



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:40 PM GMT

PDB ID : 3UKR
Title : Crystal structure of Bos taurus Arp2/3 complex with bound inhibitor CK-666
Authors : Nolen, B.J.; Han, M.
Deposited on : 2011-11-09
Resolution : 2.48 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

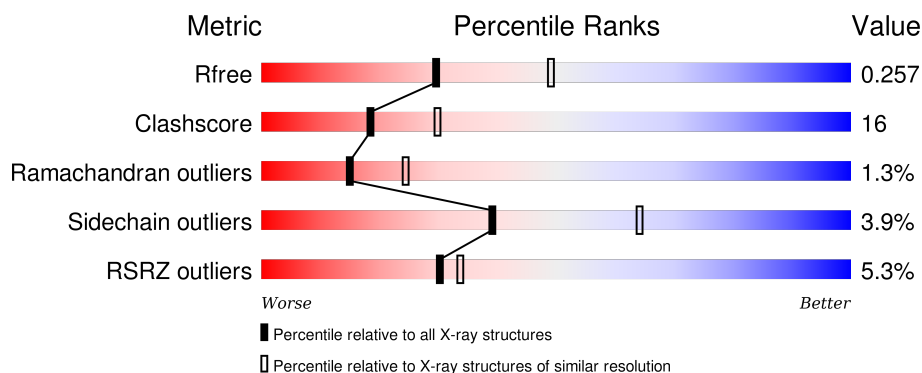
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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

Mol	Chain	Length	Quality of chain
1	A	418	<div> <div>5%</div> <div>71%</div> <div>23%</div> <div>• •</div> </div>
2	B	394	<div> <div>8%</div> <div>27%</div> <div>19%</div> <div>•</div> <div>51%</div> </div>
3	C	372	<div> <div>3%</div> <div>66%</div> <div>26%</div> <div>• 6%</div> </div>
4	D	300	<div> <div>%</div> <div>74%</div> <div>20%</div> <div>• 6%</div> </div>
5	E	178	<div> <div>6%</div> <div>57%</div> <div>34%</div> <div>6% •</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	168	<div><div>%</div><div><div></div><div>77%</div><div>21%</div><div>••</div></div></div>
7	G	151	<div><div>9%</div><div><div></div><div>64%</div><div>23%</div><div>•</div><div>10%</div></div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13746 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3187	2048	534	589	16			

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	0	0
			1527	982	257	284	4			

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	349	Total	C	N	O	S	0	0	0
			2716	1721	480	496	19			

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	282	Total	C	N	O	S	0	0	0
			2279	1449	395	427	8			

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	173	Total	C	N	O	S	0	0	0
			1401	902	235	255	9			

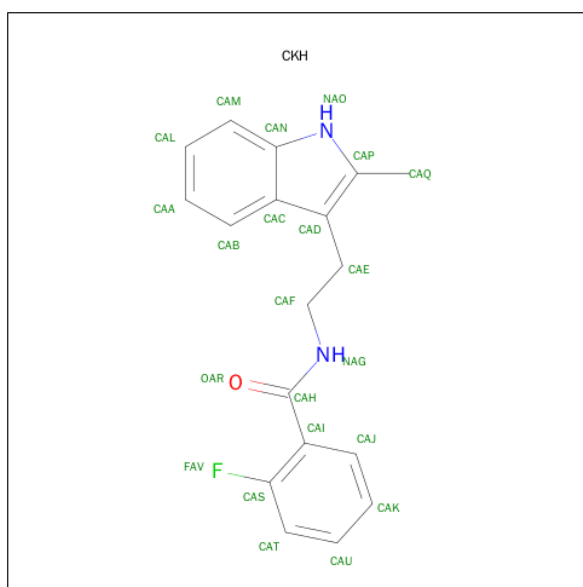
- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	167	Total	C	N	O	S	0	0	0
			1363	871	239	244	9			

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	136	Total	C	N	O	S	0	0	0
			1030	647	181	199	3			

- Molecule 8 is 2-FLUORO-N-[2-(2-METHYL-1H-INDOL-3-YL)ETHYL]BENZAMIDE (three-letter code: CKH) (formula: C₁₈H₁₇FN₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	F	N	O	0	0
			22	18	1	2	1		


- Molecule 9 is water.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	45	Total	O	0	0
			45	45		
9	B	11	Total	O	0	0
			11	11		
9	C	51	Total	O	0	0
			51	51		
9	D	51	Total	O	0	0
			51	51		

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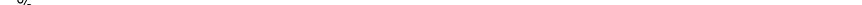
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	6	Total 6	O 6	0	0
9	F	46	Total 46	O 46	0	0
9	G	11	Total 11	O 11	0	0

- Chain C: 

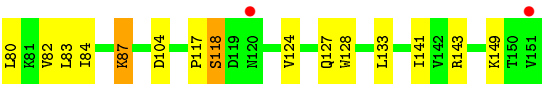
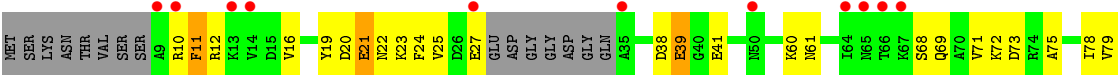
- Chain D: 
- 
- | Position | Amino Acid | Frequency (%) |
|----------|------------|---------------|
| 1 | M1 | 100 |
| 2 | I2 | 100 |
| 3 | L3 | 100 |
| 4 | D37 | 100 |
| 5 | Y43 | 100 |
| 6 | H44 | 100 |
| 7 | I45 | 100 |
| 8 | T53 | 100 |
| 9 | K54 | 100 |
| 10 | V55 | 100 |
| 11 | M56 | 100 |
| 12 | V57 | 100 |
| 13 | S58 | 100 |
| 14 | I59 | 100 |
| 15 | L67 | 100 |
| 16 | E74 | 100 |
| 17 | L75 | 100 |
| 18 | L84 | 100 |
| 19 | L116 | 100 |
| 20 | G120 | 100 |
| 21 | F121 | 100 |
| 22 | A122 | 100 |
| 23 | S123 | 100 |
| 24 | V124 | 100 |
| 25 | F129 | 100 |
| 26 | Q130 | 100 |
| 27 | E133 | 100 |
| 28 | E134 | 100 |
| 29 | G135 | 100 |
| 30 | K136 | 100 |
| 31 | E137 | 100 |
| 32 | R147 | 100 |
| 33 | E150 | 100 |
| 34 | K158 | 100 |
| 35 | D159 | 100 |
| 36 | R160 | 100 |
| 37 | M182 | 100 |
| 38 | Q183 | 100 |
| 39 | G188 | 100 |
| 40 | R199 | 100 |
| 41 | Q197 | 100 |
| 42 | V198 | 100 |
| 43 | L199 | 100 |
| 44 | F200 | 100 |
| 45 | S201 | 100 |
| 46 | H202 | 100 |
| 47 | P205 | 100 |
| 48 | D211 | 100 |
| 49 | T212 | 100 |
| 50 | D213 | 100 |
| 51 | A214 | 100 |
| 52 | Y222 | 100 |
| 53 | I223 | 100 |
| 54 | T224 | 100 |
| 55 | F225 | 100 |
| 56 | V226 | 100 |
| 57 | L227 | 100 |
| 58 | F228 | 100 |
| 59 | P229 | 100 |
| 60 | R230 | 100 |
| 61 | H231 | 100 |
| 62 | T232 | 100 |
| 63 | N233 | 100 |
| 64 | A234 | 100 |
| 65 | S235 | 100 |
| 66 | A236 | 100 |
| 67 | R237 | 100 |
| 68 | R248 | 100 |
| 69 | S258 | 100 |
| 70 | I262 | 100 |
| 71 | H263 | 100 |
| 72 | M266 | 100 |
| 73 | R267 | 100 |
| 74 | L274 | 100 |
| 75 | L277 | 100 |
| 76 | N278 | 100 |
| 77 | R281 | 100 |
| 78 | P282 | 100 |
| 79 | ASP | 100 |
| 80 | ALA | 100 |
| 81 | GLU | 100 |
| 82 | LYS | 100 |
| 83 | LYS | 100 |
| 84 | GLU | 100 |
| 85 | LYS | 100 |
| 86 | THR | 100 |
| 87 | THR | 100 |
| 88 | ILE | 100 |
| 89 | THR | 100 |
| 90 | GLY | 100 |
| 91 | LYS | 100 |
| 92 | THR | 100 |
| 93 | PHE | 100 |
| 94 | L199 | 100 |

