Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:02 am BST

PDB ID	:	5NF1
Title	:	crystal structure of variants
Authors	:	Linde, M.; Rajendran, C.; Babinger, P.; Sterner, R.
Deposited on	:	2017-03-13
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

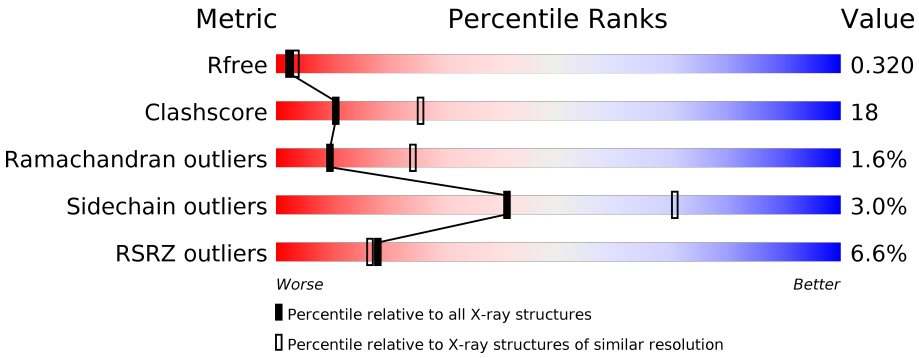
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	256	58% 32% • 9%
1	B	256	3% 52% 33% • 14%
1	C	256	2% 66% 20% • 12%
1	D	256	5% 56% 31% 13%
1	E	256	12% 54% 37% • 7%
1	F	256	13% 53% 36% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9975 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 Geranylgeranylglyceryl phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1730	1089	294	337	10			
1	B	221	Total	C	N	O	S	0	0	0
			1590	1002	266	314	8			
1	C	226	Total	C	N	O	S	0	0	0
			1628	1036	273	309	10			
1	D	224	Total	C	N	O	S	0	0	0
			1610	1017	276	308	9			
1	E	237	Total	C	N	O	S	0	0	0
			1708	1073	286	339	10			
1	F	231	Total	C	N	O	S	0	0	0
			1666	1055	277	325	9			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O26652
A	2	PHE	-	expression tag	UNP O26652
A	3	LYS	-	expression tag	UNP O26652
A	141	ALA	TRP	conflict	UNP O26652
A	249	LEU	-	expression tag	UNP O26652
A	250	GLU	-	expression tag	UNP O26652
A	251	HIS	-	expression tag	UNP O26652
A	252	HIS	-	expression tag	UNP O26652
A	253	HIS	-	expression tag	UNP O26652
A	254	HIS	-	expression tag	UNP O26652
A	255	HIS	-	expression tag	UNP O26652
A	256	HIS	-	expression tag	UNP O26652
B	1	MET	-	initiating methionine	UNP O26652
B	2	PHE	-	expression tag	UNP O26652
B	3	LYS	-	expression tag	UNP O26652
B	141	ALA	TRP	conflict	UNP O26652
B	249	LEU	-	expression tag	UNP O26652

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Chain	Residue	Modelled	Actual	Comment	Reference
B	250	GLU	-	expression tag	UNP O26652
B	251	HIS	-	expression tag	UNP O26652
B	252	HIS	-	expression tag	UNP O26652
B	253	HIS	-	expression tag	UNP O26652
B	254	HIS	-	expression tag	UNP O26652
B	255	HIS	-	expression tag	UNP O26652
B	256	HIS	-	expression tag	UNP O26652
C	1	MET	-	initiating methionine	UNP O26652
C	2	PHE	-	expression tag	UNP O26652
C	3	LYS	-	expression tag	UNP O26652
C	141	ALA	TRP	conflict	UNP O26652
C	249	LEU	-	expression tag	UNP O26652
C	250	GLU	-	expression tag	UNP O26652
C	251	HIS	-	expression tag	UNP O26652
C	252	HIS	-	expression tag	UNP O26652
C	253	HIS	-	expression tag	UNP O26652
C	254	HIS	-	expression tag	UNP O26652
C	255	HIS	-	expression tag	UNP O26652
C	256	HIS	-	expression tag	UNP O26652
D	1	MET	-	initiating methionine	UNP O26652
D	2	PHE	-	expression tag	UNP O26652
D	3	LYS	-	expression tag	UNP O26652
D	141	ALA	TRP	conflict	UNP O26652
D	249	LEU	-	expression tag	UNP O26652
D	250	GLU	-	expression tag	UNP O26652
D	251	HIS	-	expression tag	UNP O26652
D	252	HIS	-	expression tag	UNP O26652
D	253	HIS	-	expression tag	UNP O26652
D	254	HIS	-	expression tag	UNP O26652
D	255	HIS	-	expression tag	UNP O26652
D	256	HIS	-	expression tag	UNP O26652
E	1	MET	-	initiating methionine	UNP O26652
E	2	PHE	-	expression tag	UNP O26652
E	3	LYS	-	expression tag	UNP O26652
E	141	ALA	TRP	conflict	UNP O26652
E	249	LEU	-	expression tag	UNP O26652
E	250	GLU	-	expression tag	UNP O26652
E	251	HIS	-	expression tag	UNP O26652
E	252	HIS	-	expression tag	UNP O26652
E	253	HIS	-	expression tag	UNP O26652
E	254	HIS	-	expression tag	UNP O26652
E	255	HIS	-	expression tag	UNP O26652

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Chain	Residue	Modelled	Actual	Comment	Reference
E	256	HIS	-	expression tag	UNP O26652
F	1	MET	-	initiating methionine	UNP O26652
F	2	PHE	-	expression tag	UNP O26652
F	3	LYS	-	expression tag	UNP O26652
F	141	ALA	TRP	conflict	UNP O26652
F	249	LEU	-	expression tag	UNP O26652
F	250	GLU	-	expression tag	UNP O26652
F	251	HIS	-	expression tag	UNP O26652
F	252	HIS	-	expression tag	UNP O26652
F	253	HIS	-	expression tag	UNP O26652
F	254	HIS	-	expression tag	UNP O26652
F	255	HIS	-	expression tag	UNP O26652
F	256	HIS	-	expression tag	UNP O26652

- Molecule 2 is water.

