



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:40 AM GMT

PDB ID : 3MP3
Title : Crystal Structure of Human Lyase in complex with inhibitor HG-CoA
Authors : Fu, Z.; Runquist, J.A.; Montgomery, C.; Mizioro, H.M.; Kim, J.-J.P.
Deposited on : 2010-04-24
Resolution : 2.40 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

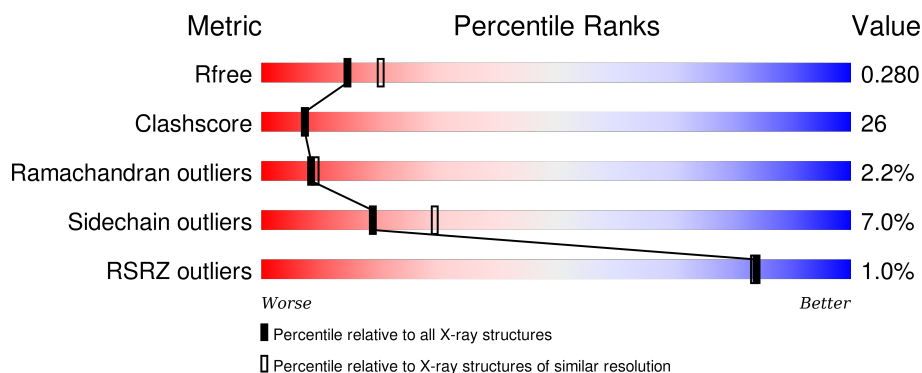
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




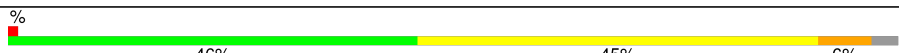
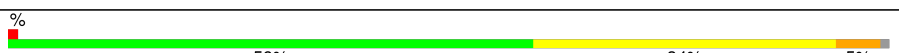
The reported resolution of this entry is 2.40 Å.

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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 $\leq 5\%$. 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	298	 63% 32% ...
1	B	298	 2% 61% 34% . .
1	C	298	 53% 42% . .
1	D	298	 % 46% 45% 6% .
1	E	298	 % 59% 34% 5% .

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Mol	Chain	Length	Quality of chain
1	F	298	<div> <div></div> <div>%</div> <div>48%</div> <div>46%</div> <div>6%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3HG	A	400	-	-	-	X

2 Entry composition [i](#)

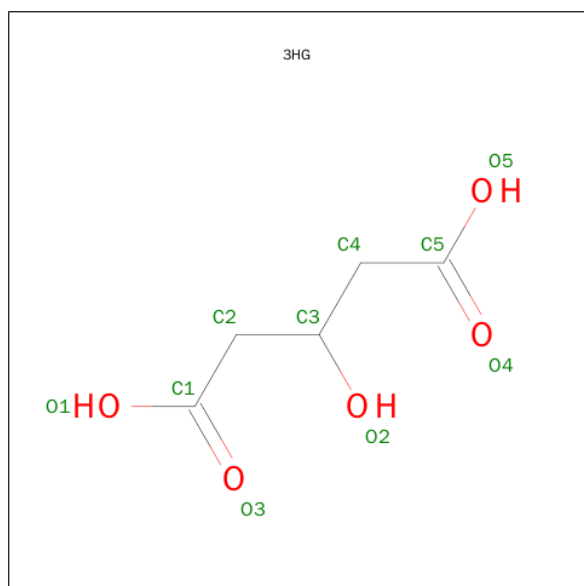
There are 5 unique types of molecules in this entry. The entry contains 13597 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hydroxymethylglutaryl-CoA lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2189	1390	365	417	17			
1	B	296	Total	C	N	O	S	0	0	0
			2189	1390	365	417	17			
1	C	296	Total	C	N	O	S	0	0	0
			2189	1390	365	417	17			
1	D	289	Total	C	N	O	S	0	0	0
			2142	1361	357	408	16			
1	E	296	Total	C	N	O	S	0	0	0
			2189	1390	365	417	17			
1	F	296	Total	C	N	O	S	0	0	0
			2189	1390	365	417	17			

- Molecule 2 is 3-HYDROXYPENTANEDIOIC ACID (three-letter code: 3HG) (formula: C₅H₈O₅).

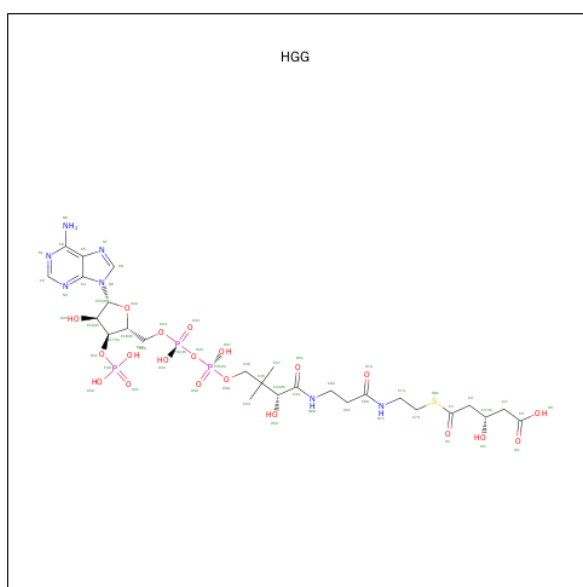


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (3R,5S,9R,21S)-1-[(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-4-HYDROXY-3-(PHOSPHONOOXY)TETRAHYDROFURAN-2-YL]-3,5,9,21-TETRAHYDROXY-8,8-DIMETHYL-10,14,19-TRIOXO-2,4,6-TRIOXA-18-THIA-11,15-DIAZA-3,5-DIPHOSPHATRICOSAN-23-OIC ACID 3,5-DIOXIDE (three-letter code: HGG) (formula: C₂₆H₄₂N₇O₂₀P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	0	0
			57	26	7	20	3	1		

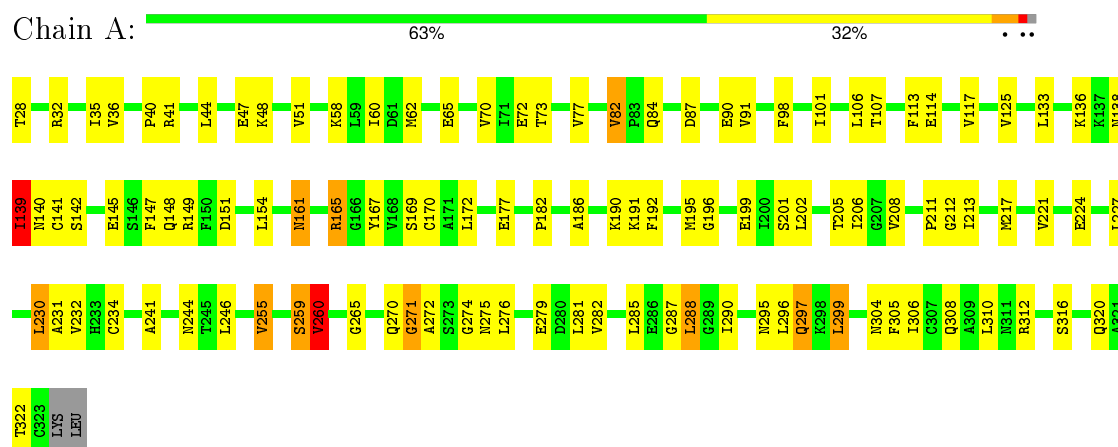
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	100	Total 100	O 100	0	0
5	B	70	Total 70	O 70	0	0
5	C	70	Total 70	O 70	0	0
5	D	65	Total 65	O 65	0	0
5	E	74	Total 74	O 74	0	0
5	F	58	Total 58	O 58	0	0

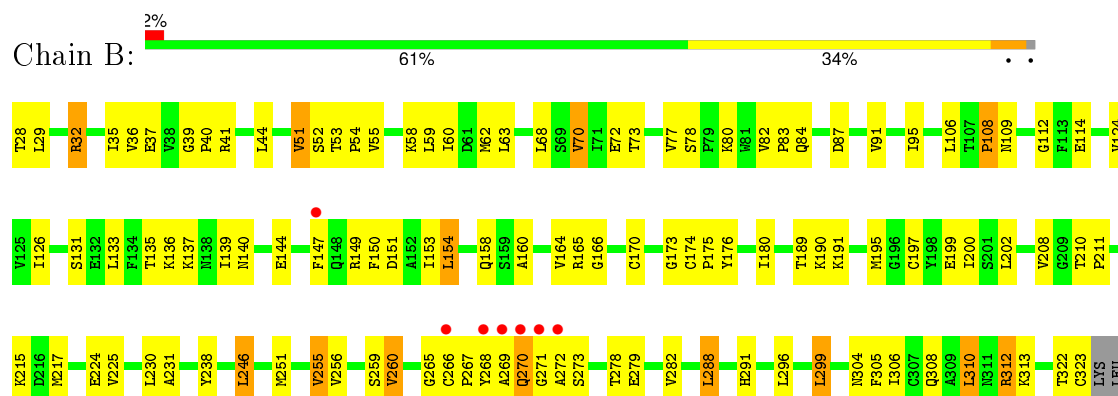
3 Residue-property plots

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

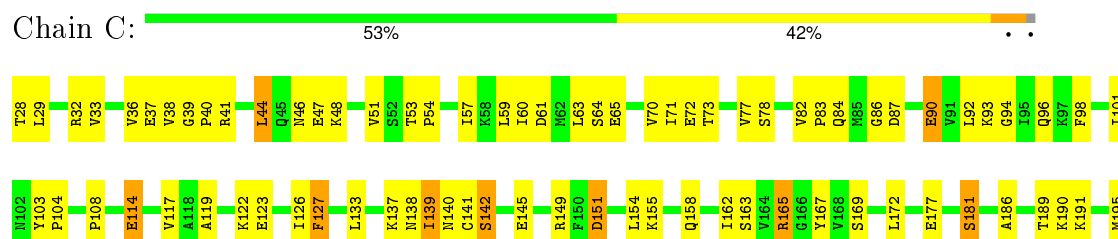
• Molecule 1: Hydroxymethylglutaryl-CoA lyase