- Chain E:
-

- Chain F: 



● Molecule 7: Actin-related protein 2/3 complex subunit 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.19Å 129.69Å 205.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.48 46.54 – 2.48	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.48) 84.4 (46.54-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.261 0.218 , 0.257	Depositor DCC
R_{free} test set	4698 reflections (5.56%)	DCC
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 93952 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13746	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.38	0/3268	0.59	0/4437
2	B	0.36	0/1554	0.59	0/2100
3	C	0.38	0/2785	0.64	1/3777 (0.0%)
4	D	0.39	0/2328	0.60	0/3143
5	E	0.32	0/1435	0.57	0/1936
6	F	0.40	0/1385	0.63	0/1858
7	G	0.32	0/1042	0.54	0/1401
All	All	0.37	0/13797	0.60	1/18652 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	11	ILE	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3187	0	3117	78	0
2	B	1527	0	1551	96	0
3	C	2716	0	2666	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2279	0	2248	50	0
5	E	1401	0	1405	63	0
6	F	1363	0	1402	38	0
7	G	1030	0	1047	39	0
8	B	22	0	17	2	0
9	A	45	0	0	3	0
9	B	11	0	0	0	0
9	C	51	0	0	2	0
9	D	51	0	0	3	0
9	E	6	0	0	0	0
9	F	46	0	0	1	0
9	G	11	0	0	0	0
All	All	13746	0	13453	419	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 16.

