Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:49 PM GMT

PDB ID	:	1M7W
Title	:	HNF4a ligand binding domain with bound fatty acid
Authors	:	Dhe-Paganon, S.; Duda, K.; Iwamoto, M.; Chi, Y.I.; Shoelson, S.E.
Deposited on	:	2002-07-22
Resolution	:	2.80 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 (i)) were used in the production of this report:

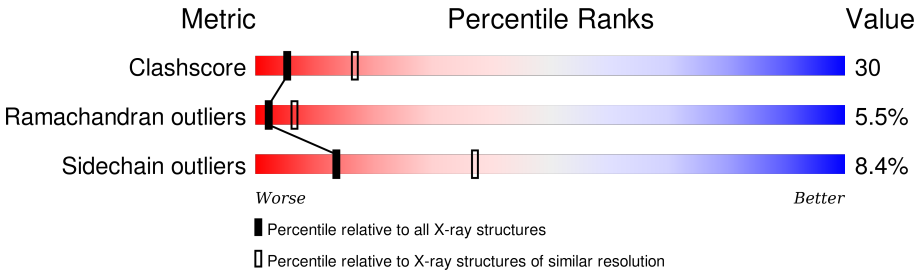
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	51% 29% 8% • 11%
1	B	250	38% 38% 10% 13%
1	C	250	42% 38% 7% • 12%
1	D	250	43% 39% 6% 12%

2 Entry composition

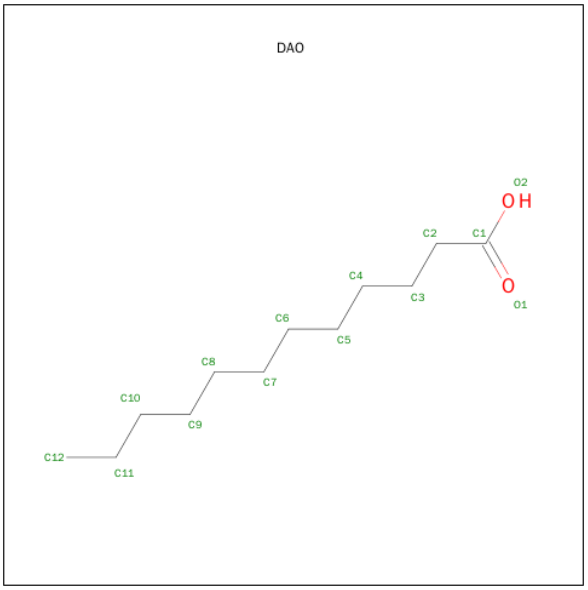
There are 3 unique types of molecules in this entry. The entry contains 7176 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hepatocyte nuclear factor 4-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1777	1140	298	329	10			
1	B	218	Total	C	N	O	S	0	0	0
			1745	1122	293	320	10			
1	C	220	Total	C	N	O	S	0	0	0
			1759	1131	295	323	10			
1	D	221	Total	C	N	O	S	0	0	0
			1765	1134	296	325	10			

- Molecule 2 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	12	2		
2	B	1	Total	C	O	0	0
			14	12	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 14 12 2	0	0
2	D	1	Total C O 14 12 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	17	Total O 17 17	0	0
3	B	22	Total O 22 22	0	0
3	C	19	Total O 19 19	0	0
3	D	16	Total O 16 16	0	0

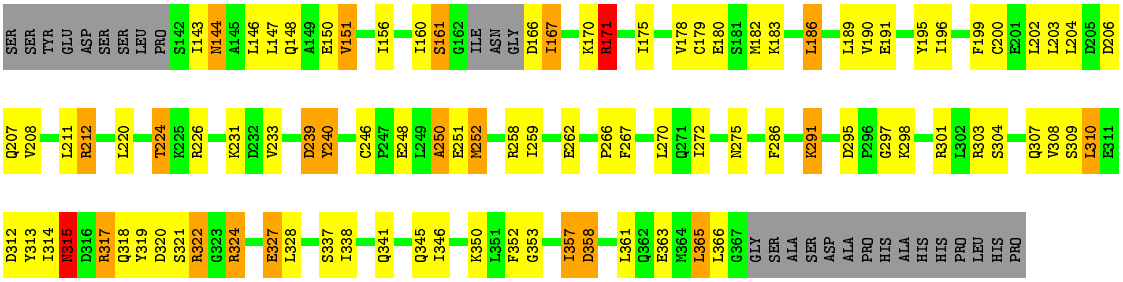
3 Residue-property plots (i)

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

Note EDS was not executed.

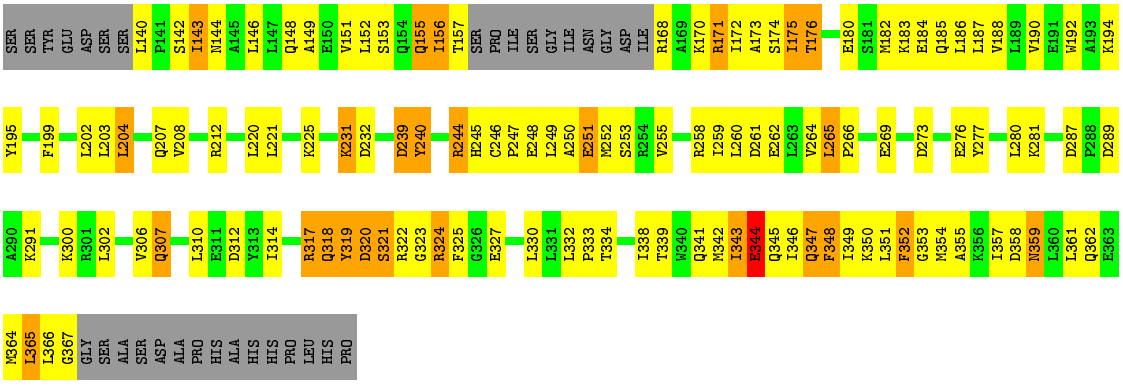
- Molecule 1: Hepatocyte nuclear factor 4-alpha

Chain A:



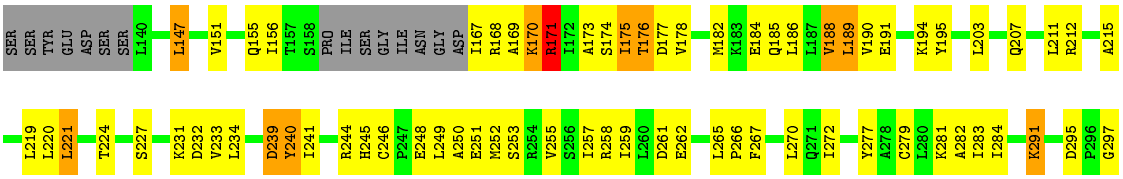
- Molecule 1: Hepatocyte nuclear factor 4-alpha

