



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:38 AM GMT

PDB ID : 1DML
Title : CRYSTAL STRUCTURE OF HERPES SIMPLEX UL42 BOUND TO THE
C-TERMINUS OF HSV POL
Authors : Zuccola, H.J.; Filman, D.J.; Coen, D.M.; Hogle, J.M.
Deposited on : 1999-12-14
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

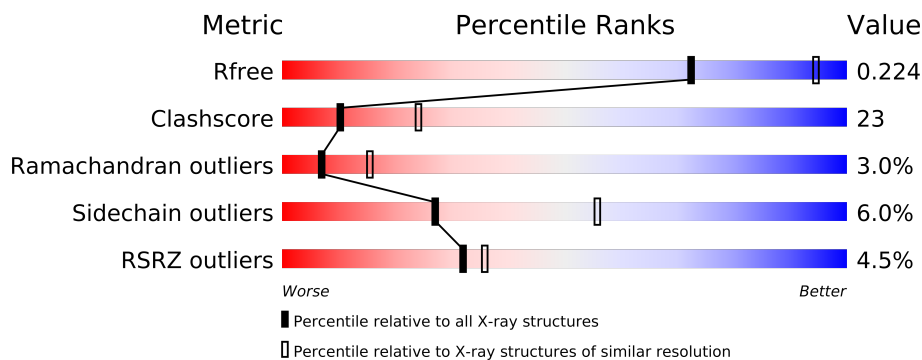
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	319	
1	C	319	
1	E	319	
1	G	319	
2	B	36	
2	D	36	
2	F	36	
2	H	36	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9414 atoms, of which 0 are hydrogen and 0 are deuterium.

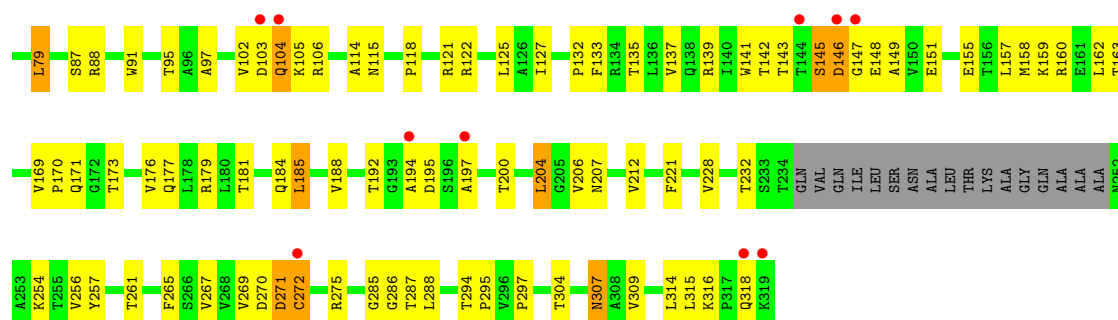
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA POLYMERASE PROCESSIVITY FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2059	1309	362	381	7			
1	C	272	Total	C	N	O	S	0	0	0
			2087	1325	368	387	7			
1	E	275	Total	C	N	O	S	0	0	0
			2108	1336	370	395	7			
1	G	275	Total	C	N	O	S	0	0	0
			2108	1336	370	395	7			

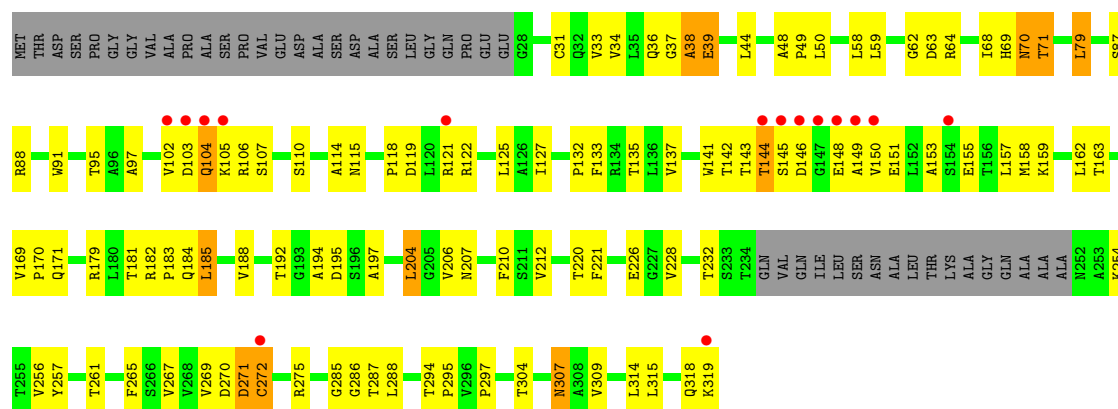
- Molecule 2 is a protein called DNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	36	Total	C	N	O	S	0	0	0
			263	159	53	50	1			
2	D	36	Total	C	N	O	S	0	0	0
			263	159	53	50	1			
2	F	36	Total	C	N	O	S	0	0	0
			263	159	53	50	1			
2	H	36	Total	C	N	O	S	0	0	0
			263	159	53	50	1			



• Molecule 1: DNA POLYMERASE PROCESSIVITY FACTOR

Chain G:



• Molecule 2: DNA POLYMERASE

Chain B:



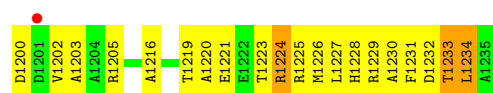
• Molecule 2: DNA POLYMERASE

Chain D:



• Molecule 2: DNA POLYMERASE

Chain F:



• Molecule 2: DNA POLYMERASE

Chain H:

D1200	D1201	V1202	A1203	A1204	R1205	L1206	R1207	A1208	F1211	A1216	T1219	A1220	E1221	E1222	T1223	R1224	R1225	M1226	L1227	H1228	R1229	A1230	F1231	D1232	T1233	L1234	A1235

