D:269:LEU:HD13	1:D:271:ILE:HD11	1.71	0.71
1:D:289:VAL:HG21	1:D:323:ILE:HD12	1.72	0.71
1:E:259:LYS:HB3	1:E:259:LYS:NZ	2.06	0.71
1:B:151:MSE:HE2	1:B:155:LEU:HG	1.73	0.70
1:C:315:ASP:O	1:C:319:HIS:HD2	1.73	0.70
1:F:269:LEU:HD21	1:F:289:VAL:HG23	1.73	0.70
1:C:278:MSE:HE2	1:C:306:ALA:HA	1.71	0.70
1:D:168:ILE:HD11	1:D:173:ALA:HB2	1.73	0.69
1:C:148:LYS:O	1:C:156:MSE:HE2	1.93	0.69
1:C:188:GLN:HB2	1:C:224:ILE:HG21	1.74	0.69
1:F:164:THR:O	1:F:164:THR:HG22	1.92	0.69
1:E:271:ILE:HD13	1:E:316:LEU:CD2	2.20	0.68
1:A:323:ILE:HD13	1:A:323:ILE:O	1.94	0.68
1:C:278:MSE:HA	1:C:278:MSE:HE3	1.75	0.68
1:F:253:LEU:HD23	3:F:56:HOH:O	1.94	0.68
1:A:269:LEU:HD21	1:A:323:ILE:CD1	2.24	0.67
1:F:226:LEU:CD1	1:F:233:ILE:HG12	2.24	0.67
1:F:273:ASP:OD2	1:F:294:GLY:HA3	1.94	0.67
1:E:188:GLN:HE21	1:E:189:HIS:CE1	2.13	0.67
1:E:271:ILE:CD1	1:E:316:LEU:HD21	2.24	0.67
1:C:188:GLN:HB2	1:C:224:ILE:CG2	2.24	0.66
1:F:148:LYS:HB3	1:F:156:MSE:HG3	1.75	0.66
1:C:152:SER:HB3	1:C:247:GLY:HA3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:ASP:OD1	1:E:300:GLU:HG3	1.97	0.65
1:E:166:MSE:SE	1:E:167:SER:H	2.30	0.65
1:F:148:LYS:HE2	3:F:335:HOH:O	1.97	0.65
1:E:157:LEU:O	1:E:161:SER:HB2	1.97	0.65
1:D:289:VAL:HG21	1:D:323:ILE:HD11	1.78	0.64
1:D:136:GLU:OE2	1:D:175:ARG:HD2	1.97	0.64
1:F:219:ILE:HG12	1:F:242:ASP:OD2	1.96	0.64
1:C:132:ALA:HA	1:C:179:LYS:HG2	1.79	0.64
1:E:181:ALA:O	1:E:185:GLU:HG3	1.97	0.63
1:C:245:SER:HB2	1:C:246:TYR:CE2	2.33	0.63
1:D:269:LEU:HD11	1:D:323:ILE:HD13	1.78	0.63
1:B:239:VAL:HG13	1:B:243:ASP:HB2	1.80	0.63
1:B:130:LYS:HG2	1:B:142:MSE:SE	2.49	0.62
1:E:148:LYS:HB3	1:E:156:MSE:HG3	1.81	0.62
1:B:142:MSE:CE	1:F:124:GLN:HE22	2.06	0.62
1:E:229:LEU:C	1:E:230:LYS:HD2	2.19	0.62
1:E:233:ILE:HG23	1:E:234:ASN:N	2.15	0.62
1:F:172:GLN:NE2	3:F:96:HOH:O	2.31	0.62
1:E:140:LEU:HD21	1:E:160:LEU:HD22	1.79	0.62
1:D:239:VAL:HG12	1:D:253:LEU:HD12	1.82	0.62
1:F:278:MSE:HE2	1:F:290:GLY:HA3	1.82	0.62
1:E:140:LEU:CD2	1:E:160:LEU:HD22	2.30	0.62
1:E:148:LYS:CB	1:E:156:MSE:HG3	2.31	0.61
1:F:124:GLN:HE21	1:F:190:GLN:HE21	1.46	0.61
1:E:233:ILE:HG23	1:E:234:ASN:H	1.65	0.61
1:B:157:LEU:HD12	1:B:157:LEU:C	2.21	0.61
1:E:232:ASP:HB3	1:E:235:LYS:CD	2.31	0.60
1:D:144:ARG:NH2	1:D:163:GLU:OE2	2.35	0.60
1:D:289:VAL:CG2	1:D:323:ILE:HD11	2.32	0.60
