Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:08 AM GMT

PDB ID	:	2FRP
Title	:	Bacteriophage HK97 Expansion Intermediate IV
Authors	:	Gan, L.; Speir, J.A.; Conway, J.F.; Lander, G.; Cheng, N.; Firek, B.A.; Hendrix, R.W.; Duda, R.L.; Liljas, L.; Johnson, J.E.
Deposited on	:	2006-01-19
Resolution	:	7.50 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 (i) symbol.

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

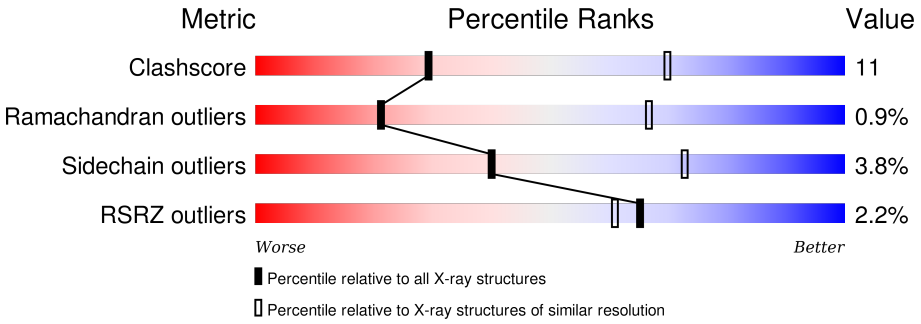
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 7.50 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))
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	282	70% 28%
1	B	282	74% 23%
1	C	282	78% 21%
1	D	282	76% 22%
1	E	282	74% 25%
1	F	282	63% 25% 9%
1	G	282	6% 60% 23% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14631 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 Major capsid protein.

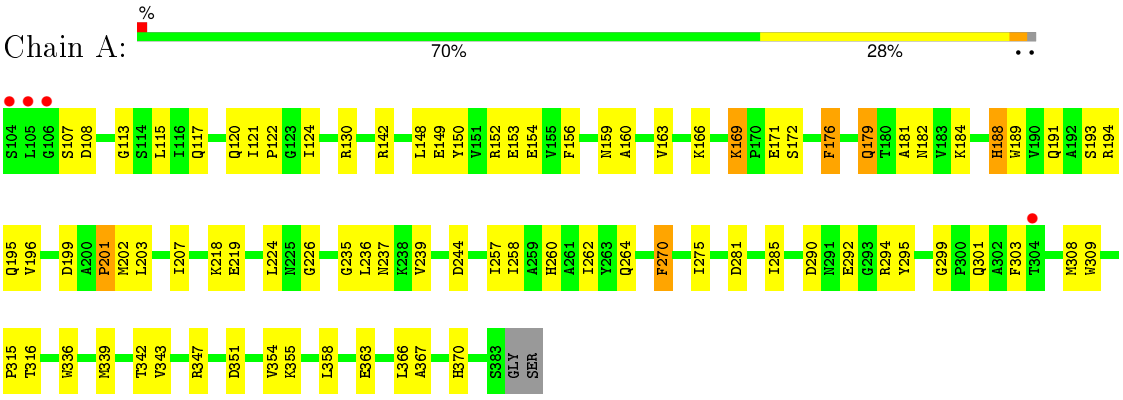
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	B	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	C	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	D	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	E	280	Total	C	N	O	S	0	0	0
			2151	1344	375	422	10			
1	F	256	Total	C	N	O	S	0	0	0
			1986	1241	349	388	8			
1	G	243	Total	C	N	O	S	0	0	0
			1890	1181	333	368	8			

3 Residue-property plots (i)

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

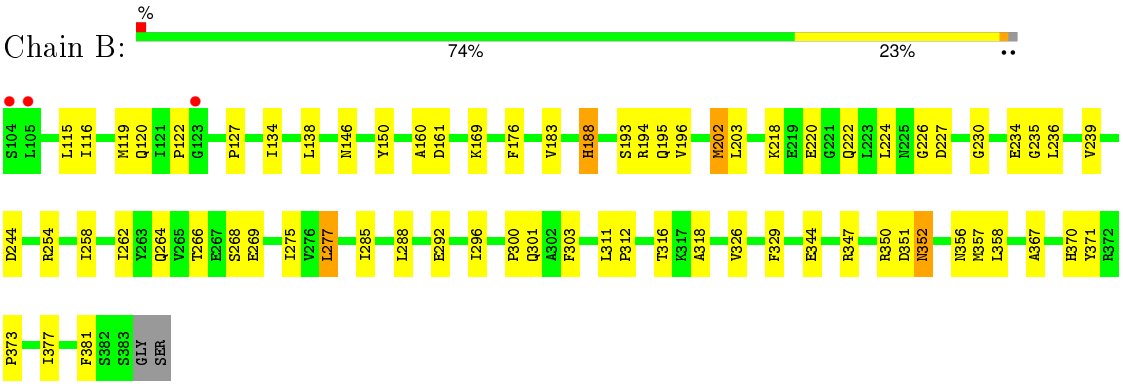
- Molecule 1: Major capsid protein

Chain A:



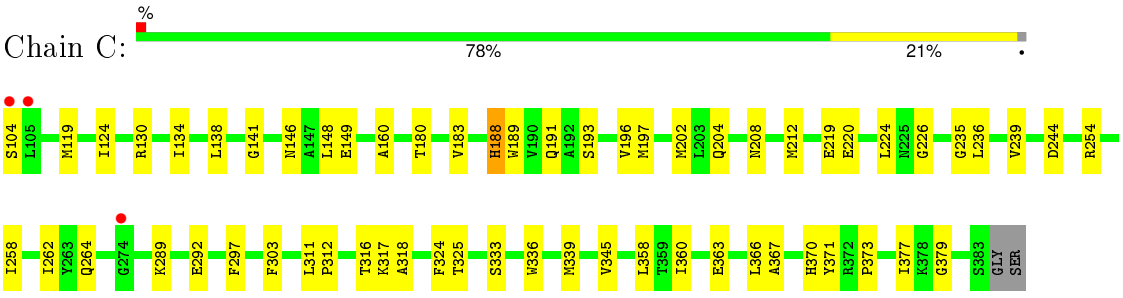
- Molecule 1: Major capsid protein

Chain B:

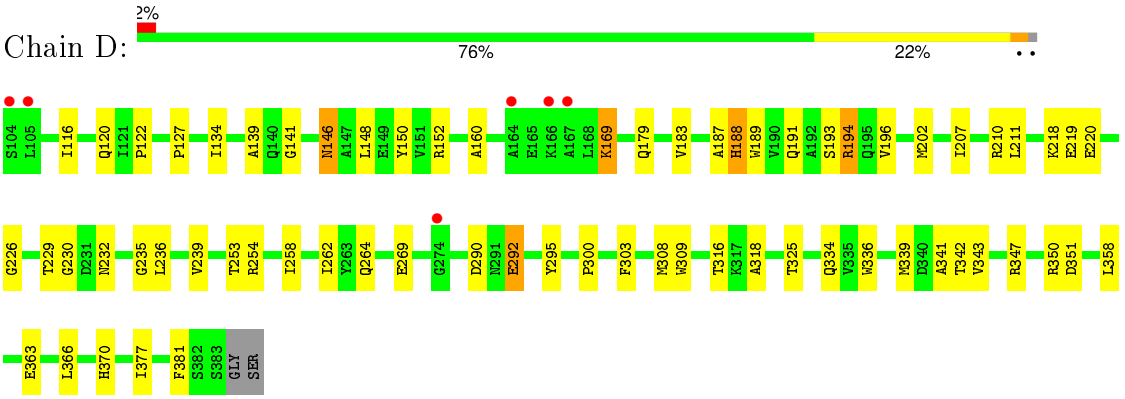


- Molecule 1: Major capsid protein

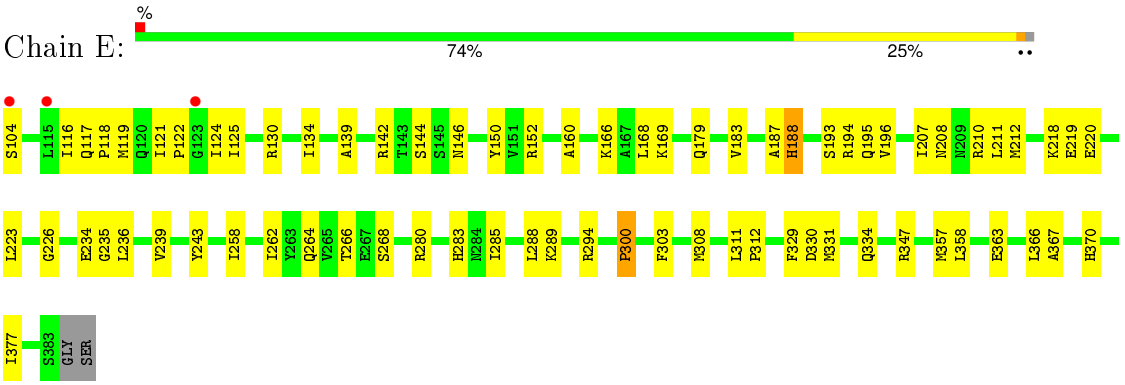
Chain C:



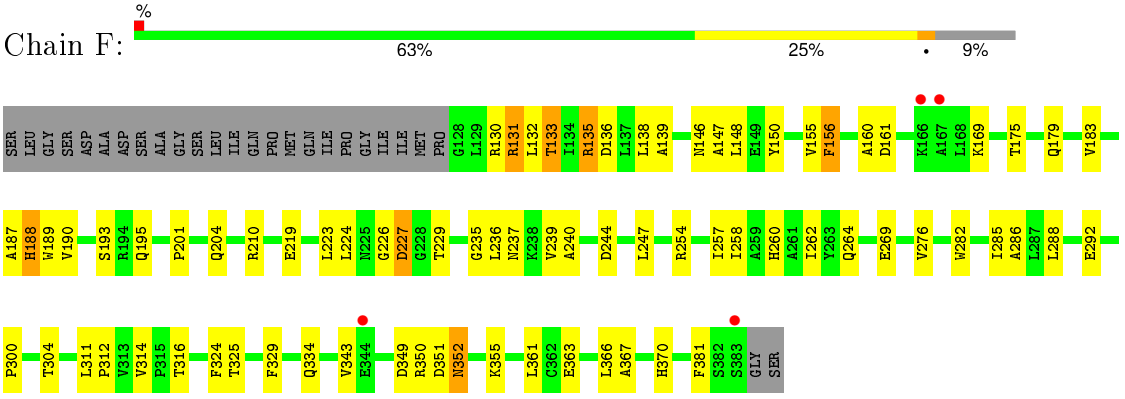
- Molecule 1: Major capsid protein



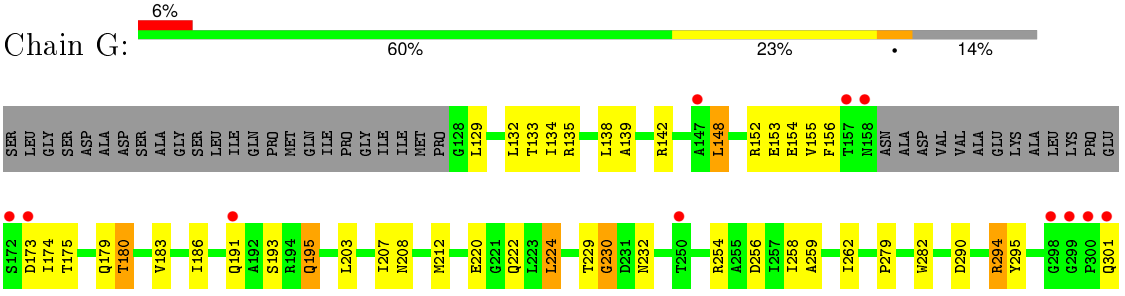
- Molecule 1: Major capsid protein

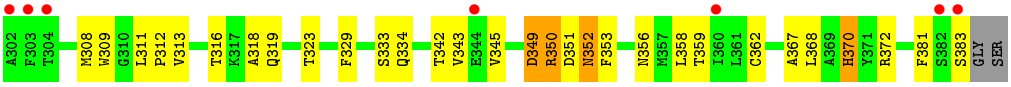


- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein




A302
F303
T304
M308
W309
G310
L311
P312
V313
T316
K317
A318
Q319
T323
F329
S333
Q334
T342
V343
E344
V345
D349
R350
D351
N352
F353
N356
M357
L358
T359
I360
L361
C362
A367
L368
A369
H370
Y371
R372
F381
S382
S383
GLY
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	1009.80Å 1009.80Å 732.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 7.50 40.16 – 7.51	Depositor EDS
% Data completeness (in resolution range)	64.7 (40.00-7.50) 64.9 (40.16-7.51)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 7.33Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.421 , (Not available) 0.363 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	152.8	Xtriage
Anisotropy	0.763	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 176.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 305905 reflections	Xtriage
F_o,F_c correlation	0.13	EDS
Total number of atoms	14631	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.30	0/2188	0.50	0/2969
1	B	0.32	1/2188 (0.0%)	0.49	0/2969
1	C	0.28	0/2188	0.48	0/2969
1	D	0.34	1/2188 (0.0%)	0.49	0/2969
1	E	0.28	0/2188	0.51	0/2969
1	F	0.28	0/2020	0.50	0/2740
1	G	0.49	1/1922 (0.1%)	0.63	4/2605 (0.2%)
All	All	0.33	3/14882 (0.0%)	0.51	4/20190 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	180	THR	C-N	-17.02	0.94	1.34
1	D	169	LYS	CE-NZ	8.56	1.70	1.49
1	B	356	ASN	CG-ND2	8.00	1.52	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	148	LEU	O-C-N	12.69	143.00	122.70
1	G	148	LEU	CA-C-N	-9.85	95.54	117.20
1	G	148	LEU	C-N-CA	-7.34	103.35	121.70
1	G	180	THR	O-C-N	-5.36	114.13	122.70

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	2151	0	2119	57	0
1	B	2151	0	2119	54	0
1	C	2151	0	2119	48	0
1	D	2151	0	2119	52	0
1	E	2151	0	2119	51	0
1	F	1986	0	1951	60	0
1	G	1890	0	1850	51	0
All	All	14631	0	14396	327	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 11.