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.32Å 100.07Å 129.53Å 90.00° 100.62° 90.00°	Depositor
Resolution (Å)	12.00 – 2.70 29.87 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.6 (12.00-2.70) 99.9 (29.87-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.21 (at 2.51Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.230 , 0.281 0.190 , 0.224	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 17.7	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 47173 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9414	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.37 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7625e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0/2097	0.71	2/2851 (0.1%)
1	C	0.41	0/2125	0.70	2/2889 (0.1%)
1	E	0.39	0/2146	0.65	0/2918
1	G	0.38	0/2146	0.64	0/2918
2	B	0.41	0/265	0.56	0/354
2	D	0.40	0/265	0.56	0/354
2	F	0.38	0/265	0.52	0/354
2	H	0.39	0/265	0.55	0/354
All	All	0.40	0/9574	0.66	4/12992 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	GLU	N-CA-C	-6.85	92.49	111.00
1	C	155	GLU	N-CA-C	-6.85	92.50	111.00
1	A	136	LEU	CA-CB-CG	5.30	127.49	115.30
1	C	136	LEU	CA-CB-CG	5.27	127.43	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2059	0	2104	100	0
1	C	2087	0	2130	96	0
1	E	2108	0	2150	104	0
1	G	2108	0	2150	104	0
2	B	263	0	256	18	0
2	D	263	0	256	20	0
2	F	263	0	256	25	0
2	H	263	0	256	22	0
All	All	9414	0	9558	444	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (444) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:121:ARG:HH11	1:G:143:THR:HG22	1.18	1.06
1:A:267:VAL:HG11	1:A:315:LEU:HD13	1.34	1.05
1:G:171:GLN:HA	2:H:1233:THR:HG21	1.39	1.04
1:C:149:ALA:HB3	1:C:152:LEU:HD22	1.41	0.99
1:E:286:GLY:HA2	1:E:304:THR:HG23	1.44	0.99
1:C:267:VAL:HG11	1:C:315:LEU:HD13	1.41	0.99
1:G:307:ASN:HD21	1:G:309:VAL:HG22	1.28	0.98
1:E:307:ASN:HD21	1:E:309:VAL:HG22	1.32	0.95
1:C:248:GLN:HG3	1:C:249:ALA:H	1.33	0.93
1:G:286:GLY:HA2	1:G:304:THR:HG23	1.51	0.92
1:E:171:GLN:HA	2:F:1233:THR:HG21	1.53	0.91
1:E:307:ASN:HD22	1:E:309:VAL:H	1.18	0.90
1:G:121:ARG:NH1	1:G:143:THR:HG22	1.89	0.88
1:G:70:ASN:ND2	1:G:71:THR:H	1.72	0.88
1:G:307:ASN:HD22	1:G:309:VAL:H	1.19	0.87
1:C:303:ALA:HB3	1:C:308:ALA:HB1	1.54	0.86
1:E:70:ASN:ND2	1:E:71:THR:H	1.73	0.85
1:A:303:ALA:HB3	1:A:308:ALA:HB1	1.57	0.85
1:G:144:THR:HG22	1:G:145:SER:H	1.40	0.84
1:C:200:THR:HB	1:C:269:VAL:HG12	1.60	0.83
1:A:200:THR:HB	1:A:269:VAL:HG12	1.61	0.83
1:E:228:VAL:O	1:E:232:THR:HG23	1.80	0.81
1:E:171:GLN:HE22	2:F:1226:MET:CE	1.94	0.80
1:E:102:VAL:HG22	1:E:159:LYS:HD3	1.63	0.80
1:E:50:LEU:HD21	1:E:309:VAL:HG11	1.65	0.78
1:G:307:ASN:ND2	1:G:309:VAL:HG22	1.97	0.78
1:G:102:VAL:HG22	1:G:159:LYS:HD3	1.66	0.77
1:E:307:ASN:ND2	1:E:309:VAL:H	1.82	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:267:VAL:HA	1:E:318:GLN:NE2	2.00	0.77
1:G:228:VAL:O	1:G:232:THR:HG23	1.83	0.77
1:G:267:VAL:HA	1:G:318:GLN:NE2	1.99	0.76
1:A:122:ARG:CZ	1:A:148:GLU:HG2	2.16	0.76
1:G:307:ASN:ND2	1:G:309:VAL:H	1.84	0.75
1:E:307:ASN:ND2	1:E:309:VAL:HG22	2.01	0.74
1:A:207:ASN:HD21	1:A:209:LYS:HB2	1.52	0.74
1:G:50:LEU:HD21	1:G:309:VAL:HG11	1.69	0.74
1:C:31:CYS:HB2	1:C:127:ILE:HB	1.69	0.74
1:G:70:ASN:HD22	1:G:71:THR:H	1.36	0.74
1:A:31:CYS:HB2	1:A:127:ILE:HB	1.69	0.74
2:B:1230:ALA:O	2:B:1234:LEU:HB2	1.88	0.73
1:A:141:TRP:HE1	1:A:152:LEU:HD21	1.53	0.73
1:A:267:VAL:HG11	1:A:315:LEU:CD1	2.17	0.73
1:C:132:PRO:HB2	1:C:163:THR:HA	1.71	0.73
1:C:39:GLU:HG3	1:C:87:SER:N	2.04	0.72
1:G:121:ARG:HH11	1:G:143:THR:CG2	1.99	0.72
1:G:171:GLN:HE22	2:H:1226:MET:CE	2.03	0.72
1:A:39:GLU:HG3	1:A:87:SER:N	2.05	0.71
1:C:207:ASN:HD21	1:C:209:LYS:HB2	1.55	0.71
2:D:1230:ALA:O	2:D:1234:LEU:HB2	1.91	0.70
1:C:162:LEU:O	1:C:164:SER:N	2.22	0.70
1:C:179:ARG:O	1:C:256:VAL:HG23	1.91	0.70
1:A:179:ARG:O	1:A:256:VAL:HG23	1.91	0.70
2:B:1201:ASP:O	2:B:1205:ARG:HG3	1.92	0.69
1:A:162:LEU:O	1:A:164:SER:N	2.22	0.69
1:G:155:GLU:O	1:G:157:LEU:HD22	1.93	0.69
1:A:132:PRO:HB2	1:A:163:THR:HA	1.75	0.68
1:A:118:PRO:HB3	2:F:1225:ARG:HH21	1.56	0.68
1:E:70:ASN:HD22	1:E:71:THR:H	1.40	0.68
1:E:62:GLY:HA2	1:E:91:TRP:CE2	2.29	0.68
1:E:294:THR:HB	1:E:295:PRO:HD2	1.76	0.67
1:G:62:GLY:HA2	1:G:91:TRP:CE2	2.29	0.67
1:C:297:PRO:HB2	1:C:315:LEU:HB2	1.76	0.66