1:F:269:LEU:HD11	1:F:323:ILE:CG1	2.32	0.60
1:B:264:PRO:HG2	1:B:267:GLU:HG3	1.84	0.60
1:F:226:LEU:HD12	1:F:233:ILE:HG12	1.83	0.59
1:F:204:LEU:HD23	1:F:204:LEU:C	2.23	0.59
1:C:316:LEU:HD11	1:C:323:ILE:CD1	2.31	0.59
1:F:269:LEU:HD21	1:F:289:VAL:CG2	2.33	0.59
1:C:269:LEU:HD11	1:C:323:ILE:HD12	1.84	0.58
1:F:269:LEU:HD11	1:F:323:ILE:HG12	1.84	0.58
1:D:185:GLU:HG2	1:D:224:ILE:HD11	1.85	0.58
1:A:278:MSE:SE	1:A:306:ALA:HB2	2.54	0.58
1:C:278:MSE:HE2	1:C:306:ALA:CA	2.33	0.57
1:B:289:VAL:HG21	1:B:323:ILE:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:LEU:HD21	1:F:211:TRP:NE1	2.19	0.57
1:D:244:VAL:HG21	1:D:253:LEU:HD13	1.86	0.57
1:B:227:LYS:HE2	3:B:348:HOH:O	2.04	0.57
1:A:151:MSE:HE3	1:A:156:MSE:CA	2.28	0.56
1:F:204:LEU:HD23	1:F:205:ASP:N	2.20	0.56
1:E:166:MSE:O	1:E:167:SER:CB	2.54	0.56
1:F:226:LEU:HD12	1:F:233:ILE:CG1	2.35	0.56
1:B:239:VAL:HG12	1:B:253:LEU:HD12	1.86	0.56
1:D:216:SER:O	1:D:241:ARG:HB2	2.06	0.56
1:F:244:VAL:HG21	1:F:253:LEU:CD2	2.35	0.56
1:A:297:ASP:HB3	3:E:364:HOH:O	2.05	0.56
1:A:161:SER:OG	1:A:168:ILE:HD13	2.06	0.55
1:A:151:MSE:CE	1:A:156:MSE:HG2	2.33	0.55
1:D:151:MSE:HE2	1:D:155:LEU:CB	2.37	0.55
1:E:151:MSE:HE3	1:E:276:TRP:CZ3	2.41	0.55
1:E:166:MSE:O	1:E:167:SER:HB3	2.07	0.55
1:C:115:ASP:CB	1:C:121:SER:OG	2.52	0.55
1:D:151:MSE:HE2	1:D:155:LEU:HB3	1.87	0.55
1:C:245:SER:HB2	1:C:246:TYR:CD2	2.42	0.55
1:B:315:ASP:O	1:B:319:HIS:HD2	1.90	0.55
1:B:284:CYS:O	1:B:285:LYS:HB2	2.06	0.55
1:B:181:ALA:O	1:B:185:GLU:HG3	2.07	0.55
1:F:124:GLN:HE21	1:F:190:GLN:NE2	2.06	0.54
1:E:237:ASN:ND2	1:E:261:ILE:HG22	2.22	0.54
1:C:116:GLY:HA3	1:C:122:VAL:HG23	1.88	0.54
1:B:182:GLN:O	1:B:186:ARG:HG3	2.07	0.54
1:F:278:MSE:HE1	1:F:289:VAL:CA	2.37	0.54
1:C:164:THR:HB	1:C:166:MSE:HG3	1.89	0.54
1:E:273:ASP:OD2	1:E:294:GLY:HA3	2.06	0.54
1:E:239:VAL:CG1	1:E:253:LEU:HD12	2.36	0.54
1:F:312:ASP:HB2	1:F:313:PRO:CD	2.38	0.54
1:F:239:VAL:HG13	1:F:243:ASP:HB2	1.90	0.54
1:F:315:ASP:O	1:F:319:HIS:HD2	1.91	0.54
1:F:201:LEU:O	1:F:204:LEU:HD22	2.08	0.53
1:D:140:LEU:CD1	1:D:160:LEU:HD13	2.38	0.53
1:F:278:MSE:CE	1:F:290:GLY:CA	2.84	0.53
1:A:239:VAL:CG1	1:A:253:LEU:HD12	2.33	0.53
1:C:297:ASP:HB2	1:D:297:ASP:OD2	2.08	0.53
1:B:169:THR:O	1:B:173:ALA:HB2	2.09	0.53