All (419) 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)
3:C:183:THR:HG22	3:C:185:TRP:H	1.18	1.04
7:G:23:LYS:HG2	7:G:24:PHE:H	1.28	0.96
3:C:142:ARG:NH2	7:G:25:VAL:H	1.64	0.94
2:B:175:LEU:HD12	2:B:178:LEU:HD12	1.48	0.92
3:C:142:ARG:HH22	7:G:25:VAL:H	0.93	0.90
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.51	0.90
3:C:142:ARG:HH22	7:G:25:VAL:N	1.69	0.89
7:G:87:LYS:H	7:G:87:LYS:HE3	1.37	0.89
4:D:197:GLN:HE21	4:D:199:LEU:HD11	1.34	0.89
2:B:205:ASN:HD22	2:B:208:ALA:H	1.17	0.88
2:B:158:ASP:OD1	2:B:304:SER:HB3	1.75	0.86
2:B:330:LEU:HG	2:B:336:LYS:NZ	1.89	0.86
5:E:82:LEU:HD23	5:E:148:VAL:HG21	1.56	0.86
5:E:15:LEU:HD21	5:E:63:GLU:HG3	1.61	0.82
2:B:267:GLN:HG2	7:G:12:ARG:HH12	1.45	0.81
2:B:177:HIS:O	2:B:178:LEU:HB2	1.81	0.79
3:C:107:ASN:ND2	3:C:109:LYS:H	1.80	0.79
3:C:183:THR:HG22	3:C:185:TRP:N	1.98	0.79
6:F:31:GLU:OE2	6:F:32:ARG:HG3	1.82	0.79
1:A:243:ASN:ND2	5:E:47:TYR:HE1	1.81	0.78
3:C:284:ARG:HD3	3:C:286:ASP:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:10:ARG:O	7:G:11:PHE:HB3	1.84	0.78
2:B:194:ILE:HG12	2:B:213:VAL:HG21	1.66	0.77
1:A:39:GLU:HG3	1:A:39:GLU:O	1.84	0.76
4:D:228:PHE:H	4:D:231:HIS:HD2	1.31	0.76
2:B:327:GLU:HG3	2:B:328:ARG:N	2.02	0.74
1:A:289:ASN:ND2	1:A:291:ASP:H	1.86	0.74
2:B:163:VAL:HG22	2:B:164:THR:H	1.52	0.74
2:B:180:ARG:HH12	2:B:285:THR:HA	1.52	0.73
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.70	0.73
1:A:191:LYS:HE2	1:A:303:VAL:HG22	1.71	0.73
6:F:4:THR:HG23	6:F:55:ARG:HE	1.54	0.72
2:B:329:VAL:HG13	2:B:330:LEU:HD22	1.72	0.72
5:E:28:PHE:HE1	5:E:142:LEU:HD22	1.55	0.71
5:E:18:ASN:ND2	5:E:118:ALA:H	1.88	0.71
5:E:60:ILE:HD11	5:E:116:ILE:HD13	1.72	0.71
7:G:68:SER:O	7:G:71:VAL:HG12	1.90	0.71
6:F:158:ARG:O	6:F:162:GLU:HG3	1.91	0.70
2:B:329:VAL:HG13	2:B:330:LEU:CD2	2.21	0.70
1:A:79:ARG:HG3	1:A:84:GLU:OE1	1.92	0.70
4:D:189:ARG:NH2	4:D:197:GLN:HG3	2.07	0.69
2:B:340:PHE:CE2	2:B:342:ILE:HD11	2.27	0.69
3:C:107:ASN:HD22	3:C:107:ASN:C	1.96	0.69
7:G:87:LYS:N	7:G:87:LYS:HE3	2.07	0.69
5:E:18:ASN:HD21	5:E:118:ALA:H	1.41	0.69
2:B:327:GLU:HG3	2:B:328:ARG:H	1.56	0.68
2:B:336:LYS:HE2	2:B:337:LEU:N	2.07	0.68
2:B:345:GLU:HG3	2:B:346:ASP:N	2.08	0.68
1:A:274:GLU:OE1	1:A:274:GLU:N	2.27	0.68
3:C:297:THR:HG22	3:C:298:ALA:H	1.58	0.67
7:G:75:ALA:O	7:G:79:VAL:HG23	1.95	0.67
2:B:282:LEU:HD21	2:B:301:ILE:HD13	1.76	0.66
3:C:183:THR:CG2	3:C:185:TRP:H	2.02	0.66
2:B:290:ASP:HB2	2:B:293:THR:OG1	1.95	0.66
2:B:163:VAL:HG22	2:B:164:THR:N	2.10	0.65
6:F:58:LYS:HA	6:F:58:LYS:HE2	1.77	0.65
2:B:175:LEU:N	2:B:175:LEU:HD23	2.11	0.65
4:D:278:ASN:HB3	9:D:427:HOH:O	1.96	0.65
6:F:86:LEU:HB3	6:F:149:MET:HE2	1.78	0.65
2:B:330:LEU:HG	2:B:336:LYS:HZ2	1.60	0.65
2:B:274:GLU:OE1	2:B:275:GLY:N	2.23	0.65
1:A:289:ASN:HD22	1:A:291:ASP:H	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:TRP:O	3:C:131:TRP:HE3	1.80	0.64
5:E:152:GLN:HB2	5:E:155:LYS:HD2	1.79	0.64
5:E:56:LYS:HG3	5:E:170:ASN:ND2	2.13	0.64
2:B:336:LYS:HE2	2:B:336:LYS:C	2.18	0.64
6:F:86:LEU:HB3	6:F:149:MET:CE	2.28	0.64
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.80	0.64
1:A:262:ILE:O	1:A:263:SER:HB3	1.96	0.64
2:B:329:VAL:C	2:B:330:LEU:HD22	2.18	0.64
2:B:205:ASN:ND2	2:B:208:ALA:H	1.91	0.63
5:E:119:LYS:HB2	5:E:120:PRO:HD2	1.81	0.63
3:C:72:THR:HA	3:C:98:ALA:HB1	1.81	0.63
4:D:121:PHE:O	4:D:124:VAL:HG12	1.98	0.63
1:A:223:THR:O	1:A:227:VAL:HG23	1.98	0.63
1:A:389:GLU:HA	1:A:392:GLN:OE1	1.98	0.63
7:G:23:LYS:HG2	7:G:24:PHE:N	2.09	0.63
5:E:18:ASN:HD21	5:E:118:ALA:N	1.96	0.63
7:G:38:ASP:HB3	7:G:41:GLU:HB3	1.80	0.63
1:A:321:LEU:HD12	1:A:369:THR:HG22	1.81	0.62
1:A:257:THR:HG22	1:A:268:SER:HB3	1.81	0.62
5:E:152:GLN:HB3	5:E:155:LYS:NZ	2.13	0.62
1:A:194:PRO:C	1:A:195:ILE:HD12	2.20	0.62
4:D:3:LEU:HD11	6:F:167:ASN:ND2	2.14	0.62
3:C:371:ILE:HG22	3:C:372:VAL:HG23	1.82	0.62
2:B:177:HIS:O	2:B:178:LEU:CB	2.47	0.62
3:C:358:ASP:OD1	3:C:360:ARG:HG2	2.00	0.62
2:B:345:GLU:HG3	2:B:346:ASP:H	1.65	0.61
2:B:175:LEU:CD1	2:B:178:LEU:HD12	2.26	0.61
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.65	0.61
5:E:86:ASN:C	5:E:154:ASP:HA	2.20	0.61
2:B:198:LEU:HD23	2:B:202:TYR:O	1.99	0.61
1:A:176:HIS:HD2	1:A:192:HIS:CD2	2.18	0.61
4:D:266:MET:HE3	6:F:93:PHE:CD1	2.36	0.61
5:E:97:THR:O	5:E:101:THR:HG23	2.00	0.61
1:A:116:PRO:O	1:A:117:LEU:HB2	2.01	0.60
4:D:281:ARG:HH12	6:F:102:PHE:HZ	1.48	0.60
5:E:75:ILE:HG23	5:E:144:LEU:HD11	1.83	0.60
6:F:130:LYS:HE2	6:F:130:LYS:HA	1.82	0.60
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.32	0.59
1:A:19:LEU:HG	1:A:29:PHE:HB2	1.83	0.59
6:F:4:THR:HG23	6:F:55:ARG:HH21	1.67	0.59
2:B:235:LEU:HD23	6:F:107:LYS:NZ	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:87:SER:HA	5:E:153:ASN:OD1	2.02	0.58