2:D:1201:ASP:O	2:D:1205:ARG:HG3	1.95	0.66
1:A:39:GLU:CD	1:A:39:GLU:H	1.99	0.66
1:A:286:GLY:HA2	1:A:304:THR:HG23	1.77	0.66
1:C:151:GLU:O	1:C:153:ALA:N	2.29	0.66
1:C:39:GLU:CD	1:C:39:GLU:H	1.99	0.66
2:H:1219:THR:O	2:H:1223:THR:HG22	1.95	0.66
1:C:140:ILE:O	1:C:154:SER:HA	1.96	0.65
1:E:127:ILE:HD12	1:E:127:ILE:N	2.12	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:153:ALA:O	1:C:154:SER:HB3	1.97	0.65
1:C:41:ASN:O	1:C:45:GLN:HG3	1.96	0.65
1:A:140:ILE:O	1:A:154:SER:HA	1.96	0.65
1:A:41:ASN:O	1:A:45:GLN:HG3	1.97	0.65
1:C:194:ALA:HB2	1:C:275:ARG:HH21	1.61	0.65
1:C:286:GLY:HA2	1:C:304:THR:HG23	1.78	0.65
1:E:143:THR:HA	1:E:148:GLU:O	1.96	0.65
1:A:297:PRO:HB2	1:A:315:LEU:HB2	1.77	0.65
1:G:144:THR:HB	1:G:150:VAL:HG21	1.80	0.64
2:F:1219:THR:O	2:F:1223:THR:HG22	1.97	0.64
1:G:267:VAL:HA	1:G:318:GLN:HE22	1.61	0.64
1:A:39:GLU:HG3	1:A:87:SER:CA	2.27	0.64
1:G:148:GLU:HG3	1:G:149:ALA:H	1.62	0.64
1:G:294:THR:HB	1:G:295:PRO:HD2	1.80	0.64
1:A:153:ALA:O	1:A:154:SER:HB3	1.97	0.64
1:C:39:GLU:HG3	1:C:87:SER:CA	2.29	0.63
1:G:171:GLN:CA	2:H:1233:THR:HG21	2.23	0.63
1:E:188:VAL:HG13	1:E:212:VAL:HG21	1.81	0.63
1:C:200:THR:HB	1:C:269:VAL:CG1	2.29	0.63
1:A:207:ASN:ND2	1:A:209:LYS:HB2	2.13	0.63
1:G:122:ARG:HB3	1:G:141:TRP:HB2	1.81	0.63
1:E:102:VAL:O	1:E:106:ARG:HB2	1.99	0.63
1:G:39:GLU:HG3	1:G:87:SER:CA	2.30	0.62
1:E:297:PRO:HG2	1:E:315:LEU:HB2	1.81	0.62
1:A:223:ALA:O	1:A:224:ARG:HB2	1.99	0.62
1:G:102:VAL:O	1:G:106:ARG:HB2	2.00	0.62
1:E:70:ASN:HD22	1:E:71:THR:N	1.98	0.61
1:C:207:ASN:ND2	1:C:209:LYS:HB2	2.14	0.61
1:G:314:LEU:HD12	2:H:1205:ARG:CZ	2.30	0.61
1:C:248:GLN:HG3	1:C:249:ALA:N	2.11	0.61
1:A:61:MET:HG2	1:A:66:ILE:HG12	1.83	0.61
1:A:101:LEU:HD23	1:A:107:SER:HB2	1.82	0.61
1:C:223:ALA:O	1:C:224:ARG:HB2	2.00	0.61
1:G:127:ILE:N	1:G:127:ILE:HD12	2.16	0.61
1:E:122:ARG:HB3	1:E:141:TRP:HB2	1.81	0.61
1:G:70:ASN:HD22	1:G:71:THR:N	1.98	0.61
1:A:200:THR:HB	1:A:269:VAL:CG1	2.30	0.61
1:E:267:VAL:HA	1:E:318:GLN:HE22	1.62	0.61
1:E:39:GLU:HG3	1:E:87:SER:CA	2.31	0.60
1:A:39:GLU:HG2	1:A:87:SER:OG	2.00	0.60
1:A:194:ALA:HB2	1:A:275:ARG:HH21	1.67	0.60
1:G:103:ASP:HB3	1:G:106:ARG:HD3	1.82	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:122:ARG:HB3	1:C:141:TRP:HB2	1.82	0.60
1:C:101:LEU:HD23	1:C:107:SER:HB2	1.83	0.60
1:C:267:VAL:HG11	1:C:315:LEU:CD1	2.23	0.60
1:E:36:GLN:NE2	1:E:122:ARG:NH1	2.49	0.60
1:E:103:ASP:HB3	1:E:106:ARG:HD3	1.84	0.60
1:G:36:GLN:NE2	1:G:122:ARG:NH1	2.50	0.59
1:E:155:GLU:O	1:E:157:LEU:HD22	2.01	0.59
1:A:127:ILE:HD12	1:A:127:ILE:N	2.18	0.59
1:C:61:MET:HG2	1:C:66:ILE:HG12	1.85	0.59
1:C:39:GLU:HG2	1:C:87:SER:OG	2.01	0.59
2:B:1225:ARG:O	2:B:1229:ARG:HG3	2.03	0.59
1:G:179:ARG:O	1:G:256:VAL:HG13	2.03	0.59
1:A:115:ASN:HD22	2:F:1228:HIS:CG	2.21	0.58
1:C:103:ASP:OD2	1:C:106:ARG:HD3	2.04	0.58
1:A:286:GLY:CA	1:A:304:THR:HG23	2.33	0.58
1:A:115:ASN:ND2	2:F:1228:HIS:CE1	2.72	0.58
1:E:314:LEU:HD12	2:F:1205:ARG:CZ	2.33	0.58
1:C:127:ILE:HD12	1:C:127:ILE:N	2.19	0.58
2:H:1200:ASP:OD1	2:H:1202:VAL:HG22	2.03	0.58
1:E:37:GLY:O	1:E:38:ALA:CB	2.52	0.58
1:G:297:PRO:HG2	1:G:315:LEU:HB2	1.84	0.58
2:H:1220:ALA:O	2:H:1224:ARG:HB3	2.04	0.58
1:G:162:LEU:O	1:G:163:THR:HB	2.04	0.57
1:G:37:GLY:O	1:G:38:ALA:CB	2.51	0.57
2:F:1200:ASP:OD1	2:F:1202:VAL:HG22	2.03	0.57
1:A:149:ALA:HB3	1:A:152:LEU:HD13	1.86	0.57
1:C:39:GLU:CG	1:C:87:SER:OG	2.52	0.57
1:A:103:ASP:OD2	1:A:106:ARG:HD3	2.04	0.57
1:G:221:PHE:HA	1:G:254:LYS:HG2	1.87	0.57
1:A:263:ARG:HH11	1:A:263:ARG:HG3	1.69	0.57
1:E:145:SER:O	1:E:146:ASP:HB2	2.05	0.56
1:E:179:ARG:O	1:E:256:VAL:HG13	2.04	0.56
2:D:1225:ARG:O	2:D:1229:ARG:HG3	2.04	0.56
1:E:221:PHE:HA	1:E:254:LYS:HG2	1.87	0.56
1:C:286:GLY:CA	1:C:304:THR:HG23	2.35	0.56
1:E:169:VAL:HG23	1:E:170:PRO:HD2	1.86	0.56
1:A:39:GLU:CG	1:A:87:SER:OG	2.53	0.56
1:C:318:GLN:O	1:C:319:LYS:HB2	2.06	0.56
1:C:139:ARG:NE	1:C:150:VAL:HG13	2.21	0.56
1:A:122:ARG:HB3	1:A:141:TRP:HB2	1.88	0.56
2:D:1221:GLU:O	2:D:1225:ARG:HG2	2.05	0.56
1:G:206:VAL:HG12	1:G:207:ASN:ND2	2.21	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:185:LEU:HD12	1:E:285:GLY:HA2	1.87	0.56
1:E:121:ARG:CZ	1:E:149:ALA:HB2	2.36	0.56
1:E:39:GLU:HG3	1:E:87:SER:N	2.21	0.55
1:G:195:ASP:OD2	1:G:197:ALA:HB3	2.06	0.55
1:C:33:VAL:HB	1:C:125:LEU:HB2	1.88	0.55
2:F:1220:ALA:O	2:F:1224:ARG:HB3	2.06	0.55