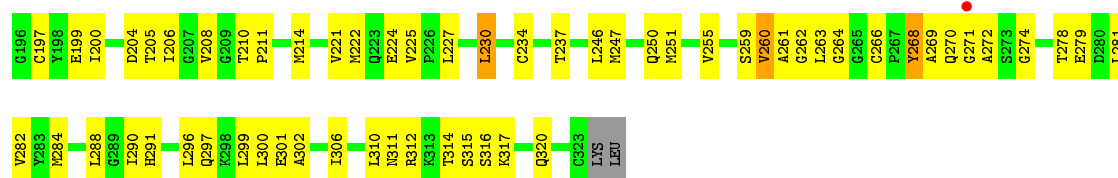


• Molecule 1: Hydroxymethylglutaryl-CoA lyase

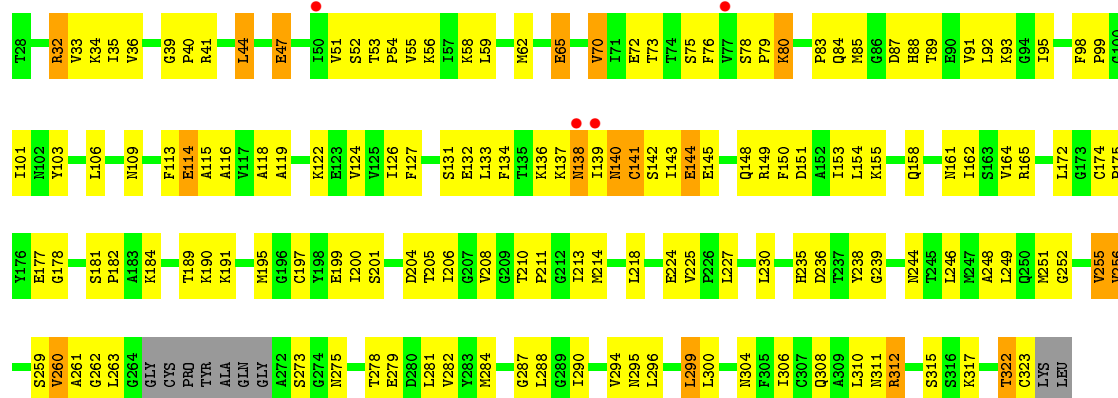


• Molecule 1: Hydroxymethylglutaryl-CoA lyase

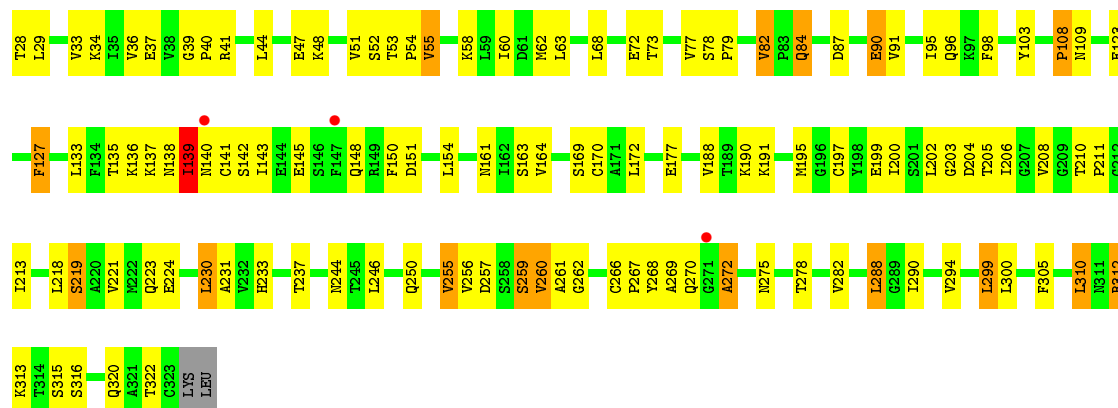




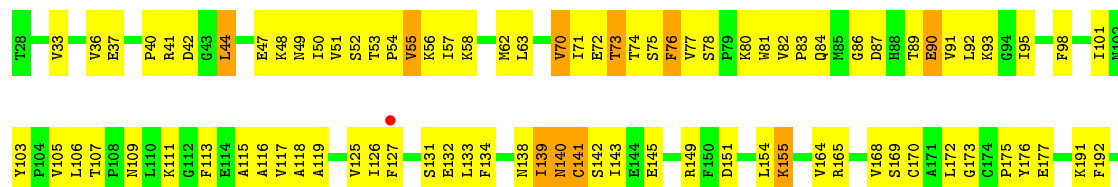
• Molecule 1: Hydroxymethylglutaryl-CoA lyase

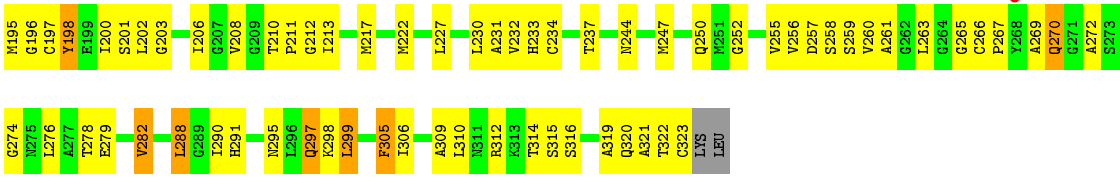


• Molecule 1: Hydroxymethylglutaryl-CoA lyase



• Molecule 1: Hydroxymethylglutaryl-CoA lyase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.37Å 117.00Å 86.87Å 90.00° 112.31° 90.00°	Depositor
Resolution (Å)	29.70 – 2.40 39.17 – 2.39	Depositor EDS
% Data completeness (in resolution range)	93.3 (29.70-2.40) 77.2 (39.17-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.281 0.212 , 0.280	Depositor DCC
R_{free} test set	6749 reflections (10.14%)	DCC
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 66824 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13597	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HGG, MG, 3HG

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	0.41	0/2224	0.64	0/3011
1	B	0.39	0/2224	0.63	0/3011
1	C	0.39	0/2224	0.63	0/3011
1	D	0.38	0/2174	0.60	0/2941
1	E	0.38	0/2224	0.62	0/3011
1	F	0.36	0/2224	0.58	0/3011
All	All	0.38	0/13294	0.62	0/17996

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 [i](#)

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	2189	0	2244	92	0
1	B	2189	0	2244	93	0
1	C	2189	0	2244	139	0
1	D	2142	0	2203	136	0
1	E	2189	0	2244	104	0
1	F	2189	0	2244	138	0
2	A	10	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	B	57	0	37	10	0
5	A	100	0	0	6	0
5	B	70	0	0	3	0
5	C	70	0	0	7	0
5	D	65	0	0	3	0
5	E	74	0	0	4	0
5	F	58	0	0	3	0
All	All	13597	0	13466	686	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 26.