3:C:370:LYS:O	3:C:371:ILE:HB	2.02	0.58
5:E:150:ASP:O	5:E:152:GLN:N	2.37	0.58
2:B:343:ARG:HH11	2:B:343:ARG:HG3	1.68	0.58
3:C:359:VAL:O	3:C:363:GLU:HG3	2.04	0.58
2:B:329:VAL:O	2:B:329:VAL:HG22	2.03	0.58
5:E:130:ARG:HG3	5:E:130:ARG:HH11	1.69	0.57
2:B:205:ASN:HD22	2:B:208:ALA:N	1.97	0.57
2:B:327:GLU:HA	2:B:332:GLY:H	1.69	0.57
5:E:95:MET:HA	5:E:95:MET:CE	2.35	0.57
6:F:86:LEU:HD22	6:F:149:MET:HE3	1.84	0.57
6:F:79:ALA:HB3	6:F:83:GLU:OE2	2.03	0.57
2:B:166:ILE:O	2:B:168:PRO:HD3	2.03	0.57
3:C:200:SER:HB3	9:C:408:HOH:O	2.05	0.57
2:B:329:VAL:O	2:B:330:LEU:HD22	2.04	0.57
3:C:126:GLU:HB2	3:C:131:TRP:CZ3	2.40	0.57
1:A:129:ILE:O	1:A:133:SER:HB2	2.05	0.57
4:D:233:ASN:OD1	4:D:235:SER:N	2.34	0.57
7:G:60:LYS:HG2	7:G:61:ASN:ND2	2.20	0.56
2:B:326:LEU:HD23	2:B:326:LEU:C	2.25	0.56
3:C:107:ASN:HD22	3:C:108:GLU:N	2.03	0.56
3:C:3:TYR:HB2	3:C:324:LEU:HG	1.85	0.56
4:D:53:THR:C	4:D:54:LYS:HD2	2.26	0.56
3:C:221:SER:HB2	3:C:223:ASP:OD1	2.05	0.56
1:A:352:GLU:C	1:A:354:SER:H	2.07	0.56
5:E:134:GLN:O	5:E:138:GLN:HG3	2.05	0.56
6:F:4:THR:CG2	6:F:55:ARG:HH21	2.19	0.56
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.87	0.56
2:B:163:VAL:HG21	2:B:181:ARG:HH22	1.71	0.55
2:B:163:VAL:HG21	2:B:181:ARG:NH2	2.21	0.55
4:D:59:ILE:HB	4:D:116:LEU:HD13	1.87	0.55
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.88	0.55
4:D:248:ARG:C	4:D:248:ARG:HD3	2.26	0.55
3:C:156:LEU:HD11	3:C:183:THR:HG21	1.89	0.55
3:C:26:CYS:SG	3:C:55:VAL:HB	2.47	0.55
4:D:183:GLN:HB3	9:D:442:HOH:O	2.07	0.55
2:B:325:TYR:CD1	2:B:329:VAL:HG11	2.42	0.55
2:B:287:GLN:O	2:B:294:ARG:NH2	2.38	0.55
4:D:133:GLU:O	4:D:133:GLU:HG2	2.06	0.55
3:C:363:GLU:OE2	3:C:371:ILE:HD12	2.06	0.54
2:B:257:GLU:HA	2:B:260:GLU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:182:MET:HG3	4:D:200:PHE:CD1	2.41	0.54
4:D:197:GLN:NE2	4:D:199:LEU:HD11	2.13	0.54
5:E:133:LEU:O	5:E:137:ARG:HG3	2.06	0.54
6:F:99:GLU:HG3	9:F:220:HOH:O	2.07	0.54
3:C:263:HIS:CD2	6:F:21:CYS:HB3	2.42	0.54
3:C:365:ALA:C	3:C:366:LEU:HD12	2.28	0.54
2:B:330:LEU:HG	2:B:336:LYS:CE	2.38	0.54
2:B:250:ARG:HD2	8:B:401:CKH:H3	1.89	0.54
2:B:318:GLU:HG3	2:B:344:ILE:HD12	1.90	0.54
3:C:84:ARG:HG2	3:C:84:ARG:HH11	1.73	0.54
1:A:85:ASP:OD2	1:A:88:LEU:HD22	2.08	0.54
1:A:243:ASN:HD22	5:E:47:TYR:HE1	1.55	0.54
1:A:343:VAL:HG22	1:A:363:ILE:HD11	1.90	0.53
5:E:88:LYS:O	5:E:92:GLU:HG3	2.08	0.53
1:A:191:LYS:CE	1:A:303:VAL:HG22	2.36	0.53
5:E:152:GLN:CB	5:E:155:LYS:HD2	2.39	0.53
3:C:32:VAL:HG22	3:C:58:ILE:HD11	1.90	0.53
1:A:155:SER:HB2	1:A:370:HIS:HB3	1.90	0.53
7:G:117:PRO:O	7:G:118:SER:HB3	2.09	0.53
2:B:225:TYR:CZ	2:B:319:ARG:HD2	2.44	0.53
7:G:87:LYS:N	7:G:87:LYS:CD	2.72	0.53
1:A:343:VAL:HG13	1:A:363:ILE:HD11	1.91	0.53
7:G:71:VAL:HG13	7:G:72:LYS:N	2.24	0.53
1:A:151:ALA:O	1:A:154:THR:HG22	2.09	0.53
3:C:90:LEU:HD23	3:C:91:VAL:H	1.73	0.53
5:E:56:LYS:HG3	5:E:170:ASN:HD21	1.74	0.53
3:C:102:VAL:HA	3:C:112:ALA:O	2.09	0.52
2:B:235:LEU:HD23	6:F:107:LYS:HZ1	1.73	0.52
2:B:336:LYS:HE2	2:B:337:LEU:HA	1.91	0.52
6:F:80:ASP:OD1	6:F:82:ILE:HG22	2.10	0.52
5:E:105:ILE:HG12	5:E:108:GLU:OE1	2.10	0.52
1:A:243:ASN:ND2	5:E:47:TYR:CE1	2.71	0.52
1:A:263:SER:O	1:A:265:LYS:N	2.42	0.52
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.39	0.52
4:D:160:ARG:HB3	4:D:160:ARG:NH1	2.25	0.52
2:B:345:GLU:CG	2:B:346:ASP:N	2.73	0.52
1:A:388:PRO:O	1:A:392:GLN:OE1	2.27	0.52
2:B:345:GLU:CG	2:B:346:ASP:H	2.23	0.52
1:A:237:ASP:OD2	1:A:240:LYS:HG3	2.09	0.51
7:G:60:LYS:HE2	7:G:61:ASN:HD21	1.76	0.51
3:C:144:THR:H	6:F:28:GLN:NE2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:87:LYS:N	7:G:87:LYS:CE	2.73	0.51
6:F:4:THR:HG23	6:F:55:ARG:NE	2.22	0.51
5:E:144:LEU:O	5:E:148:VAL:HG23	2.10	0.51
3:C:185:TRP:CZ2	3:C:231:ALA:HB2	2.45	0.51
1:A:153:TRP:HA	1:A:158:VAL:HG21	1.92	0.51
5:E:167:GLN:NE2	5:E:172:SER:HB2	2.26	0.51
3:C:107:ASN:C	3:C:107:ASN:ND2	2.63	0.51
3:C:107:ASN:HD22	3:C:109:LYS:H	1.54	0.51
4:D:233:ASN:OD1	4:D:235:SER:HB3	2.11	0.51
5:E:85:CYS:SG	5:E:149:PHE:HZ	2.34	0.51
2:B:336:LYS:HE2	2:B:337:LEU:CA	2.41	0.50
1:A:289:ASN:HD22	1:A:289:ASN:C	2.14	0.50
1:A:116:PRO:HG2	1:A:178:ILE:HD13	1.93	0.50
5:E:78:CYS:O	5:E:82:LEU:HB2	2.11	0.50
1:A:257:THR:HG22	1:A:268:SER:CB	2.42	0.50
3:C:254:THR:HA	3:C:340:ALA:O	2.11	0.50
1:A:38:LYS:HE2	1:A:72:TYR:CZ	2.46	0.50
1:A:392:GLN:N	1:A:392:GLN:OE1	2.45	0.50
1:A:393:VAL:HG21	1:A:414:PHE:CD2	2.47	0.50
2:B:334:VAL:HG21	7:G:19:TYR:CE1	2.46	0.50
4:D:199:LEU:HB2	4:D:224:THR:HB	1.93	0.50
1:A:143:VAL:HG12	9:A:516:HOH:O	2.12	0.50
5:E:60:ILE:HD11	5:E:116:ILE:HG21	1.93	0.50
3:C:185:TRP:CE2	3:C:231:ALA:HB2	2.47	0.49
3:C:228:LEU:HD23	3:C:228:LEU:C	2.33	0.49
2:B:330:LEU:HG	2:B:336:LYS:HD3	1.94	0.49
4:D:129:PHE:HD2	4:D:237:ARG:HG3	1.77	0.49