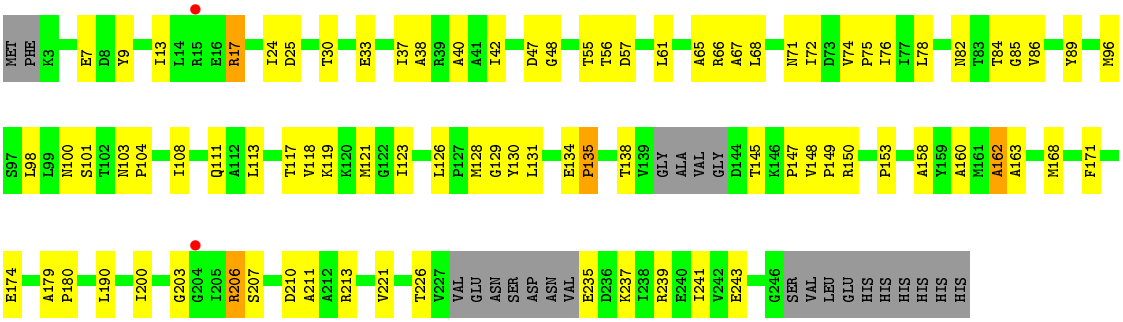
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	8	Total O 8 8	0	0
2	B	6	Total O 6 6	0	0
2	C	20	Total O 20 20	0	0
2	D	5	Total O 5 5	0	0
2	E	2	Total O 2 2	0	0
2	F	2	Total O 2 2	0	0

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

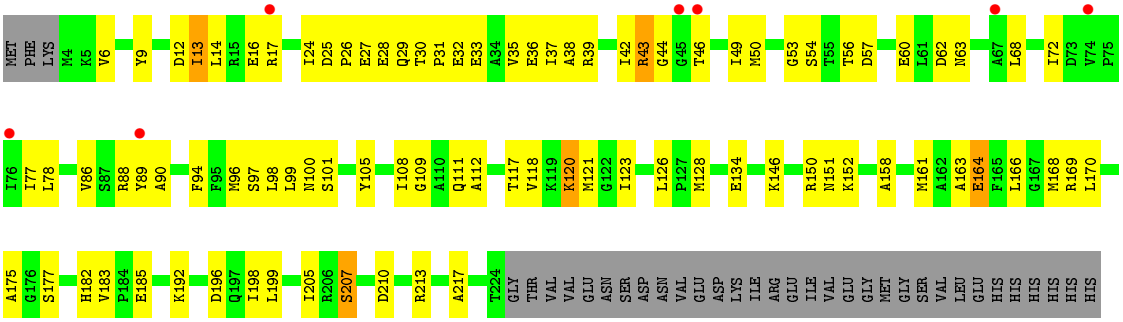
- Molecule 1: Geranylgeranylglyceryl phosphate synthase

Chain A:



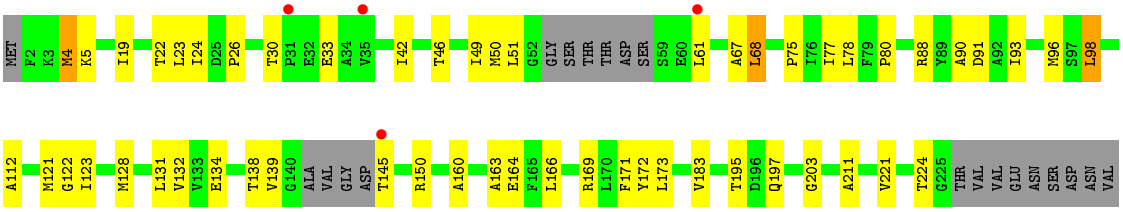
- Molecule 1: Geranylgeranylglyceryl phosphate synthase

Chain B:



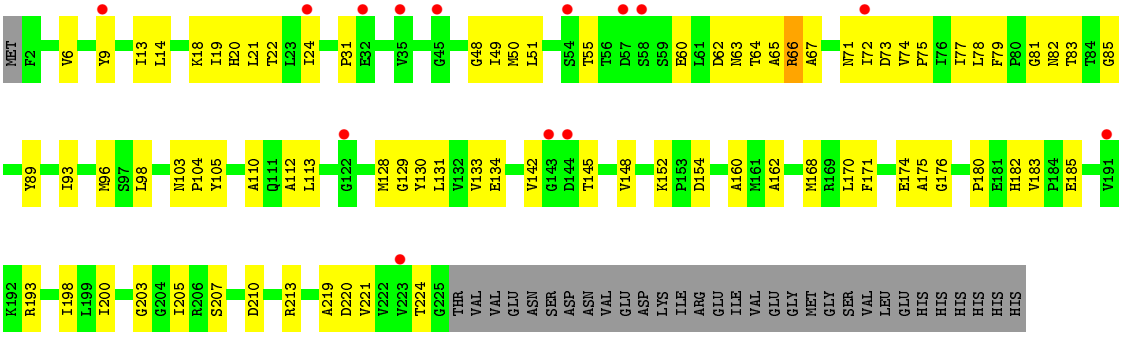
- Molecule 1: Geranylgeranylglyceryl phosphate synthase

Chain C:



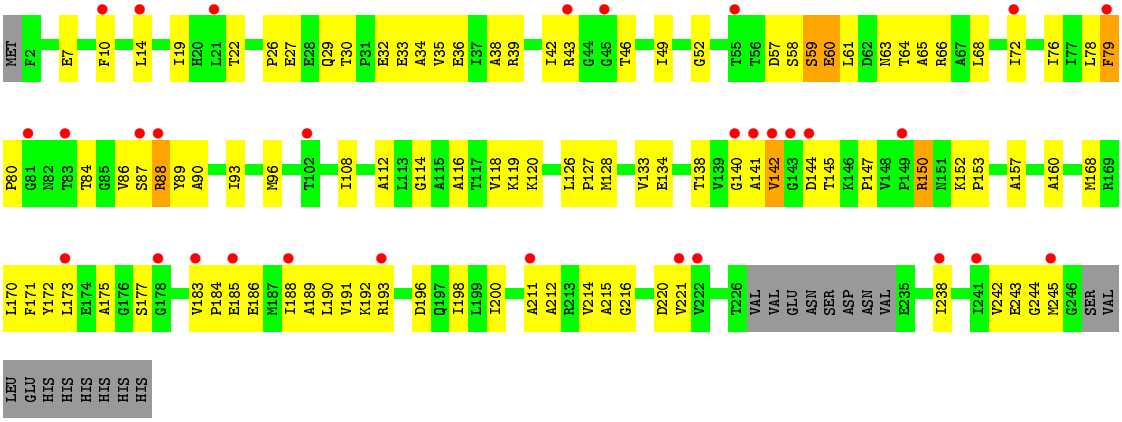
• Molecule 1: Geranylgeranylglyceryl phosphate synthase

Chain D:



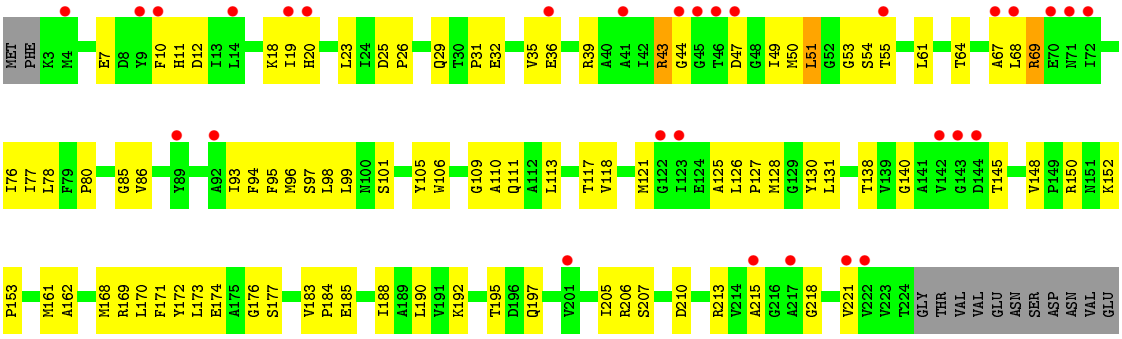
• Molecule 1: Geranylgeranylglyceryl phosphate synthase

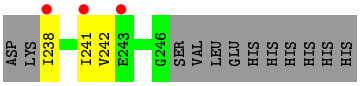
Chain E:



• Molecule 1: Geranylgeranylglyceryl phosphate synthase

Chain F:




ASP
LYS
I238
I241
V242
E243
G246
SER
VAL
LEU
GLU
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.20Å 62.78Å 136.26Å 90.00° 96.35° 90.00°	Depositor
Resolution (Å)	47.96 – 2.70 47.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.9 (47.96-2.70) 89.9 (47.96-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.232 , 0.321 0.232 , 0.320	Depositor DCC
R_{free} test set	1752 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	58.5	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 67.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9975	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.50	0/1756	0.68	0/2381
1	B	0.46	0/1617	0.67	0/2205
1	C	0.48	0/1653	0.66	0/2245
1	D	0.44	0/1638	0.63	0/2230
1	E	0.39	0/1734	0.57	0/2359
1	F	0.38	0/1692	0.58	0/2302
All	All	0.44	0/10090	0.63	0/13722

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	1730	0	1717	55	0
1	B	1590	0	1537	70	0
1	C	1628	0	1596	38	0
1	D	1610	0	1575	65	0
1	E	1708	0	1654	68	0
1	F	1666	0	1637	81	0
2	A	8	0	0	0	0
2	B	6	0	0	1	0
2	C	20	0	0	3	0
2	D	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2	0	0	2	0
2	F	2	0	0	0	0
All	All	9975	0	9716	363	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 18.