All (686) 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:47:GLU:HG2	1:D:310:LEU:HD21	1.46	0.98
1:E:211:PRO:HG2	1:F:288:LEU:HD11	1.44	0.96
1:D:263:LEU:HD11	1:D:306:ILE:HD12	1.48	0.96
1:E:84:GLN:NE2	1:E:84:GLN:H	1.65	0.94
1:E:51:VAL:HB	1:E:55:VAL:HG21	1.48	0.93
1:D:92:LEU:HD23	1:D:119:ALA:HB3	1.51	0.92
1:C:266:CYS:HB3	1:C:269:ALA:HB3	1.52	0.91
1:A:190:LYS:HD3	1:A:224:GLU:HB3	1.56	0.87
1:C:48:LYS:H	1:C:48:LYS:HD2	1.40	0.87
1:D:142:SER:HB2	1:D:145:GLU:HB2	1.57	0.86
1:A:48:LYS:HD2	1:A:48:LYS:N	1.90	0.86
1:F:52:SER:OG	1:F:55:VAL:HG12	1.77	0.85
1:C:93:LYS:HE3	1:C:119:ALA:HA	1.57	0.84
1:C:149:ARG:HH11	1:E:161:ASN:HD22	1.21	0.84
1:E:63:LEU:HD21	1:E:260:VAL:HG11	1.60	0.83
1:C:36:VAL:HA	1:C:70:VAL:HG13	1.61	0.83
1:A:48:LYS:HD2	1:A:48:LYS:H	1.40	0.83
1:E:68:LEU:HD13	1:E:294:VAL:HG21	1.61	0.83
1:B:28:THR:HG22	1:B:29:LEU:H	1.44	0.83
1:A:288:LEU:HD11	1:B:211:PRO:HG2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:GLU:HG2	1:C:310:LEU:HD21	1.61	0.82
1:C:28:THR:HG22	1:C:29:LEU:H	1.43	0.82
1:D:52:SER:OG	1:D:55:VAL:HG23	1.80	0.82
1:D:59:LEU:HD22	1:D:306:ILE:HG21	1.61	0.81
1:D:190:LYS:HD2	1:D:224:GLU:HB3	1.62	0.81
1:B:265:GLY:O	1:B:267:PRO:HD3	1.81	0.81
1:E:28:THR:HG22	1:E:29:LEU:H	1.46	0.81
1:C:84:GLN:CD	1:C:84:GLN:H	1.85	0.80
1:E:84:GLN:HE21	1:E:84:GLN:H	1.30	0.80
1:E:260:VAL:HG23	1:E:261:ALA:H	1.46	0.80
1:A:36:VAL:HA	1:A:70:VAL:HG13	1.64	0.79
1:E:51:VAL:HG13	1:E:310:LEU:HD13	1.64	0.79
1:C:39:GLY:HA3	1:C:260:VAL:HG23	1.63	0.79
1:C:33:VAL:HG23	1:C:290:ILE:HG21	1.65	0.78
1:F:134:PHE:O	1:F:138:ASN:HB2	1.83	0.77
1:E:52:SER:O	1:E:55:VAL:HG23	1.82	0.77
1:E:141:CYS:HB2	1:E:145:GLU:HB2	1.66	0.77
1:F:50:ILE:HG22	1:F:84:GLN:HG3	1.67	0.77
1:F:138:ASN:HD22	1:F:139:ILE:HG12	1.51	0.76
1:D:138:ASN:ND2	1:D:139:ILE:HG13	2.00	0.76
1:F:278:THR:O	1:F:282:VAL:HG12	1.84	0.76
1:F:279:GLU:HG3	1:F:299:LEU:HD13	1.67	0.76
1:D:151:ASP:O	1:D:155:LYS:HB2	1.84	0.76
1:C:60:ILE:HD13	1:C:73:THR:HG23	1.67	0.76
1:F:306:ILE:O	1:F:310:LEU:HD13	1.85	0.76
1:F:133:LEU:HD13	1:F:177:GLU:HG2	1.68	0.75
1:C:270:GLN:O	1:C:272:ALA:N	2.19	0.75
1:B:58:LYS:HZ3	1:B:62:MET:HE2	1.52	0.74
1:D:109:ASN:HA	1:D:153:ILE:HD11	1.68	0.74
1:E:270:GLN:HG3	1:F:321:ALA:O	1.88	0.74
1:A:47:GLU:HG2	1:A:310:LEU:HD21	1.69	0.74
1:E:154:LEU:CD1	1:E:195:MET:HB3	2.18	0.74
1:B:322:THR:O	1:B:323:CYS:HB2	1.87	0.73
1:C:59:LEU:HD13	1:C:306:ILE:HB	1.70	0.73
1:F:113:PHE:O	1:F:117:VAL:HG23	1.87	0.73
1:E:40:PRO:HG2	1:E:72:GLU:O	1.89	0.73
1:C:264:GLY:O	1:C:274:GLY:HA3	1.88	0.73
1:F:75:SER:O	1:F:77:VAL:HG12	1.88	0.72
1:A:206:ILE:HG13	1:A:208:VAL:HG13	1.72	0.72
1:B:77:VAL:HG11	4:B:399:HGG:H61	1.72	0.72
1:C:40:PRO:HG2	1:C:72:GLU:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PHE:CE1	1:A:191:LYS:HG2	2.25	0.71
1:A:141:CYS:HA	1:A:145:GLU:OE2	1.89	0.71
1:E:316:SER:O	1:E:320:GLN:HG3	1.90	0.71
1:B:133:LEU:HD23	1:B:176:TYR:HB3	1.71	0.71
1:E:237:THR:HG23	1:E:272:ALA:HB3	1.73	0.71
1:C:83:PRO:HD2	1:C:84:GLN:HE22	1.56	0.71
1:F:90:GLU:CD	1:F:90:GLU:H	1.93	0.71
1:D:172:LEU:HD12	1:D:204:ASP:HB2	1.73	0.71
1:E:58:LYS:HD3	1:E:305:PHE:CZ	2.25	0.70
1:F:36:VAL:HG13	1:F:70:VAL:HG22	1.73	0.70
1:F:58:LYS:HD3	1:F:305:PHE:CZ	2.27	0.70
1:A:36:VAL:HG22	1:A:70:VAL:HG11	1.74	0.70
1:A:138:ASN:C	1:A:139:ILE:HG12	2.12	0.70
1:F:33:VAL:HG23	1:F:290:ILE:HG21	1.73	0.70
1:B:150:PHE:O	1:B:154:LEU:HD12	1.92	0.70
1:F:51:VAL:HG23	1:F:56:LYS:HE3	1.74	0.70
1:C:284:MET:O	1:C:288:LEU:HB2	1.92	0.70
1:C:262:GLY:HA3	1:C:315:SER:HB2	1.73	0.69
1:A:62:MET:HE3	1:A:305:PHE:CD2	2.27	0.69
1:C:149:ARG:HH11	1:E:161:ASN:ND2	1.89	0.69
1:D:59:LEU:HD22	1:D:306:ILE:CG2	2.22	0.69
1:B:108:PRO:HG2	1:B:109:ASN:H	1.56	0.69
1:E:91:VAL:O	1:E:95:ILE:HG23	1.93	0.69
1:D:322:THR:O	1:D:323:CYS:HB2	1.91	0.69
1:C:149:ARG:NH1	1:E:161:ASN:HD22	1.91	0.69
1:D:263:LEU:CD1	1:D:306:ILE:HD12	2.23	0.69
1:B:109:ASN:ND2	4:B:399:HGG:H57A	2.06	0.69
1:E:48:LYS:HD3	5:E:668:HOH:O	1.91	0.69
1:A:36:VAL:HA	1:A:70:VAL:CG1	2.23	0.68
1:F:74:THR:H	1:F:105:VAL:HG12	1.59	0.68
1:A:259:SER:HB2	1:A:275:ASN:HB2	1.75	0.68
1:C:37:GLU:HG2	1:C:63:LEU:HD13	1.76	0.68
1:E:53:THR:N	1:E:54:PRO:HD2	2.09	0.68
1:E:278:THR:HG22	1:E:299:LEU:HD11	1.76	0.68
1:B:278:THR:HG22	1:B:299:LEU:HD11	1.76	0.67
1:F:52:SER:O	1:F:55:VAL:HG13	1.92	0.67
1:C:82:VAL:HG23	1:C:84:GLN:OE1	1.94	0.67
1:E:300:LEU:HD13	1:E:322:THR:HG21	1.76	0.67
1:F:36:VAL:HG21	1:F:165:ARG:HH22	1.59	0.67
1:F:53:THR:N	1:F:54:PRO:HD2	2.10	0.66
1:C:48:LYS:HD2	1:C:48:LYS:N	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:HD13	1:B:306:ILE:HB	1.77	0.66
1:C:211:PRO:HG2	1:D:288:LEU:HD21	1.77	0.66
1:B:112:GLY:CA	4:B:399:HGG:N6	2.59	0.66
1:F:155:LYS:N	1:F:155:LYS:HE2	2.11	0.66
1:F:87:ASP:O	1:F:91:VAL:HG23	1.95	0.66
1:D:92:LEU:HD23	1:D:119:ALA:CB	2.26	0.66
1:F:98:PHE:HB2	1:F:101:ILE:HD12	1.77	0.65
1:D:76:PHE:CZ	1:D:116:ALA:HA	2.31	0.65
1:F:55:VAL:HG23	1:F:305:PHE:CE2	2.31	0.65
1:F:297:GLN:HB3	5:F:560:HOH:O	1.97	0.65
1:C:93:LYS:CE	1:C:119:ALA:HA	2.26	0.65
1:A:161:ASN:HD21	1:F:149:ARG:HH22	1.45	0.65
1:D:200:ILE:N	1:D:200:ILE:HD12	2.11	0.65
1:D:191:LYS:O	1:D:195:MET:HB2	1.97	0.64
1:E:37:GLU:HG2	1:E:63:LEU:HD13	1.79	0.64
1:E:154:LEU:HD13	1:E:195:MET:HB3	1.79	0.64
1:F:202:LEU:HD13	1:F:217:MET:SD	2.37	0.64
1:B:58:LYS:NZ	1:B:62:MET:HE2	2.12	0.64
1:F:106:LEU:HD12	1:F:106:LEU:N	2.13	0.64
1:B:144:GLU:OE1	1:B:147:PHE:HD1	1.81	0.64
1:A:58:LYS:HD3	1:A:305:PHE:CZ	2.32	0.64
1:B:112:GLY:HA2	4:B:399:HGG:N6	2.11	0.64
1:F:81:TRP:O	1:F:83:PRO:HD3	1.97	0.64
1:D:165:ARG:NH2	1:D:199:GLU:OE2	2.31	0.64
1:A:40:PRO:HG2	1:A:72:GLU:O	1.97	0.64
1:F:316:SER:O	1:F:320:GLN:HG3	1.97	0.64
1:C:96:GLN:HB2	1:C:98:PHE:HE1	1.62	0.64
1:C:151:ASP:HB3	5:C:573:HOH:O	1.97	0.64
1:C:278:THR:O	1:C:282:VAL:HG13	1.98	0.63
1:C:317:LYS:HA	1:C:320:GLN:OE1	1.98	0.63
1:C:127:PHE:N	1:C:127:PHE:CD1	2.65	0.63
1:E:51:VAL:HB	1:E:55:VAL:CG2	2.28	0.63
1:E:169:SER:HB2	1:E:205:THR:OG1	1.98	0.63
1:F:154:LEU:HD13	1:F:195:MET:HB3	1.79	0.63
1:F:78:SER:HB2	1:F:80:LYS:HG3	1.81	0.63
1:A:169:SER:HB2	1:A:205:THR:OG1	1.99	0.62
1:B:304:ASN:O	1:B:308:GLN:HG3	1.99	0.62
1:D:115:ALA:O	1:D:118:ALA:HB3	2.00	0.62
1:C:57:ILE:HD13	1:C:94:GLY:HA3	1.82	0.62
1:F:138:ASN:HD22	1:F:139:ILE:H	1.46	0.62
1:D:33:VAL:HG23	1:D:290:ILE:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:HD13	1:B:217:MET:SD	2.40	0.62
1:D:246:LEU:O	1:D:246:LEU:HD13	1.99	0.62
1:F:47:GLU:HG2	1:F:310:LEU:HD23	1.82	0.62
1:E:28:THR:HG22	1:E:29:LEU:N	2.15	0.62
1:C:38:VAL:HG12	1:C:72:GLU:HB2	1.81	0.61
1:B:40:PRO:HG2	1:B:72:GLU:O	2.01	0.61
1:C:154:LEU:HD13	1:C:195:MET:HG2	1.83	0.61
1:A:316:SER:O	1:A:320:GLN:HG3	2.00	0.61
1:F:172:LEU:HD22	1:F:213:ILE:HG22	1.83	0.61
1:B:112:GLY:CA	4:B:399:HGG:HN6A	2.14	0.61
1:D:278:THR:HG22	1:D:299:LEU:HD11	1.82	0.61
1:C:288:LEU:HD13	1:D:211:PRO:HG2	1.83	0.60
1:E:33:VAL:HG23	1:E:290:ILE:HG21	1.81	0.60
1:C:60:ILE:CD1	1:C:73:THR:HG23	2.31	0.60
1:F:231:ALA:HA	1:F:255:VAL:HG13	1.81	0.60
1:F:279:GLU:HA	1:F:282:VAL:HG13	1.83	0.60
1:D:210:THR:HB	1:D:211:PRO:HD2	1.83	0.60
1:B:151:ASP:HB3	5:B:985:HOH:O	2.01	0.60
1:A:295:ASN:OD1	1:A:297:GLN:HG2	2.01	0.60
1:A:297:GLN:H	1:A:297:GLN:CD	2.04	0.60
1:A:172:LEU:HD22	1:A:213:ILE:HG22	1.84	0.60
1:C:263:LEU:HD11	1:C:306:ILE:HG12	1.82	0.60
1:C:77:VAL:HG11	1:C:82:VAL:HG11	1.82	0.60
1:A:260:VAL:O	1:A:279:GLU:OE1	2.18	0.60
1:D:62:MET:HA	1:D:65:GLU:OE2	2.01	0.60
1:B:291:HIS:HB2	5:B:961:HOH:O	2.00	0.60
1:C:261:ALA:HB1	1:C:314:THR:OG1	2.02	0.60
1:F:133:LEU:HD13	1:F:177:GLU:CG	2.31	0.60
1:D:59:LEU:HD13	1:D:306:ILE:CG2	2.31	0.60