1:D:140:LEU:CD2	1:D:164:THR:HG21	2.38	0.53
1:A:293:SER:HA	1:E:143:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ARG:HH11	1:C:175:ARG:HB2	1.74	0.53
1:A:143:TRP:HZ2	1:A:144:ARG:NH1	2.07	0.53
1:F:278:MSE:HE3	1:F:306:ALA:CA	2.35	0.52
1:F:278:MSE:CE	1:F:306:ALA:CB	2.66	0.52
1:E:230:LYS:N	1:E:230:LYS:HD2	2.25	0.52
1:D:264:PRO:HD2	1:D:267:GLU:OE1	2.10	0.52
1:E:166:MSE:SE	1:E:167:SER:N	2.93	0.52
1:A:140:LEU:HD22	1:A:160:LEU:HD21	1.91	0.52
1:F:239:VAL:HG12	1:F:253:LEU:CD1	2.40	0.52
1:F:278:MSE:HE3	1:F:306:ALA:HB1	1.83	0.52
1:C:164:THR:N	1:C:165:GLY:CA	2.59	0.51
1:D:169:THR:HB	1:D:172:GLN:HB2	1.91	0.51
1:A:303:ARG:HH11	1:A:303:ARG:HB2	1.76	0.51
1:C:278:MSE:HE1	1:C:288:GLY:C	2.31	0.51
1:D:156:MSE:O	1:D:160:LEU:HG	2.10	0.51
1:C:269:LEU:HD21	1:C:289:VAL:CG2	2.40	0.51
1:A:169:THR:HG22	1:A:172:GLN:N	2.21	0.51
1:B:232:ASP:HB3	1:B:235:LYS:HB2	1.93	0.51
1:C:223:THR:O	1:C:227:LYS:HG2	2.11	0.51
1:E:191:ILE:HD13	1:E:225:ASN:ND2	2.26	0.51
1:E:232:ASP:CG	1:E:235:LYS:HD2	2.31	0.50
1:C:181:ALA:O	1:C:185:GLU:HG3	2.11	0.50
1:C:269:LEU:HD21	1:C:289:VAL:HG23	1.93	0.50
1:B:223:THR:O	1:B:227:LYS:HG2	2.11	0.50
1:D:269:LEU:HD21	1:D:289:VAL:HG23	1.93	0.50
1:B:169:THR:HG22	1:B:170:ASP:N	2.22	0.50
1:E:222:ALA:O	1:E:226:LEU:HG	2.12	0.50
1:A:297:ASP:CG	1:E:297:ASP:CG	2.71	0.50
1:B:253:LEU:HD22	3:B:47:HOH:O	2.11	0.50
1:A:148:LYS:HB3	1:A:151:MSE:CE	2.32	0.49
1:E:259:LYS:HB3	1:E:259:LYS:HZ2	1.76	0.49
1:C:249:PRO:HG3	1:C:276:TRP:CE3	2.46	0.49
1:D:239:VAL:CG1	1:D:253:LEU:HD12	2.41	0.49
1:D:151:MSE:HE3	1:D:155:LEU:HG	1.92	0.49
1:E:259:LYS:HB3	1:E:259:LYS:HZ3	1.77	0.49
1:C:278:MSE:CE	1:C:306:ALA:HA	2.41	0.49
1:B:291:LEU:HA	1:B:310:TYR:O	2.13	0.49
1:C:184:TYR:CD2	1:C:221:THR:HG22	2.48	0.49
1:D:116:GLY:HA3	1:D:122:VAL:HG23	1.95	0.49
1:D:269:LEU:HD11	1:D:323:ILE:HD12	1.95	0.49
1:E:312:ASP:HB2	1:E:313:PRO:CD	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:HD21	1:A:323:ILE:HD11	1.94	0.49
1:B:273:ASP:OD2	1:B:294:GLY:HA3	2.13	0.49
1:C:278:MSE:HE2	1:C:306:ALA:N	2.28	0.49
1:E:269:LEU:HD21	1:E:289:VAL:CG2	2.43	0.49
1:A:249:PRO:HG3	1:A:276:TRP:CE3	2.48	0.49
1:B:142:MSE:HG2	1:F:123:TYR:CG	2.47	0.48
1:F:112:PHE:CE1	1:F:271:ILE:HD13	2.47	0.48
1:A:151:MSE:HE3	1:A:156:MSE:CG	2.40	0.48
1:C:249:PRO:HG3	1:C:276:TRP:HE3	1.78	0.48