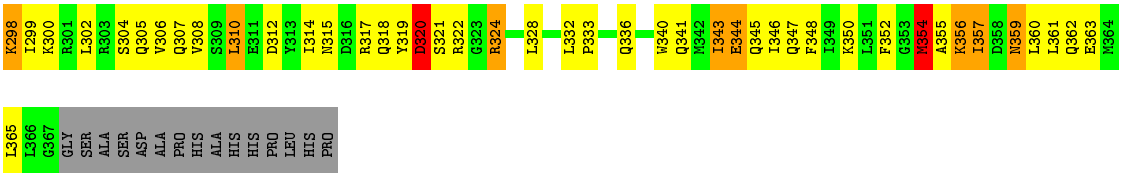
Chain B:



- Molecule 1: Hepatocyte nuclear factor 4-alpha

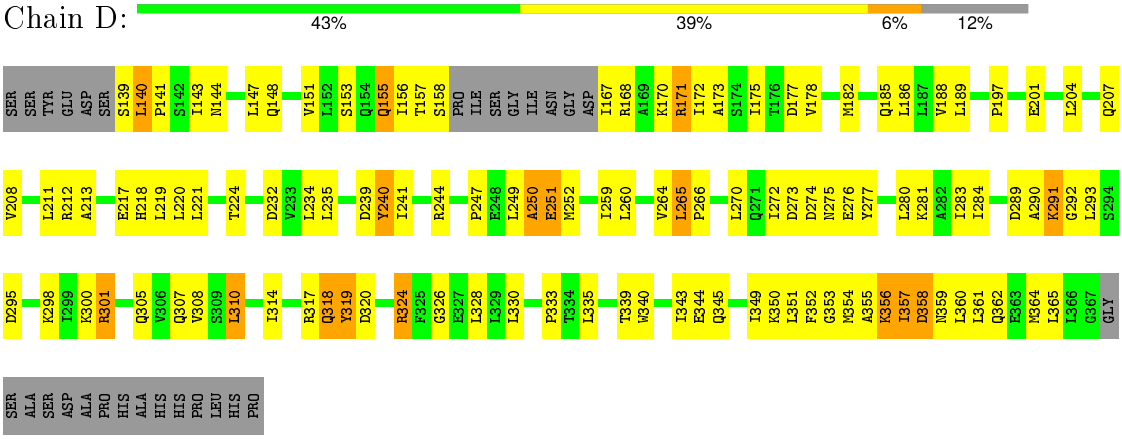
Chain C:





- Molecule 1: Hepatocyte nuclear factor 4-alpha

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	102.29Å 102.29Å 227.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7176	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAO

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	0.40	0/1803	0.63	0/2435
1	B	0.40	0/1771	0.64	0/2392
1	C	0.41	0/1785	0.68	1/2411 (0.0%)
1	D	0.39	0/1791	0.63	0/2419
All	All	0.40	0/7150	0.65	1/9657 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	347	GLN	N-CA-C	-5.43	96.33	111.00

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	1777	0	1834	89	0
1	B	1745	0	1806	119	0
1	C	1759	0	1822	119	0
1	D	1765	0	1827	117	0
2	A	14	0	23	1	0
2	B	14	0	23	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	14	0	23	1	0
2	D	14	0	23	1	0
3	A	17	0	0	3	0
3	B	22	0	0	3	0
3	C	19	0	0	3	0
3	D	16	0	0	3	0
All	All	7176	0	7381	435	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 30.