1:C:133:LEU:HD13	1:C:177:GLU:HG2	1.82	0.60
1:A:82:VAL:HG23	1:A:84:GLN:OE1	2.02	0.60
1:E:288:LEU:HD11	1:F:211:PRO:HG2	1.84	0.59
1:C:151:ASP:O	1:C:155:LYS:HD3	2.01	0.59
1:C:165:ARG:NH2	1:C:199:GLU:OE2	2.32	0.59
1:B:322:THR:O	1:B:323:CYS:CB	2.50	0.59
1:D:246:LEU:C	1:D:246:LEU:HD13	2.22	0.59
1:C:127:PHE:N	1:C:127:PHE:HD1	2.01	0.59
1:A:138:ASN:O	1:A:139:ILE:HG23	2.03	0.59
1:D:131:SER:HB3	1:D:134:PHE:HB3	1.85	0.59
1:F:89:THR:O	1:F:93:LYS:HG3	2.02	0.59
1:C:28:THR:HG22	1:C:29:LEU:N	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:VAL:CG2	1:C:296:LEU:HD13	2.32	0.59
1:E:133:LEU:HB3	1:E:177:GLU:HG3	1.84	0.59
1:C:282:VAL:HG21	1:C:296:LEU:HD13	1.85	0.59
1:E:312:ARG:HD3	1:E:313:LYS:O	2.03	0.59
1:D:140:ASN:O	1:D:141:CYS:HB3	2.02	0.59
1:A:139:ILE:HB	1:A:141:CYS:HG	1.67	0.59
1:F:227:LEU:HA	1:F:230:LEU:HD23	1.83	0.59
1:B:53:THR:N	1:B:54:PRO:HD2	2.17	0.59
1:D:175:PRO:HD3	1:D:206:ILE:HD13	1.83	0.58
1:D:36:VAL:HG13	1:D:70:VAL:HG22	1.85	0.58
1:D:34:LYS:HD3	1:D:70:VAL:HG11	1.85	0.58
1:F:206:ILE:HG13	1:F:208:VAL:HG22	1.84	0.58
1:E:84:GLN:HG2	5:E:570:HOH:O	2.03	0.58
1:E:221:VAL:HG12	1:E:230:LEU:HD21	1.85	0.58
1:D:154:LEU:O	1:D:158:GLN:HG3	2.02	0.58
1:B:109:ASN:HD22	4:B:399:HGG:H57A	1.67	0.58
1:C:221:VAL:HG12	1:C:230:LEU:HD21	1.85	0.58
1:F:87:ASP:O	1:F:90:GLU:HG2	2.04	0.58
1:D:227:LEU:HD21	1:D:252:GLY:HA3	1.84	0.57
1:F:106:LEU:CD1	1:F:106:LEU:H	2.17	0.57
1:C:96:GLN:HB2	1:C:98:PHE:CE1	2.39	0.57
1:A:98:PHE:HB2	1:A:101:ILE:HD12	1.86	0.57
1:C:44:LEU:HD11	1:C:306:ILE:HD11	1.87	0.57
1:D:109:ASN:CA	1:D:153:ILE:HD11	2.34	0.57
1:E:260:VAL:HG23	1:E:261:ALA:N	2.19	0.57
1:C:28:THR:CG2	1:C:29:LEU:H	2.12	0.57
1:A:141:CYS:HB2	1:A:145:GLU:CB	2.35	0.57
1:B:87:ASP:O	1:B:91:VAL:HG23	2.04	0.57
1:F:131:SER:O	1:F:143:ILE:HD11	2.05	0.57
1:A:65:GLU:HG3	1:A:98:PHE:CZ	2.40	0.57
1:F:201:SER:HA	1:F:231:ALA:HB3	1.86	0.57
1:D:53:THR:N	1:D:54:PRO:HD2	2.19	0.57
1:C:297:GLN:O	1:C:301:GLU:HG3	2.04	0.57
1:E:87:ASP:O	1:E:91:VAL:HG23	2.05	0.56
1:B:28:THR:HG22	1:B:29:LEU:N	2.18	0.56
1:C:84:GLN:N	1:C:84:GLN:CD	2.58	0.56
1:E:82:VAL:O	1:E:82:VAL:HG22	2.04	0.56
1:C:186:ALA:HA	1:C:221:VAL:HG22	1.87	0.56
1:D:83:PRO:HG2	1:D:84:GLN:NE2	2.20	0.56
1:B:52:SER:OG	1:B:55:VAL:HG23	2.05	0.56
1:A:77:VAL:HG11	1:A:82:VAL:HG13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:ALA:CB	1:E:255:VAL:HG22	2.36	0.56
1:E:191:LYS:O	1:E:195:MET:HG3	2.06	0.56
1:A:77:VAL:CG1	1:A:82:VAL:HG13	2.35	0.56
1:F:142:SER:H	1:F:145:GLU:HB2	1.71	0.56
1:B:190:LYS:HD3	1:B:224:GLU:HB3	1.87	0.56
1:C:32:ARG:HB3	1:C:291:HIS:HB3	1.87	0.56
1:F:200:ILE:N	1:F:200:ILE:HD12	2.21	0.56
1:E:52:SER:OG	1:E:55:VAL:HG22	2.06	0.56
1:F:106:LEU:HD12	1:F:106:LEU:H	1.70	0.56
1:D:91:VAL:O	1:D:95:ILE:HG23	2.05	0.56
1:D:59:LEU:CD2	1:D:306:ILE:HG21	2.33	0.56
1:D:41:ARG:C	1:D:41:ARG:HD2	2.27	0.56
1:D:151:ASP:OD1	1:D:155:LYS:HD3	2.06	0.56
1:A:77:VAL:HG11	1:A:82:VAL:CG1	2.36	0.56
1:D:89:THR:O	1:D:93:LYS:HG3	2.06	0.56
1:E:138:ASN:O	1:E:139:ILE:HG23	2.06	0.55
1:B:139:ILE:O	1:B:140:ASN:HB3	2.06	0.55
1:E:63:LEU:HD21	1:E:260:VAL:CG1	2.35	0.55
1:A:271:GLY:HA2	5:A:505:HOH:O	2.05	0.55
1:C:83:PRO:HG2	1:C:84:GLN:NE2	2.21	0.55
1:C:234:CYS:HB3	5:C:817:HOH:O	2.06	0.55
1:E:41:ARG:HD2	1:E:41:ARG:C	2.26	0.55
1:C:172:LEU:HD11	1:C:214:MET:HE2	1.88	0.55
1:C:123:GLU:HG3	1:C:163:SER:CB	2.36	0.55
1:F:258:SER:HB2	1:F:276:LEU:O	2.07	0.55
1:F:131:SER:HB3	1:F:134:PHE:HB3	1.88	0.55
1:C:133:LEU:HD13	1:C:177:GLU:CG	2.36	0.55
1:F:74:THR:OG1	1:F:75:SER:N	2.39	0.55
1:E:230:LEU:O	1:E:255:VAL:HG13	2.07	0.55
1:F:261:ALA:HB1	1:F:314:THR:OG1	2.06	0.54
1:C:139:ILE:HD13	1:C:139:ILE:N	2.22	0.54
1:C:41:ARG:HD2	1:C:41:ARG:C	2.28	0.54
1:C:77:VAL:HB	1:C:108:PRO:HG3	1.90	0.54
1:B:35:ILE:CD1	1:B:282:VAL:HG12	2.37	0.54
1:C:126:ILE:HD11	1:C:197:CYS:SG	2.47	0.54
1:E:262:GLY:HA3	1:E:315:SER:HB2	1.90	0.54
1:D:39:GLY:HA3	1:D:260:VAL:HG23	1.89	0.54
1:E:51:VAL:HG13	1:E:310:LEU:CD1	2.35	0.54
1:B:191:LYS:HE2	1:B:195:MET:SD	2.47	0.54
1:D:114:GLU:HG3	5:D:729:HOH:O	2.07	0.54
1:E:36:VAL:HB	1:E:257:ASP:OD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:MET:HE3	1:B:305:PHE:CD2	2.42	0.54
1:E:172:LEU:HD22	1:E:213:ILE:HG22	1.90	0.54
1:E:84:GLN:HE21	1:E:84:GLN:N	2.03	0.53
1:C:142:SER:OG	1:C:145:GLU:HG3	2.07	0.53
1:F:51:VAL:HG22	5:F:770:HOH:O	2.08	0.53
1:A:107:THR:HG21	1:A:113:PHE:HA	1.90	0.53
1:B:174:CYS:SG	1:B:175:PRO:HD2	2.49	0.53
1:D:75:SER:HB3	1:D:85:MET:HG3	1.90	0.53
1:F:37:GLU:HG2	1:F:63:LEU:HD13	1.90	0.53
1:E:135:THR:HG22	1:E:141:CYS:O	2.07	0.53
1:F:76:PHE:CZ	1:F:116:ALA:HA	2.44	0.53
1:E:145:GLU:HA	1:E:148:GLN:OE1	2.09	0.53
1:A:297:GLN:N	1:A:297:GLN:NE2	2.56	0.53
1:B:91:VAL:O	1:B:95:ILE:HG23	2.08	0.53
1:C:191:LYS:HE2	1:C:195:MET:CE	2.37	0.53
1:B:126:ILE:O	1:B:166:GLY:HA2	2.07	0.53
1:F:210:THR:C	1:F:244:ASN:HD21	2.12	0.53
1:D:122:LYS:O	1:D:162:ILE:HG23	2.08	0.53
1:D:230:LEU:O	1:D:255:VAL:HG13	2.08	0.53
1:A:87:ASP:O	1:A:91:VAL:HG23	2.09	0.53
1:C:259:SER:OG	1:C:263:LEU:HB2	2.09	0.53
1:D:279:GLU:HG3	1:D:299:LEU:HD13	1.91	0.53
1:E:206:ILE:HG13	1:E:208:VAL:HG13	1.91	0.53
1:C:114:GLU:OE2	1:C:114:GLU:N	2.42	0.53
1:C:47:GLU:HG2	1:C:310:LEU:CD2	2.38	0.52
1:D:136:LYS:O	1:D:140:ASN:HA	2.08	0.52
1:B:189:THR:HG22	1:B:225:VAL:HG21	1.91	0.52
1:D:145:GLU:HA	1:D:148:GLN:HG2	1.91	0.52
1:E:58:LYS:O	1:E:62:MET:HG3	2.09	0.52
1:D:84:GLN:CD	1:D:84:GLN:H	2.13	0.52
1:D:236:ASP:OD1	1:D:239:GLY:HA2	2.09	0.52
1:B:60:ILE:HD13	1:B:73:THR:HG23	1.91	0.52
1:C:247:MET:O	1:C:251:MET:HG2	2.08	0.52
1:F:127:PHE:HZ	1:F:139:ILE:HD11	1.73	0.52
1:E:77:VAL:HG11	1:E:82:VAL:HG11	1.92	0.52
1:F:78:SER:HB2	1:F:80:LYS:CG	2.39	0.52
1:C:133:LEU:HD13	1:C:177:GLU:OE1	2.10	0.52
1:E:259:SER:HB2	1:E:275:ASN:HB2	1.91	0.52
1:F:227:LEU:HD21	1:F:252:GLY:HA3	1.92	0.52
1:C:172:LEU:HD12	1:C:204:ASP:HB2	1.91	0.52
1:D:139:ILE:HG23	1:D:149:ARG:HH12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:O	1:A:117:VAL:HG23	2.10	0.52
1:B:231:ALA:CB	1:B:255:VAL:HG22	2.40	0.52
1:B:266:CYS:SG	1:B:269:ALA:HB3	2.50	0.52
1:A:259:SER:HB2	1:A:275:ASN:CB	2.40	0.51
1:C:210:THR:HG21	1:D:287:GLY:HA3	1.91	0.51
1:F:142:SER:HB3	1:F:145:GLU:OE1	2.10	0.51
1:E:211:PRO:HG2	1:F:288:LEU:CD1	2.29	0.51
1:F:62:MET:HE3	1:F:305:PHE:CD2	2.44	0.51
1:A:141:CYS:HB2	1:A:145:GLU:HB3	1.93	0.51
1:F:151:ASP:OD1	1:F:155:LYS:HE3	2.10	0.51
1:B:260:VAL:O	1:B:279:GLU:OE1	2.28	0.51
1:A:288:LEU:CD1	1:B:211:PRO:HG2	2.38	0.51
1:A:139:ILE:HB	1:A:141:CYS:SG	2.50	0.51
1:F:91:VAL:O	1:F:95:ILE:HG23	2.10	0.51
1:C:127:PHE:H	1:C:127:PHE:HD1	1.57	0.51
1:D:73:THR:OG1	1:D:103:TYR:HB3	2.10	0.51
1:B:147:PHE:CZ	1:B:191:LYS:HG2	2.46	0.51
1:C:122:LYS:NZ	1:C:122:LYS:HB3	2.25	0.51
1:F:75:SER:O	1:F:77:VAL:N	2.44	0.51
1:F:198:TYR:H	1:F:198:TYR:HD1	1.59	0.51
1:C:117:VAL:HG22	1:C:162:ILE:HD11	1.92	0.51
1:E:48:LYS:N	1:E:48:LYS:HD2	2.25	0.51
1:D:143:ILE:HG23	1:D:144:GLU:H	1.76	0.51
1:A:65:GLU:HG3	1:A:98:PHE:HZ	1.75	0.51
1:A:35:ILE:CD1	1:A:282:VAL:HG12	2.41	0.51
1:E:200:ILE:N	1:E:200:ILE:HD12	2.26	0.51
1:A:182:PRO:HD2	5:A:575:HOH:O	2.11	0.51
1:E:60:ILE:HD13	1:E:73:THR:HG23	1.93	0.51
1:A:133:LEU:HD13	1:A:177:GLU:HG2	1.93	0.51
1:D:189:THR:HG22	1:D:225:VAL:HG21	1.93	0.51
1:A:191:LYS:O	1:A:195:MET:HB2	2.10	0.50
1:B:32:ARG:NH1	1:B:291:HIS:CD2	2.80	0.50
1:E:58:LYS:HD3	1:E:305:PHE:CE1	2.47	0.50
1:A:82:VAL:O	1:A:82:VAL:HG22	2.11	0.50
1:F:266:CYS:SG	1:F:269:ALA:HB3	2.52	0.50
1:E:123:GLU:HG3	1:E:163:SER:HB2	1.94	0.50
1:B:251:MET:HA	1:B:251:MET:CE	2.42	0.50
1:B:231:ALA:HB2	1:B:255:VAL:HG22	1.93	0.50
1:B:251:MET:HE2	1:B:251:MET:HA	1.94	0.50
1:A:281:LEU:O	1:A:285:LEU:HG	2.12	0.50