2:B:160:GLY:O	2:B:185:ALA:HB1	2.12	0.49
3:C:178:GLU:O	3:C:179:ARG:C	2.51	0.49
7:G:39:GLU:HG2	7:G:78:ILE:HD11	1.94	0.49
3:C:253:ILE:HB	3:C:342:CYS:HB3	1.93	0.49
4:D:188:GLY:HA3	6:F:165:LEU:CD2	2.42	0.49
3:C:119:VAL:HG22	3:C:120:ILE:N	2.27	0.49
1:A:258:GLY:C	1:A:259:ILE:HD12	2.32	0.49
3:C:142:ARG:NH2	7:G:25:VAL:N	2.41	0.49
5:E:95:MET:HG2	5:E:141:GLY:O	2.13	0.49
2:B:334:VAL:HG22	2:B:334:VAL:O	2.12	0.49
4:D:134:GLU:OE2	4:D:136:LYS:HE2	2.12	0.49
4:D:74:GLU:N	4:D:74:GLU:OE1	2.43	0.49
3:C:92:ILE:HG22	3:C:94:ARG:HG3	1.94	0.49
5:E:91:GLY:O	5:E:95:MET:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:VAL:HG22	1:A:363:ILE:CD1	2.41	0.49
2:B:191:ARG:HG3	2:B:206:HIS:CE1	2.47	0.49
7:G:23:LYS:CG	7:G:24:PHE:H	2.09	0.49
5:E:139:GLU:O	5:E:142:LEU:HD23	2.11	0.49
1:A:120:PRO:HB3	1:A:409:ARG:HG2	1.95	0.49
1:A:183:GLY:HA3	1:A:413:VAL:HG21	1.95	0.49
1:A:340:LYS:HG2	1:A:365:VAL:HB	1.95	0.49
1:A:174:VAL:HG12	1:A:175:THR:N	2.28	0.48
5:E:82:LEU:CD2	5:E:148:VAL:HG21	2.37	0.48
5:E:95:MET:HA	5:E:95:MET:HE3	1.94	0.48
2:B:163:VAL:CG2	2:B:164:THR:H	2.24	0.48
4:D:158:LYS:HD3	4:D:158:LYS:C	2.33	0.48
1:A:91:ARG:O	1:A:94:GLU:HB2	2.13	0.48
2:B:330:LEU:HG	2:B:336:LYS:HZ1	1.76	0.48
3:C:370:LYS:O	3:C:371:ILE:CB	2.61	0.48
5:E:32:ALA:CB	5:E:135:GLN:OE1	2.61	0.48
3:C:140:PRO:O	3:C:142:ARG:HG3	2.13	0.48
4:D:263:HIS:O	4:D:267:ARG:HG3	2.14	0.48
4:D:202:HIS:HD2	9:D:435:HOH:O	1.97	0.48
7:G:20:ASP:C	7:G:22:ASN:H	2.17	0.48
3:C:282:GLY:HA2	3:C:370:LYS:HE3	1.96	0.48
3:C:84:ARG:HG2	3:C:84:ARG:NH1	2.29	0.48
5:E:60:ILE:CD1	5:E:116:ILE:HD13	2.42	0.48
4:D:205:PRO:HB3	4:D:222:TYR:CZ	2.49	0.48
2:B:337:LEU:HD21	7:G:16:VAL:HG13	1.96	0.48
2:B:155:VAL:HG21	2:B:286:ILE:HD11	1.95	0.48
4:D:37:ASP:HB2	4:D:43:TYR:HE1	1.78	0.48
2:B:181:ARG:HB2	2:B:181:ARG:NH1	2.29	0.48
3:C:143:SER:OG	3:C:162:CYS:HB2	2.13	0.48
3:C:269:LEU:HD22	3:C:369:LEU:HD11	1.96	0.48
2:B:205:ASN:HB3	2:B:208:ALA:HB3	1.96	0.47
7:G:83:LEU:HD22	7:G:128:TRP:CD2	2.49	0.47
4:D:158:LYS:HG3	4:D:159:ASP:CG	2.34	0.47
2:B:239:VAL:HG23	2:B:240:LEU:HD13	1.96	0.47
1:A:348:LYS:HE2	1:A:352:GLU:OE2	2.15	0.47
1:A:216:PRO:HB2	1:A:219:GLN:HB2	1.97	0.47
3:C:76:ALA:HB2	3:C:93:LEU:HD11	1.95	0.47
6:F:4:THR:CG2	6:F:55:ARG:HE	2.23	0.47
4:D:263:HIS:HD2	4:D:266:MET:CE	2.27	0.47
2:B:302:VAL:HG13	2:B:302:VAL:O	2.15	0.47
2:B:175:LEU:O	2:B:177:HIS:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ILE:HG13	2:B:213:VAL:HG11	1.96	0.47
1:A:289:ASN:HD22	1:A:290:PRO:N	2.12	0.47
5:E:153:ASN:OD1	5:E:154:ASP:N	2.46	0.47
2:B:180:ARG:HH12	2:B:285:THR:CA	2.25	0.47
3:C:10:PRO:HB3	3:C:350:MET:HA	1.96	0.47
5:E:74:TYR:CE1	5:E:137:ARG:HD2	2.50	0.47
6:F:43:SER:HB2	6:F:46:LEU:HD12	1.96	0.47
2:B:334:VAL:HG21	7:G:19:TYR:CZ	2.50	0.47
5:E:16:ILE:O	5:E:16:ILE:HG23	2.15	0.47
2:B:340:PHE:CD2	2:B:342:ILE:HD11	2.50	0.46
2:B:175:LEU:O	2:B:177:HIS:O	2.32	0.46
4:D:197:GLN:HB3	4:D:226:VAL:HB	1.98	0.46
1:A:307:CYS:HB3	1:A:308:PRO:HD2	1.97	0.46
6:F:4:THR:HG23	6:F:55:ARG:NH2	2.30	0.46
5:E:71:ILE:O	5:E:75:ILE:HG13	2.16	0.46
6:F:130:LYS:CE	6:F:130:LYS:HA	2.45	0.46
6:F:128:LYS:O	6:F:132:VAL:HG23	2.15	0.46
5:E:22:LEU:HD23	5:E:41:ILE:HB	1.96	0.46
3:C:101:CYS:O	3:C:113:VAL:HA	2.15	0.46
5:E:9:MET:SD	5:E:63:GLU:HG2	2.55	0.46
6:F:82:ILE:O	6:F:86:LEU:HG	2.15	0.46
5:E:86:ASN:O	5:E:87:SER:HB3	2.14	0.46
3:C:247:LEU:HA	3:C:262:GLY:HA3	1.97	0.46
1:A:143:VAL:HG13	1:A:146:VAL:HG23	1.96	0.46
4:D:228:PHE:H	4:D:231:HIS:CD2	2.21	0.46
1:A:239:VAL:HG23	1:A:240:LYS:N	2.30	0.46
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.50	0.46
4:D:84:LEU:C	4:D:84:LEU:HD23	2.37	0.46
7:G:78:ILE:O	7:G:82:VAL:HG23	2.15	0.46
6:F:22:LEU:HD21	6:F:70:VAL:HG23	1.96	0.46
3:C:72:THR:HA	3:C:98:ALA:CB	2.45	0.46
5:E:23:PRO:HG3	5:E:33:PRO:HB2	1.98	0.46
3:C:7:LEU:HD12	3:C:9:GLU:HB2	1.97	0.46
4:D:160:ARG:HH11	4:D:160:ARG:HB3	1.81	0.45
1:A:90:GLU:HB3	9:A:509:HOH:O	2.16	0.45
2:B:278:VAL:HG13	2:B:279:ALA:N	2.31	0.45
4:D:274:LEU:O	4:D:278:ASN:ND2	2.46	0.45
3:C:69:THR:O	3:C:76:ALA:HA	2.17	0.45
5:E:145:CYS:C	5:E:147:LYS:H	2.19	0.45
2:B:163:VAL:CG2	2:B:164:THR:N	2.79	0.45
5:E:87:SER:N	5:E:154:ASP:HA	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:105:ARG:HG2	6:F:105:ARG:HH11	1.82	0.45
3:C:74:ARG:HD2	6:F:31:GLU:CG	2.47	0.45
6:F:86:LEU:HD13	6:F:149:MET:HB3	1.97	0.45
1:A:359:LYS:N	1:A:360:PRO:HD3	2.32	0.45
2:B:170:TYR:O	2:B:171:GLU:C	2.54	0.45
1:A:349:LEU:O	1:A:353:LEU:HD23	2.17	0.45
2:B:330:LEU:HG	2:B:336:LYS:CD	2.47	0.45
6:F:38:VAL:HG12	6:F:69:SER:OG	2.17	0.45
1:A:274:GLU:HA	1:A:277:LEU:HB2	1.98	0.44
2:B:246:LEU:HB3	2:B:247:PRO:HD2	1.99	0.44
2:B:239:VAL:HG23	2:B:240:LEU:CD1	2.47	0.44
2:B:299:LYS:NZ	2:B:300:HIS:HE1	2.15	0.44
4:D:263:HIS:HD2	4:D:266:MET:HE1	1.80	0.44