All (363) 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:D:205:ILE:HD11	1:D:224:THR:HG22	1.27	1.15
1:F:98:LEU:HD21	1:F:106:TRP:HB3	1.45	0.95
1:D:170:LEU:HD22	1:D:198:ILE:HB	1.55	0.88
1:A:138:THR:HG22	1:B:152:LYS:HE2	1.58	0.85
1:C:26:PRO:HG2	1:C:61:LEU:HG	1.58	0.84
1:E:30:THR:HG22	1:E:33:GLU:HB2	1.60	0.84
1:D:205:ILE:HD11	1:D:224:THR:CG2	2.07	0.84
1:F:78:LEU:CB	1:F:93:ILE:HD12	2.08	0.83
1:E:19:ILE:HB	1:E:221:VAL:HG12	1.60	0.83
1:C:164:GLU:OE1	2:C:301:HOH:O	1.99	0.81
1:F:207:SER:HB2	1:F:210:ASP:H	1.46	0.79
1:D:182:HIS:HB3	1:D:205:ILE:HG22	1.63	0.79
1:B:39:ARG:NH1	1:B:39:ARG:O	2.17	0.77
1:D:20:HIS:HE1	1:D:22:THR:HG22	1.49	0.77
1:F:78:LEU:HB2	1:F:93:ILE:HD12	1.66	0.77
1:B:134:GLU:OE1	1:B:150:ARG:HG3	1.88	0.74
1:E:185:GLU:HA	1:E:188:ILE:HD12	1.70	0.72
1:B:39:ARG:HH12	1:B:43:ARG:N	1.88	0.72
1:E:59:SER:O	1:E:63:ASN:ND2	2.23	0.71
1:F:35:VAL:HG12	1:F:68:LEU:HD12	1.72	0.71
1:E:170:LEU:HD22	1:E:198:ILE:HB	1.73	0.71
1:D:20:HIS:CE1	1:D:22:THR:HG22	2.25	0.71
1:F:210:ASP:OD1	1:F:213:ARG:NH2	2.24	0.70
1:F:78:LEU:HB3	1:F:93:ILE:HD12	1.72	0.70
1:E:243:GLU:N	1:E:243:GLU:OE1	2.25	0.70
1:E:150:ARG:N	2:E:302:HOH:O	2.23	0.70
1:F:68:LEU:HB3	1:F:76:ILE:HD13	1.73	0.69
1:F:98:LEU:CD2	1:F:106:TRP:HB3	2.23	0.69
1:B:97:SER:O	1:B:99:LEU:HD12	1.91	0.69
1:A:207:SER:HB2	1:A:210:ASP:H	1.58	0.68
1:D:200:ILE:HG23	1:D:221:VAL:CG2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:GLU:O	1:E:190:LEU:HG	1.93	0.67
1:F:19:ILE:HG23	1:F:221:VAL:HG22	1.76	0.67
1:B:56:THR:OG1	1:B:57:ASP:N	2.28	0.66
1:F:54:SER:OG	1:F:55:THR:N	2.27	0.66
1:A:30:THR:HG23	1:A:33:GLU:H	1.61	0.66
1:E:26:PRO:HG2	1:E:61:LEU:HD12	1.77	0.66
1:F:51:LEU:HD22	1:F:76:ILE:HG22	1.78	0.66
1:F:80:PRO:HG3	1:F:93:ILE:HD11	1.79	0.65
1:A:98:LEU:HG	1:A:101:SER:HB2	1.78	0.65
1:F:64:THR:O	1:F:68:LEU:HD13	1.97	0.64
1:E:211:ALA:HA	1:E:214:VAL:HG12	1.79	0.64
1:F:205:ILE:HD12	1:F:210:ASP:HB3	1.77	0.64
1:F:18:LYS:HD2	1:F:215:ALA:HB1	1.78	0.64
1:D:31:PRO:HB3	1:D:63:ASN:O	1.97	0.64
1:D:65:ALA:HB1	1:D:89:TYR:HB2	1.80	0.64
1:B:12:ASP:O	1:B:14:LEU:N	2.31	0.63
1:F:32:GLU:O	1:F:35:VAL:HG22	1.98	0.63
1:B:35:VAL:HA	1:B:68:LEU:HD21	1.80	0.63
1:B:182:HIS:ND1	1:B:183:VAL:O	2.31	0.62
1:E:78:LEU:HD11	1:E:87:SER:H	1.64	0.62
1:D:207:SER:HB2	1:D:210:ASP:H	1.63	0.62
1:D:24:ILE:HG13	1:D:49:ILE:HD11	1.80	0.62
1:F:127:PRO:HB2	1:F:168:MET:HA	1.81	0.62
1:B:30:THR:HG22	1:B:31:PRO:HD2	1.81	0.62
1:E:36:GLU:OE1	1:E:39:ARG:NH1	2.32	0.62
1:F:195:THR:HG22	1:F:197:GLN:HG2	1.82	0.62
1:E:108:ILE:HG12	1:F:99:LEU:HB3	1.82	0.62
1:A:24:ILE:HG22	1:A:25:ASP:H	1.64	0.61
1:B:32:GLU:O	1:B:35:VAL:N	2.32	0.61
1:B:175:ALA:HB2	1:B:183:VAL:HG23	1.82	0.61
1:C:24:ILE:O	1:C:51:LEU:HA	2.00	0.61
1:F:140:GLY:O	1:F:145:THR:HG22	1.99	0.61
1:B:33:GLU:O	1:B:37:ILE:HG13	2.00	0.61
1:F:95:PHE:HE2	1:F:118:VAL:HG21	1.65	0.61
1:E:76:ILE:HD11	1:E:90:ALA:HA	1.83	0.61
1:F:192:LYS:NZ	1:F:218:GLY:O	2.24	0.61
1:C:23:LEU:HD12	1:C:50:MET:O	2.01	0.60
1:B:120:LYS:HE3	1:B:121:MET:HE3	1.81	0.60
1:D:174:GLU:OE2	1:D:176:GLY:N	2.27	0.60
1:E:27:GLU:HA	1:E:60:GLU:OE2	2.01	0.60
1:E:134:GLU:HB2	1:E:150:ARG:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:LEU:HG	1:F:101:SER:HB2	1.84	0.60
1:C:33:GLU:OE1	1:C:33:GLU:N	2.34	0.60
1:E:173:LEU:HD23	1:E:183:VAL:HG11	1.84	0.60
1:F:78:LEU:HB3	1:F:93:ILE:CD1	2.33	0.59
1:F:35:VAL:O	1:F:39:ARG:HG3	2.02	0.59
1:C:78:LEU:HB2	1:C:93:ILE:HG13	1.84	0.59
1:F:51:LEU:CD2	1:F:76:ILE:HG22	2.33	0.59
1:E:145:THR:HG23	1:E:147:PRO:HD3	1.84	0.59
1:E:112:ALA:HA	1:F:162:ALA:HB2	1.85	0.59
1:D:205:ILE:HB	1:D:210:ASP:HB3	1.85	0.58
1:F:185:GLU:HA	1:F:188:ILE:HD12	1.85	0.58
1:C:169:ARG:NE	2:C:304:HOH:O	2.28	0.58
1:B:42:ILE:HA	1:B:46:THR:HG22	1.84	0.58
1:E:157:ALA:HA	1:E:191:VAL:HG12	1.84	0.58
1:C:90:ALA:HB3	1:C:123:ILE:HD11	1.84	0.58
1:F:19:ILE:CD1	1:F:47:ASP:HB2	2.34	0.58
1:D:131:LEU:HD21	1:D:148:VAL:HG21	1.86	0.58
1:D:48:GLY:HA2	1:D:74:VAL:HB	1.87	0.57
1:D:19:ILE:HG12	1:D:221:VAL:HG12	1.86	0.57
1:E:150:ARG:NH1	1:E:184:PRO:HG3	2.19	0.57