All (435) 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:340:TRP:NE1	3:D:48:HOH:O	1.86	1.07
1:C:291:LYS:HD2	1:C:291:LYS:H	1.24	1.01
1:C:324:ARG:HG2	1:C:324:ARG:HH11	1.25	1.01
1:D:356:LYS:HA	1:D:356:LYS:HE3	1.41	1.00
1:C:170:LYS:O	1:C:171:ARG:HB2	1.64	0.98
1:B:361:LEU:O	1:B:365:LEU:HB2	1.63	0.96
1:D:173:ALA:HB2	1:D:240:TYR:HB3	1.50	0.94
1:A:324:ARG:HG2	1:A:324:ARG:HH11	1.30	0.92
1:D:220:LEU:O	1:D:224:THR:HG22	1.70	0.92
1:D:340:TRP:CE2	3:D:48:HOH:O	2.17	0.91
1:B:357:ILE:O	1:B:361:LEU:HG	1.72	0.90
1:A:322:ARG:HH11	1:A:322:ARG:HG2	1.34	0.90
1:D:324:ARG:HG2	1:D:324:ARG:HH11	1.38	0.88
1:B:252:MET:SD	1:B:345:GLN:HG2	2.14	0.87
1:B:345:GLN:O	1:B:348:PHE:HB2	1.74	0.86
1:D:218:HIS:HD2	1:D:281:LYS:HE2	1.42	0.85
1:C:291:LYS:N	1:C:291:LYS:HD2	1.92	0.84
1:B:168:ARG:HD2	1:B:170:LYS:HE2	1.58	0.84
1:B:355:ALA:HA	1:B:358:ASP:HB3	1.61	0.82
1:B:173:ALA:HB2	1:B:240:TYR:HB3	1.59	0.82
1:A:304:SER:O	1:A:308:VAL:HG23	1.79	0.82
1:A:175:ILE:HD12	1:A:175:ILE:H	1.42	0.82
1:C:360:LEU:HA	1:C:363:GLU:HB2	1.63	0.81
1:C:168:ARG:HH11	1:C:168:ARG:HA	1.44	0.80
1:D:147:LEU:O	1:D:151:VAL:HG23	1.81	0.80
1:C:281:LYS:HE2	3:C:41:HOH:O	1.81	0.80
1:C:291:LYS:CD	1:C:291:LYS:H	1.90	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ALA:O	1:C:251:GLU:HB3	1.82	0.77
1:C:248:GLU:CD	1:C:248:GLU:H	1.88	0.77
1:B:185:GLN:O	1:B:188:VAL:HG22	1.84	0.76
1:C:307:GLN:HG3	1:C:308:VAL:N	2.01	0.76
1:B:314:ILE:HG22	1:B:321:SER:HB2	1.70	0.73
1:B:324:ARG:HH11	1:B:324:ARG:HG2	1.53	0.73
1:C:221:LEU:O	1:C:224:THR:HG22	1.90	0.72
1:B:232:ASP:OD1	1:B:244:ARG:HD3	1.90	0.72
1:C:175:ILE:HD12	1:C:175:ILE:H	1.55	0.72
1:A:324:ARG:NH1	1:A:324:ARG:HG2	2.04	0.71
1:C:168:ARG:CA	1:C:168:ARG:HH11	2.03	0.71
1:D:357:ILE:O	1:D:358:ASP:HB2	1.90	0.71
1:D:170:LYS:O	1:D:171:ARG:HB3	1.91	0.71
1:C:265:LEU:HB3	1:C:266:PRO:HD3	1.72	0.71
1:C:151:VAL:O	1:C:155:GLN:HG3	1.91	0.71
1:C:307:GLN:HG3	1:C:308:VAL:H	1.57	0.70
1:B:180:GLU:O	1:B:184:GLU:HG3	1.91	0.70
1:D:234:LEU:HG	1:D:260:LEU:HD21	1.74	0.70
1:B:343:ILE:HG22	1:B:344:GLU:N	2.06	0.70
1:C:175:ILE:HD12	1:C:175:ILE:N	2.06	0.70
1:B:249:LEU:O	1:B:253:SER:HB2	1.92	0.69
1:C:324:ARG:NH1	1:C:324:ARG:HG2	2.02	0.69
1:C:312:ASP:HA	1:C:315:ASN:HD21	1.57	0.69
1:C:336:GLN:O	1:C:340:TRP:HD1	1.76	0.69
1:D:356:LYS:CE	1:D:356:LYS:HA	2.21	0.68
1:C:314:ILE:O	1:C:317:ARG:HB2	1.92	0.68
1:C:186:LEU:HD13	1:C:219:LEU:HD11	1.74	0.68
1:B:310:LEU:O	1:B:314:ILE:HG12	1.92	0.68
1:A:312:ASP:HA	1:A:315:ASN:HB2	1.73	0.68
1:C:356:LYS:HE2	1:C:356:LYS:HA	1.76	0.68
1:C:295:ASP:OD2	1:C:298:LYS:HB2	1.94	0.67
1:B:248:GLU:CD	1:B:248:GLU:H	1.98	0.67
1:D:272:ILE:HD11	1:D:328:LEU:HD22	1.77	0.67
1:C:310:LEU:O	1:C:314:ILE:HG12	1.93	0.66
1:D:239:ASP:O	1:D:240:TYR:HB2	1.95	0.66
1:C:239:ASP:O	1:C:240:TYR:HB2	1.95	0.66
1:D:298:LYS:HA	1:D:301:ARG:NH1	2.09	0.66
1:B:170:LYS:O	1:B:171:ARG:HB3	1.95	0.66
1:C:312:ASP:HA	1:C:315:ASN:ND2	2.11	0.66
1:A:312:ASP:O	1:A:315:ASN:HB2	1.96	0.66
1:B:204:LEU:O	1:B:208:VAL:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:ARG:CG	1:C:324:ARG:HH11	2.04	0.65
1:D:186:LEU:HG	1:D:364:MET:CE	2.26	0.65
1:D:276:GLU:OE1	1:D:324:ARG:NH1	2.24	0.65
1:D:357:ILE:HG22	1:D:358:ASP:N	2.11	0.65
1:D:144:ASN:O	1:D:148:GLN:HG2	1.97	0.65
1:B:190:VAL:O	1:B:194:LYS:HG2	1.97	0.65
1:B:246:CYS:SG	1:B:249:LEU:HB2	2.37	0.64
1:A:322:ARG:HH11	1:A:322:ARG:CG	2.10	0.64
1:A:220:LEU:HD22	1:A:259:ILE:HD11	1.79	0.64
1:B:265:LEU:HD22	1:B:269:GLU:OE2	1.98	0.64
1:C:357:ILE:O	1:C:360:LEU:HB2	1.97	0.63
1:A:148:GLN:HA	1:A:151:VAL:HG12	1.80	0.63
1:B:151:VAL:O	1:B:155:GLN:HB2	1.96	0.63
1:D:324:ARG:CG	1:D:324:ARG:HH11	2.10	0.63
1:C:345:GLN:O	1:C:348:PHE:HB2	1.98	0.63
1:D:155:GLN:O	1:D:158:SER:N	2.30	0.63
1:A:202:LEU:HD22	1:A:298:LYS:HE3	1.80	0.63
1:D:351:LEU:C	1:D:352:PHE:HD2	2.01	0.63
1:B:258:ARG:HH11	1:B:341:GLN:NE2	1.96	0.63
1:B:232:ASP:HB3	1:B:244:ARG:HB2	1.80	0.62
1:C:356:LYS:O	1:C:357:ILE:HG13	1.99	0.62
1:D:185:GLN:O	1:D:188:VAL:HG22	1.99	0.62
1:A:212:ARG:HG2	1:A:363:GLU:O	1.99	0.62
1:D:349:ILE:HG23	1:D:355:ALA:HB3	1.81	0.62
1:C:255:VAL:O	1:C:259:ILE:HG13	1.99	0.62
1:C:258:ARG:HH11	1:C:341:GLN:NE2	1.97	0.62
1:A:199:PHE:CZ	1:A:207:GLN:HB3	2.35	0.62
1:A:291:LYS:NZ	1:A:291:LYS:H	1.98	0.61
1:C:250:ALA:C	1:C:252:MET:H	2.04	0.61
1:D:186:LEU:HG	1:D:364:MET:HE2	1.83	0.61
1:D:295:ASP:OD2	1:D:298:LYS:HB2	2.00	0.61
1:B:261:ASP:O	1:B:265:LEU:HB2	2.01	0.60
1:B:225:LYS:HB2	1:B:277:TYR:CE1	2.36	0.60
1:D:283:ILE:HD11	1:D:307:GLN:HA	1.83	0.60
1:B:255:VAL:O	1:B:259:ILE:HG13	2.00	0.60
1:A:291:LYS:HZ1	1:A:291:LYS:H	1.47	0.60
1:D:252:MET:HB3	2:D:703:DAO:H102	1.81	0.60
1:D:156:ILE:O	1:D:156:ILE:HG22	2.01	0.60
1:A:179:CYS:O	1:A:183:LYS:HG3	2.02	0.60
1:C:346:ILE:C	1:C:348:PHE:N	2.53	0.60