1:E:164:VAL:O	1:E:197:CYS:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:SER:HB2	1:D:54:PRO:HD2	1.94	0.50
1:C:33:VAL:HG23	1:C:290:ILE:CG2	2.39	0.50
1:B:312:ARG:HD3	1:B:313:LYS:O	2.12	0.50
1:C:154:LEU:O	1:C:158:GLN:HG3	2.12	0.49
1:E:266:CYS:HB3	1:E:269:ALA:HB3	1.93	0.49
1:F:33:VAL:HG23	1:F:290:ILE:CG2	2.41	0.49
1:B:173:GLY:HA2	1:B:180:ILE:HG12	1.93	0.49
1:B:39:GLY:HA2	1:B:259:SER:OG	2.12	0.49
1:B:165:ARG:HD2	1:B:199:GLU:OE2	2.13	0.49
1:B:39:GLY:HA3	1:B:260:VAL:HG23	1.94	0.49
1:D:174:CYS:SG	1:D:175:PRO:HD2	2.52	0.49
1:D:150:PHE:O	1:D:154:LEU:HB2	2.11	0.49
1:D:133:LEU:HD13	1:D:177:GLU:HG2	1.95	0.49
1:F:109:ASN:OD1	1:F:111:LYS:HB3	2.11	0.49
1:E:47:GLU:HG2	1:E:310:LEU:HD21	1.94	0.49
1:B:37:GLU:HG2	1:B:63:LEU:HD13	1.93	0.49
1:F:259:SER:OG	1:F:263:LEU:HB2	2.12	0.49
1:D:51:VAL:O	1:D:56:LYS:NZ	2.45	0.49
1:C:211:PRO:CG	1:D:288:LEU:HD21	2.43	0.49
1:D:143:ILE:HG23	1:D:144:GLU:N	2.26	0.49
1:E:154:LEU:HD11	1:E:195:MET:HB3	1.91	0.49
1:E:90:GLU:CD	1:E:90:GLU:H	2.15	0.49
1:E:82:VAL:HA	1:E:84:GLN:HE22	1.78	0.49
1:C:302:ALA:O	1:C:306:ILE:HG22	2.13	0.48
1:F:279:GLU:HA	1:F:282:VAL:CG1	2.43	0.48
1:F:165:ARG:NH1	1:F:201:SER:HB2	2.28	0.48
1:A:58:LYS:HD3	1:A:305:PHE:CE1	2.48	0.48
1:B:124:VAL:CG2	1:B:164:VAL:HG22	2.43	0.48
1:E:139:ILE:HD12	1:E:141:CYS:SG	2.53	0.48
1:D:208:VAL:HG12	1:D:238:TYR:CE2	2.48	0.48
1:F:269:ALA:O	1:F:270:GLN:O	2.31	0.48
1:E:53:THR:N	1:E:54:PRO:CD	2.76	0.48
1:D:35:ILE:CD1	1:D:282:VAL:HG12	2.44	0.48
1:B:170:CYS:HA	1:B:173:GLY:O	2.14	0.48
1:C:138:ASN:HB2	1:C:139:ILE:HD13	1.94	0.48
1:C:247:MET:HE3	1:C:250:GLN:HE21	1.78	0.48
1:B:133:LEU:HG	1:B:137:LYS:NZ	2.29	0.48
1:D:83:PRO:HG2	1:D:84:GLN:HE22	1.77	0.48
1:A:202:LEU:HD13	1:A:217:MET:SD	2.54	0.48
1:C:139:ILE:HB	1:C:149:ARG:NH2	2.28	0.48
1:F:73:THR:OG1	1:F:103:TYR:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:THR:HG23	1:B:139:ILE:HD11	1.95	0.48
1:C:172:LEU:HD21	1:C:214:MET:HA	1.95	0.48
1:C:73:THR:OG1	1:C:103:TYR:HB3	2.14	0.48
1:F:106:LEU:CD1	1:F:106:LEU:N	2.74	0.48
1:C:222:MET:HG2	1:C:227:LEU:HD13	1.95	0.48
1:A:306:ILE:O	1:A:310:LEU:HB2	2.12	0.48
1:C:98:PHE:HB2	1:C:101:ILE:HD12	1.96	0.48
1:E:169:SER:O	1:E:170:CYS:HB2	2.14	0.48
1:A:279:GLU:HG3	1:A:299:LEU:HD13	1.96	0.48
1:D:205:THR:HA	1:D:235:HIS:CD2	2.49	0.48
1:D:248:ALA:O	1:D:251:MET:HB2	2.14	0.48
1:F:222:MET:HG2	1:F:227:LEU:HD13	1.96	0.47
1:E:288:LEU:HD11	1:F:212:GLY:H	1.78	0.47
1:D:133:LEU:HD22	1:D:177:GLU:HG2	1.95	0.47
1:B:51:VAL:HG13	1:B:310:LEU:CD1	2.44	0.47
1:D:306:ILE:O	1:D:310:LEU:HB2	2.14	0.47
1:F:265:GLY:N	1:F:274:GLY:HA3	2.29	0.47
1:D:126:ILE:HD11	1:D:197:CYS:SG	2.54	0.47
1:B:59:LEU:O	1:B:63:LEU:HG	2.14	0.47
1:C:141:CYS:HB2	1:C:145:GLU:HB2	1.96	0.47
1:D:85:MET:O	1:D:88:HIS:HD2	1.97	0.47
1:B:200:ILE:HD12	1:B:200:ILE:N	2.29	0.47
1:F:232:VAL:HG22	1:F:234:CYS:SG	2.54	0.47
1:C:169:SER:HB2	1:C:205:THR:OG1	2.13	0.47
1:E:136:LYS:NZ	1:E:142:SER:HB3	2.29	0.47
1:D:132:GLU:HG2	1:D:143:ILE:HB	1.97	0.47
1:F:131:SER:C	1:F:143:ILE:HD11	2.35	0.47
1:F:211:PRO:N	1:F:244:ASN:HD21	2.13	0.47
1:D:174:CYS:N	1:D:178:GLY:O	2.46	0.47
1:C:172:LEU:HD11	1:C:214:MET:CE	2.43	0.47
1:E:199:GLU:C	1:E:200:ILE:HD12	2.35	0.47
1:A:28:THR:HA	5:A:864:HOH:O	2.15	0.47
1:B:270:GLN:O	1:B:272:ALA:N	2.47	0.47
1:F:82:VAL:HG22	1:F:82:VAL:O	2.14	0.47
1:C:40:PRO:HA	1:C:44:LEU:HD22	1.96	0.47
1:C:306:ILE:HD11	1:C:310:LEU:HD22	1.96	0.47
1:A:141:CYS:HB2	1:A:145:GLU:HB2	1.95	0.47
1:D:33:VAL:CG2	1:D:290:ILE:HG21	2.44	0.47
1:A:287:GLY:HA3	1:B:210:THR:HG21	1.97	0.47
1:A:60:ILE:HD13	1:A:73:THR:HG23	1.96	0.47
1:C:190:LYS:HD3	1:C:224:GLU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:ASN:ND2	1:F:139:ILE:H	2.12	0.47
1:D:284:MET:O	1:D:288:LEU:HD23	2.14	0.47
1:F:63:LEU:HB2	1:F:71:ILE:HD13	1.97	0.47
1:C:206:ILE:HG13	1:C:208:VAL:HG13	1.97	0.47
1:F:170:CYS:HA	1:F:173:GLY:O	2.15	0.47
1:F:310:LEU:HD12	1:F:310:LEU:N	2.30	0.47
1:C:181:SER:HB2	5:C:1017:HOH:O	2.15	0.47
1:A:231:ALA:CB	1:A:255:VAL:HG22	2.45	0.47
1:C:71:ILE:O	1:C:104:PRO:HD2	2.15	0.47
1:C:48:LYS:CD	1:C:48:LYS:H	2.19	0.47
1:D:143:ILE:HD11	1:D:184:LYS:HZ1	1.80	0.47
1:C:77:VAL:HG13	1:C:82:VAL:HG13	1.95	0.47
1:C:133:LEU:HD12	1:C:133:LEU:N	2.29	0.47
1:B:60:ILE:CD1	1:B:73:THR:HG23	2.45	0.47
1:B:282:VAL:CG2	1:B:296:LEU:HD13	2.45	0.46
1:D:259:SER:CB	1:D:275:ASN:HB2	2.45	0.46
1:B:126:ILE:HD11	1:B:197:CYS:SG	2.55	0.46
1:F:164:VAL:O	1:F:197:CYS:HA	2.15	0.46
1:F:203:GLY:HA2	1:F:233:HIS:O	2.15	0.46
1:A:322:THR:HG23	5:A:728:HOH:O	2.14	0.46
1:E:190:LYS:HD3	1:E:224:GLU:HB3	1.96	0.46
1:D:214:MET:HE2	1:D:244:ASN:HB3	1.96	0.46
1:A:288:LEU:HB3	1:A:290:ILE:HG13	1.96	0.46
1:C:53:THR:O	1:C:57:ILE:HG13	2.15	0.46
1:C:189:THR:HG22	1:C:225:VAL:HG21	1.98	0.46
1:F:126:ILE:HD11	1:F:197:CYS:SG	2.56	0.46
1:F:247:MET:CE	1:F:250:GLN:HE21	2.29	0.46
1:C:77:VAL:CG1	1:C:82:VAL:HG11	2.46	0.46
1:D:41:ARG:HG3	1:D:106:LEU:HD13	1.98	0.46
1:C:77:VAL:CG1	1:C:82:VAL:CG1	2.94	0.46
1:D:58:LYS:HG2	1:D:62:MET:HE2	1.97	0.46
1:F:169:SER:O	1:F:170:CYS:HB2	2.14	0.46
1:F:295:ASN:OD1	1:F:298:LYS:HG3	2.16	0.46
1:C:200:ILE:HD12	1:C:200:ILE:N	2.30	0.46
1:C:247:MET:CE	1:C:250:GLN:HE21	2.29	0.46
1:B:68:LEU:HD22	1:B:68:LEU:H	1.80	0.46
1:F:81:TRP:O	1:F:83:PRO:CD	2.63	0.46
1:F:175:PRO:HD3	1:F:206:ILE:HG21	1.98	0.46
1:F:115:ALA:O	1:F:118:ALA:HB3	2.15	0.46
1:F:52:SER:O	1:F:55:VAL:CG1	2.62	0.46
1:F:127:PHE:CZ	1:F:139:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:399:HGG:O36	4:B:399:HGG:H19	2.15	0.46
1:F:95:ILE:HD12	1:F:103:TYR:CD1	2.51	0.46
1:C:53:THR:N	1:C:54:PRO:HD2	2.31	0.46
1:C:191:LYS:HE2	1:C:195:MET:HE3	1.98	0.46
1:A:125:VAL:HG22	1:A:165:ARG:HB3	1.98	0.46
1:C:46:ASN:HB3	5:C:682:HOH:O	2.16	0.46
1:D:263:LEU:HD23	1:D:312:ARG:NH1	2.31	0.45
1:E:51:VAL:CG1	1:E:310:LEU:HD13	2.40	0.45
1:D:172:LEU:HD22	1:D:213:ILE:HG22	1.99	0.45
1:A:297:GLN:N	1:A:297:GLN:CD	2.68	0.45
1:F:92:LEU:HD23	1:F:119:ALA:HB3	1.97	0.45
1:D:256:VAL:CG2	1:D:281:LEU:HD21	2.46	0.45
1:D:144:GLU:O	1:D:148:GLN:HG2	2.15	0.45
1:C:36:VAL:HG13	1:C:70:VAL:HG22	1.97	0.45
1:B:58:LYS:HD3	1:B:305:PHE:CZ	2.51	0.45
1:C:260:VAL:O	1:C:279:GLU:OE1	2.35	0.45
1:B:41:ARG:HD3	1:B:106:LEU:HD22	1.98	0.45
1:E:77:VAL:CG1	1:E:82:VAL:HG11	2.46	0.45
1:C:210:THR:HG23	5:C:818:HOH:O	2.17	0.45
1:C:268:TYR:N	1:C:268:TYR:CD1	2.85	0.45
1:D:40:PRO:HA	1:D:44:LEU:HD22	1.99	0.45
1:C:306:ILE:O	1:C:310:LEU:HB2	2.17	0.45
1:F:77:VAL:HG22	1:F:78:SER:N	2.31	0.45
1:E:172:LEU:HD12	1:E:204:ASP:HB2	1.97	0.45
1:D:40:PRO:HG2	1:D:72:GLU:O	2.16	0.45
1:F:168:VAL:HG23	1:F:200:ILE:CG2	2.47	0.45
1:C:117:VAL:HG22	1:C:162:ILE:CD1	2.47	0.45
1:F:230:LEU:HD22	1:F:230:LEU:N	2.31	0.45
1:C:123:GLU:HG3	1:C:163:SER:HB2	1.98	0.45
1:A:282:VAL:HG21	1:A:296:LEU:HD13	1.99	0.45
1:F:40:PRO:HA	1:F:44:LEU:HD22	1.99	0.45
1:A:154:LEU:HD13	1:A:195:MET:HG2	1.99	0.45
1:C:92:LEU:HD23	1:C:119:ALA:HB3	1.99	0.45
1:A:227:LEU:HA	1:A:230:LEU:HD22	1.99	0.45
1:D:145:GLU:OE1	1:D:145:GLU:N	2.49	0.44
1:E:135:THR:O	1:E:139:ILE:HG13	2.17	0.44
1:A:58:LYS:HG2	1:A:62:MET:HE2	1.99	0.44
1:D:282:VAL:CG2	1:D:296:LEU:HD13	2.47	0.44
1:F:266:CYS:HA	1:F:267:PRO:HD3	1.87	0.44
1:E:96:GLN:HB2	1:E:98:PHE:HE1	1.82	0.44
1:C:191:LYS:HE2	1:C:195:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:VAL:C	1:D:262:GLY:H	2.19	0.44
1:A:154:LEU:HD22	1:A:196:GLY:HA3	1.99	0.44
1:C:247:MET:HE3	1:C:247:MET:HA	1.98	0.44
1:A:136:LYS:HE3	1:A:142:SER:HA	2.00	0.44
1:C:37:GLU:OE2	1:C:260:VAL:N	2.51	0.44
1:F:165:ARG:NH1	1:F:257:ASP:OD1	2.50	0.44
1:B:154:LEU:O	1:B:158:GLN:HG3	2.17	0.44
1:D:199:GLU:C	1:D:200:ILE:HD12	2.37	0.44