1:C:275:ILE:HG22	1:C:279:LEU:HD22	1.96	0.48
1:C:121:SER:HA	1:C:124:GLN:OE1	2.13	0.48
1:A:143:TRP:CZ2	1:A:144:ARG:NH1	2.82	0.48
1:C:298:ILE:O	1:C:302:GLU:HG3	2.13	0.48
1:B:157:LEU:HD12	1:B:157:LEU:O	2.14	0.48
1:A:140:LEU:HD23	1:A:145:ILE:HG13	1.96	0.48
1:E:269:LEU:HD21	1:E:289:VAL:HG23	1.95	0.48
1:E:223:THR:O	1:E:227:LYS:HG2	2.14	0.48
1:D:151:MSE:HE2	1:D:155:LEU:C	2.34	0.47
1:D:140:LEU:HD21	1:D:164:THR:HG21	1.96	0.47
1:D:121:SER:HB2	1:D:184:TYR:OH	2.14	0.47
1:D:269:LEU:HD21	1:D:323:ILE:CD1	2.40	0.47
1:A:169:THR:CG2	1:A:172:GLN:H	2.25	0.47
1:F:204:LEU:CD2	1:F:211:TRP:CD1	2.89	0.47
1:C:184:TYR:OH	1:C:191:ILE:HD13	2.14	0.47
1:C:200:LEU:O	1:C:204:LEU:HG	2.14	0.47
1:A:178:GLU:O	1:A:182:GLN:HG3	2.15	0.47
1:A:148:LYS:CG	1:A:151:MSE:HE2	2.45	0.47
1:D:151:MSE:CE	1:D:155:LEU:CG	2.90	0.47
1:E:117:THR:HG23	1:E:291:LEU:HD22	1.96	0.47
1:B:231:LEU:HG	1:B:236:ILE:HG21	1.96	0.47
1:B:152:SER:HB3	1:B:155:LEU:HB2	1.97	0.46
1:F:164:THR:O	1:F:164:THR:CG2	2.62	0.46
1:A:315:ASP:O	1:A:319:HIS:HD2	1.97	0.46
1:E:166:MSE:CG	1:E:167:SER:N	2.78	0.46
1:F:148:LYS:O	1:F:151:MSE:HB2	2.16	0.46
1:D:129:TRP:CD2	1:D:156:MSE:HE1	2.50	0.46
1:E:158:LYS:O	1:E:161:SER:HB3	2.16	0.46
1:C:148:LYS:HB3	1:C:156:MSE:HG3	1.97	0.46
1:C:293:SER:HA	1:D:143:TRP:CD1	2.51	0.46
1:A:185:GLU:HG2	1:A:224:ILE:HD11	1.96	0.46
1:B:143:TRP:CD1	1:F:293:SER:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:VAL:HG21	1:C:253:LEU:HD22	1.96	0.46
1:F:278:MSE:CE	1:F:289:VAL:C	2.73	0.46
1:A:144:ARG:HE	1:A:163:GLU:CD	2.19	0.46
1:E:315:ASP:O	1:E:319:HIS:HD2	1.99	0.46
1:B:148:LYS:HB3	1:B:156:MSE:HG2	1.96	0.46
1:E:140:LEU:HD23	1:E:144:ARG:HB2	1.97	0.46
1:E:152:SER:HB2	1:E:241:ARG:HD3	1.96	0.46
1:F:147:ARG:NH2	1:F:163:GLU:OE1	2.49	0.46
1:E:151:MSE:HE3	1:E:276:TRP:CH2	2.50	0.45
1:D:273:ASP:OD2	1:D:294:GLY:HA3	2.16	0.45
1:A:191:ILE:HD13	1:A:225:ASN:ND2	2.32	0.45
1:D:279:LEU:HD13	1:D:304:ALA:HB1	1.99	0.45
1:A:184:TYR:CD2	1:A:221:THR:HG22	2.52	0.45
1:D:140:LEU:HD13	1:D:160:LEU:HD13	1.99	0.45
1:B:117:THR:HG23	1:B:291:LEU:HD22	1.99	0.45
1:C:113:ASP:HB3	1:C:272:GLY:HA2	1.97	0.45
1:C:175:ARG:NH1	1:C:175:ARG:HB2	2.31	0.45
1:C:312:ASP:HB2	1:C:313:PRO:CD	2.46	0.45
1:D:153:GLY:HA2	1:D:156:MSE:HG2	1.99	0.45
1:A:260:LYS:HE3	1:A:260:LYS:HB2	1.71	0.45