1:B:244:ARG:HD2	1:B:260:LEU:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:LEU:HD13	1:C:361:LEU:O	2.02	0.60
1:C:343:ILE:HG22	1:C:344:GLU:N	2.15	0.59
1:D:173:ALA:HB1	1:D:177:ASP:HB2	1.82	0.59
1:D:270:LEU:HD13	1:D:328:LEU:HD23	1.82	0.59
1:A:322:ARG:NH1	1:A:322:ARG:HG2	2.11	0.59
1:B:142:SER:O	1:B:144:ASN:N	2.36	0.59
1:C:221:LEU:HD22	1:C:277:TYR:HE1	1.67	0.59
1:A:160:ILE:O	1:A:161:SER:O	2.20	0.59
1:A:203:LEU:HD23	3:A:39:HOH:O	2.02	0.58
1:B:172:ILE:HG21	1:B:248:GLU:HG3	1.86	0.58
1:D:330:LEU:O	1:D:333:PRO:HD2	2.03	0.58
1:C:346:ILE:C	1:C:348:PHE:H	2.05	0.58
1:D:155:GLN:O	1:D:156:ILE:C	2.40	0.58
1:B:291:LYS:NZ	1:B:291:LYS:HB2	2.19	0.58
1:A:304:SER:HA	1:A:307:GLN:HG2	1.85	0.57
1:D:350:LYS:NZ	1:D:362:GLN:HE22	2.02	0.57
1:C:348:PHE:O	1:C:352:PHE:N	2.33	0.57
1:D:173:ALA:HB2	1:D:240:TYR:CB	2.30	0.57
1:B:276:GLU:OE1	1:B:324:ARG:NH1	2.37	0.57
1:C:295:ASP:O	1:C:298:LYS:HB3	2.04	0.57
1:D:167:ILE:N	1:D:170:LYS:HD3	2.20	0.57
1:D:220:LEU:HD22	1:D:259:ILE:HD11	1.86	0.57
1:B:322:ARG:HG3	1:B:322:ARG:HH11	1.69	0.57
1:B:324:ARG:NH1	1:B:324:ARG:HG2	2.19	0.57
1:C:147:LEU:O	1:C:151:VAL:HG23	2.05	0.57
1:D:350:LYS:HG3	1:D:357:ILE:HG12	1.85	0.57
1:C:253:SER:O	1:C:257:ILE:HG13	2.05	0.57
1:A:365:LEU:O	1:A:366:LEU:HD23	2.04	0.57
1:A:147:LEU:HD22	1:A:275:ASN:OD1	2.05	0.57
1:B:355:ALA:O	1:B:359:ASN:HB2	2.04	0.56
1:D:324:ARG:HG2	1:D:324:ARG:NH1	2.14	0.56
1:C:354:MET:O	1:C:356:LYS:N	2.39	0.56
1:B:244:ARG:HD2	1:B:260:LEU:HD13	1.88	0.56
1:B:355:ALA:O	1:B:359:ASN:N	2.39	0.56
1:A:314:ILE:O	1:A:315:ASN:C	2.43	0.56
1:A:246:CYS:SG	1:A:248:GLU:HG2	2.46	0.56
1:A:357:ILE:O	1:A:358:ASP:CB	2.53	0.56
1:C:252:MET:SD	1:C:345:GLN:NE2	2.79	0.56
1:D:232:ASP:OD2	1:D:244:ARG:HD2	2.05	0.56
1:A:258:ARG:HH11	1:A:341:GLN:NE2	2.03	0.56
1:C:173:ALA:HB2	1:C:240:TYR:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ILE:HD11	1:C:191:GLU:OE1	2.06	0.55
1:D:197:PRO:O	1:D:201:GLU:HG3	2.07	0.55
1:B:346:ILE:C	1:B:348:PHE:N	2.60	0.55
1:B:171:ARG:O	1:B:240:TYR:HA	2.07	0.55
1:B:318:GLN:O	1:B:320:ASP:N	2.40	0.55
1:B:252:MET:HE1	1:B:346:ILE:HA	1.88	0.55
1:D:208:VAL:CG1	1:D:212:ARG:HD3	2.37	0.55
1:A:267:PHE:CE1	1:A:272:ILE:HD12	2.42	0.55
1:A:220:LEU:O	1:A:224:THR:HG23	2.07	0.55
1:C:178:VAL:HG21	1:C:249:LEU:HD11	1.88	0.55
1:D:221:LEU:HD13	1:D:277:TYR:CE1	2.42	0.54
1:C:221:LEU:HD22	1:C:277:TYR:CE1	2.42	0.54
1:D:186:LEU:CD1	1:D:219:LEU:HD11	2.38	0.54
1:B:287:ASP:OD1	1:B:289:ASP:N	2.35	0.54
1:C:324:ARG:CG	1:C:324:ARG:NH1	2.67	0.54
1:D:239:ASP:O	1:D:240:TYR:CB	2.56	0.54
1:B:343:ILE:O	1:B:346:ILE:N	2.39	0.54
1:B:273:ASP:HB3	3:B:42:HOH:O	2.08	0.54
1:B:346:ILE:O	1:B:348:PHE:N	2.41	0.54
1:C:156:ILE:HG22	1:C:156:ILE:O	2.08	0.54
1:B:192:TRP:CE2	1:B:281:LYS:HD3	2.43	0.54
1:B:347:GLN:O	1:B:351:LEU:HB2	2.08	0.54
1:A:270:LEU:O	1:A:324:ARG:NH2	2.26	0.54
1:A:322:ARG:NH1	1:A:322:ARG:CG	2.70	0.53
1:B:170:LYS:O	1:B:171:ARG:CB	2.55	0.53
1:D:276:GLU:CD	1:D:324:ARG:HH12	2.11	0.53
1:D:218:HIS:CD2	1:D:281:LYS:HE2	2.33	0.53
1:B:204:LEU:HD13	1:C:184:GLU:HB3	1.91	0.53
1:C:185:GLN:HA	1:C:188:VAL:CG1	2.38	0.53
1:D:170:LYS:HG3	1:D:239:ASP:OD2	2.09	0.53
1:B:239:ASP:O	1:B:240:TYR:HB2	2.08	0.53
1:B:322:ARG:HG3	1:B:322:ARG:NH1	2.24	0.53
3:A:51:HOH:O	1:B:300:LYS:HE2	2.10	0.52
1:B:323:GLY:O	1:B:327:GLU:HB2	2.09	0.52
1:D:213:ALA:HA	1:D:291:LYS:HZ1	1.73	0.52
1:B:183:LYS:HE2	1:C:212:ARG:NH1	2.24	0.52
1:A:252:MET:HG2	2:A:700:DAO:H123	1.91	0.52
1:B:172:ILE:HG21	1:B:248:GLU:CG	2.39	0.52
1:B:146:LEU:O	1:B:149:ALA:N	2.41	0.52
1:B:346:ILE:C	1:B:348:PHE:H	2.12	0.52
1:C:203:LEU:O	1:C:207:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ASP:HB3	1:A:298:LYS:HE2	1.92	0.52
1:D:307:GLN:HG3	1:D:308:VAL:N	2.25	0.52
1:D:349:ILE:CG2	1:D:355:ALA:HB3	2.39	0.51
1:C:174:SER:O	1:C:175:ILE:C	2.48	0.51
1:C:250:ALA:C	1:C:252:MET:N	2.63	0.51
1:A:320:ASP:C	1:A:322:ARG:H	2.13	0.51
1:B:148:GLN:O	1:B:152:LEU:HG	2.11	0.51
1:D:318:GLN:O	1:D:319:TYR:O	2.28	0.51
1:D:247:PRO:HA	1:D:250:ALA:HB2	1.91	0.51
1:B:320:ASP:O	1:B:321:SER:HB3	2.10	0.51
1:C:315:ASN:C	1:C:317:ARG:H	2.13	0.51
1:C:252:MET:HA	1:C:345:GLN:NE2	2.26	0.51
1:A:202:LEU:CD2	1:A:298:LYS:HE3	2.41	0.51
1:B:220:LEU:HD12	1:B:339:THR:OG1	2.10	0.51
1:B:349:ILE:HA	1:B:352:PHE:HB3	1.92	0.51
1:A:143:ILE:HG13	1:A:309:SER:HB3	1.93	0.51
1:A:291:LYS:HB2	1:A:291:LYS:HZ2	1.75	0.51
1:A:220:LEU:CD2	1:A:259:ILE:HD11	2.40	0.50
1:D:265:LEU:HB2	1:D:266:PRO:HD3	1.93	0.50
1:D:310:LEU:O	1:D:314:ILE:HG12	2.11	0.50
1:D:186:LEU:HD12	1:D:219:LEU:HD21	1.93	0.50
1:D:173:ALA:HB1	1:D:177:ASP:CB	2.41	0.50
1:B:208:VAL:HG12	1:B:212:ARG:HD3	1.93	0.50
1:B:250:ALA:O	1:B:251:GLU:CB	2.60	0.50
1:D:280:LEU:O	1:D:284:ILE:HG13	2.11	0.50
1:B:355:ALA:HA	1:B:358:ASP:CB	2.38	0.50
1:C:185:GLN:HA	1:C:188:VAL:HG13	1.92	0.50
1:C:270:LEU:HD13	1:C:328:LEU:CD2	2.41	0.50
1:A:357:ILE:O	1:A:358:ASP:HB2	2.12	0.50