1:A:177:GLN:O	1:A:258:GLY:HA3	2.05	0.55
1:E:162:LEU:O	1:E:163:THR:HB	2.04	0.55
1:E:195:ASP:OD2	1:E:197:ALA:HB3	2.07	0.55
1:E:267:VAL:HG21	1:E:315:LEU:HD13	1.89	0.55
1:E:79:LEU:HG	1:E:309:VAL:HG12	1.89	0.55
1:A:318:GLN:O	1:A:319:LYS:HB2	2.06	0.55
1:C:122:ARG:NH2	1:C:148:GLU:HG2	2.21	0.55
1:G:185:LEU:HD12	1:G:285:GLY:HA2	1.89	0.55
1:C:162:LEU:C	1:C:164:SER:H	2.10	0.55
1:A:162:LEU:C	1:A:164:SER:H	2.10	0.55
1:C:267:VAL:CG1	1:C:315:LEU:HD22	2.37	0.54
1:A:115:ASN:HD21	2:F:1228:HIS:CE1	2.26	0.54
1:G:63:ASP:O	1:G:64:ARG:HB3	2.08	0.54
2:D:1225:ARG:HG3	2:D:1225:ARG:HH11	1.72	0.54
1:C:263:ARG:HG3	1:C:263:ARG:HH11	1.72	0.54
1:G:132:PRO:HB2	1:G:163:THR:HA	1.88	0.54
2:B:1221:GLU:O	2:B:1225:ARG:HG2	2.08	0.54
1:C:194:ALA:HB2	1:C:275:ARG:NH2	2.23	0.54
1:C:156:THR:C	1:C:157:LEU:HD12	2.28	0.54
1:C:151:GLU:C	1:C:152:LEU:HD23	2.28	0.54
1:G:295:PRO:HG2	2:H:1208:ALA:O	2.07	0.54
1:G:79:LEU:HG	1:G:309:VAL:HG12	1.90	0.54
1:G:70:ASN:ND2	1:G:71:THR:N	2.49	0.53
2:H:1202:VAL:HG23	2:H:1203:ALA:N	2.23	0.53
1:G:169:VAL:HG23	1:G:170:PRO:HD2	1.89	0.53
1:E:70:ASN:ND2	1:E:71:THR:N	2.49	0.53
1:E:121:ARG:HD3	1:E:143:THR:OG1	2.09	0.53
1:E:132:PRO:HB2	1:E:163:THR:HA	1.89	0.53
1:C:251:ALA:C	1:C:253:ALA:H	2.11	0.53
1:G:39:GLU:HG3	1:G:87:SER:N	2.23	0.53
1:E:206:VAL:HG12	1:E:207:ASN:ND2	2.23	0.53
1:A:171:GLN:HB2	2:B:1229:ARG:NH1	2.24	0.53
1:C:85:GLN:HG3	1:C:307:ASN:OD1	2.08	0.53
1:A:141:TRP:HE1	1:A:152:LEU:CD2	2.21	0.53
1:G:188:VAL:HG13	1:G:212:VAL:HG21	1.90	0.53
1:A:33:VAL:HB	1:A:125:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1225:ARG:HH11	2:B:1225:ARG:HG3	1.74	0.53
1:A:156:THR:C	1:A:157:LEU:HD12	2.29	0.53
1:C:171:GLN:HB2	2:D:1229:ARG:NH1	2.24	0.52
1:A:223:ALA:O	1:A:224:ARG:CB	2.57	0.52
1:C:223:ALA:O	1:C:224:ARG:CB	2.57	0.52
1:E:63:ASP:O	1:E:64:ARG:HB3	2.09	0.52
1:A:270:ASP:HA	1:A:316:LYS:HE3	1.90	0.52
1:A:85:GLN:HG3	1:A:307:ASN:OD1	2.09	0.52
1:E:31:CYS:HB2	1:E:127:ILE:HB	1.91	0.52
1:C:177:GLN:O	1:C:258:GLY:HA3	2.09	0.52
1:A:30:PRO:CB	1:A:92:ARG:HD3	2.40	0.52
1:G:314:LEU:HB2	2:H:1205:ARG:NH2	2.24	0.52
1:G:31:CYS:HB2	1:G:127:ILE:HB	1.91	0.52
1:A:150:VAL:N	1:A:152:LEU:HD22	2.25	0.52
1:E:121:ARG:NH2	1:E:149:ALA:HB2	2.25	0.52
1:E:185:LEU:HD12	1:E:285:GLY:CA	2.40	0.52
1:E:261:THR:O	1:E:261:THR:HG22	2.10	0.51
1:A:90:ARG:NH2	1:A:92:ARG:HD2	2.25	0.51
1:A:163:THR:HB	1:G:133:PHE:CG	2.46	0.51
1:G:39:GLU:HG3	1:G:87:SER:HA	1.92	0.51
1:G:115:ASN:O	1:G:118:PRO:HD3	2.11	0.51
1:G:171:GLN:HA	2:H:1233:THR:CG2	2.27	0.51
1:E:269:VAL:O	1:E:269:VAL:HG13	2.10	0.51
1:E:39:GLU:HG3	1:E:87:SER:HA	1.93	0.51
1:C:90:ARG:NH2	1:C:92:ARG:HD2	2.26	0.51
1:E:69:HIS:CD2	1:E:70:ASN:N	2.79	0.50
1:G:71:THR:O	1:G:71:THR:HG22	2.11	0.50
2:F:1202:VAL:HG23	2:F:1203:ALA:N	2.24	0.50
1:C:152:LEU:HG	1:C:153:ALA:N	2.27	0.50
1:C:145:SER:HB3	1:C:153:ALA:HB2	1.93	0.50
2:D:1221:GLU:OE1	2:D:1224:ARG:HD3	2.11	0.50
1:G:69:HIS:CD2	1:G:70:ASN:N	2.80	0.50
1:G:269:VAL:HG13	1:G:269:VAL:O	2.12	0.50
1:A:267:VAL:CG1	1:A:315:LEU:HD22	2.42	0.50
1:G:256:VAL:HG12	1:G:257:TYR:N	2.26	0.50
1:E:104:GLN:OE1	1:E:105:LYS:HE3	2.12	0.50
1:C:248:GLN:O	1:C:251:ALA:HB3	2.11	0.50
1:G:169:VAL:HG21	2:H:1230:ALA:HB1	1.92	0.50
1:G:185:LEU:HD12	1:G:285:GLY:CA	2.42	0.49
1:C:270:ASP:HA	1:C:316:LYS:HE3	1.94	0.49
1:C:164:SER:OG	1:E:160:ARG:NE	2.40	0.49
1:E:288:LEU:N	1:E:288:LEU:HD23	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:261:THR:O	1:G:261:THR:HG22	2.12	0.49
1:C:59:LEU:O	1:C:97:ALA:HA	2.13	0.49
1:A:115:ASN:ND2	2:F:1228:HIS:CD2	2.80	0.49
1:G:169:VAL:HG21	2:H:1230:ALA:CB	2.43	0.49
1:E:256:VAL:HG12	1:E:257:TYR:N	2.28	0.49
1:G:34:VAL:HG21	1:G:88:ARG:HH21	1.78	0.49
1:C:152:LEU:HG	1:C:153:ALA:H	1.78	0.49
1:E:34:VAL:HG21	1:E:88:ARG:HH21	1.78	0.49
1:A:59:LEU:O	1:A:97:ALA:HA	2.13	0.48
1:A:194:ALA:HB2	1:A:275:ARG:NH2	2.28	0.48
1:G:267:VAL:HG21	1:G:315:LEU:HD13	1.94	0.48
2:D:1217:GLY:HA3	1:E:137:VAL:HG21	1.95	0.48
1:C:30:PRO:CB	1:C:92:ARG:HD3	2.43	0.48
1:G:48:ALA:HB3	1:G:49:PRO:CD	2.43	0.48
1:G:270:ASP:O	1:G:271:ASP:O	2.32	0.48
1:E:33:VAL:HB	1:E:125:LEU:HB2	1.95	0.48
1:G:104:GLN:OE1	1:G:105:LYS:HE3	2.13	0.48
1:E:171:GLN:HE22	2:F:1226:MET:HE1	1.78	0.48
1:A:133:PHE:HB3	1:A:160:ARG:HH22	1.77	0.48
1:G:48:ALA:HB3	1:G:49:PRO:HD3	1.96	0.48
1:G:58:LEU:HD11	1:G:97:ALA:HB1	1.96	0.48