7:G:87:LYS:N	7:G:87:LYS:HD3	2.33	0.44
5:E:18:ASN:ND2	5:E:118:ALA:N	2.57	0.44
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.53	0.44
1:A:158:VAL:O	1:A:158:VAL:HG23	2.18	0.44
2:B:166:ILE:HD13	2:B:282:LEU:HA	1.97	0.44
1:A:284:HIS:N	1:A:285:PRO:HD3	2.33	0.44
4:D:258:SER:O	4:D:262:ILE:HG12	2.17	0.44
4:D:75:LEU:C	4:D:75:LEU:HD23	2.38	0.44
2:B:325:TYR:HA	2:B:329:VAL:HG12	1.99	0.44
5:E:82:LEU:HD13	5:E:95:MET:SD	2.57	0.44
4:D:212:THR:C	4:D:214:ALA:H	2.21	0.44
2:B:334:VAL:HG21	7:G:19:TYR:CD1	2.52	0.44
1:A:205:GLN:NE2	1:A:220:SER:OG	2.48	0.44
3:C:82:LYS:HD2	3:C:87:LYS:HG3	2.00	0.44
2:B:325:TYR:O	2:B:329:VAL:HG12	2.18	0.44
5:E:22:LEU:HA	5:E:23:PRO:HD3	1.82	0.44
3:C:258:LEU:HB2	3:C:270:PHE:HB2	2.00	0.44
4:D:45:ILE:HA	4:D:56:MET:O	2.18	0.44
5:E:75:ILE:O	5:E:79:LEU:HG	2.17	0.44
5:E:112:PRO:O	5:E:113:LEU:HB2	2.17	0.44
3:C:14:HIS:H	3:C:331:GLN:HE22	1.66	0.44
7:G:80:LEU:O	7:G:84:ILE:HD13	2.18	0.44
3:C:189:MET:HA	3:C:195:MET:HE1	2.00	0.44
3:C:146:LEU:HD11	3:C:162:CYS:SG	2.58	0.44
7:G:133:LEU:HD13	7:G:141:ILE:HD11	1.99	0.43
4:D:182:MET:HG3	4:D:200:PHE:CE1	2.52	0.43
1:A:389:GLU:CA	1:A:392:GLN:OE1	2.65	0.43
5:E:74:TYR:CE1	5:E:98:LEU:HD12	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:124:VAL:O	7:G:127:GLN:HB2	2.18	0.43
4:D:263:HIS:HA	4:D:266:MET:HE2	2.01	0.43
4:D:67:LEU:HD13	4:D:120:CYS:O	2.18	0.43
3:C:129:ASN:HB2	3:C:131:TRP:CZ3	2.54	0.43
2:B:322:LYS:HD3	7:G:16:VAL:HG11	2.01	0.43
2:B:323:GLN:HB3	7:G:11:PHE:O	2.18	0.43
3:C:170:SER:HB2	3:C:195:MET:HE3	1.99	0.43
2:B:232:LYS:HB3	2:B:232:LYS:HE2	1.81	0.43
2:B:164:THR:HB	2:B:182:LEU:HB3	2.00	0.43
2:B:247:PRO:HG2	8:B:401:CKH:H6	2.01	0.43
4:D:75:LEU:HD13	4:D:123:SER:N	2.33	0.43
6:F:60:LYS:HE3	6:F:112:TYR:CE2	2.54	0.43
7:G:104:ASP:OD2	7:G:143:ARG:NE	2.39	0.43
3:C:225:THR:HG22	3:C:241:ALA:HA	2.01	0.43
2:B:295:SER:O	2:B:299:LYS:HG2	2.19	0.42
3:C:30:HIS:HB2	9:C:402:HOH:O	2.19	0.42
5:E:18:ASN:CG	5:E:118:ALA:H	2.22	0.42
1:A:313:ARG:CZ	1:A:363:ILE:HG22	2.50	0.42
4:D:158:LYS:O	4:D:158:LYS:HD3	2.18	0.42
3:C:107:ASN:ND2	3:C:109:LYS:HB2	2.34	0.42
3:C:12:SER:HB2	3:C:26:CYS:HB3	2.01	0.42
5:E:102:ASN:HD21	5:E:130:ARG:NE	2.17	0.42
1:A:300:VAL:O	1:A:304:ILE:HG13	2.19	0.42
7:G:10:ARG:O	7:G:11:PHE:CB	2.60	0.42
1:A:143:VAL:CG1	1:A:146:VAL:HG23	2.49	0.42
1:A:30:ILE:HD13	1:A:375:TYR:CZ	2.55	0.42
7:G:149:LYS:HE3	7:G:149:LYS:HB2	1.89	0.42
1:A:39:GLU:CG	1:A:39:GLU:O	2.62	0.42
2:B:290:ASP:HB2	2:B:293:THR:HG1	1.84	0.42
1:A:259:ILE:N	1:A:259:ILE:HD12	2.34	0.42
1:A:369:THR:HA	1:A:373:GLN:OE1	2.20	0.42
1:A:259:ILE:HG23	1:A:265:LYS:O	2.20	0.41
5:E:120:PRO:HG3	5:E:126:ASP:OD1	2.19	0.41
1:A:38:LYS:NZ	1:A:71:THR:CG2	2.83	0.41
5:E:121:ALA:HB3	5:E:125:GLU:OE2	2.20	0.41
3:C:185:TRP:HE3	3:C:235:MET:CE	2.33	0.41
3:C:347:THR:OG1	3:C:355:SER:HB2	2.20	0.41
3:C:321:LEU:HD11	6:F:129:HIS:CE1	2.56	0.41
3:C:151:HIS:CE1	3:C:152:PRO:HG2	2.56	0.41
2:B:303:LEU:HD21	2:B:344:ILE:HG21	2.02	0.41
4:D:137:GLU:OE2	4:D:158:LYS:HE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:138:PHE:O	6:F:142:ILE:HG23	2.20	0.41
1:A:19:LEU:HD23	1:A:19:LEU:N	2.35	0.41
3:C:119:VAL:HG22	3:C:120:ILE:H	1.86	0.41
1:A:228:LYS:O	1:A:232:SER:HB2	2.19	0.41
2:B:194:ILE:CG1	2:B:213:VAL:HG21	2.44	0.41
1:A:91:ARG:HD2	9:A:501:HOH:O	2.21	0.41
4:D:45:ILE:HG12	4:D:57:VAL:HG22	2.03	0.41
4:D:282:PRO:HD3	6:F:125:GLN:O	2.21	0.41
2:B:325:TYR:O	2:B:327:GLU:N	2.54	0.41
6:F:31:GLU:OE2	6:F:32:ARG:CG	2.63	0.41
1:A:343:VAL:O	1:A:347:LEU:HD13	2.20	0.41
1:A:339:LEU:HD23	1:A:365:VAL:HG13	2.03	0.41
5:E:44:GLU:HG2	5:E:48:TYR:CE2	2.55	0.41
1:A:348:LYS:HG2	1:A:352:GLU:OE2	2.21	0.41
3:C:370:LYS:HB2	3:C:370:LYS:HE2	1.97	0.40
3:C:266:PHE:CD1	3:C:284:ARG:HG3	2.57	0.40
1:A:240:LYS:O	1:A:244:LYS:HG3	2.21	0.40
1:A:307:CYS:HB3	1:A:308:PRO:CD	2.52	0.40
5:E:132:TYR:CE2	5:E:136:LEU:HD11	2.57	0.40
5:E:161:THR:O	5:E:161:THR:HG22	2.22	0.40
2:B:212:THR:O	2:B:216:ILE:HG13	2.21	0.40
3:C:207:GLY:O	3:C:219:TRP:HA	2.21	0.40
3:C:219:TRP:CE2	3:C:227:CYS:HB2	2.57	0.40
7:G:71:VAL:CG1	7:G:72:LYS:N	2.84	0.40
3:C:370:LYS:H	3:C:370:LYS:HZ3	1.69	0.40
1:A:352:GLU:C	1:A:354:SER:N	2.74	0.40
7:G:23:LYS:CG	7:G:24:PHE:N	2.77	0.40
2:B:325:TYR:O	2:B:326:LEU:C	2.60	0.40
1:A:53:LYS:O	1:A:56:ASP:OD2	2.39	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	395/418 (94%)	373 (94%)	19 (5%)	3 (1%)	24	39
2	B	191/394 (48%)	168 (88%)	16 (8%)	7 (4%)	4	4
3	C	343/372 (92%)	321 (94%)	20 (6%)	2 (1%)	30	48
4	D	280/300 (93%)	268 (96%)	10 (4%)	2 (1%)	26	43
5	E	171/178 (96%)	156 (91%)	12 (7%)	3 (2%)	11	16
6	F	165/168 (98%)	160 (97%)	4 (2%)	1 (1%)	30	48
7	G	132/151 (87%)	123 (93%)	6 (4%)	3 (2%)	8	11
All	All	1677/1981 (85%)	1569 (94%)	87 (5%)	21 (1%)	15	24