1:A:144:ASN:O	1:A:148:GLN:HG2	2.11	0.50
1:B:352:PHE:CD1	1:B:353:GLY:N	2.80	0.50
1:B:334:THR:O	1:B:338:ILE:HG13	2.12	0.49
1:A:310:LEU:O	1:A:314:ILE:HG13	2.12	0.49
1:A:312:ASP:CA	1:A:315:ASN:HB2	2.41	0.49
1:B:265:LEU:CB	1:B:266:PRO:HD3	2.42	0.49
1:D:317:ARG:O	1:D:318:GLN:HB2	2.12	0.49
1:C:251:GLU:O	1:C:345:GLN:NE2	2.46	0.49
1:B:140:LEU:HD12	1:B:140:LEU:C	2.32	0.49
1:B:260:LEU:O	1:B:264:VAL:HB	2.12	0.49
1:A:327:GLU:OE1	1:B:307:GLN:NE2	2.45	0.49
1:A:270:LEU:HD11	1:A:327:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:MET:HB3	2:B:701:DAO:H121	1.93	0.49
1:C:174:SER:O	1:C:176:THR:N	2.46	0.49
1:B:168:ARG:HB2	1:B:170:LYS:HG2	1.93	0.49
1:D:186:LEU:HD13	1:D:219:LEU:HD11	1.95	0.49
1:D:291:LYS:HD2	1:D:291:LYS:N	2.27	0.49
1:A:175:ILE:H	1:A:175:ILE:CD1	2.17	0.49
1:C:220:LEU:HD21	1:C:259:ILE:CD1	2.42	0.49
1:A:156:ILE:HD13	1:A:195:TYR:OH	2.12	0.49
1:A:310:LEU:O	1:A:310:LEU:HD22	2.13	0.48
1:B:220:LEU:HD22	1:B:259:ILE:HD11	1.95	0.48
1:D:249:LEU:O	1:D:250:ALA:C	2.50	0.48
1:B:245:HIS:C	1:B:247:PRO:HD3	2.33	0.48
1:B:281:LYS:HE2	3:B:44:HOH:O	2.13	0.48
1:C:189:LEU:HD23	1:C:189:LEU:O	2.13	0.48
1:A:204:LEU:O	1:A:208:VAL:HG23	2.13	0.48
1:D:324:ARG:NH1	1:D:324:ARG:CG	2.71	0.48
1:D:352:PHE:O	1:D:354:MET:HG3	2.13	0.48
1:B:183:LYS:HE2	1:C:212:ARG:HH11	1.79	0.48
1:A:252:MET:HG3	1:A:345:GLN:HG3	1.95	0.48
1:C:302:LEU:O	1:C:305:GLN:HB3	2.13	0.48
1:A:220:LEU:HD22	1:A:259:ILE:CD1	2.43	0.48
1:D:339:THR:O	1:D:343:ILE:HG13	2.14	0.48
1:A:286:PHE:O	1:A:303:ARG:HD3	2.14	0.48
1:D:298:LYS:HA	1:D:301:ARG:HH12	1.76	0.48
1:A:317:ARG:O	1:A:318:GLN:HB2	2.13	0.48
1:B:239:ASP:O	1:B:240:TYR:O	2.32	0.48
1:B:314:ILE:O	1:B:317:ARG:HD3	2.13	0.48
1:C:246:CYS:SG	1:C:249:LEU:HB2	2.54	0.48
1:A:231:LYS:O	1:A:233:VAL:HG23	2.13	0.48
1:A:146:LEU:HD23	1:A:196:ILE:HD12	1.95	0.48
1:C:227:SER:OG	1:C:234:LEU:HA	2.14	0.48
1:C:282:ALA:HB3	1:C:306:VAL:HG11	1.95	0.47
1:D:340:TRP:O	1:D:344:GLU:HG3	2.14	0.47
1:C:248:GLU:CD	1:C:248:GLU:N	2.65	0.47
1:D:361:LEU:O	1:D:365:LEU:HB2	2.14	0.47
1:D:239:ASP:O	1:D:240:TYR:CD2	2.68	0.47
1:B:252:MET:HB3	2:B:701:DAO:C12	2.44	0.47
1:D:272:ILE:HA	1:D:276:GLU:OE2	2.15	0.47
1:C:356:LYS:HE2	1:C:356:LYS:CA	2.44	0.47
1:B:152:LEU:HB2	1:B:195:TYR:CE2	2.50	0.47
1:D:178:VAL:O	1:D:182:MET:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:MET:HA	1:C:345:GLN:HE22	1.79	0.47
1:D:170:LYS:O	1:D:171:ARG:CB	2.62	0.47
1:D:260:LEU:HA	1:D:264:VAL:HB	1.97	0.47
1:A:313:TYR:CD2	1:A:313:TYR:C	2.87	0.47
1:A:239:ASP:O	1:A:240:TYR:HB2	2.15	0.47
1:A:250:ALA:O	1:A:251:GLU:HB2	2.15	0.47
1:C:343:ILE:O	1:C:345:GLN:N	2.48	0.46
1:A:203:LEU:H	1:A:203:LEU:HD22	1.79	0.46
1:A:350:LYS:HB2	1:A:357:ILE:HG13	1.96	0.46
1:C:178:VAL:HG12	1:C:182:MET:HE2	1.97	0.46
1:C:190:VAL:CG1	1:C:194:LYS:HD2	2.45	0.46
1:A:212:ARG:HD2	1:A:363:GLU:OE2	2.15	0.46
1:C:318:GLN:HG2	1:C:319:TYR:H	1.81	0.46
1:A:170:LYS:O	1:A:171:ARG:CB	2.64	0.46
1:D:148:GLN:O	1:D:151:VAL:N	2.49	0.46
1:C:167:ILE:HG23	1:C:167:ILE:O	2.14	0.46
1:D:207:GLN:O	1:D:211:LEU:HD12	2.14	0.46
1:D:340:TRP:HD1	3:D:47:HOH:O	1.98	0.46
1:C:322:ARG:CZ	1:D:308:VAL:HG11	2.45	0.46
1:A:226:ARG:NH1	3:A:29:HOH:O	2.48	0.46
1:B:302:LEU:O	1:B:306:VAL:HG23	2.15	0.46
1:A:361:LEU:O	1:A:365:LEU:HB2	2.16	0.46
1:C:359:ASN:HA	1:C:359:ASN:HD22	1.48	0.46
1:B:362:GLN:O	1:B:366:LEU:HG	2.15	0.46
1:A:166:ASP:O	1:A:167:ILE:HG13	2.16	0.46
1:B:174:SER:O	1:B:176:THR:N	2.49	0.46
1:B:143:ILE:HG22	1:B:144:ASN:HD22	1.81	0.46
1:C:320:ASP:O	1:C:321:SER:OG	2.22	0.46
1:D:239:ASP:O	1:D:240:TYR:HD2	1.99	0.46
1:C:186:LEU:HD12	1:C:186:LEU:HA	1.77	0.46
1:D:250:ALA:O	1:D:251:GLU:CB	2.63	0.46
1:A:304:SER:O	1:A:307:GLN:HG3	2.16	0.45
1:A:258:ARG:HH11	1:A:341:GLN:HE21	1.64	0.45
1:A:297:GLY:O	1:A:301:ARG:HB2	2.15	0.45
1:D:350:LYS:HZ3	1:D:362:GLN:HE22	1.63	0.45
1:B:365:LEU:C	1:B:367:GLY:H	2.20	0.45
1:D:314:ILE:HD12	1:D:324:ARG:HG2	1.99	0.45
1:C:250:ALA:O	1:C:251:GLU:CB	2.57	0.45
1:B:258:ARG:O	1:B:262:GLU:HB2	2.17	0.45
1:B:220:LEU:HD21	1:B:342:MET:SD	2.56	0.45
1:A:180:GLU:HA	1:A:183:LYS:HE3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:VAL:HG13	1:D:212:ARG:HD3	1.97	0.45
1:D:143:ILE:HG21	1:D:275:ASN:HB3	1.98	0.45
1:C:170:LYS:O	1:C:171:ARG:CB	2.46	0.45
1:C:189:LEU:HD22	1:C:211:LEU:HD23	1.98	0.45
1:C:231:LYS:O	1:C:232:ASP:HB2	2.16	0.45
1:D:140:LEU:HA	1:D:141:PRO:HD3	1.80	0.45
1:C:344:GLU:OE1	1:D:340:TRP:HZ3	2.00	0.45
1:B:231:LYS:HD3	1:B:232:ASP:HB2	1.98	0.45
1:D:189:LEU:HD13	1:D:189:LEU:C	2.37	0.45
1:D:290:ALA:HB3	1:D:293:LEU:HG	1.99	0.45
1:C:155:GLN:O	1:C:156:ILE:HD13	2.17	0.45
1:B:182:MET:O	1:B:186:LEU:HB2	2.16	0.45
1:D:352:PHE:N	1:D:352:PHE:CD2	2.85	0.45
1:B:203:LEU:O	1:B:207:GLN:HG3	2.17	0.45
1:D:270:LEU:HD13	1:D:328:LEU:CD2	2.45	0.44
1:D:186:LEU:HG	1:D:364:MET:HE1	1.99	0.44
1:D:249:LEU:O	1:D:250:ALA:O	2.34	0.44