1:C:114:LEU:HD21	1:C:225:ASN:HB2	1.98	0.45
1:C:116:GLY:CA	1:C:122:VAL:HG23	2.46	0.45
1:F:258:ALA:HB1	1:F:263:ALA:O	2.16	0.45
1:B:285:LYS:HA	1:B:285:LYS:HD2	1.68	0.44
1:D:140:LEU:HD11	1:D:160:LEU:HD13	1.98	0.44
1:C:184:TYR:OH	1:C:191:ILE:CD1	2.65	0.44
1:E:312:ASP:HB2	1:E:313:PRO:HD2	1.99	0.44
1:A:249:PRO:HG3	1:A:276:TRP:HE3	1.82	0.44
1:E:279:LEU:HD13	1:E:304:ALA:HB1	2.00	0.44
1:F:239:VAL:HG13	1:F:243:ASP:CB	2.47	0.44
1:D:275:ILE:HD11	1:D:300:GLU:HB3	2.00	0.44
1:B:135:ALA:CB	1:B:179:LYS:HE3	2.48	0.44
1:A:148:LYS:HD2	1:A:151:MSE:CE	2.46	0.44
1:E:166:MSE:HG2	1:E:167:SER:N	2.33	0.44
1:F:249:PRO:HG3	1:F:276:TRP:CE3	2.52	0.44
1:C:155:LEU:HA	1:C:155:LEU:HD12	1.81	0.43
1:A:169:THR:HG22	1:A:171:GLU:N	2.33	0.43
1:C:188:GLN:CB	1:C:224:ILE:HG21	2.46	0.43
1:A:169:THR:CG2	1:A:170:ASP:N	2.81	0.43
1:B:245:SER:HB3	1:B:246:TYR:CE2	2.53	0.43
1:E:289:VAL:HG21	1:E:323:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:LYS:HE3	1:E:158:LYS:HB3	1.79	0.43
1:C:156:MSE:HE1	3:C:29:HOH:O	2.19	0.43
1:B:312:ASP:HB2	1:B:313:PRO:CD	2.49	0.43
1:C:143:TRP:CD1	1:D:293:SER:HA	2.53	0.43
1:A:112:PHE:CE1	1:A:271:ILE:HD12	2.54	0.42
1:F:312:ASP:HB2	1:F:313:PRO:HD2	2.00	0.42
1:D:315:ASP:O	1:D:319:HIS:HD2	2.02	0.42
1:A:144:ARG:NH2	1:A:163:GLU:OE2	2.53	0.42
1:A:231:LEU:HG	1:A:236:ILE:HG21	2.02	0.42
1:E:110:PHE:O	1:E:211:TRP:HA	2.20	0.42
1:B:285:LYS:NZ	3:B:62:HOH:O	2.52	0.42
1:A:231:LEU:HA	1:A:231:LEU:HD12	1.84	0.42
1:A:169:THR:HG21	1:A:171:GLU:OE1	2.20	0.42
1:D:140:LEU:HD23	1:D:164:THR:HG21	2.02	0.42
1:C:188:GLN:HB2	1:C:224:ILE:HG23	1.99	0.41
1:A:171:GLU:HG3	1:A:171:GLU:H	1.59	0.41
1:E:157:LEU:HD12	1:E:157:LEU:HA	1.91	0.41
1:E:189:HIS:CD2	1:F:206:LYS:HB2	2.55	0.41
1:F:320:LEU:HD12	1:F:320:LEU:HA	1.76	0.41
1:C:149:ILE:HD13	1:C:156:MSE:HE1	2.02	0.41
1:F:269:LEU:HD11	1:F:323:ILE:HG13	2.01	0.41
1:E:148:LYS:HB2	1:E:156:MSE:HG3	2.02	0.41
1:C:184:TYR:CZ	1:C:191:ILE:HD11	2.55	0.41
1:E:110:PHE:HB2	1:E:211:TRP:HB3	2.02	0.41
1:B:254:PHE:CE2	1:B:280:ALA:HB3	2.55	0.41
1:D:110:PHE:O	1:D:211:TRP:HA	2.20	0.41
1:A:148:LYS:HD2	1:A:151:MSE:HE2	2.02	0.41
1:C:185:GLU:HA	1:C:224:ILE:CD1	2.50	0.41
1:A:121:SER:HB2	1:A:184:TYR:OH	2.20	0.41
1:B:298:ILE:HG23	1:B:299:GLY:N	2.36	0.41
1:C:219:ILE:HG12	1:C:242:ASP:OD2	2.20	0.41