1:D:98:LEU:HD13	1:D:130:TYR:HD1	1.69	0.57
1:D:6:VAL:HG11	1:D:75:PRO:HB3	1.85	0.57
1:E:68:LEU:HD23	1:E:72:ILE:HD11	1.85	0.57
1:F:43:ARG:HD3	1:F:44:GLY:N	2.19	0.57
1:B:33:GLU:HG2	1:B:37:ILE:HG13	1.86	0.57
1:B:33:GLU:O	1:B:37:ILE:N	2.24	0.57
1:F:31:PRO:HA	1:F:64:THR:HG23	1.86	0.57
1:B:38:ALA:O	1:B:42:ILE:HD12	2.05	0.57
1:D:78:LEU:HD11	1:D:93:ILE:HD12	1.87	0.57
1:F:78:LEU:CB	1:F:93:ILE:CD1	2.81	0.57
1:B:134:GLU:OE1	1:B:150:ARG:CG	2.53	0.56
1:B:33:GLU:HA	1:B:36:GLU:HB2	1.88	0.56
1:F:150:ARG:CZ	1:F:184:PRO:HG3	2.35	0.56
1:E:153:PRO:HB2	1:E:190:LEU:HD12	1.87	0.56
1:A:67:ALA:O	1:A:71:ASN:ND2	2.32	0.56
1:B:13:ILE:HG22	1:B:17:ARG:H	1.69	0.56
1:C:134:GLU:HB3	1:C:150:ARG:HG3	1.88	0.56
1:C:195:THR:OG1	1:C:197:GLN:HG2	2.05	0.56
1:D:79:PHE:HE1	1:D:96:MET:HE1	1.71	0.56
1:E:22:THR:OG1	1:E:49:ILE:HD13	2.06	0.55
1:F:10:PHE:CE1	1:F:19:ILE:HG12	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:VAL:O	1:C:145:THR:HG21	2.06	0.55
1:C:211:ALA:HB2	1:C:241:ILE:HG23	1.87	0.55
1:E:200:ILE:HG23	1:E:221:VAL:HG23	1.89	0.55
1:B:13:ILE:HG23	1:B:16:GLU:HB3	1.88	0.55
1:D:79:PHE:CE1	1:D:96:MET:HE1	2.42	0.55
1:F:171:PHE:HB2	1:F:197:GLN:HE21	1.72	0.55
1:A:48:GLY:HA2	1:A:74:VAL:CG1	2.36	0.55
1:B:13:ILE:HG22	1:B:17:ARG:N	2.21	0.55
1:D:60:GLU:N	1:D:60:GLU:OE1	2.40	0.55
1:F:10:PHE:HE1	1:F:19:ILE:HG12	1.72	0.55
1:F:78:LEU:HD13	1:F:86:VAL:HA	1.89	0.55
1:F:171:PHE:HB2	1:F:197:GLN:NE2	2.22	0.54
1:A:134:GLU:HG2	1:A:149:PRO:HA	1.88	0.54
1:B:185:GLU:HB3	1:B:217:ALA:HB2	1.89	0.54
1:C:42:ILE:HA	1:C:46:THR:HG22	1.88	0.54
1:C:4:MET:HG2	1:C:5:LYS:N	2.23	0.54
1:F:23:LEU:HD12	1:F:50:MET:O	2.07	0.54
1:D:98:LEU:HD21	1:D:145:THR:HG22	1.90	0.54
1:E:14:LEU:HD23	1:E:14:LEU:O	2.07	0.54
1:C:96:MET:HA	1:C:128:MET:O	2.06	0.54
1:D:134:GLU:OE2	2:D:301:HOH:O	2.19	0.54
1:C:160:ALA:HA	1:C:171:PHE:CE1	2.42	0.54
1:D:154:ASP:HB2	2:D:304:HOH:O	2.07	0.53
1:A:179:ALA:O	1:A:206:ARG:NH2	2.41	0.53
1:D:31:PRO:HA	1:D:64:THR:HG22	1.90	0.53
1:E:38:ALA:O	1:E:42:ILE:HG23	2.08	0.53
1:F:26:PRO:HG2	1:F:61:LEU:HD12	1.91	0.53
1:F:78:LEU:HD22	1:F:85:GLY:O	2.08	0.53
1:A:74:VAL:HG13	1:A:75:PRO:HD2	1.91	0.53
1:E:39:ARG:HA	1:E:42:ILE:HG12	1.91	0.53
1:A:56:THR:OG1	1:A:57:ASP:N	2.42	0.53
1:A:66:ARG:HG3	1:A:89:TYR:CE1	2.44	0.53
1:A:145:THR:O	1:A:147:PRO:HD3	2.09	0.52
1:A:111:GLN:OE1	1:A:111:GLN:N	2.38	0.52
1:B:117:THR:O	1:B:120:LYS:HG3	2.09	0.52
1:E:138:THR:HG22	1:E:142:VAL:HG23	1.91	0.52
1:B:96:MET:HB3	1:B:128:MET:HB3	1.91	0.52
1:B:39:ARG:NH1	1:B:42:ILE:HB	2.25	0.52
1:E:80:PRO:HG3	1:E:93:ILE:HD11	1.91	0.52
1:E:116:ALA:O	1:E:120:LYS:HG2	2.09	0.52
1:F:105:TYR:HA	1:F:109:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:ARG:HE	1:F:69:ARG:C	2.13	0.52
1:A:135:PRO:HG2	1:A:180:PRO:HD2	1.93	0.51
1:D:129:GLY:HA2	1:D:168:MET:HE1	1.92	0.51
1:E:32:GLU:HA	1:E:35:VAL:HG12	1.91	0.51
1:D:98:LEU:HD13	1:D:130:TYR:CD1	2.44	0.51
1:D:9:TYR:O	1:D:13:ILE:HG13	2.09	0.51
1:A:9:TYR:CZ	1:A:13:ILE:HD11	2.45	0.51
1:F:131:LEU:HD21	1:F:148:VAL:HG21	1.92	0.51
1:A:130:TYR:OH	1:A:174:GLU:OE1	2.28	0.51
1:D:200:ILE:HG12	1:D:221:VAL:HG22	1.91	0.51
1:D:82:ASN:OD1	1:D:83:THR:N	2.39	0.51
1:A:134:GLU:HG3	1:A:150:ARG:HG3	1.93	0.51
1:A:239:ARG:HG2	1:A:243:GLU:OE2	2.10	0.51
1:B:111:GLN:H	1:B:111:GLN:CD	2.14	0.51
1:F:169:ARG:C	1:F:170:LEU:HD12	2.31	0.51
1:B:50:MET:HA	1:B:77:ILE:O	2.10	0.50
1:B:88:ARG:NH1	1:B:89:TYR:OH	2.45	0.50
1:D:79:PHE:HD1	1:D:96:MET:HE3	1.76	0.50
1:E:39:ARG:NH2	1:E:43:ARG:HH12	2.09	0.50
1:A:200:ILE:HG12	1:A:221:VAL:HB	1.92	0.50
1:F:19:ILE:CG2	1:F:221:VAL:HG22	2.41	0.50
1:C:183:VAL:N	2:C:306:HOH:O	2.33	0.50
1:D:200:ILE:HA	1:D:221:VAL:HG22	1.94	0.50
1:B:33:GLU:HG3	1:B:36:GLU:HB2	1.94	0.50
1:C:236:ASP:N	1:C:236:ASP:OD1	2.44	0.50
1:C:163:ALA:HA	1:C:166:LEU:HD12	1.94	0.50
1:F:19:ILE:HD12	1:F:20:HIS:H	1.77	0.50
1:B:68:LEU:O	1:B:72:ILE:HG12	2.12	0.49
1:D:200:ILE:HG23	1:D:221:VAL:HG23	1.94	0.49
1:E:189:ALA:O	1:E:193:ARG:HG3	2.12	0.49
1:F:195:THR:CG2	1:F:197:GLN:HG2	2.40	0.49
1:B:56:THR:HG22	1:F:113:LEU:O	2.11	0.49