1:A:286:GLY:N	1:A:304:THR:HG23	2.29	0.47
1:E:270:ASP:O	1:E:271:ASP:O	2.32	0.47
2:B:1221:GLU:OE1	2:B:1224:ARG:HD3	2.14	0.47
1:G:33:VAL:HB	1:G:125:LEU:HB2	1.97	0.47
1:E:58:LEU:HD11	1:E:97:ALA:HB1	1.95	0.47
2:D:1219:THR:O	2:D:1223:THR:HG23	2.14	0.47
1:E:71:THR:HG22	1:E:71:THR:O	2.13	0.47
2:D:1225:ARG:HG3	2:D:1225:ARG:NH1	2.30	0.47
1:G:144:THR:HB	1:G:150:VAL:CG2	2.45	0.47
1:G:36:GLN:NE2	1:G:122:ARG:HH11	2.12	0.47
1:G:195:ASP:N	1:G:272:CYS:HB3	2.30	0.47
1:E:195:ASP:N	1:E:272:CYS:HB3	2.29	0.47
1:G:104:GLN:HG2	1:G:105:LYS:HG3	1.97	0.47
1:E:169:VAL:HG21	2:F:1230:ALA:HB1	1.97	0.47
1:C:171:GLN:C	2:D:1233:THR:HG21	2.35	0.47
1:C:98:PHE:CE2	1:C:136:LEU:HB2	2.49	0.47
1:C:153:ALA:O	1:C:154:SER:CB	2.62	0.46
2:B:1225:ARG:NH1	2:B:1225:ARG:HG3	2.31	0.46
1:C:117:TYR:HB3	1:C:120:LEU:HB2	1.97	0.46
1:C:139:ARG:HE	1:C:150:VAL:HG13	1.80	0.46
1:E:36:GLN:NE2	1:E:122:ARG:HH11	2.13	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:63:ASP:OD1	2:F:1224:ARG:NE	2.48	0.46
1:G:39:GLU:CG	1:G:87:SER:OG	2.63	0.46
1:A:133:PHE:HB3	1:A:160:ARG:NH2	2.30	0.46
1:G:288:LEU:N	1:G:288:LEU:HD23	2.30	0.46
1:A:98:PHE:CE2	1:A:136:LEU:HB2	2.50	0.46
1:A:263:ARG:HD3	1:A:264:THR:O	2.15	0.46
1:A:105:LYS:HG3	1:E:173:THR:HB	1.97	0.46
1:C:267:VAL:CG1	1:C:315:LEU:HB3	2.46	0.46
1:G:170:PRO:HG3	2:H:1234:LEU:HD11	1.97	0.46
2:F:1221:GLU:N	2:F:1221:GLU:OE1	2.40	0.46
1:G:39:GLU:HG2	1:G:87:SER:OG	2.16	0.46
1:A:137:VAL:HG22	1:A:158:MET:HG2	1.97	0.46
1:C:133:PHE:HB3	1:C:160:ARG:HH22	1.80	0.46
1:A:269:VAL:HG13	1:A:272:CYS:HB2	1.98	0.46
2:B:1229:ARG:O	2:B:1233:THR:HG23	2.16	0.46
1:A:171:GLN:C	2:B:1233:THR:HG21	2.37	0.46
1:G:179:ARG:NH2	1:G:226:GLU:OE2	2.48	0.46
1:E:169:VAL:HG21	2:F:1230:ALA:CB	2.46	0.46
1:E:115:ASN:O	1:E:118:PRO:HD3	2.15	0.46
1:G:204:LEU:HB2	1:G:265:PHE:CE2	2.51	0.46
2:H:1229:ARG:O	2:H:1232:ASP:HB2	2.16	0.46
2:B:1219:THR:O	2:B:1223:THR:HG23	2.16	0.46
1:A:267:VAL:HG13	1:A:315:LEU:HB3	1.98	0.45
1:G:63:ASP:O	1:G:64:ARG:CB	2.64	0.45
2:D:1218:ALA:HB3	2:D:1223:THR:HG22	1.98	0.45
2:B:1218:ALA:HB3	2:B:1223:THR:HG22	1.98	0.45
1:C:286:GLY:N	1:C:304:THR:HG23	2.32	0.45
2:F:1229:ARG:O	2:F:1232:ASP:HB2	2.16	0.45
1:A:96:ALA:HB2	1:A:134:ARG:NH2	2.31	0.45
2:H:1227:LEU:O	2:H:1231:PHE:HD1	1.99	0.45
1:A:150:VAL:N	1:A:152:LEU:CD2	2.80	0.45
1:A:263:ARG:C	1:A:263:ARG:HD3	2.36	0.45
1:G:188:VAL:O	1:G:192:THR:HG23	2.16	0.45
1:A:274:MET:HA	1:A:313:PHE:CE2	2.52	0.45
1:C:269:VAL:HG13	1:C:272:CYS:HB2	1.98	0.45
1:A:185:LEU:HD22	1:A:189:LEU:HG	1.99	0.45
1:C:137:VAL:HG22	1:C:158:MET:HG2	1.97	0.45
1:A:267:VAL:CG1	1:A:315:LEU:HB3	2.47	0.45
1:A:171:GLN:OE1	2:B:1229:ARG:NH1	2.50	0.45
1:C:90:ARG:HG3	1:C:90:ARG:HH11	1.82	0.45
1:G:206:VAL:HG12	1:G:207:ASN:CG	2.37	0.45
1:C:133:PHE:HB3	1:C:160:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:107:SER:HB3	1:G:110:SER:OG	2.16	0.45
1:C:185:LEU:HD22	1:C:189:LEU:HG	1.99	0.45
1:G:137:VAL:HG22	1:G:158:MET:HG2	1.99	0.45
2:F:1224:ARG:CG	2:F:1224:ARG:HH11	2.30	0.45
1:E:206:VAL:HG12	1:E:207:ASN:CG	2.36	0.45
1:A:90:ARG:HG3	1:A:90:ARG:HH11	1.82	0.45
1:A:39:GLU:CD	1:A:39:GLU:N	2.70	0.44
1:C:274:MET:HA	1:C:313:PHE:CE2	2.52	0.44
1:G:59:LEU:HD22	1:G:68:ILE:HG12	1.98	0.44
1:E:52:THR:HB	1:E:55:LEU:HD12	1.99	0.44
1:C:267:VAL:HG13	1:C:315:LEU:HB3	1.99	0.44
1:E:184:GLN:O	1:E:188:VAL:HG23	2.18	0.44
1:G:184:GLN:O	1:G:188:VAL:HG23	2.17	0.44
1:C:96:ALA:HB2	1:C:134:ARG:NH2	2.33	0.44
1:C:122:ARG:CZ	1:C:148:GLU:HG2	2.48	0.44
1:E:104:GLN:HG2	1:E:105:LYS:HG3	1.99	0.44
1:E:137:VAL:HG22	1:E:158:MET:HG2	2.00	0.44
1:G:151:GLU:O	1:G:153:ALA:N	2.50	0.44
2:H:1221:GLU:N	2:H:1221:GLU:OE1	2.42	0.43
1:C:207:ASN:HD21	1:C:209:LYS:HE2	1.83	0.43
2:F:1227:LEU:O	2:F:1231:PHE:HD1	2.01	0.43
1:A:224:ARG:HD2	1:A:255:THR:CG2	2.48	0.43
1:A:207:ASN:HD21	1:A:209:LYS:HE2	1.84	0.43
2:D:1207:ARG:HH21	1:E:158:MET:CE	2.31	0.43
1:E:48:ALA:HB3	1:E:49:PRO:CD	2.48	0.43
1:E:169:VAL:CG2	1:E:170:PRO:HD2	2.49	0.43
1:C:149:ALA:O	1:C:150:VAL:HB	2.19	0.43
1:E:204:LEU:HB2	1:E:265:PHE:CE2	2.53	0.43
1:C:79:LEU:HD13	1:C:309:VAL:HG12	2.00	0.43
1:A:223:ALA:HB1	1:A:261:THR:HB	2.01	0.43
1:A:115:ASN:ND2	2:F:1228:HIS:NE2	2.67	0.43
1:G:63:ASP:OD1	2:H:1224:ARG:NE	2.52	0.42
1:C:263:ARG:HD3	1:C:264:THR:O	2.19	0.42
1:C:267:VAL:HG11	1:C:315:LEU:HD22	2.00	0.42
1:E:64:ARG:HD2	1:E:64:ARG:HA	1.82	0.42