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	SER
1	A	264	LYS
2	B	329	VAL
7	G	11	PHE
2	B	171	GLU
2	B	290	ASP
2	B	326	LEU
3	C	371	ILE
4	D	237	ARG
6	F	102	PHE
2	B	178	LEU
3	C	50	GLU
5	E	151	PRO
5	E	153	ASN
1	A	353	LEU
2	B	328	ARG
5	E	87	SER
2	B	176	PRO
4	D	213	ASP
7	G	21	GLU
7	G	118	SER

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	344/363 (95%)	332 (96%)	12 (4%)	43	69
2	B	165/345 (48%)	152 (92%)	13 (8%)	15	27
3	C	296/313 (95%)	285 (96%)	11 (4%)	41	67
4	D	248/264 (94%)	244 (98%)	4 (2%)	70	89
5	E	153/159 (96%)	144 (94%)	9 (6%)	24	42
6	F	152/155 (98%)	150 (99%)	2 (1%)	76	91
7	G	109/123 (89%)	103 (94%)	6 (6%)	27	46
All	All	1467/1722 (85%)	1410 (96%)	57 (4%)	39	64

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	19	LEU
1	A	88	LEU
1	A	191	LYS
1	A	206	GLN
1	A	230	ARG
1	A	289	ASN
1	A	335	LEU
1	A	343	VAL
1	A	344	ASP
1	A	363	ILE
1	A	394	CYS
2	B	158	ASP
2	B	161	ASP
2	B	173	PHE
2	B	175	LEU
2	B	176	PRO
2	B	182	LEU
2	B	200	ARG
2	B	220	LEU
2	B	235	LEU
2	B	257	GLU
2	B	290	ASP
2	B	297	PHE
2	B	336	LYS
3	C	8	VAL
3	C	30	HIS