All (327) 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:169:LYS:CE	1:D:169:LYS:NZ	1.70	1.54
1:F:224:LEU:HD11	1:F:276:VAL:HG11	1.52	0.89
1:G:138:LEU:HD23	1:G:329:PHE:HB3	1.56	0.88
1:G:345:VAL:HB	1:G:358:LEU:HD21	1.56	0.87
1:A:218:LYS:HE2	1:B:161:ASP:OD1	1.77	0.84
1:G:316:THR:HG22	1:G:318:ALA:H	1.41	0.83
1:G:319:GLN:HE21	1:G:323:THR:HB	1.43	0.82
1:B:218:LYS:HE3	1:B:222:GLN:NE2	1.95	0.82
1:G:229:THR:HG23	1:G:230:GLY:H	1.45	0.80
1:G:368:LEU:HG	1:G:370:HIS:HE1	1.52	0.75
1:A:153:GLU:HA	1:A:176:PHE:HB3	1.71	0.73
1:E:194:ARG:HH12	1:E:347:ARG:NE	1.86	0.73
1:E:218:LYS:HE2	1:F:161:ASP:OD1	1.90	0.72
1:C:219:GLU:HG3	1:C:366:LEU:HD11	1.70	0.72
1:C:149:GLU:HG2	1:C:180:THR:HG22	1.72	0.72
1:D:316:THR:HG22	1:D:318:ALA:H	1.54	0.71
1:F:133:THR:HG22	1:F:136:ASP:H	1.53	0.71
1:E:130:ARG:HA	1:F:269:GLU:HG2	1.71	0.71
1:G:148:LEU:O	1:G:180:THR:HA	1.90	0.70
1:A:179:GLN:HA	1:A:179:GLN:HE21	1.55	0.69
1:E:121:ILE:HD12	1:F:150:TYR:HB3	1.73	0.69
1:F:236:LEU:HD23	1:F:370:HIS:HE1	1.58	0.68
1:A:347:ARG:HB3	1:A:358:LEU:HD12	1.74	0.68
1:D:127:PRO:HD2	1:D:210:ARG:HH21	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:HIS:ND1	1:B:160:ALA:HB2	2.10	0.66
1:D:254:ARG:HB3	1:D:381:PHE:HE2	1.59	0.66
1:A:124:ILE:HD11	1:B:176:PHE:HE2	1.60	0.66
1:B:226:GLY:H	1:B:235:GLY:HA3	1.61	0.65
1:G:368:LEU:HG	1:G:370:HIS:CE1	2.31	0.65
1:B:301:GLN:HE22	1:C:297:PHE:HA	1.62	0.64
1:A:244:ASP:HB2	1:A:264:GLN:NE2	2.11	0.64
1:A:130:ARG:HA	1:B:269:GLU:HG2	1.79	0.63
1:F:133:THR:HG23	1:F:135:ARG:HB3	1.79	0.63
1:G:193:SER:HB2	1:G:195:GLN:NE2	2.13	0.63
1:A:226:GLY:H	1:A:235:GLY:HA3	1.64	0.62
1:B:183:VAL:HG22	1:B:367:ALA:HB2	1.81	0.62
1:A:160:ALA:HB2	1:F:188:HIS:ND1	2.14	0.62
1:G:183:VAL:HG22	1:G:367:ALA:HB2	1.81	0.62
1:D:236:LEU:HD23	1:D:370:HIS:HE1	1.65	0.61
1:E:193:SER:HB3	1:E:196:VAL:HG23	1.81	0.61
1:B:275:ILE:HG23	1:B:326:VAL:HG22	1.82	0.61
1:D:239:VAL:HG21	1:D:370:HIS:CD2	2.36	0.61
1:A:236:LEU:HD23	1:A:370:HIS:HE1	1.66	0.61
1:C:189:TRP:HZ3	1:C:191:GLN:HB2	1.65	0.61
1:B:239:VAL:HG21	1:B:370:HIS:CD2	2.36	0.61
1:F:244:ASP:HB3	1:F:247:LEU:HG	1.82	0.60
1:B:218:LYS:HE3	1:B:222:GLN:HE21	1.63	0.60
1:B:218:LYS:CE	1:B:222:GLN:NE2	2.64	0.60
1:F:244:ASP:HB2	1:F:264:GLN:NE2	2.17	0.60
1:F:130:ARG:C	1:F:132:LEU:H	2.05	0.59
1:G:134:ILE:HD12	1:G:220:GLU:HG2	1.84	0.59
1:F:286:ALA:HB1	1:F:304:THR:HG21	1.84	0.59
1:F:183:VAL:HG22	1:F:367:ALA:HB2	1.85	0.59
1:D:229:THR:HG22	1:D:232:ASN:HD22	1.66	0.59
1:D:189:TRP:HZ3	1:D:191:GLN:HB2	1.67	0.59
1:B:347:ARG:HB3	1:B:358:LEU:HD12	1.85	0.59
1:G:254:ARG:HB3	1:G:381:PHE:HZ	1.68	0.59
1:A:189:TRP:CD1	1:B:169:LYS:HB2	2.38	0.58
1:C:104:SER:HB3	1:E:166:LYS:NZ	2.18	0.58
1:A:239:VAL:HG21	1:A:370:HIS:CD2	2.38	0.58
1:F:133:THR:CG2	1:F:136:ASP:H	2.17	0.58
1:B:316:THR:HG22	1:B:318:ALA:H	1.68	0.58
1:A:189:TRP:HZ3	1:A:191:GLN:HB2	1.68	0.58
1:E:116:ILE:HD12	1:F:146:ASN:HB2	1.86	0.58
1:E:183:VAL:HG22	1:E:367:ALA:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:ASN:O	1:D:183:VAL:HG12	2.04	0.57
1:C:316:THR:HG22	1:C:318:ALA:H	1.69	0.57
1:E:264:GLN:HB3	1:E:377:ILE:HD13	1.85	0.57
1:B:236:LEU:HD23	1:B:370:HIS:HE1	1.70	0.57
1:C:226:GLY:HA3	1:C:235:GLY:H	1.69	0.57
1:D:264:GLN:HB3	1:D:377:ILE:HD13	1.86	0.56
1:C:130:ARG:HA	1:D:269:GLU:HG2	1.86	0.56
1:E:119:MET:HB3	1:F:148:LEU:HD23	1.87	0.56
1:E:187:ALA:HB2	1:E:363:GLU:HA	1.87	0.56
1:E:239:VAL:HG21	1:E:370:HIS:CD2	2.40	0.56
1:C:197:MET:HE1	1:C:204:GLN:HB2	1.85	0.56
1:F:138:LEU:HD23	1:F:329:PHE:HB3	1.86	0.56
1:C:236:LEU:HD23	1:C:370:HIS:HE1	1.70	0.56
1:F:227:ASP:HB3	1:F:229:THR:HG22	1.88	0.56
1:D:134:ILE:HB	1:D:220:GLU:HG3	1.88	0.56
1:D:139:ALA:HB3	1:D:334:GLN:HB2	1.88	0.56
1:F:150:TYR:CE1	1:F:179:GLN:HB2	2.41	0.55
1:A:336:TRP:HB2	1:A:367:ALA:HB3	1.87	0.55
1:A:188:HIS:CE1	1:B:160:ALA:HB2	2.42	0.55
1:B:193:SER:HB3	1:B:196:VAL:HG23	1.89	0.55
1:G:156:PHE:CD1	1:G:174:ILE:HG12	2.41	0.55
1:E:243:TYR:HA	1:E:264:GLN:HE22	1.70	0.55
1:F:239:VAL:HG21	1:F:370:HIS:CD2	2.41	0.54
1:C:188:HIS:ND1	1:D:160:ALA:HB2	2.23	0.54
1:F:236:LEU:HD23	1:F:370:HIS:CE1	2.42	0.54
1:A:107:SER:O	1:A:113:GLY:HA3	2.07	0.54
1:C:141:GLY:O	1:C:336:TRP:HA	2.07	0.54
1:A:142:ARG:HB3	1:A:142:ARG:NH1	2.23	0.54
1:F:201:PRO:O	1:F:204:GLN:HB3	2.08	0.54
1:B:244:ASP:HB2	1:B:264:GLN:NE2	2.23	0.53
1:G:132:LEU:HD13	1:G:312:PRO:HB3	1.90	0.53
1:A:193:SER:HB3	1:A:196:VAL:HG23	1.89	0.53
1:D:141:GLY:O	1:D:336:TRP:HA	2.08	0.53
1:F:224:LEU:HD23	1:F:237:ASN:ND2	2.24	0.53
1:E:188:HIS:ND1	1:F:160:ALA:HB2	2.22	0.53
1:F:350:ARG:HG3	1:F:351:ASP:H	1.72	0.53
1:D:229:THR:CG2	1:D:232:ASN:HD22	2.22	0.53
1:B:264:GLN:HB3	1:B:377:ILE:HD13	1.90	0.53
1:C:134:ILE:HB	1:C:220:GLU:HG3	1.91	0.53
1:C:239:VAL:HG21	1:C:370:HIS:CD2	2.44	0.52
1:E:188:HIS:HB3	1:F:160:ALA:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:VAL:HG22	1:C:367:ALA:HB2	1.90	0.52
1:G:153:GLU:HG3	1:G:372:ARG:NH1	2.25	0.52
1:B:352:ASN:HA	1:B:357:MET:HB2	1.90	0.52
1:D:254:ARG:HB3	1:D:381:PHE:CE2	2.43	0.51