1:C:119:ASP:HB3	1:C:143:THR:OG1	2.18	0.42
1:C:149:ALA:C	1:C:151:GLU:H	2.22	0.42
1:A:180:LEU:HD23	1:A:256:VAL:CG2	2.49	0.42
1:C:176:VAL:HG12	1:C:177:GLN:N	2.35	0.42
1:A:95:THR:HG21	2:B:1223:THR:OG1	2.19	0.42
2:B:1215:GLY:H	2:B:1223:THR:CG2	2.32	0.42
1:E:48:ALA:HB3	1:E:49:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:141:TRP:CE2	1:E:151:GLU:HG3	2.55	0.42
1:E:63:ASP:O	1:E:64:ARG:CB	2.66	0.42
2:D:1207:ARG:HH21	1:E:158:MET:HE2	1.84	0.42
1:E:176:VAL:HG12	1:E:177:GLN:N	2.35	0.42
1:G:144:THR:HG22	1:G:145:SER:N	2.20	0.42
1:C:185:LEU:O	1:C:189:LEU:HG	2.19	0.42
1:A:48:ALA:HB3	1:A:49:PRO:CD	2.49	0.42
1:G:318:GLN:HB2	1:G:319:LYS:H	1.62	0.42
1:E:139:ARG:HD2	1:E:151:GLU:OE2	2.19	0.42
1:G:170:PRO:CG	2:H:1234:LEU:HD11	2.50	0.42
1:E:181:THR:OG1	1:E:184:GLN:HG3	2.20	0.42
1:C:30:PRO:CA	1:C:92:ARG:HD3	2.50	0.42
1:A:100:SER:HA	1:A:108:LEU:HD12	2.02	0.42
1:C:95:THR:HG21	2:D:1223:THR:OG1	2.20	0.42
1:A:169:VAL:CG2	1:A:170:PRO:HD2	2.50	0.42
1:A:117:TYR:HB3	1:A:120:LEU:HB2	2.02	0.42
1:A:180:LEU:HD23	1:A:256:VAL:HG23	2.00	0.42
1:E:39:GLU:HG2	1:E:87:SER:OG	2.20	0.42
1:G:181:THR:OG1	1:G:184:GLN:HG3	2.20	0.42
1:A:115:ASN:HD22	2:F:1228:HIS:CD2	2.38	0.41
1:A:188:VAL:HG13	1:A:212:VAL:HG21	2.02	0.41
2:B:1227:LEU:O	2:B:1231:PHE:HD1	2.02	0.41
1:E:59:LEU:HD22	1:E:68:ILE:HG12	2.02	0.41
1:E:142:THR:O	1:E:149:ALA:HA	2.20	0.41
2:H:1202:VAL:CG2	2:H:1203:ALA:N	2.83	0.41
1:C:171:GLN:HB2	2:D:1229:ARG:HH11	1.85	0.41
1:E:307:ASN:ND2	1:E:309:VAL:HG13	2.35	0.41
1:E:267:VAL:CG2	1:E:315:LEU:HD13	2.49	0.41
1:A:151:GLU:O	1:A:152:LEU:O	2.38	0.41
1:C:224:ARG:HD2	1:C:255:THR:CG2	2.50	0.41
1:C:263:ARG:C	1:C:263:ARG:HD3	2.41	0.41
2:H:1206:LEU:O	2:H:1211:PHE:HB2	2.21	0.41
1:E:170:PRO:HG3	2:F:1234:LEU:HD11	2.03	0.41
1:G:127:ILE:N	1:G:127:ILE:CD1	2.84	0.41
1:G:265:PHE:CD1	1:G:265:PHE:C	2.93	0.41
1:A:185:LEU:O	1:A:189:LEU:HG	2.20	0.41
1:E:307:ASN:ND2	1:E:307:ASN:C	2.74	0.41
1:A:182:ARG:N	1:A:183:PRO:HD2	2.35	0.41
1:G:307:ASN:ND2	1:G:307:ASN:C	2.74	0.41
1:C:172:GLY:O	2:D:1233:THR:CG2	2.68	0.41
1:A:181:THR:HG23	1:A:184:GLN:OE1	2.20	0.41
1:E:102:VAL:O	1:E:103:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:162:LEU:C	1:C:164:SER:N	2.71	0.41
1:A:162:LEU:C	1:A:164:SER:N	2.72	0.41
1:E:192:THR:HG22	1:E:200:THR:HG21	2.03	0.41
1:C:223:ALA:HB1	1:C:261:THR:HB	2.03	0.41
1:G:169:VAL:CG2	1:G:170:PRO:HD2	2.51	0.41
1:A:30:PRO:CA	1:A:92:ARG:HD3	2.50	0.41
1:C:70:ASN:HD22	1:C:70:ASN:HA	1.52	0.41
1:C:271:ASP:O	1:C:271:ASP:OD1	2.38	0.41
1:A:200:THR:O	1:A:268:VAL:HA	2.20	0.41
1:A:148:GLU:C	1:A:150:VAL:H	2.23	0.41
2:F:1202:VAL:CG2	2:F:1203:ALA:N	2.84	0.41
1:E:265:PHE:CD1	1:E:265:PHE:C	2.93	0.41
1:G:194:ALA:HB2	1:G:275:ARG:HD3	2.02	0.41
2:D:1200:ASP:CG	2:D:1201:ASP:N	2.74	0.41
1:E:143:THR:HG23	1:E:147:GLY:HA2	2.02	0.41
1:G:64:ARG:HD2	1:G:64:ARG:HA	1.82	0.41
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.98	0.41
1:G:210:PHE:O	1:G:220:THR:HA	2.21	0.41
1:C:210:PHE:O	1:C:220:THR:HA	2.21	0.41
1:A:169:VAL:HG22	1:A:170:PRO:HD2	2.03	0.40
1:G:182:ARG:N	1:G:183:PRO:HD2	2.36	0.40
1:E:194:ALA:HB2	1:E:275:ARG:HD3	2.03	0.40
1:E:188:VAL:O	1:E:192:THR:HG23	2.21	0.40
1:A:171:GLN:HB2	2:B:1229:ARG:HH11	1.86	0.40
2:B:1215:GLY:H	2:B:1223:THR:HG21	1.85	0.40
1:C:182:ARG:N	1:C:183:PRO:HD2	2.36	0.40
1:E:315:LEU:O	1:E:316:LYS:C	2.59	0.40
1:E:132:PRO:HD2	1:E:133:PHE:CE1	2.57	0.40
1:C:64:ARG:HD3	2:D:1228:HIS:CE1	2.57	0.40
1:A:39:GLU:HG3	1:A:87:SER:HA	2.01	0.40
2:D:1234:LEU:HD12	2:D:1234:LEU:HA	1.97	0.40
1:G:132:PRO:HD2	1:G:133:PHE:CE1	2.56	0.40
1:G:119:ASP:HB2	1:G:142:THR:OG1	2.21	0.40
1:E:314:LEU:HB2	2:F:1205:ARG:NH2	2.36	0.40
1:A:259:GLU:HG2	1:A:260:ASN:ND2	2.36	0.40
1:G:142:THR:O	1:G:149:ALA:HA	2.21	0.40
1:E:39:GLU:CG	1:E:87:SER:OG	2.69	0.40
2:H:1224:ARG:CG	2:H:1224:ARG:HH11	2.35	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	263/319 (82%)	237 (90%)	18 (7%)	8 (3%)	7	15
1	C	268/319 (84%)	240 (90%)	16 (6%)	12 (4%)	4	7
1	E	271/319 (85%)	243 (90%)	21 (8%)	7 (3%)	8	20
1	G	271/319 (85%)	238 (88%)	28 (10%)	5 (2%)	13	31
2	B	34/36 (94%)	33 (97%)	0	1 (3%)	7	16
2	D	34/36 (94%)	33 (97%)	0	1 (3%)	7	16
2	F	34/36 (94%)	31 (91%)	2 (6%)	1 (3%)	7	16
2	H	34/36 (94%)	30 (88%)	3 (9%)	1 (3%)	7	16
All	All	1209/1420 (85%)	1085 (90%)	88 (7%)	36 (3%)	7	15