1:D:151:MSE:HE1	1:D:159:SER:HB2	2.02	0.41
1:C:279:LEU:HD13	1:C:304:ALA:HB1	2.02	0.41
1:E:291:LEU:HA	1:E:310:TYR:O	2.21	0.41
1:A:312:ASP:HB2	1:A:313:PRO:CD	2.51	0.41
1:B:123:TYR:CG	1:F:142:MSE:HG2	2.56	0.41
1:B:216:SER:O	1:B:241:ARG:HB2	2.21	0.41
1:A:269:LEU:CD1	1:A:323:ILE:HD12	2.40	0.41
1:C:188:GLN:HB3	1:C:224:ILE:HD13	2.03	0.41
1:A:297:ASP:OD2	1:E:297:ASP:OD1	2.38	0.41
1:E:152:SER:CB	1:E:241:ARG:HD3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:SER:CB	1:C:246:TYR:CE2	3.03	0.40
1:D:269:LEU:CD1	1:D:323:ILE:HD13	2.49	0.40
1:D:269:LEU:HD21	1:D:289:VAL:CG2	2.52	0.40
1:C:312:ASP:HB2	1:C:313:PRO:HD2	2.03	0.40
1:F:263:ALA:HA	1:F:264:PRO:HD2	1.93	0.40
1:A:216:SER:O	1:A:241:ARG:HB2	2.21	0.40
1:C:143:TRP:CE2	1:C:144:ARG:HG3	2.56	0.40
1:A:147:ARG:NH2	1:A:163:GLU:OE2	2.55	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	212/233 (91%)	208 (98%)	4 (2%)	0	100	100
1	B	205/233 (88%)	191 (93%)	13 (6%)	1 (0%)	34	35
1	C	208/233 (89%)	200 (96%)	8 (4%)	0	100	100
1	D	212/233 (91%)	206 (97%)	6 (3%)	0	100	100
1	E	218/233 (94%)	206 (94%)	11 (5%)	1 (0%)	34	35
1	F	217/233 (93%)	213 (98%)	4 (2%)	0	100	100
All	All	1272/1398 (91%)	1224 (96%)	46 (4%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	167	SER
1	B	156	MSE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	176/185 (95%)	161 (92%)	15 (8%)	13	13
1	B	169/185 (91%)	158 (94%)	11 (6%)	21	23
1	C	171/185 (92%)	162 (95%)	9 (5%)	28	32
1	D	176/185 (95%)	166 (94%)	10 (6%)	25	29
1	E	179/185 (97%)	166 (93%)	13 (7%)	17	18
1	F	178/185 (96%)	166 (93%)	12 (7%)	20	21
All	All	1049/1110 (94%)	979 (93%)	70 (7%)	20	21

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	LEU
1	A	156	MSE
1	A	157	LEU
1	A	159	SER
1	A	160	LEU
1	A	169	THR
1	A	204	LEU
1	A	231	LEU
1	A	252	ASP
1	A	253	LEU
1	A	279	LEU
1	A	291	LEU
1	A	297	ASP
1	A	307	LEU
1	A	323	ILE
1	B	114	LEU
1	B	140	LEU
1	B	155	LEU
1	B	231	LEU
1	B	252	ASP
1	B	253	LEU
1	B	259	LYS

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Mol	Chain	Res	Type
1	B	279	LEU
1	B	291	LEU
1	B	323	ILE
1	B	325	SER
1	C	140	LEU
1	C	142	MSE
1	C	166	MSE
1	C	175	ARG
1	C	246	TYR
1	C	252	ASP
1	C	269	LEU
1	C	279	LEU
1	C	297	ASP
1	D	168	ILE
1	D	170	ASP
1	D	201	LEU
1	D	204	LEU
1	D	230	LYS
1	D	252	ASP
1	D	253	LEU