1:C:188:HIS:HB3	1:D:160:ALA:HA	1.91	0.51
1:E:210:ARG:HB3	1:F:156:PHE:HE2	1.74	0.51
1:G:208:ASN:O	1:G:212:MET:HG2	2.10	0.51
1:C:208:ASN:O	1:C:212:MET:HG2	2.10	0.51
1:C:339:MET:HE3	1:C:363:GLU:HG3	1.92	0.51
1:G:229:THR:HG23	1:G:230:GLY:N	2.21	0.51
1:G:254:ARG:HB3	1:G:381:PHE:CZ	2.44	0.51
1:G:154:GLU:HB2	1:G:175:THR:HB	1.93	0.51
1:F:351:ASP:HB3	1:F:355:LYS:HD3	1.93	0.51
1:D:226:GLY:H	1:D:235:GLY:HA3	1.76	0.51
1:A:224:LEU:HD13	1:A:237:ASN:HD22	1.76	0.51
1:G:133:THR:HG22	1:G:135:ARG:H	1.76	0.51
1:B:218:LYS:CE	1:B:222:GLN:HE21	2.22	0.51
1:E:223:LEU:O	1:E:236:LEU:HD13	2.11	0.51
1:F:226:GLY:H	1:F:235:GLY:HA3	1.75	0.51
1:D:116:ILE:HG21	1:E:146:ASN:HB2	1.93	0.50
1:F:343:VAL:HA	1:F:361:LEU:O	2.12	0.50
1:D:120:GLN:O	1:D:122:PRO:HD3	2.12	0.50
1:F:282:TRP:O	1:F:285:ILE:HB	2.11	0.50
1:E:226:GLY:H	1:E:235:GLY:HA3	1.77	0.50
1:D:193:SER:HB3	1:D:196:VAL:HG23	1.93	0.50
1:E:236:LEU:HD12	1:E:370:HIS:HE1	1.77	0.50
1:C:244:ASP:HB2	1:C:264:GLN:NE2	2.26	0.50
1:A:166:LYS:HE3	1:E:104:SER:HB2	1.92	0.50
1:D:139:ALA:HB3	1:D:334:GLN:CB	2.41	0.50
1:B:188:HIS:ND1	1:C:160:ALA:HB2	2.27	0.50
1:C:124:ILE:HD12	1:C:124:ILE:N	2.27	0.50
1:G:139:ALA:HB3	1:G:334:GLN:CB	2.42	0.50
1:E:168:LEU:HD23	1:E:169:LYS:N	2.27	0.49
1:F:132:LEU:HB3	1:F:314:VAL:HG12	1.94	0.49
1:C:264:GLN:HB3	1:C:377:ILE:HD13	1.94	0.49
1:B:188:HIS:HB3	1:C:160:ALA:HA	1.94	0.49
1:B:115:LEU:HD12	1:B:115:LEU:N	2.27	0.49
1:A:218:LYS:HG3	1:A:218:LYS:O	2.12	0.49
1:G:191:GLN:OE1	1:G:350:ARG:NH1	2.45	0.49
1:A:163:VAL:HG21	1:A:169:LYS:HG3	1.95	0.49
1:A:169:LYS:HB3	1:F:189:TRP:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ILE:O	1:A:262:ILE:HG13	2.12	0.49
1:E:124:ILE:HG22	1:E:125:ILE:N	2.28	0.49
1:A:292:GLU:HG3	1:B:292:GLU:HG2	1.95	0.49
1:E:283:HIS:NE2	1:F:260:HIS:HA	2.28	0.49
1:D:236:LEU:HD23	1:D:370:HIS:CE1	2.48	0.48
1:D:150:TYR:CE1	1:D:179:GLN:HB2	2.48	0.48
1:E:219:GLU:HG3	1:E:366:LEU:HD11	1.94	0.48
1:E:139:ALA:O	1:E:334:GLN:HG3	2.12	0.48
1:A:120:GLN:O	1:A:122:PRO:HD3	2.12	0.48
1:C:119:MET:HB3	1:D:148:LEU:HD23	1.94	0.48
1:C:292:GLU:HG2	1:D:292:GLU:OE2	2.13	0.48
1:A:121:ILE:HG13	1:B:150:TYR:HB3	1.95	0.48
1:G:153:GLU:HG3	1:G:372:ARG:CZ	2.44	0.48
1:G:186:ILE:HG21	1:G:222:GLN:HG3	1.95	0.48
1:D:188:HIS:ND1	1:E:160:ALA:HB2	2.28	0.48
1:B:288:LEU:O	1:B:296:ILE:HG12	2.14	0.48
1:E:266:THR:C	1:E:268:SER:H	2.17	0.48
1:D:254:ARG:O	1:D:258:ILE:HD12	2.13	0.48
1:D:347:ARG:HG2	1:D:358:LEU:CD1	2.43	0.48
1:A:194:ARG:CZ	1:A:347:ARG:NH1	2.76	0.48
1:C:345:VAL:HG12	1:C:360:ILE:HG12	1.94	0.47
1:D:218:LYS:O	1:D:218:LYS:HG3	2.14	0.47
1:C:130:ARG:HD2	1:C:317:LYS:HB2	1.96	0.47
1:B:350:ARG:HB3	1:B:351:ASP:H	1.47	0.47
1:B:119:MET:HB3	1:C:148:LEU:HD23	1.96	0.47
1:B:236:LEU:HD23	1:B:370:HIS:CE1	2.49	0.47
1:A:160:ALA:HA	1:F:188:HIS:HB3	1.97	0.47
1:G:139:ALA:HB3	1:G:334:GLN:HB2	1.96	0.47
1:G:349:ASP:OD1	1:G:350:ARG:HG2	2.15	0.47
1:B:218:LYS:NZ	1:B:222:GLN:NE2	2.62	0.47
1:G:258:ILE:O	1:G:262:ILE:HG13	2.15	0.47
1:D:189:TRP:CZ3	1:D:191:GLN:HB2	2.47	0.47
1:A:150:TYR:HE2	1:A:181:ALA:HB2	1.80	0.47
1:C:324:PHE:CZ	1:C:379:GLY:HA3	2.50	0.47
1:C:197:MET:CE	1:C:204:GLN:HB2	2.45	0.46
1:D:194:ARG:NH2	1:D:347:ARG:NH2	2.62	0.46
1:A:224:LEU:HD13	1:A:237:ASN:ND2	2.30	0.46
1:D:342:THR:HG22	1:D:343:VAL:N	2.30	0.46
1:D:188:HIS:CE1	1:E:160:ALA:HB2	2.49	0.46
1:F:285:ILE:O	1:F:288:LEU:HG	2.16	0.46
1:D:350:ARG:HB3	1:D:351:ASP:H	1.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ILE:HD11	1:B:381:PHE:HZ	1.81	0.46
1:G:229:THR:CG2	1:G:232:ASN:HD22	2.29	0.46
1:C:325:THR:HA	1:C:377:ILE:O	2.16	0.46
1:C:124:ILE:HD12	1:C:124:ILE:H	1.81	0.46
1:A:172:SER:O	1:F:190:VAL:HG22	2.15	0.46
1:A:188:HIS:HB3	1:B:160:ALA:HA	1.98	0.46
1:E:285:ILE:O	1:E:288:LEU:HG	2.16	0.46
1:A:219:GLU:HG3	1:A:366:LEU:HD11	1.98	0.46
1:D:341:ALA:HA	1:D:363:GLU:O	2.16	0.46
1:C:226:GLY:H	1:C:235:GLY:HA3	1.81	0.45
1:B:116:ILE:HG21	1:C:146:ASN:HB2	1.98	0.45
1:F:258:ILE:O	1:F:262:ILE:HG13	2.16	0.45
1:B:275:ILE:HG22	1:B:277:LEU:HD11	1.99	0.45
1:B:134:ILE:HD12	1:B:220:GLU:HG2	1.98	0.45
1:F:155:VAL:H	1:F:175:THR:HB	1.81	0.45
1:E:234:GLU:HG2	1:E:239:VAL:CG2	2.46	0.45
1:G:155:VAL:H	1:G:175:THR:HB	1.81	0.45
1:D:295:TYR:CE1	1:D:300:PRO:HG3	2.51	0.45
1:C:254:ARG:O	1:C:258:ILE:HD13	2.17	0.45
1:F:139:ALA:O	1:F:334:GLN:HG3	2.16	0.45
1:C:104:SER:HB3	1:E:166:LYS:HZ2	1.81	0.45
1:D:258:ILE:O	1:D:262:ILE:HG13	2.16	0.45
1:B:285:ILE:O	1:B:288:LEU:HG	2.17	0.45
1:B:134:ILE:HD12	1:B:220:GLU:CG	2.47	0.45
1:A:154:GLU:H	1:A:176:PHE:HA	1.82	0.45
1:B:194:ARG:HD2	1:B:347:ARG:NH1	2.32	0.45
1:E:130:ARG:HA	1:F:269:GLU:CG	2.44	0.44
1:D:229:THR:HG23	1:D:230:GLY:N	2.32	0.44
1:F:133:THR:CG2	1:F:135:ARG:HB3	2.43	0.44
1:A:258:ILE:HG21	1:A:275:ILE:HD13	1.98	0.44
1:B:138:LEU:HD23	1:B:329:PHE:HB3	1.99	0.44
1:A:290:ASP:OD2	1:A:294:ARG:HB2	2.17	0.44
1:E:264:GLN:HE21	1:E:377:ILE:HG12	1.83	0.44
1:B:120:GLN:O	1:B:122:PRO:HD3	2.17	0.44
1:F:193:SER:OG	1:F:195:GLN:HG2	2.18	0.44
1:D:207:ILE:O	1:D:211:LEU:HD23	2.17	0.44