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	LEU
1	A	223	ALA
1	A	270	ASP
1	A	272	CYS
2	B	1216	ALA
1	C	152	LEU
1	C	223	ALA
1	C	270	ASP
1	C	272	CYS
2	D	1216	ALA
1	E	38	ALA
1	E	145	SER
1	E	271	ASP
1	G	38	ALA
1	G	271	ASP
1	A	114	ALA
1	A	224	ARG
1	C	114	ALA
1	C	224	ARG

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Mol	Chain	Res	Type
1	C	248	GLN
1	E	272	CYS
2	F	1216	ALA
1	G	272	CYS
2	H	1216	ALA
1	A	154	SER
1	A	163	THR
1	C	154	SER
1	C	161	GLU
1	E	104	GLN
1	E	146	ASP
1	G	104	GLN
1	G	114	ALA
1	C	150	VAL
1	C	163	THR
1	E	114	ALA
1	C	284	GLY

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	228/266 (86%)	214 (94%)	14 (6%)	26	54
1	C	229/266 (86%)	216 (94%)	13 (6%)	29	58
1	E	235/266 (88%)	224 (95%)	11 (5%)	36	69
1	G	235/266 (88%)	222 (94%)	13 (6%)	30	60
2	B	22/22 (100%)	20 (91%)	2 (9%)	14	30
2	D	22/22 (100%)	20 (91%)	2 (9%)	14	30
2	F	22/22 (100%)	19 (86%)	3 (14%)	5	13
2	H	22/22 (100%)	19 (86%)	3 (14%)	5	13
All	All	1015/1152 (88%)	954 (94%)	61 (6%)	27	56