1:A:297:GLN:HE21	1:A:297:GLN:CA	2.29	0.44
1:B:131:SER:HG	1:B:174:CYS:HG	1.64	0.44
1:C:37:GLU:CG	1:C:63:LEU:HD13	2.47	0.44
1:B:144:GLU:OE1	1:B:147:PHE:CD1	2.67	0.44
1:D:206:ILE:HG13	1:D:208:VAL:HG22	1.98	0.44
1:D:87:ASP:O	1:D:91:VAL:HG23	2.18	0.44
1:D:78:SER:OG	1:D:80:LYS:HG2	2.18	0.44
1:A:148:GLN:O	1:A:151:ASP:HB3	2.18	0.44
1:D:200:ILE:N	1:D:200:ILE:CD1	2.81	0.44
1:A:84:GLN:CD	1:A:84:GLN:H	2.21	0.44
1:D:113:PHE:CD2	1:D:124:VAL:HG11	2.53	0.44
1:F:106:LEU:O	1:F:107:THR:HG23	2.17	0.44
1:F:306:ILE:O	1:F:309:ALA:HB3	2.17	0.44
1:F:133:LEU:HD22	1:F:177:GLU:HG2	1.98	0.44
1:D:154:LEU:HD23	1:D:164:VAL:HG21	1.99	0.44
1:D:259:SER:O	1:D:260:VAL:O	2.36	0.44
1:E:267:PRO:C	1:E:269:ALA:H	2.20	0.44
1:F:237:THR:HG23	1:F:272:ALA:HB3	2.00	0.44
1:E:73:THR:OG1	1:E:103:TYR:HB3	2.17	0.44
1:E:108:PRO:HG2	1:E:109:ASN:H	1.83	0.44
1:E:77:VAL:HG13	1:E:82:VAL:HG13	2.00	0.43
1:F:310:LEU:CD1	1:F:310:LEU:N	2.81	0.43
1:A:147:PHE:HD1	1:A:191:LYS:HZ3	1.65	0.43
1:F:230:LEU:O	1:F:255:VAL:CG1	2.66	0.43
1:D:259:SER:HB3	1:D:275:ASN:HB2	2.00	0.43
1:A:265:GLY:HA2	1:A:274:GLY:CA	2.47	0.43
1:B:44:LEU:HD12	1:B:44:LEU:HA	1.86	0.43
1:F:139:ILE:HG22	1:F:149:ARG:HH22	1.83	0.43
1:D:140:ASN:HD22	1:D:141:CYS:N	2.16	0.43
1:F:133:LEU:N	1:F:133:LEU:HD12	2.33	0.43
1:D:210:THR:CB	1:D:211:PRO:HD2	2.46	0.43
1:B:208:VAL:HG12	1:B:238:TYR:CE2	2.52	0.43
1:F:322:THR:O	1:F:323:CYS:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:HIS:HB2	5:F:608:HOH:O	2.18	0.43
1:E:77:VAL:HG13	1:E:82:VAL:CG1	2.48	0.43
1:C:191:LYS:O	1:C:195:MET:HB2	2.18	0.43
1:D:279:GLU:HG2	1:D:300:LEU:HD23	1.99	0.43
1:A:241:ALA:HB1	1:A:276:LEU:HD13	2.00	0.43
1:D:165:ARG:NH1	1:D:201:SER:HB2	2.33	0.43
1:C:237:THR:O	1:D:317:LYS:HB3	2.18	0.43
1:B:109:ASN:OD1	4:B:399:HGG:N7	2.50	0.43
1:A:141:CYS:SG	1:A:149:ARG:NH2	2.92	0.43
1:F:247:MET:HE3	1:F:247:MET:O	2.18	0.43
1:A:106:LEU:HD12	1:A:125:VAL:HB	1.99	0.43
1:A:90:GLU:N	1:A:90:GLU:OE1	2.42	0.43
1:D:32:ARG:HD3	5:D:819:HOH:O	2.18	0.43
1:D:278:THR:O	1:D:282:VAL:HG13	2.18	0.43
1:B:36:VAL:HA	1:B:70:VAL:HG13	2.00	0.43
1:C:36:VAL:HG22	1:C:70:VAL:HG11	2.00	0.43
1:A:51:VAL:CG1	1:A:310:LEU:HD13	2.49	0.43
1:C:114:GLU:OE2	1:C:114:GLU:CA	2.66	0.43
1:F:41:ARG:HG3	1:F:106:LEU:HD13	2.01	0.43
1:F:41:ARG:HB2	1:F:72:GLU:O	2.19	0.43
1:C:133:LEU:O	1:C:137:LYS:CG	2.67	0.43
1:A:182:PRO:HG3	5:A:791:HOH:O	2.18	0.43
1:A:133:LEU:HD13	1:A:177:GLU:CG	2.49	0.43
1:B:83:PRO:HG2	1:B:84:GLN:NE2	2.33	0.43
1:F:106:LEU:HA	1:F:125:VAL:HB	2.01	0.43
1:F:154:LEU:HD22	1:F:196:GLY:HA3	2.01	0.43
1:B:136:LYS:O	1:B:140:ASN:HA	2.19	0.43
1:D:80:LYS:N	1:D:80:LYS:HD3	2.34	0.43
1:E:267:PRO:HD2	5:E:685:HOH:O	2.17	0.43
1:B:68:LEU:HD22	1:B:68:LEU:N	2.34	0.43
1:D:33:VAL:HG23	1:D:290:ILE:CG2	2.46	0.42
1:B:32:ARG:NH2	5:B:649:HOH:O	2.50	0.42
1:D:134:PHE:C	1:D:134:PHE:CD1	2.92	0.42
1:A:212:GLY:H	1:B:288:LEU:CD1	2.32	0.42
1:E:82:VAL:HG23	1:E:84:GLN:OE1	2.19	0.42
1:D:279:GLU:O	1:D:282:VAL:HG22	2.20	0.42
1:E:127:PHE:O	1:E:150:PHE:HZ	2.02	0.42
1:E:218:LEU:O	1:E:219:SER:C	2.58	0.42
1:F:41:ARG:HD2	1:F:41:ARG:C	2.39	0.42
1:A:169:SER:O	1:A:170:CYS:HB2	2.20	0.42
1:A:211:PRO:HD3	1:A:244:ASN:ND2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:ASN:O	1:F:141:CYS:HB3	2.19	0.42
1:C:51:VAL:HG13	1:C:310:LEU:HD13	2.01	0.42
1:A:139:ILE:O	1:A:141:CYS:N	2.52	0.42
1:D:206:ILE:HG13	1:D:208:VAL:HG13	2.01	0.42
1:B:124:VAL:HG23	1:B:164:VAL:HG22	2.00	0.42
1:A:41:ARG:HD2	1:A:41:ARG:C	2.39	0.42
1:B:78:SER:OG	1:B:80:LYS:HB2	2.20	0.42
1:F:191:LYS:O	1:F:195:MET:HG3	2.19	0.42
1:D:218:LEU:HD12	1:D:251:MET:HG3	2.00	0.42
1:A:234:CYS:HB3	5:A:523:HOH:O	2.18	0.42
1:C:82:VAL:HG22	1:C:82:VAL:O	2.20	0.42
1:D:322:THR:HG22	1:D:323:CYS:N	2.34	0.42
1:E:219:SER:O	1:E:223:GLN:HG2	2.20	0.42
1:D:59:LEU:HD13	1:D:306:ILE:HG23	2.02	0.42
1:D:127:PHE:CE2	1:D:139:ILE:HD11	2.55	0.42
1:B:53:THR:N	1:B:54:PRO:CD	2.81	0.42
1:F:261:ALA:O	1:F:315:SER:HB2	2.20	0.42
1:D:311:ASN:O	1:D:311:ASN:OD1	2.38	0.42
1:C:83:PRO:CD	1:C:84:GLN:HE22	2.28	0.42
1:A:165:ARG:NH2	1:A:199:GLU:OE2	2.52	0.42
1:A:232:VAL:HG13	1:A:234:CYS:SG	2.59	0.42
1:F:57:ILE:HG23	1:F:95:ILE:HA	2.02	0.41
1:A:279:GLU:HB2	1:A:316:SER:OG	2.20	0.41
1:B:246:LEU:HD22	1:B:246:LEU:O	2.20	0.41
1:C:316:SER:O	1:C:320:GLN:HG3	2.20	0.41
1:D:143:ILE:CD1	1:D:184:LYS:NZ	2.84	0.41
1:C:206:ILE:HG12	1:C:206:ILE:H	1.61	0.41
1:F:134:PHE:HA	1:F:176:TYR:HD1	1.85	0.41
1:C:210:THR:HB	1:C:211:PRO:HD2	2.02	0.41
1:D:36:VAL:HG13	1:D:70:VAL:CG2	2.49	0.41
4:B:399:HGG:H57	4:B:399:HGG:O34	2.21	0.41
1:F:316:SER:HB3	1:F:319:ALA:CB	2.50	0.41
1:D:235:HIS:CE1	1:D:275:ASN:OD1	2.74	0.41
1:D:78:SER:HA	1:D:79:PRO:HD3	1.90	0.41
1:E:140:ASN:HD22	1:E:140:ASN:N	2.18	0.41
1:F:133:LEU:HD13	1:F:177:GLU:OE1	2.20	0.41
1:B:77:VAL:CG1	1:B:78:SER:N	2.83	0.41
1:D:134:PHE:HB2	1:D:174:CYS:SG	2.60	0.41
1:D:260:VAL:O	1:D:262:GLY:N	2.53	0.41
1:A:265:GLY:N	1:A:274:GLY:HA3	2.36	0.41
1:E:78:SER:HA	1:E:79:PRO:HD3	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:THR:N	1:F:54:PRO:CD	2.80	0.41
1:C:133:LEU:O	1:C:137:LYS:HG2	2.19	0.41
1:A:304:ASN:O	1:A:308:GLN:HG3	2.21	0.41
1:C:87:ASP:O	1:C:90:GLU:HG2	2.21	0.41
1:E:68:LEU:H	1:E:68:LEU:HD22	1.85	0.41
1:B:150:PHE:C	1:B:154:LEU:HD12	2.40	0.41
1:F:316:SER:HB3	1:F:319:ALA:HB3	2.03	0.41
1:F:244:ASN:HA	1:F:244:ASN:HD22	1.69	0.41
1:F:42:ASP:OD1	1:F:233:HIS:NE2	2.53	0.41
1:D:181:SER:HA	1:D:182:PRO:HD3	1.93	0.41
1:B:28:THR:HG22	1:B:29:LEU:HG	2.02	0.41
1:C:279:GLU:HG2	1:C:300:LEU:HD23	2.02	0.41
1:F:132:GLU:CD	1:F:143:ILE:HD12	2.41	0.41
1:F:98:PHE:HD1	1:F:103:TYR:OH	2.03	0.41
1:C:61:ASP:HA	1:C:64:SER:HB2	2.03	0.41
1:D:246:LEU:HA	1:D:249:LEU:HD12	2.02	0.41
1:C:133:LEU:HD12	1:C:133:LEU:H	1.86	0.41
1:A:201:SER:HA	1:A:231:ALA:HB3	2.03	0.41
1:A:186:ALA:HA	1:A:221:VAL:HG22	2.02	0.41
1:D:47:GLU:HA	1:D:47:GLU:OE1	2.21	0.41
1:E:145:GLU:HG2	5:E:1022:HOH:O	2.20	0.41
1:E:39:GLY:N	1:E:40:PRO:HD2	2.35	0.41
1:B:199:GLU:C	1:B:200:ILE:HD12	2.41	0.41
1:C:77:VAL:CG2	1:C:78:SER:N	2.83	0.40
1:D:141:CYS:SG	1:D:149:ARG:NH2	2.94	0.40
1:B:39:GLY:N	1:B:40:PRO:HD2	2.35	0.40
1:E:231:ALA:HB2	1:E:255:VAL:HG22	2.03	0.40
1:D:122:LYS:C	1:D:162:ILE:HG23	2.41	0.40
1:B:215:LYS:HE3	1:B:251:MET:HE1	2.02	0.40
1:C:281:LEU:HD12	1:C:281:LEU:O	2.21	0.40
1:B:112:GLY:HA3	4:B:399:HGG:HN6A	1.84	0.40
1:E:203:GLY:HA2	1:E:233:HIS:O	2.22	0.40
1:E:210:THR:C	1:E:244:ASN:HD21	2.25	0.40
1:C:61:ASP:CG	1:C:96:GLN:H	2.24	0.40
1:D:304:ASN:O	1:D:308:GLN:HG3	2.22	0.40
1:D:98:PHE:CB	1:D:101:ILE:HD12	2.51	0.40
1:D:99:PRO:HD2	5:D:1010:HOH:O	2.20	0.40
1:B:37:GLU:CG	1:B:63:LEU:HD13	2.51	0.40
1:D:214:MET:CE	1:D:244:ASN:HB3	2.51	0.40
1:C:86:GLY:HA2	5:C:554:HOH:O	2.20	0.40
5:C:869:HOH:O	1:E:34:LYS:HE2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:VAL:HG23	1:F:305:PHE:HE2	1.81	0.40
1:E:29:LEU:HD23	1:E:250:GLN:HA	2.04	0.40
1:E:139:ILE:C	1:E:141:CYS:H	2.25	0.40
1:F:77:VAL:CG2	1:F:78:SER:N	2.84	0.40
1:C:61:ASP:O	1:C:65:GLU:HG3	2.21	0.40
1:D:282:VAL:HG21	1:D:296:LEU:HD13	2.03	0.40
1:E:133:LEU:O	1:E:137:LYS:HG3	2.21	0.40
1:E:231:ALA:HB1	1:E:255:VAL:HG22	2.00	0.40
1:B:149:ARG:O	1:B:153:ILE:HG13	2.21	0.40
1:D:294:VAL:HG12	1:D:295:ASN:N	2.36	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	294/298 (99%)	272 (92%)	16 (5%)	6 (2%)	9	11
1	B	294/298 (99%)	272 (92%)	16 (5%)	6 (2%)	9	11
1	C	294/298 (99%)	263 (90%)	27 (9%)	4 (1%)	14	19
1	D	285/298 (96%)	254 (89%)	25 (9%)	6 (2%)	9	10
1	E	294/298 (99%)	273 (93%)	15 (5%)	6 (2%)	9	11
1	F	294/298 (99%)	249 (85%)	35 (12%)	10 (3%)	5	4
All	All	1755/1788 (98%)	1583 (90%)	134 (8%)	38 (2%)	8	9