1:F:98:LEU:HA	1:F:130:TYR:O	2.12	0.49
1:B:118:VAL:HG13	1:B:123:ILE:HG22	1.93	0.49
1:F:51:LEU:HD22	1:F:76:ILE:CG2	2.42	0.49
1:A:96:MET:HA	1:A:128:MET:O	2.13	0.49
1:E:27:GLU:OE2	2:E:301:HOH:O	2.20	0.49
1:B:192:LYS:HB2	1:B:199:LEU:HD23	1.94	0.49
1:C:224:THR:HG21	1:C:241:ILE:HD13	1.95	0.49
1:A:55:THR:HG21	1:D:113:LEU:HD13	1.95	0.49
1:E:96:MET:HA	1:E:128:MET:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:PHE:C	1:F:12:ASP:H	2.17	0.49
1:B:163:ALA:HB1	1:B:168:MET:HB2	1.94	0.48
1:B:207:SER:H	1:B:210:ASP:HB2	1.78	0.48
1:B:30:THR:CG2	1:B:31:PRO:HD2	2.43	0.48
1:A:55:THR:HG23	1:A:82:ASN:ND2	2.28	0.48
1:B:169:ARG:HG3	1:B:169:ARG:HH11	1.78	0.48
1:E:57:ASP:OD1	1:E:58:SER:N	2.46	0.48
1:E:30:THR:CG2	1:E:33:GLU:HB2	2.39	0.48
1:E:64:THR:O	1:E:68:LEU:HD12	2.14	0.48
1:A:160:ALA:HA	1:A:171:PHE:CE1	2.48	0.48
1:C:98:LEU:HD11	1:C:132:VAL:HG23	1.95	0.48
1:F:49:ILE:HB	1:F:76:ILE:HG23	1.96	0.48
1:B:26:PRO:HB2	1:B:60:GLU:HG3	1.94	0.48
1:B:96:MET:HA	1:B:128:MET:O	2.13	0.48
1:D:55:THR:OG1	1:D:82:ASN:HB2	2.13	0.48
1:D:75:PRO:HB2	1:D:77:ILE:HD11	1.96	0.48
1:D:18:LYS:HD3	1:D:219:ALA:O	2.13	0.48
1:E:119:LYS:HD2	1:F:161:MET:SD	2.54	0.48
1:E:160:ALA:HA	1:E:171:PHE:CE2	2.48	0.48
1:E:215:ALA:HB2	1:E:245:MET:HG2	1.96	0.48
1:C:121:MET:O	1:C:123:ILE:N	2.38	0.48
1:F:130:TYR:HD1	1:F:172:TYR:HB3	1.78	0.48
1:D:160:ALA:HA	1:D:171:PHE:CE1	2.49	0.47
1:F:174:GLU:HG3	1:F:176:GLY:H	1.78	0.47
1:B:98:LEU:HG	1:B:101:SER:HB2	1.95	0.47
1:A:129:GLY:HA2	1:A:168:MET:HE1	1.96	0.47
1:A:65:ALA:HB1	1:A:89:TYR:HB2	1.96	0.47
1:D:185:GLU:HG2	1:D:213:ARG:HG3	1.95	0.47
1:F:96:MET:HA	1:F:128:MET:O	2.14	0.47
1:A:239:ARG:CG	1:A:243:GLU:OE2	2.63	0.47
1:A:82:ASN:OD1	1:A:84:THR:HG22	2.14	0.47
1:E:127:PRO:HB2	1:E:168:MET:HA	1.96	0.47
1:E:212:ALA:O	1:E:216:GLY:N	2.44	0.47
1:B:94:PHE:HE1	1:B:126:LEU:HD12	1.78	0.47
1:C:131:LEU:HD22	1:C:171:PHE:HZ	1.80	0.47
1:E:175:ALA:HB2	1:E:183:VAL:HG22	1.95	0.47
1:B:78:LEU:HD13	1:B:86:VAL:HA	1.97	0.47
1:D:175:ALA:HB3	1:D:203:GLY:HA3	1.97	0.47
1:E:242:VAL:N	1:E:243:GLU:OE1	2.48	0.47
1:E:200:ILE:HG23	1:E:221:VAL:CG2	2.44	0.47
1:B:105:TYR:HA	1:B:109:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:GLU:OE2	2:B:301:HOH:O	2.21	0.47
1:B:42:ILE:O	1:B:44:GLY:N	2.48	0.47
1:D:24:ILE:CG1	1:D:49:ILE:HD11	2.43	0.46
1:E:42:ILE:HA	1:E:46:THR:HG22	1.97	0.46
1:E:243:GLU:CD	1:E:244:GLY:N	2.69	0.46
1:A:211:ALA:HB2	1:A:241:ILE:HG23	1.98	0.46
1:B:31:PRO:HG3	1:B:63:ASN:ND2	2.30	0.46
1:F:69:ARG:NE	1:F:69:ARG:O	2.40	0.46
1:F:78:LEU:HB2	1:F:93:ILE:CD1	2.42	0.46
1:D:72:ILE:HG22	1:D:73:ASP:H	1.80	0.46
1:F:207:SER:N	1:F:210:ASP:HB2	2.31	0.46
1:F:173:LEU:HD23	1:F:183:VAL:HG11	1.98	0.46
1:F:19:ILE:HD12	1:F:20:HIS:N	2.30	0.46
1:B:170:LEU:HG	1:B:198:ILE:HB	1.98	0.46
1:A:37:ILE:HG21	1:A:226:THR:HG23	1.97	0.45
1:F:206:ARG:O	1:F:241:ILE:HD11	2.16	0.45
1:A:118:VAL:HG13	1:A:123:ILE:HG23	1.99	0.45
1:B:90:ALA:HB3	1:B:123:ILE:HD11	1.99	0.45
1:B:38:ALA:HB1	1:B:49:ILE:HD11	1.99	0.45
1:A:7:GLU:HG3	1:A:126:LEU:HD22	1.98	0.45
1:A:168:MET:HE3	1:C:166:LEU:HD22	1.97	0.45
1:B:213:ARG:HG3	1:B:213:ARG:HH11	1.81	0.45
1:D:78:LEU:HD13	1:D:85:GLY:O	2.17	0.45
1:E:78:LEU:HD13	1:E:86:VAL:HA	1.97	0.45
1:D:105:TYR:CZ	1:D:110:ALA:HB2	2.51	0.45
1:D:96:MET:HA	1:D:128:MET:O	2.17	0.45
1:D:133:VAL:HG11	1:D:183:VAL:HG13	1.98	0.45
1:D:19:ILE:CG1	1:D:221:VAL:HG12	2.46	0.45
1:B:158:ALA:HA	1:B:161:MET:HE3	1.99	0.45
1:C:75:PRO:HA	1:C:91:ASP:OD2	2.17	0.45
1:E:58:SER:OG	1:E:84:THR:HB	2.17	0.45
1:B:25:ASP:OD1	1:B:54:SER:HB2	2.16	0.44
1:C:30:THR:HG23	1:C:33:GLU:OE1	2.16	0.44
1:E:66:ARG:HH21	1:E:88:ARG:HH12	1.64	0.44
1:A:72:ILE:HD11	1:A:76:ILE:HD11	1.98	0.44
1:E:7:GLU:HB2	1:E:126:LEU:HD21	1.98	0.44
1:A:38:ALA:O	1:A:42:ILE:HD12	2.18	0.44
1:E:133:VAL:HG12	1:E:134:GLU:H	1.83	0.44
1:E:198:ILE:HA	1:E:220:ASP:OD2	2.17	0.44
1:F:105:TYR:CZ	1:F:110:ALA:HB2	2.53	0.44
1:F:25:ASP:O	1:F:29:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:GLU:HG2	1:D:213:ARG:CG	2.47	0.44
1:D:60:GLU:O	1:D:64:THR:HG23	2.17	0.44