1:F:311:LEU:HA	1:F:312:PRO:HD3	1.90	0.43
1:G:352:ASN:O	1:G:356:ASN:N	2.51	0.43
1:G:138:LEU:HD22	1:G:333:SER:O	2.19	0.43
1:G:279:PRO:HD3	1:G:316:THR:O	2.18	0.43
1:C:189:TRP:CZ3	1:C:191:GLN:HB2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:ASN:O	1:E:212:MET:HG2	2.18	0.43
1:A:270:PHE:HA	1:A:270:PHE:HD2	1.68	0.43
1:A:347:ARG:HB3	1:A:358:LEU:CD1	2.46	0.43
1:C:311:LEU:HA	1:C:312:PRO:HD3	1.90	0.43
1:G:203:LEU:O	1:G:207:ILE:HG13	2.17	0.43
1:G:282:TRP:CE3	1:G:313:VAL:HG11	2.53	0.43
1:F:349:ASP:O	1:F:352:ASN:HB2	2.18	0.43
1:A:152:ARG:CZ	1:A:179:GLN:HG3	2.48	0.43
1:G:350:ARG:HG2	1:G:350:ARG:H	1.47	0.43
1:D:254:ARG:HH21	1:D:381:PHE:HB3	1.83	0.43
1:B:234:GLU:HG2	1:B:239:VAL:CG2	2.48	0.43
1:D:339:MET:HE3	1:D:363:GLU:HG3	2.01	0.43
1:A:339:MET:HE3	1:A:363:GLU:HG3	2.00	0.43
1:C:239:VAL:HG12	1:C:373:PRO:HB3	2.01	0.43
1:B:258:ILE:HD11	1:B:381:PHE:CZ	2.54	0.43
1:G:152:ARG:HG2	1:G:370:HIS:O	2.19	0.42
1:C:264:GLN:HB3	1:C:377:ILE:CD1	2.49	0.42
1:F:131:ARG:HH21	1:F:316:THR:HA	1.84	0.42
1:D:264:GLN:HB3	1:D:377:ILE:CD1	2.48	0.42
1:E:258:ILE:HD12	1:E:308:MET:HE1	2.01	0.42
1:C:193:SER:HB3	1:C:196:VAL:HG23	2.01	0.42
1:D:187:ALA:HB3	1:E:169:LYS:HE2	2.02	0.42
1:B:119:MET:HB3	1:C:148:LEU:CD2	2.49	0.42
1:B:254:ARG:O	1:B:258:ILE:HD13	2.19	0.42
1:D:295:TYR:HE1	1:D:300:PRO:HG3	1.84	0.42
1:C:258:ILE:O	1:C:262:ILE:HG13	2.19	0.42
1:E:117:GLN:HA	1:E:118:PRO:HD3	1.91	0.42
1:G:308:MET:HG2	1:G:309:TRP:CD1	2.55	0.42
1:B:277:LEU:N	1:B:277:LEU:HD12	2.34	0.42
1:D:325:THR:HA	1:D:377:ILE:O	2.18	0.42
1:G:152:ARG:NE	1:G:179:GLN:HG3	2.35	0.42
1:F:324:PHE:HB3	1:F:381:PHE:HE1	1.84	0.42
1:A:199:ASP:O	1:A:201:PRO:HD3	2.19	0.42
1:E:119:MET:HB3	1:F:148:LEU:CD2	2.49	0.42
1:A:159:ASN:H	1:A:172:SER:HB3	1.85	0.42
1:F:254:ARG:HB3	1:F:381:PHE:HE2	1.84	0.42
1:D:308:MET:HG2	1:D:309:TRP:CD1	2.54	0.42
1:A:342:THR:HG22	1:A:343:VAL:N	2.34	0.42
1:E:311:LEU:HA	1:E:312:PRO:HD3	1.92	0.42
1:G:311:LEU:HA	1:G:312:PRO:HD3	1.88	0.42
1:F:350:ARG:HG3	1:F:351:ASP:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:ALA:HB2	1:F:363:GLU:HA	2.01	0.42
1:A:281:ASP:O	1:A:285:ILE:HG13	2.20	0.42
1:F:219:GLU:HG3	1:F:366:LEU:HD11	2.01	0.42
1:E:121:ILE:HA	1:E:122:PRO:HD3	1.92	0.41
1:F:223:LEU:O	1:F:236:LEU:HG	2.20	0.41
1:E:150:TYR:CE1	1:E:179:GLN:HB2	2.55	0.41
1:A:153:GLU:CA	1:A:176:PHE:HB3	2.46	0.41
1:F:147:ALA:HA	1:F:183:VAL:HG23	2.02	0.41
1:A:182:ASN:HB2	1:A:184:LYS:HE2	2.02	0.41
1:C:371:TYR:CD1	1:C:371:TYR:N	2.88	0.41
1:G:342:THR:HG22	1:G:343:VAL:N	2.36	0.41
1:G:224:LEU:HD21	1:G:319:GLN:OE1	2.19	0.41
1:F:130:ARG:C	1:F:132:LEU:N	2.73	0.41
1:E:234:GLU:HG2	1:E:239:VAL:HG22	2.01	0.41
1:C:197:MET:HG3	1:C:358:LEU:HD23	2.02	0.41
1:G:259:ALA:HA	1:G:262:ILE:HD12	2.02	0.41
1:E:134:ILE:HB	1:E:220:GLU:HG3	2.02	0.41
1:A:295:TYR:HB2	1:A:299:GLY:HA2	2.03	0.41
1:C:289:LYS:NZ	1:D:253:THR:HG23	2.35	0.41
1:B:264:GLN:HB3	1:B:377:ILE:CD1	2.51	0.41
1:G:203:LEU:HD21	1:G:207:ILE:HD11	2.02	0.41
1:G:294:ARG:HD3	1:G:295:TYR:H	1.85	0.41
1:G:351:ASP:O	1:G:353:PHE:N	2.54	0.41
1:G:358:LEU:HD23	1:G:359:THR:N	2.36	0.41
1:B:234:GLU:HG2	1:B:239:VAL:HG23	2.03	0.41
1:A:354:VAL:O	1:A:354:VAL:HG12	2.21	0.41
1:D:219:GLU:HG3	1:D:366:LEU:HD11	2.03	0.41
1:A:171:GLU:HB2	1:F:189:TRP:CZ2	2.55	0.41
1:E:357:MET:HG3	1:E:358:LEU:H	1.85	0.41
1:D:226:GLY:N	1:D:235:GLY:HA3	2.35	0.41
1:G:139:ALA:O	1:G:334:GLN:HB2	2.20	0.41
1:A:258:ILE:N	1:A:258:ILE:HD12	2.36	0.41
1:F:257:ILE:O	1:F:260:HIS:HB2	2.21	0.41
1:C:292:GLU:O	1:D:290:ASP:HB2	2.21	0.41
1:G:343:VAL:HG22	1:G:362:CYS:SG	2.61	0.41
1:E:187:ALA:HB3	1:F:169:LYS:HE2	2.03	0.41
1:B:266:THR:C	1:B:268:SER:H	2.22	0.41
1:E:329:PHE:C	1:E:331:MET:H	2.24	0.41
1:A:203:LEU:O	1:A:207:ILE:HG13	2.20	0.41
1:F:210:ARG:HD2	1:F:210:ARG:HA	1.97	0.41
1:B:311:LEU:HA	1:B:312:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PHE:N	1:A:176:PHE:CD1	2.89	0.40
1:G:135:ARG:HH11	1:G:135:ARG:HG3	1.85	0.40
1:A:351:ASP:OD1	1:A:355:LYS:HE2	2.22	0.40
1:A:308:MET:HG2	1:A:309:TRP:CD1	2.55	0.40
1:E:207:ILE:O	1:E:211:LEU:HD13	2.21	0.40
1:G:193:SER:HB2	1:G:195:GLN:HE22	1.86	0.40
1:B:202:MET:HG2	1:B:203:LEU:N	2.36	0.40
1:F:276:VAL:HB	1:F:325:THR:HB	2.03	0.40
1:E:194:ARG:HH22	1:E:347:ARG:CZ	2.34	0.40
1:E:258:ILE:O	1:E:262:ILE:HG13	2.22	0.40
1:A:257:ILE:O	1:A:260:HIS:HB2	2.22	0.40
1:E:289:LYS:HA	1:E:294:ARG:O	2.21	0.40
1:G:193:SER:HB2	1:G:195:GLN:HE21	1.85	0.40
1:C:138:LEU:HD22	1:C:333:SER:HB2	2.04	0.40
1:B:258:ILE:O	1:B:262:ILE:HG13	2.21	0.40
1:B:371:TYR:O	1:B:373:PRO:HD3	2.22	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	278/282 (99%)	249 (90%)	27 (10%)	2 (1%)	26	71
1	B	278/282 (99%)	252 (91%)	22 (8%)	4 (1%)	14	58
1	C	278/282 (99%)	258 (93%)	20 (7%)	0	100	100
1	D	278/282 (99%)	256 (92%)	22 (8%)	0	100	100
1	E	278/282 (99%)	246 (88%)	29 (10%)	3 (1%)	17	63
1	F	254/282 (90%)	229 (90%)	21 (8%)	4 (2%)	12	56
1	G	239/282 (85%)	208 (87%)	27 (11%)	4 (2%)	11	55
All	All	1883/1974 (95%)	1698 (90%)	168 (9%)	17 (1%)	21	67