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ILE
1	A	140	ASN

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Mol	Chain	Res	Type
1	A	260	VAL
1	A	270	GLN
1	A	272	ALA
1	B	260	VAL
1	B	273	SER
1	C	140	ASN
1	C	271	GLY
1	D	260	VAL
1	E	139	ILE
1	E	260	VAL
1	F	73	THR
1	F	76	PHE
1	F	260	VAL
1	F	270	GLN
1	B	108	PRO
1	B	160	ALA
1	B	271	GLY
1	D	138	ASN
1	D	141	CYS
1	F	48	LYS
1	F	86	GLY
1	F	139	ILE
1	F	140	ASN
1	F	141	CYS
1	A	271	GLY
1	C	260	VAL
1	D	137	LYS
1	E	272	ALA
1	D	261	ALA
1	E	143	ILE
1	B	270	GLN
1	C	142	SER
1	E	268	TYR
1	F	305	PHE
1	D	273	SER
1	E	108	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	238/240 (99%)	220 (92%)	18 (8%)	16	25
1	B	238/240 (99%)	223 (94%)	15 (6%)	22	35
1	C	238/240 (99%)	222 (93%)	16 (7%)	20	31
1	D	234/240 (98%)	218 (93%)	16 (7%)	20	31
1	E	238/240 (99%)	217 (91%)	21 (9%)	12	18
1	F	238/240 (99%)	224 (94%)	14 (6%)	24	38
All	All	1424/1440 (99%)	1324 (93%)	100 (7%)	19	29