1:D:182:HIS:HB3	1:D:205:ILE:CG2	2.42	0.44
1:B:166:LEU:HD22	1:D:168:MET:HE3	2.00	0.44
1:F:19:ILE:HD11	1:F:47:ASP:HB2	1.99	0.44
1:F:7:GLU:HG3	1:F:126:LEU:HD22	2.00	0.44
1:A:48:GLY:HA2	1:A:74:VAL:HG13	1.99	0.44
1:B:27:GLU:HA	1:B:60:GLU:HG2	1.99	0.44
1:E:10:PHE:CD1	1:E:19:ILE:HD13	2.53	0.44
1:C:80:PRO:HD2	1:C:96:MET:HE2	2.00	0.44
1:B:213:ARG:HG3	1:B:213:ARG:NH1	2.33	0.44
1:D:152:LYS:HE2	1:F:138:THR:OG1	2.18	0.44
1:D:14:LEU:HD11	1:D:220:ASP:HB3	2.00	0.43
1:F:97:SER:HA	1:F:111:GLN:NE2	2.33	0.43
1:B:39:ARG:HD2	1:B:39:ARG:HA	1.62	0.43
1:A:158:ALA:HB1	1:C:112:ALA:O	2.18	0.43
1:A:131:LEU:HD11	1:A:148:VAL:HG21	2.00	0.43
1:B:111:GLN:H	1:B:111:GLN:NE2	2.17	0.43
1:B:30:THR:HG22	1:B:31:PRO:CD	2.47	0.43
1:E:29:GLN:HG3	1:E:34:ALA:HB2	1.99	0.43
1:F:31:PRO:O	1:F:35:VAL:HG13	2.18	0.43
1:C:50:MET:HA	1:C:77:ILE:O	2.19	0.43
1:D:72:ILE:HG22	1:D:73:ASP:N	2.33	0.43
1:F:207:SER:HB2	1:F:210:ASP:N	2.25	0.43
1:A:78:LEU:HD13	1:A:86:VAL:HA	2.01	0.43
1:F:77:ILE:HG21	1:F:94:PHE:CZ	2.53	0.43
1:A:40:ALA:HB1	1:A:235:GLU:HG3	2.01	0.43
1:E:19:ILE:O	1:E:221:VAL:HA	2.19	0.43
1:E:140:GLY:HA2	1:E:145:THR:HG21	2.01	0.43
1:B:100:ASN:ND2	1:B:146:LYS:O	2.49	0.43
1:D:103:ASN:HD22	1:D:104:PRO:HD2	1.84	0.43
1:B:112:ALA:HA	1:D:162:ALA:HB2	2.01	0.42
1:A:121:MET:C	1:A:123:ILE:H	2.23	0.42
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.84	0.42
1:C:22:THR:HB	1:C:49:ILE:HD13	2.01	0.42
1:F:117:THR:O	1:F:121:MET:HG3	2.19	0.42
1:A:17:ARG:HH22	1:A:47:ASP:CG	2.20	0.42
1:C:24:ILE:HD12	1:C:49:ILE:HD12	2.01	0.42
1:F:96:MET:HB3	1:F:96:MET:HE2	1.87	0.42
1:D:182:HIS:CB	1:D:205:ILE:HG22	2.43	0.42
1:F:35:VAL:HG11	1:F:67:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ILE:HG21	1:C:68:LEU:HD21	2.01	0.42
1:C:23:LEU:HA	1:C:50:MET:HG3	2.01	0.42
1:E:114:GLY:O	1:E:118:VAL:HG12	2.20	0.42
1:E:152:LYS:HD2	1:E:152:LYS:HA	1.83	0.42
1:E:49:ILE:O	1:E:76:ILE:HA	2.19	0.42
1:D:24:ILE:HB	1:D:51:LEU:HD12	2.01	0.42
1:F:153:PRO:HB2	1:F:190:LEU:HD13	2.01	0.42
1:A:96:MET:SD	1:A:128:MET:CE	3.08	0.42
1:A:113:LEU:HD21	1:D:142:VAL:HG13	2.02	0.42
1:F:238:ILE:O	1:F:242:VAL:HG23	2.19	0.42
1:E:238:ILE:O	1:E:242:VAL:HG23	2.20	0.42
1:B:9:TYR:O	1:B:12:ASP:HB2	2.20	0.41
1:B:158:ALA:HB1	1:D:112:ALA:O	2.20	0.41
1:A:134:GLU:HA	1:A:135:PRO:C	2.40	0.41
1:B:6:VAL:O	1:B:9:TYR:HB3	2.20	0.41
1:C:195:THR:HG21	1:C:197:GLN:NE2	2.35	0.41
1:F:93:ILE:CG2	1:F:125:ALA:HA	2.51	0.41
1:E:52:GLY:HA3	1:E:79:PHE:HB3	2.02	0.41
1:A:153:PRO:HB2	1:A:190:LEU:HD23	2.02	0.41
1:B:205:ILE:HG23	1:B:210:ASP:HB3	2.02	0.41
1:C:19:ILE:O	1:C:221:VAL:HA	2.20	0.41
1:A:103:ASN:HA	1:A:104:PRO:HD3	1.96	0.41
1:F:86:VAL:HG12	1:F:121:MET:HE1	2.03	0.41
1:B:13:ILE:CG2	1:B:17:ARG:N	2.84	0.41
1:C:131:LEU:HD23	1:C:173:LEU:HD23	2.01	0.41
1:D:6:VAL:HA	1:D:9:TYR:HB3	2.02	0.41
1:E:26:PRO:HA	1:E:29:GLN:NE2	2.36	0.41
1:E:65:ALA:HB1	1:E:89:TYR:HB2	2.02	0.41
1:A:117:THR:O	1:A:121:MET:HG3	2.20	0.41
1:A:213:ARG:HA	1:A:213:ARG:NE	2.35	0.41
1:B:25:ASP:HB3	1:B:28:GLU:HB2	2.01	0.41
1:D:67:ALA:O	1:D:71:ASN:HB2	2.20	0.41
1:A:61:LEU:CD1	1:A:85:GLY:HA2	2.51	0.41
1:B:24:ILE:HD12	1:B:24:ILE:N	2.36	0.41
1:C:138:THR:N	1:F:152:LYS:HZ1	2.19	0.41
1:E:192:LYS:HA	1:E:192:LYS:HD2	1.78	0.41
1:A:162:ALA:O	1:A:163:ALA:C	2.59	0.40
1:A:200:ILE:HG12	1:A:221:VAL:CG2	2.52	0.40
1:A:68:LEU:O	1:A:72:ILE:HG12	2.21	0.40
1:D:55:THR:OG1	1:D:81:GLY:O	2.39	0.40
1:B:152:LYS:HB3	1:B:152:LYS:HE3	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:LEU:HB3	1:D:50:MET:HG3	2.03	0.40
1:E:138:THR:O	1:E:142:VAL:HG23	2.21	0.40
1:A:100:ASN:OD1	1:A:131:LEU:HD22	2.22	0.40
1:C:4:MET:HG2	1:C:5:LYS:H	1.86	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	227/256 (89%)	207 (91%)	16 (7%)	4 (2%)	8 21
1	B	219/256 (86%)	192 (88%)	23 (10%)	4 (2%)	8 21
1	C	218/256 (85%)	195 (89%)	16 (7%)	7 (3%)	4 9
1	D	222/256 (87%)	204 (92%)	16 (7%)	2 (1%)	17 40
1	E	233/256 (91%)	206 (88%)	24 (10%)	3 (1%)	12 30
1	F	227/256 (89%)	207 (91%)	18 (8%)	2 (1%)	17 40
All	All	1346/1536 (88%)	1211 (90%)	113 (8%)	22 (2%)	9 24