1:A:226:ARG:O	1:A:226:ARG:HG2	2.17	0.44
1:A:203:LEU:O	1:A:207:GLN:HG3	2.17	0.44
1:C:336:GLN:O	1:C:340:TRP:CD1	2.64	0.44
1:A:178:VAL:O	1:A:182:MET:HG3	2.17	0.44
1:C:354:MET:O	1:C:357:ILE:N	2.49	0.44
1:C:156:ILE:HG13	1:C:191:GLU:OE2	2.17	0.44
1:C:191:GLU:HG2	1:C:195:TYR:CE2	2.53	0.44
1:C:298:LYS:NZ	1:C:298:LYS:HB2	2.32	0.44
1:C:304:SER:HA	1:C:307:GLN:HG2	2.00	0.44
1:A:361:LEU:HD12	1:A:361:LEU:N	2.33	0.44
1:A:272:ILE:HG12	1:A:328:LEU:HD21	1.99	0.44
1:C:169:ALA:O	1:C:171:ARG:N	2.47	0.44
1:D:350:LYS:HB2	1:D:357:ILE:CG1	2.48	0.44
1:A:312:ASP:HA	1:A:315:ASN:CB	2.43	0.44
1:B:157:THR:HG22	1:B:188:VAL:HG12	1.99	0.44
1:D:221:LEU:HD23	1:D:335:LEU:HD22	1.99	0.43
1:B:252:MET:SD	1:B:345:GLN:CG	2.99	0.43
1:B:280:LEU:HD22	1:B:332:LEU:HD21	1.99	0.43
1:A:324:ARG:NH1	1:A:324:ARG:CG	2.69	0.43
1:C:168:ARG:CA	1:C:168:ARG:NH1	2.78	0.43
1:B:320:ASP:O	1:B:321:SER:CB	2.66	0.43
1:C:175:ILE:CD1	1:C:175:ILE:N	2.76	0.43
1:B:174:SER:O	1:B:175:ILE:C	2.57	0.43
1:B:318:GLN:HB2	1:B:319:TYR:H	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:VAL:HG12	1:A:212:ARG:CD	2.48	0.43
1:C:185:GLN:O	1:C:188:VAL:HG13	2.19	0.43
1:B:231:LYS:HD3	1:B:232:ASP:OD2	2.19	0.43
1:C:186:LEU:HD11	1:C:215:ALA:HB1	2.01	0.43
1:B:199:PHE:O	1:B:202:LEU:HB2	2.18	0.43
1:A:200:CYS:C	1:A:202:LEU:H	2.20	0.43
1:D:265:LEU:CB	1:D:266:PRO:HD3	2.48	0.43
1:D:175:ILE:HG13	1:D:175:ILE:H	1.61	0.43
1:D:310:LEU:O	1:D:310:LEU:HD23	2.19	0.43
1:C:174:SER:O	1:C:177:ASP:N	2.44	0.43
1:D:153:SER:O	1:D:156:ILE:HG13	2.18	0.43
1:D:189:LEU:CD1	1:D:211:LEU:HD23	2.49	0.43
1:C:267:PHE:CE1	1:C:272:ILE:HD12	2.53	0.43
1:D:357:ILE:HG22	1:D:358:ASP:H	1.81	0.42
1:A:220:LEU:O	1:A:224:THR:CG2	2.67	0.42
1:D:252:MET:HG3	1:D:345:GLN:NE2	2.35	0.42
1:C:361:LEU:O	1:C:365:LEU:HB2	2.19	0.42
1:C:346:ILE:O	1:C:350:LYS:HB2	2.19	0.42
1:C:362:GLN:HA	1:C:365:LEU:HB3	2.01	0.42
1:A:320:ASP:C	1:A:322:ARG:N	2.73	0.42
1:D:314:ILE:HG21	1:D:324:ARG:HB3	2.02	0.42
1:B:208:VAL:HG21	1:C:184:GLU:HG2	2.01	0.42
1:A:182:MET:O	1:A:186:LEU:HD22	2.19	0.42
1:D:320:ASP:OD1	1:D:320:ASP:N	2.52	0.42
1:B:155:GLN:HG2	1:B:156:ILE:H	1.84	0.42
1:D:326:GLY:O	1:D:330:LEU:HG	2.20	0.42
1:C:332:LEU:HA	1:C:332:LEU:HD23	1.86	0.42
1:B:310:LEU:HD12	1:B:325:PHE:CD2	2.54	0.42
1:D:204:LEU:O	1:D:208:VAL:HG23	2.19	0.42
1:D:221:LEU:CD1	1:D:277:TYR:CE1	3.03	0.42
1:A:226:ARG:O	1:A:226:ARG:CG	2.67	0.42
1:A:186:LEU:O	1:A:190:VAL:HG23	2.19	0.42
1:C:332:LEU:HB2	1:C:333:PRO:HD3	2.01	0.42
1:B:250:ALA:O	1:B:251:GLU:HB3	2.20	0.42
1:B:192:TRP:NE1	1:B:281:LYS:HD3	2.34	0.42
1:B:287:ASP:OD1	1:B:287:ASP:C	2.57	0.41
1:D:208:VAL:HG12	1:D:212:ARG:HD3	2.00	0.41
1:C:244:ARG:NH2	1:C:261:ASP:OD1	2.53	0.41
1:D:218:HIS:HD2	1:D:281:LYS:CE	2.23	0.41
1:C:346:ILE:HD11	2:C:702:DAO:C12	2.50	0.41
1:A:346:ILE:HG23	1:A:357:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.90	0.41
1:C:297:GLY:HA2	1:C:300:LYS:HE3	2.02	0.41
1:B:155:GLN:O	1:B:156:ILE:C	2.59	0.41
1:D:147:LEU:CD2	1:D:274:ASP:HB3	2.49	0.41
1:B:250:ALA:HA	1:B:253:SER:CB	2.51	0.41
1:D:235:LEU:HD12	1:D:241:ILE:HG22	2.01	0.41
1:A:180:GLU:HA	1:A:183:LYS:CE	2.51	0.41
1:B:185:GLN:OE1	1:B:188:VAL:HG21	2.21	0.41
1:B:180:GLU:HG3	3:B:58:HOH:O	2.20	0.41
1:C:233:VAL:CG1	1:C:241:ILE:HB	2.50	0.41
1:D:356:LYS:CA	1:D:356:LYS:HE3	2.29	0.41
1:B:153:SER:O	1:B:157:THR:HB	2.20	0.41
1:C:315:ASN:C	1:C:317:ARG:N	2.73	0.41
1:A:312:ASP:C	1:A:315:ASN:HB2	2.41	0.41
1:B:364:MET:SD	1:D:352:PHE:CD1	3.14	0.41
1:B:140:LEU:HD12	1:B:140:LEU:O	2.21	0.41
1:C:279:CYS:O	1:C:283:ILE:HG13	2.21	0.41
1:A:262:GLU:O	1:A:266:PRO:HG2	2.21	0.41
1:B:155:GLN:O	1:B:157:THR:N	2.54	0.41
1:B:332:LEU:HB2	1:B:333:PRO:HD3	2.03	0.41
1:D:220:LEU:HD22	1:D:259:ILE:CD1	2.49	0.40
1:B:185:GLN:HG3	2:B:701:DAO:O1	2.21	0.40
1:B:231:LYS:HD3	1:B:232:ASP:CB	2.51	0.40
1:C:317:ARG:HG3	3:C:67:HOH:O	2.21	0.40
1:B:350:LYS:O	1:B:354:MET:CG	2.69	0.40
1:C:171:ARG:NH2	3:C:23:HOH:O	2.53	0.40
1:B:358:ASP:O	1:B:362:GLN:OE1	2.39	0.40
1:A:258:ARG:CZ	1:A:338:ILE:HG12	2.52	0.40
1:C:267:PHE:CD1	1:C:272:ILE:HD12	2.56	0.40
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.93	0.40
1:A:352:PHE:N	1:A:352:PHE:CD2	2.88	0.40
1:A:146:LEU:HD23	1:A:196:ILE:CD1	2.52	0.40
1:D:139:SER:O	1:D:140:LEU:HB2	2.21	0.40
1:D:172:ILE:HG12	1:D:241:ILE:CD1	2.51	0.40
1:D:273:ASP:C	1:D:273:ASP:OD2	2.59	0.40
1:D:292:GLY:O	1:D:293:LEU:C	2.59	0.40
1:B:199:PHE:CZ	1:B:207:GLN:HB3	2.56	0.40
1:C:284:ILE:HG12	1:C:332:LEU:HD22	2.02	0.40
1:C:262:GLU:HG2	1:D:289:ASP:OD1	2.21	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	219/250 (88%)	189 (86%)	19 (9%)	11 (5%)	3	8
1	B	214/250 (86%)	180 (84%)	19 (9%)	15 (7%)	1	3
1	C	216/250 (86%)	186 (86%)	20 (9%)	10 (5%)	3	9
1	D	217/250 (87%)	183 (84%)	22 (10%)	12 (6%)	2	6
All	All	866/1000 (87%)	738 (85%)	80 (9%)	48 (6%)	2	6