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Mol	Chain	Res	Type
3	C	54	GLN
3	C	90	LEU
3	C	107	ASN
3	C	128	GLU
3	C	131	TRP
3	C	134	CYS
3	C	140	PRO
3	C	179	ARG
3	C	297	THR
4	D	116	LEU
4	D	229	PRO
4	D	230	ARG
4	D	277	LEU
5	E	22	LEU
5	E	25	ARG
5	E	82	LEU
5	E	95	MET
5	E	98	LEU
5	E	130	ARG
5	E	142	LEU
5	E	144	LEU
5	E	151	PRO
6	F	101	PHE
6	F	165	LEU
7	G	21	GLU
7	G	27	GLU
7	G	39	GLU
7	G	69	GLN
7	G	73	ASP
7	G	87	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	176	HIS
1	A	192	HIS
1	A	205	GLN
1	A	289	ASN
1	A	318	ASN
1	A	371	HIS
1	A	395	HIS

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Mol	Chain	Res	Type
1	A	410	HIS
1	A	411	ASN
2	B	205	ASN
2	B	206	HIS
2	B	267	GLN
2	B	284	ASN
2	B	287	GLN
2	B	323	GLN
3	C	22	GLN
3	C	54	GLN
3	C	65	ASN
3	C	107	ASN
3	C	303	GLN
3	C	331	GLN
4	D	140	ASN
4	D	197	GLN
4	D	202	HIS
4	D	231	HIS
4	D	263	HIS
5	E	18	ASN
5	E	83	GLN
5	E	90	GLN
5	E	102	ASN
5	E	167	GLN
6	F	28	GLN
6	F	125	GLN
6	F	154	ASN
6	F	167	ASN
7	G	61	ASN
7	G	96	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

1 ligand is 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	$\# Z > 2$
8	CKH	B	401	-	22,24,24	0.97	0	25,33,33	0.98	3 (12%)

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
8	CKH	B	401	-	-	0/10/10/10	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	401	CKH	CAT-CAS-CAI	-2.58	120.19	123.20
8	B	401	CKH	CAQ-CAP-CAD	-2.04	125.01	129.68
8	B	401	CKH	CAJ-CAI-CAS	2.30	119.17	116.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	401	CKH	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	401/418 (95%)	0.13	22 (5%) 29 32	17, 40, 77, 89	0
2	B	193/394 (48%)	0.65	31 (16%) 3 2	22, 54, 98, 105	0
3	C	349/372 (93%)	0.05	10 (2%) 55 59	21, 36, 74, 94	0
4	D	282/300 (94%)	-0.04	3 (1%) 82 84	18, 38, 57, 75	0
5	E	173/178 (97%)	0.30	11 (6%) 23 25	36, 55, 88, 96	0
6	F	167/168 (99%)	-0.16	1 (0%) 90 91	17, 30, 45, 73	0
7	G	136/151 (90%)	0.47	13 (9%) 10 11	26, 55, 82, 87	0
All	All	1701/1981 (85%)	0.16	91 (5%) 30 34	17, 41, 82, 105	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	VAL	7.2
2	B	178	LEU	6.6
2	B	173	PHE	6.5
5	E	151	PRO	5.1
5	E	85	CYS	4.9
7	G	64	ILE	4.7
1	A	360	PRO	4.4
6	F	2	THR	4.3
4	D	211	ASP	4.3
1	A	40	SER	4.2
2	B	341	LYS	4.2
2	B	174	SER	4.2
5	E	93	LYS	4.2
2	B	292	ASP	4.2
5	E	89	SER	4.2
2	B	334	VAL	4.1
1	A	417	MET	4.1

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Mol	Chain	Res	Type	RSRZ
7	G	151	VAL	3.7
2	B	293	THR	3.7
3	C	372	VAL	3.7
3	C	127	GLN	3.7
7	G	35	ALA	3.6
3	C	297	THR	3.6
3	C	367	LYS	3.6
2	B	180	ARG	3.6
2	B	288	ALA	3.5
2	B	289	ALA	3.5
1	A	359	LYS	3.5
7	G	9	ALA	3.5
3	C	302	PHE	3.5
1	A	349	LEU	3.3
7	G	13	LYS	3.3
1	A	39	GLU	3.3
1	A	156	ARG	3.3
5	E	38	ASP	3.2
7	G	10	ARG	3.2
3	C	301	ARG	3.1
1	A	213	VAL	3.1
2	B	336	LYS	3.0
2	B	181	ARG	2.9
7	G	67	LYS	2.9
2	B	170	TYR	2.9
5	E	153	ASN	2.9
7	G	65	ASN	2.8
1	A	159	GLY	2.8
2	B	171	GLU	2.8
1	A	265	LYS	2.7
5	E	121	ALA	2.7
1	A	214	GLY	2.7
2	B	332	GLY	2.7
1	A	157	GLN	2.7
1	A	262	ILE	2.7
5	E	92	GLU	2.6
2	B	333	ASP	2.6
1	A	347	LEU	2.6
3	C	304	ASN	2.6
3	C	368	ASP	2.5
2	B	297	PHE	2.5
2	B	331	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	352	GLU	2.5
2	B	346	ASP	2.4
7	G	66	THR	2.4
2	B	172	GLY	2.4
3	C	319	ALA	2.4
4	D	130	GLN	2.4
2	B	325	TYR	2.4
1	A	263	SER	2.3
2	B	326	LEU	2.3
5	E	154	ASP	2.3
2	B	176	PRO	2.3
7	G	14	VAL	2.3
4	D	212	THR	2.2
5	E	36	THR	2.2
2	B	329	VAL	2.2
2	B	166	ILE	2.2
7	G	50	ASN	2.2
2	B	276	VAL	2.2
3	C	131	TRP	2.2
2	B	281	LEU	2.2
2	B	156	VAL	2.1
1	A	52	MET	2.1
1	A	354	SER	2.1
2	B	183	ASP	2.1
1	A	216	PRO	2.1
1	A	158	VAL	2.1
7	G	27	GLU	2.1
2	B	169	VAL	2.1
2	B	339	LYS	2.1
7	G	120	ASN	2.1
1	A	70	PRO	2.1
5	E	96	TYR	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	CKH	B	401	22/22	0.95	0.13	-0.48	36,39,47,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.