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	ILE
1	C	67	ALA
1	D	66	ARG
1	B	53	GLY
1	C	4	MET
1	C	88	ARG
1	E	142	VAL
1	E	177	SER

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Mol	Chain	Res	Type
1	B	43	ARG
1	C	68	LEU
1	C	98	LEU
1	E	141	ALA
1	F	53	GLY
1	D	180	PRO
1	A	162	ALA
1	F	11	HIS
1	A	203	GLY
1	B	108	ILE
1	A	108	ILE
1	C	122	GLY
1	C	203	GLY
1	A	135	PRO

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	177/201 (88%)	174 (98%)	3 (2%)	60	84
1	B	156/201 (78%)	148 (95%)	8 (5%)	24	50
1	C	158/201 (79%)	156 (99%)	2 (1%)	69	87
1	D	157/201 (78%)	154 (98%)	3 (2%)	57	82
1	E	169/201 (84%)	161 (95%)	8 (5%)	26	54
1	F	165/201 (82%)	160 (97%)	5 (3%)	41	70
All	All	982/1206 (81%)	953 (97%)	29 (3%)	41	70

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	119	LYS
1	A	206	ARG
1	B	29	GLN

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Mol	Chain	Res	Type
1	B	62	ASP
1	B	120	LYS
1	B	151	ASN
1	B	164	GLU
1	B	177	SER
1	B	196	ASP
1	B	207	SER
1	C	172	TYR
1	C	236	ASP
1	D	62	ASP
1	D	66	ARG
1	D	193	ARG
1	E	59	SER
1	E	60	GLU
1	E	79	PHE
1	E	88	ARG
1	E	144	ASP
1	E	150	ARG
1	E	172	TYR
1	E	196	ASP
1	F	36	GLU
1	F	43	ARG
1	F	51	LEU
1	F	69	ARG
1	F	177	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	103	ASN
1	D	197	GLN
1	E	63	ASN
1	F	63	ASN
1	F	197	GLN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	233/256 (91%)	0.01	2 (0%) 84 85	30, 50, 99, 146	0
1	B	221/256 (86%)	0.24	7 (3%) 47 48	34, 62, 111, 207	0
1	C	226/256 (88%)	0.06	4 (1%) 68 70	34, 56, 101, 116	0
1	D	224/256 (87%)	0.41	14 (6%) 20 19	35, 65, 119, 154	0
1	E	237/256 (92%)	0.67	31 (13%) 3 2	44, 84, 128, 152	0
1	F	231/256 (90%)	0.80	33 (14%) 2 1	45, 85, 129, 182	0
All	All	1372/1536 (89%)	0.37	91 (6%) 18 16	30, 67, 120, 207	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	122	GLY	10.3
1	F	41	ALA	9.3
1	B	45	GLY	8.3
1	E	72	ILE	6.3
1	E	238	ILE	6.2
1	D	58	SER	6.1
1	F	89	TYR	5.6
1	F	14	LEU	5.6
1	F	123	ILE	5.2
1	F	45	GLY	4.9
1	D	144	ASP	4.5
1	E	183	VAL	4.4
1	F	19	ILE	4.4
1	F	70	GLU	4.3
1	E	143	GLY	4.1
1	F	143	GLY	4.1
1	E	178	GLY	4.1
1	F	72	ILE	3.9
1	E	142	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	193	ARG	3.8
1	F	144	ASP	3.6
1	F	217	ALA	3.5
1	E	144	ASP	3.5
1	D	45	GLY	3.4
1	C	61	LEU	3.4
1	D	223	VAL	3.4
1	E	221	VAL	3.4
1	F	4	MET	3.3
1	D	72	ILE	3.2
1	D	143	GLY	3.2
1	E	79	PHE	3.2
1	D	32	GLU	3.1
1	E	141	ALA	3.1
1	E	87	SER	3.1
1	E	211	ALA	3.0
1	E	55	THR	3.0
1	D	35	VAL	3.0
1	F	221	VAL	3.0
1	E	245	MET	3.0
1	E	21	LEU	2.9
1	F	67	ALA	2.9
1	E	43	ARG	2.9
1	E	45	GLY	2.9
1	F	142	VAL	2.9
1	F	201	VAL	2.9
1	D	191	VAL	2.8
1	C	31	PRO	2.8
1	F	9	TYR	2.8
1	E	188	ILE	2.8
1	F	71	ASN	2.8
1	F	46	THR	2.7
1	E	222	VAL	2.7
1	F	222	VAL	2.7
1	F	36	GLU	2.7
1	F	92	ALA	2.6
1	F	10	PHE	2.6
1	F	55	THR	2.6
1	B	17	ARG	2.6
1	A	15	ARG	2.5
1	E	241	ILE	2.5
1	F	47	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	67	ALA	2.5
1	E	185	GLU	2.4
1	B	76	ILE	2.4
1	C	35	VAL	2.4
1	B	46	THR	2.4
1	E	173	LEU	2.4
1	F	215	ALA	2.4
1	F	68	LEU	2.3
1	F	44	GLY	2.3
1	E	81	GLY	2.3
1	D	122	GLY	2.3
1	E	140	GLY	2.3
1	F	20	HIS	2.3
1	F	243	GLU	2.2
1	B	74	VAL	2.2
1	D	54	SER	2.2
1	E	83	THR	2.1
1	D	57	ASP	2.1
1	E	10	PHE	2.1
1	D	9	TYR	2.1
1	E	102	THR	2.1
1	B	89	TYR	2.1
1	F	238	ILE	2.0
1	F	241	ILE	2.0
1	A	204	GLY	2.0
1	C	145	THR	2.0
1	D	24	ILE	2.0
1	E	14	LEU	2.0
1	E	88	ARG	2.0
1	E	149	PRO	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.