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	SER
1	A	250	ALA
1	A	358	ASP
1	B	143	ILE
1	B	175	ILE
1	B	251	GLU
1	B	318	GLN
1	B	319	TYR
1	B	321	SER
1	B	343	ILE
1	C	175	ILE
1	C	354	MET
1	C	355	ALA
1	D	250	ALA
1	D	357	ILE
1	D	358	ASP
1	A	240	TYR
1	A	353	GLY
1	A	357	ILE
1	B	155	GLN
1	B	240	TYR
1	B	344	GLU

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Mol	Chain	Res	Type
1	C	171	ARG
1	C	343	ILE
1	C	344	GLU
1	C	357	ILE
1	D	155	GLN
1	D	251	GLU
1	D	319	TYR
1	A	167	ILE
1	A	315	ASN
1	B	156	ILE
1	B	171	ARG
1	B	320	ASP
1	B	347	GLN
1	C	170	LYS
1	D	157	THR
1	D	240	TYR
1	D	318	GLN
1	A	321	SER
1	B	244	ARG
1	C	320	ASP
1	D	140	LEU
1	A	171	ARG
1	A	319	TYR
1	C	240	TYR
1	D	171	ARG
1	D	353	GLY

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	198/220 (90%)	177 (89%)	21 (11%)	8 24
1	B	194/220 (88%)	178 (92%)	16 (8%)	14 38
1	C	196/220 (89%)	179 (91%)	17 (9%)	13 35
1	D	197/220 (90%)	185 (94%)	12 (6%)	23 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	785/880 (89%)	719 (92%)	66 (8%)	14 37