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	300	PRO
1	F	352	ASN
1	G	352	ASN
1	E	330	ASP
1	G	224	LEU
1	A	201	PRO
1	B	127	PRO
1	B	230	GLY
1	F	131	ARG
1	G	349	ASP
1	B	352	ASN
1	E	144	SER
1	F	240	ALA
1	F	300	PRO
1	G	230	GLY
1	A	315	PRO
1	B	300	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/231 (100%)	214 (93%)	16 (7%)	19	56
1	B	230/231 (100%)	221 (96%)	9 (4%)	39	72
1	C	230/231 (100%)	226 (98%)	4 (2%)	68	87
1	D	230/231 (100%)	223 (97%)	7 (3%)	48	77
1	E	230/231 (100%)	223 (97%)	7 (3%)	48	77
1	F	211/231 (91%)	205 (97%)	6 (3%)	51	78
1	G	201/231 (87%)	190 (94%)	11 (6%)	27	63
All	All	1562/1617 (97%)	1502 (96%)	60 (4%)	40	73

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASP
1	A	115	LEU
1	A	117	GLN
1	A	148	LEU
1	A	149	GLU
1	A	156	PHE
1	A	169	LYS
1	A	176	PHE
1	A	179	GLN
1	A	188	HIS
1	A	195	GLN
1	A	202	MET
1	A	270	PHE
1	A	301	GLN
1	A	303	PHE
1	A	316	THR
1	B	146	ASN
1	B	188	HIS
1	B	195	GLN
1	B	202	MET
1	B	224	LEU
1	B	227	ASP
1	B	277	LEU
1	B	303	PHE
1	B	344	GLU
1	C	188	HIS
1	C	202	MET
1	C	224	LEU
1	C	303	PHE
1	D	146	ASN
1	D	152	ARG
1	D	188	HIS
1	D	194	ARG
1	D	202	MET
1	D	292	GLU
1	D	303	PHE
1	E	142	ARG
1	E	152	ARG
1	E	188	HIS
1	E	195	GLN
1	E	280	ARG
1	E	300	PRO
1	E	303	PHE