1	D	269	LEU
1	D	279	LEU
1	D	323	ILE
1	E	140	LEU
1	E	155	LEU
1	E	157	LEU
1	E	166	MSE
1	E	174	GLU
1	E	179	LYS
1	E	230	LYS
1	E	234	ASN
1	E	253	LEU
1	E	266	ASP
1	E	269	LEU
1	E	279	LEU
1	E	297	ASP
1	F	142	MSE
1	F	155	LEU
1	F	160	LEU
1	F	166	MSE
1	F	174	GLU
1	F	204	LEU

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Mol	Chain	Res	Type
1	F	208	ASN
1	F	233	ILE
1	F	269	LEU
1	F	291	LEU
1	F	297	ASP
1	F	323	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	A	319	HIS
1	B	319	HIS
1	C	137	ASN
1	C	225	ASN
1	C	319	HIS
1	D	137	ASN
1	D	234	ASN
1	D	319	HIS
1	E	189	HIS
1	E	225	ASN
1	E	234	ASN
1	E	319	HIS
1	F	124	GLN
1	F	172	GLN
1	F	190	GLN
1	F	319	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no 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	212/233 (90%)	0.24	6 (2%)	56	55	25, 35, 53, 57	0
1	B	205/233 (87%)	0.18	4 (1%)	68	67	25, 37, 57, 72	0
1	C	207/233 (88%)	0.19	6 (2%)	55	54	27, 37, 54, 61	0
1	D	212/233 (90%)	0.17	6 (2%)	56	55	26, 39, 56, 65	0
1	E	215/233 (92%)	0.20	8 (3%)	45	44	26, 38, 53, 64	0
1	F	214/233 (91%)	0.06	2 (0%)	85	85	26, 35, 50, 56	0
All	All	1265/1398 (90%)	0.17	32 (2%)	61	60	25, 37, 54, 72	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	LEU	6.1
1	B	168	ILE	4.7
1	D	168	ILE	4.7
1	C	235	LYS	3.5
1	E	234	ASN	3.5
1	C	233	ILE	3.5
1	D	160	LEU	3.4
1	E	231	LEU	3.2
1	C	232	ASP	3.1
1	D	174	GLU	3.0
1	E	233	ILE	3.0
1	E	160	LEU	3.0
1	D	232	ASP	3.0
1	A	182	GLN	3.0
1	E	155	LEU	2.8
1	B	219	ILE	2.7
1	E	192	ILE	2.7
1	F	160	LEU	2.6
1	F	233	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	168	ILE	2.5
1	E	246	TYR	2.5
1	C	234	ASN	2.5
1	E	230	LYS	2.4
1	B	138	ILE	2.3
1	B	169	THR	2.3
1	A	153	GLY	2.2
1	A	138	ILE	2.2
1	A	234	ASN	2.2
1	C	246	TYR	2.2
1	C	107	GLN	2.1
1	D	301	LEU	2.1
1	D	162	ARG	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	CA	D	6	1/1	0.99	0.12	0.51	31,31,31,31	0
2	CA	E	1	1/1	0.99	0.13	0.50	34,34,34,34	0
2	CA	E	8	1/1	0.95	0.16	-0.11	43,43,43,43	0
2	CA	B	7	1/1	0.92	0.14	-0.14	42,42,42,42	0
2	CA	B	2	1/1	0.99	0.11	-0.22	33,33,33,33	0
2	CA	C	5	1/1	0.98	0.08	-0.89	38,38,38,38	0
2	CA	F	3	1/1	0.99	0.07	-1.54	32,32,32,32	0
2	CA	C	9	1/1	0.91	0.04	-2.36	46,46,46,46	0
2	CA	A	4	1/1	0.99	0.05	-2.59	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.