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	70	ASN
1	A	71	THR
1	A	95	THR
1	A	105	LYS
1	A	111	VAL
1	A	136	LEU
1	A	148	GLU
1	A	152	LEU
1	A	155	GLU
1	A	156	THR
1	A	185	LEU
1	A	204	LEU
1	A	263	ARG
2	B	1223	THR
2	B	1234	LEU
1	C	44	LEU
1	C	70	ASN
1	C	71	THR
1	C	95	THR
1	C	105	LYS
1	C	111	VAL
1	C	136	LEU
1	C	148	GLU
1	C	155	GLU
1	C	156	THR
1	C	185	LEU
1	C	204	LEU
1	C	263	ARG
2	D	1223	THR
2	D	1234	LEU
1	E	39	GLU
1	E	44	LEU
1	E	70	ASN
1	E	71	THR
1	E	79	LEU
1	E	95	THR
1	E	135	THR
1	E	185	LEU
1	E	204	LEU
1	E	287	THR
1	E	307	ASN
2	F	1224	ARG

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Mol	Chain	Res	Type
2	F	1233	THR
2	F	1234	LEU
1	G	39	GLU
1	G	44	LEU
1	G	70	ASN
1	G	71	THR
1	G	79	LEU
1	G	95	THR
1	G	135	THR
1	G	144	THR
1	G	146	ASP
1	G	185	LEU
1	G	204	LEU
1	G	287	THR
1	G	307	ASN
2	H	1224	ARG
2	H	1233	THR
2	H	1234	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	115	ASN
1	A	190	ASN
1	A	282	GLN
1	C	70	ASN
1	C	138	GLN
1	C	190	ASN
1	E	36	GLN
1	E	70	ASN
1	E	171	GLN
1	E	207	ASN
1	E	252	ASN
1	E	307	ASN
1	G	36	GLN
1	G	70	ASN
1	G	171	GLN
1	G	207	ASN
1	G	252	ASN
1	G	307	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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, 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	267/319 (83%)	-0.12	12 (4%) 32 36	5, 19, 64, 85	0
1	C	272/319 (85%)	-0.02	13 (4%) 29 33	5, 23, 67, 87	0
1	E	275/319 (86%)	0.01	10 (3%) 41 46	8, 29, 69, 90	0
1	G	275/319 (86%)	0.20	15 (5%) 24 26	8, 33, 76, 91	0
2	B	36/36 (100%)	-0.25	0 100 100	9, 23, 45, 69	0
2	D	36/36 (100%)	-0.12	1 (2%) 50 56	11, 23, 48, 71	0
2	F	36/36 (100%)	0.26	1 (2%) 50 56	11, 46, 68, 82	0
2	H	36/36 (100%)	0.43	3 (8%) 11 12	15, 48, 71, 86	0
All	All	1233/1420 (86%)	0.02	55 (4%) 32 36	5, 27, 69, 91	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	144	THR	7.5
1	G	146	ASP	7.0
1	C	152	LEU	6.0
1	E	146	ASP	5.5
2	H	1200	ASP	5.1
1	C	146	ASP	5.1
1	E	319	LYS	5.1
1	A	227	GLY	4.8
1	C	248	GLN	4.7
1	G	105	LYS	4.7
1	G	147	GLY	4.7
1	G	319	LYS	4.7
1	A	146	ASP	4.6
1	E	104	GLN	4.4
1	G	103	ASP	4.4
1	G	154	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	148	GLU	4.3
1	C	249	ALA	4.3
1	C	250	ALA	4.3
1	C	144	THR	4.2
1	C	319	LYS	3.9
1	G	104	GLN	3.8
1	A	144	THR	3.7
1	E	147	GLY	3.6
1	C	206	VAL	3.6
1	E	103	ASP	3.5
1	G	150	VAL	3.5
1	E	194	ALA	3.4
1	A	151	GLU	3.4
2	H	1203	ALA	3.4
1	G	272	CYS	3.2
1	G	145	SER	3.1
2	F	1201	ASP	3.1
1	A	207	ASN	3.1
1	C	252	ASN	3.0
1	A	153	ALA	3.0
1	G	121	ARG	3.0
1	E	272	CYS	3.0
1	A	143	THR	2.8
1	C	153	ALA	2.8
1	C	271	ASP	2.8
2	H	1201	ASP	2.8
1	A	152	LEU	2.8
1	G	149	ALA	2.8
1	A	150	VAL	2.7
2	D	1200	ASP	2.6
1	G	102	VAL	2.6
1	E	144	THR	2.6
1	A	92	ARG	2.5
1	E	197	ALA	2.4
1	A	145	SER	2.4
1	A	149	ALA	2.3
1	C	145	SER	2.2
1	E	318	GLN	2.0
1	C	272	CYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.