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Mol	Chain	Res	Type
1	F	133	THR
1	F	135	ARG
1	F	156	PHE
1	F	188	HIS
1	F	227	ASP
1	F	292	GLU
1	G	129	LEU
1	G	142	ARG
1	G	173	ASP
1	G	195	GLN
1	G	256	ASP
1	G	290	ASP
1	G	294	ARG
1	G	301	GLN
1	G	350	ARG
1	G	370	HIS
1	G	383	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	204	GLN
1	A	225	ASN
1	A	237	ASN
1	A	334	GLN
1	B	120	GLN
1	B	191	GLN
1	B	222	GLN
1	B	301	GLN
1	B	334	GLN
1	B	352	ASN
1	C	159	ASN
1	C	191	GLN
1	C	222	GLN
1	C	334	GLN
1	C	352	ASN
1	D	191	GLN
1	D	222	GLN
1	D	232	ASN
1	D	334	GLN
1	D	352	ASN

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Mol	Chain	Res	Type
1	E	191	GLN
1	E	208	ASN
1	E	237	ASN
1	E	291	ASN
1	E	334	GLN
1	E	352	ASN
1	F	222	GLN
1	F	260	HIS
1	F	334	GLN
1	G	195	GLN
1	G	232	ASN
1	G	237	ASN
1	G	260	HIS
1	G	319	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	280/282 (99%)	-0.08	4 (1%)	78	72	58, 58, 58, 58	0
1	B	280/282 (99%)	-0.17	3 (1%)	82	78	54, 54, 54, 54	0
1	C	280/282 (99%)	-0.08	3 (1%)	82	78	53, 53, 53, 53	0
1	D	280/282 (99%)	-0.12	6 (2%)	67	62	54, 54, 54, 54	0
1	E	280/282 (99%)	-0.18	3 (1%)	82	78	48, 48, 48, 48	0
1	F	256/282 (90%)	-0.19	4 (1%)	74	69	61, 61, 61, 61	0
1	G	243/282 (86%)	0.21	18 (7%)	17	21	99, 99, 99, 99	0
All	All	1899/1974 (96%)	-0.09	41 (2%)	65	61	48, 54, 99, 99	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	SER	5.7
1	G	299	GLY	4.9
1	B	104	SER	4.9
1	C	104	SER	4.7
1	D	104	SER	4.2
1	G	298	GLY	3.9
1	A	105	LEU	3.9
1	G	300	PRO	3.8
1	B	105	LEU	3.4
1	E	104	SER	3.2
1	G	250	THR	3.1
1	G	383	SER	3.1
1	G	191	GLN	2.9
1	G	344	GLU	2.9
1	D	167	ALA	2.8
1	G	360	ILE	2.7
1	G	302	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	105	LEU	2.6
1	F	383	SER	2.6
1	A	106	GLY	2.5
1	F	167	ALA	2.5
1	G	304	THR	2.5
1	G	301	GLN	2.5
1	E	123	GLY	2.4
1	D	164	ALA	2.3
1	G	303	PHE	2.3
1	G	158	ASN	2.3
1	D	105	LEU	2.3
1	G	382	SER	2.3
1	E	115	LEU	2.3
1	G	147	ALA	2.2
1	G	172	SER	2.2
1	F	166	LYS	2.2
1	B	123	GLY	2.2
1	C	274	GLY	2.2
1	D	274	GLY	2.1
1	D	166	LYS	2.1
1	F	344	GLU	2.1
1	A	304	THR	2.0
1	G	157	THR	2.0
1	G	173	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.