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	44	LEU
1	A	82	VAL
1	A	114	GLU
1	A	139	ILE
1	A	161	ASN
1	A	165	ARG
1	A	167	TYR
1	A	192	PHE
1	A	230	LEU
1	A	246	LEU
1	A	255	VAL
1	A	259	SER
1	A	260	VAL
1	A	288	LEU
1	A	297	GLN
1	A	299	LEU
1	A	312	ARG
1	B	32	ARG
1	B	51	VAL
1	B	70	VAL
1	B	82	VAL
1	B	114	GLU
1	B	154	LEU
1	B	230	LEU
1	B	246	LEU
1	B	255	VAL

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Mol	Chain	Res	Type
1	B	256	VAL
1	B	268	TYR
1	B	288	LEU
1	B	299	LEU
1	B	310	LEU
1	B	312	ARG
1	C	44	LEU
1	C	90	GLU
1	C	114	GLU
1	C	127	PHE
1	C	139	ILE
1	C	151	ASP
1	C	165	ARG
1	C	167	TYR
1	C	181	SER
1	C	230	LEU
1	C	246	LEU
1	C	255	VAL
1	C	268	TYR
1	C	299	LEU
1	C	311	ASN
1	C	312	ARG
1	D	32	ARG
1	D	44	LEU
1	D	47	GLU
1	D	65	GLU
1	D	70	VAL
1	D	80	LYS
1	D	114	GLU
1	D	140	ASN
1	D	144	GLU
1	D	161	ASN
1	D	255	VAL
1	D	256	VAL
1	D	299	LEU
1	D	312	ARG
1	D	315	SER
1	D	322	THR
1	E	44	LEU
1	E	55	VAL
1	E	82	VAL
1	E	84	GLN

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Mol	Chain	Res	Type
1	E	90	GLU
1	E	127	PHE
1	E	139	ILE
1	E	151	ASP
1	E	188	VAL
1	E	202	LEU
1	E	219	SER
1	E	230	LEU
1	E	246	LEU
1	E	255	VAL
1	E	256	VAL
1	E	259	SER
1	E	282	VAL
1	E	288	LEU
1	E	299	LEU
1	E	310	LEU
1	E	312	ARG
1	F	44	LEU
1	F	49	ASN
1	F	55	VAL
1	F	70	VAL
1	F	90	GLU
1	F	155	LYS
1	F	192	PHE
1	F	198	TYR
1	F	256	VAL
1	F	282	VAL
1	F	288	LEU
1	F	297	GLN
1	F	299	LEU
1	F	312	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	140	ASN
1	A	161	ASN
1	A	223	GLN
1	A	244	ASN
1	A	250	GLN
1	A	297	GLN

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Mol	Chain	Res	Type
1	A	320	GLN
1	B	46	ASN
1	B	109	ASN
1	B	138	ASN
1	B	223	GLN
1	B	244	ASN
1	B	250	GLN
1	B	291	HIS
1	B	297	GLN
1	B	311	ASN
1	C	49	ASN
1	C	84	GLN
1	C	88	HIS
1	C	138	ASN
1	C	140	ASN
1	C	223	GLN
1	C	244	ASN
1	C	250	GLN
1	C	311	ASN
1	D	84	GLN
1	D	88	HIS
1	D	138	ASN
1	D	140	ASN
1	D	161	ASN
1	D	244	ASN
1	D	250	GLN
1	D	311	ASN
1	E	84	GLN
1	E	96	GLN
1	E	102	ASN
1	E	140	ASN
1	E	161	ASN
1	E	223	GLN
1	E	244	ASN
1	E	250	GLN
1	E	275	ASN
1	E	320	GLN
1	F	46	ASN
1	F	102	ASN
1	F	138	ASN
1	F	223	GLN
1	F	244	ASN

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Mol	Chain	Res	Type
1	F	250	GLN
1	F	297	GLN
1	F	304	ASN
1	F	308	GLN
1	F	320	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	3HG	A	400	3	3,9,9	2.55	2 (66%)	2,11,11	1.47	0
4	HGG	B	399	3	46,59,59	3.60	21 (45%)	58,87,87	4.17	23 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3HG	A	400	3	-	0/4/8/8	0/0/0/0
4	HGG	B	399	3	-	0/52/75/75	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	399	HGG	C2'-C1'	-3.34	1.46	1.50
4	B	399	HGG	C57-C45	-2.85	1.47	1.53
4	B	399	HGG	C73-C74	-2.31	1.41	1.51
4	B	399	HGG	C62-N68	-2.14	1.41	1.46
2	A	400	3HG	C2-C3	2.09	1.55	1.53
4	B	399	HGG	O20-C16	2.37	1.48	1.43
4	B	399	HGG	P39-O41	2.61	1.59	1.51
4	B	399	HGG	P39-O21	2.65	1.68	1.60
4	B	399	HGG	P35-O36	2.79	1.61	1.51
4	B	399	HGG	C61-C69	3.18	1.57	1.51
4	B	399	HGG	O1'-C1'	3.22	1.26	1.21
4	B	399	HGG	C43-N68	3.37	1.40	1.33
2	A	400	3HG	C4-C3	3.42	1.57	1.53
4	B	399	HGG	O51-C43	3.62	1.30	1.23
4	B	399	HGG	C16-C17	3.71	1.61	1.53
4	B	399	HGG	O72-C69	4.05	1.31	1.23
4	B	399	HGG	O22-C15	4.30	1.46	1.41
4	B	399	HGG	C6-N1	4.50	1.59	1.37
4	B	399	HGG	C5-C4	4.87	1.51	1.40
4	B	399	HGG	C69-N71	5.78	1.47	1.33
4	B	399	HGG	C2-N1	6.74	1.46	1.33
4	B	399	HGG	C4-N3	11.21	1.52	1.35
4	B	399	HGG	C2-N3	13.14	1.55	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	399	HGG	N3-C2-N1	-13.38	118.65	128.89
4	B	399	HGG	O1'-C1'-S81	-11.15	113.99	122.83
4	B	399	HGG	C15-N9-C4	-4.79	119.72	126.94
4	B	399	HGG	O52-C44-C43	-3.82	101.61	110.38
4	B	399	HGG	O22-C18-C19	-3.74	95.95	109.32
4	B	399	HGG	C53-C45-C46	-3.60	103.84	108.50
4	B	399	HGG	C61-C69-N71	-2.46	112.18	116.46
4	B	399	HGG	C61-C62-N68	-2.17	107.12	111.88
4	B	399	HGG	O37-P35-O32	2.01	114.22	105.09
4	B	399	HGG	O20-C16-C17	2.21	117.53	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	399	HGG	O23-C19-C18	2.88	119.73	109.12
4	B	399	HGG	C16-C15-N9	2.88	118.70	114.29
4	B	399	HGG	O72-C69-N71	3.14	129.17	122.94
4	B	399	HGG	C4-C5-N7	3.20	112.42	109.48
4	B	399	HGG	C73-C74-N71	4.71	121.78	112.36
4	B	399	HGG	C73-S81-C1'	4.72	118.92	102.09
4	B	399	HGG	O32-P35-O38	4.86	115.83	102.94
4	B	399	HGG	C62-C61-C69	5.75	121.79	112.31
4	B	399	HGG	C74-N71-C69	6.46	135.49	122.79
4	B	399	HGG	C18-O22-C15	6.70	117.08	109.72
4	B	399	HGG	C2'-C1'-S81	9.92	122.28	113.36
4	B	399	HGG	O38-C46-C45	10.19	126.94	110.55
4	B	399	HGG	P39-O21-C17	12.37	151.24	121.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	399	HGG	10	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	296/298 (99%)	-0.67	0	100	100	8, 21, 44, 60	0
1	B	296/298 (99%)	-0.47	7 (2%)	62	61	10, 27, 59, 74	0
1	C	296/298 (99%)	-0.47	1 (0%)	94	94	10, 30, 52, 66	0
1	D	289/298 (96%)	-0.28	4 (1%)	78	77	17, 37, 62, 79	0
1	E	296/298 (99%)	-0.56	3 (1%)	84	83	11, 26, 56, 69	0
1	F	296/298 (99%)	-0.21	2 (0%)	89	88	16, 42, 64, 73	0
All	All	1769/1788 (98%)	-0.44	17 (0%)	84	83	8, 29, 59, 79	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	269	ALA	3.7
1	E	140	ASN	3.7
1	B	268	TYR	3.6
1	E	271	GLY	3.5
1	D	138	ASN	3.1
1	F	268	TYR	3.0
1	F	127	PHE	2.9
1	C	271	GLY	2.9
1	B	266	CYS	2.8
1	B	270	GLN	2.8
1	B	272	ALA	2.7
1	D	50	ILE	2.5
1	D	139	ILE	2.5
1	E	147	PHE	2.3
1	B	147	PHE	2.2
1	D	77	VAL	2.2
1	B	271	GLY	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	3HG	A	400	10/10	0.69	0.27	2.92	61,63,66,67	0
4	HGG	B	399	57/57	0.88	0.18	1.63	58,79,96,97	0
3	MG	F	406	1/1	0.96	0.14	1.12	30,30,30,30	0
3	MG	A	403	1/1	0.95	0.12	-	16,16,16,16	0
3	MG	E	402	1/1	0.98	0.19	-	13,13,13,13	0
3	MG	C	404	1/1	0.95	0.21	-	15,15,15,15	0
3	MG	B	401	1/1	0.98	0.18	-	17,17,17,17	0
3	MG	D	405	1/1	0.96	0.12	-	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.