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	150	GLU
1	A	151	VAL
1	A	171	ARG
1	A	186	LEU
1	A	189	LEU
1	A	191	GLU
1	A	206	ASP
1	A	212	ARG
1	A	224	THR
1	A	239	ASP
1	A	252	MET
1	A	291	LYS
1	A	310	LEU
1	A	315	ASN
1	A	317	ARG
1	A	322	ARG
1	A	324	ARG
1	A	327	GLU
1	A	337	SER
1	A	365	LEU
1	B	176	THR
1	B	187	LEU
1	B	204	LEU
1	B	221	LEU
1	B	231	LYS
1	B	239	ASP
1	B	265	LEU
1	B	307	GLN
1	B	312	ASP
1	B	317	ARG
1	B	324	ARG
1	B	344	GLU
1	B	348	PHE
1	B	352	PHE
1	B	359	ASN
1	B	365	LEU

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Mol	Chain	Res	Type
1	C	147	LEU
1	C	171	ARG
1	C	176	THR
1	C	188	VAL
1	C	189	LEU
1	C	221	LEU
1	C	239	ASP
1	C	245	HIS
1	C	291	LYS
1	C	298	LYS
1	C	299	ILE
1	C	310	LEU
1	C	320	ASP
1	C	324	ARG
1	C	354	MET
1	C	356	LYS
1	C	359	ASN
1	D	168	ARG
1	D	217	GLU
1	D	265	LEU
1	D	291	LYS
1	D	300	LYS
1	D	301	ARG
1	D	305	GLN
1	D	310	LEU
1	D	324	ARG
1	D	356	LYS
1	D	359	ASN
1	D	360	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	GLN
1	A	315	ASN
1	A	336	GLN
1	A	341	GLN
1	A	347	GLN
1	A	362	GLN
1	B	144	ASN
1	B	148	GLN
1	B	268	GLN

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Mol	Chain	Res	Type
1	B	341	GLN
1	B	345	GLN
1	C	154	GLN
1	C	268	GLN
1	C	315	ASN
1	C	341	GLN
1	C	345	GLN
1	C	359	ASN
1	D	207	GLN
1	D	214	HIS
1	D	218	HIS
1	D	268	GLN
1	D	305	GLN
1	D	336	GLN
1	D	341	GLN
1	D	345	GLN
1	D	362	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

4 ligands are modelled in this entry.

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	DAO	A	700	-	10,13,13	0.38	0	10,13,13	0.34	0
2	DAO	B	701	-	10,13,13	0.28	0	10,13,13	0.49	0
2	DAO	C	702	-	10,13,13	0.24	0	10,13,13	0.41	0
2	DAO	D	703	-	10,13,13	0.24	0	10,13,13	0.31	0

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	DAO	A	700	-	-	0/9/11/11	0/0/0/0
2	DAO	B	701	-	-	0/9/11/11	0/0/0/0
2	DAO	C	702	-	-	0/9/11/11	0/0/0/0
2	DAO	D	703	-	-	0/9/11/11	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	DAO	1	0
2	B	701	DAO	3	0
2	C	702	DAO	1	0
2	D	703	DAO	1	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.