Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2023 – 12:39 PM EDT

PDB ID	:	3BUO
Title	:	Crystal structure of c-Cbl-TKB domain complexed with its binding motif in EGF receptor'
Authors	:	Ng, C.; Jackson, R.A.; Buschdorf, J.P.; Sun, Q.; Guy, G.R.; Sivaraman, J.
Deposited on	:	2008-01-03
Resolution	:	2.60 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

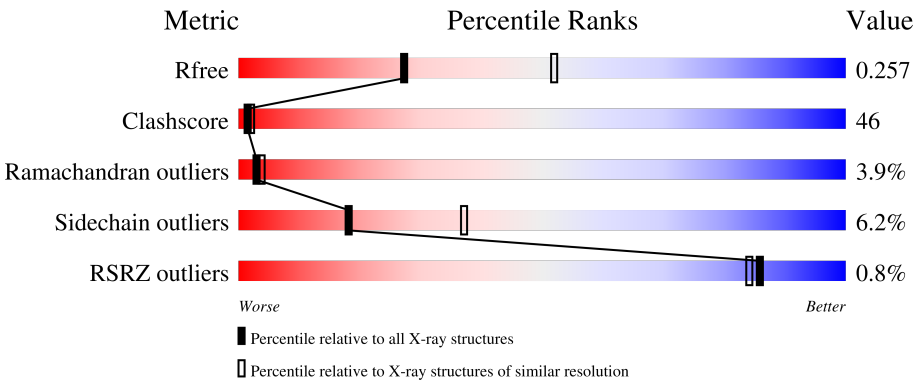
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	13	15%; 31%, 31%, 23%, 15%
1	C	13	15%; 31%, 31%, 23%, 15%
2	B	329	38%, 48%, 6%, 8%
2	D	329	36%, 49%, 6%, 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5405 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 13-meric peptide from Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	11	95	57	15	22	1	0	0	0
1	C	11	95	57	15	22	1	0	0	0

- Molecule 2 is a protein called E3 ubiquitin-protein ligase CBL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	304	2490	1612	424	441	13	0	0	0
2	D	304	2490	1612	424	441	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	SER	GLY	cloning artifact	UNP P22681
D	24	SER	GLY	cloning artifact	UNP P22681

- Molecule 3 is water.

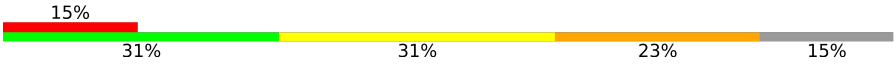
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	6	6	6	0	0
3	B	111	111	111	0	0
3	C	6	6	6	0	0
3	D	112	112	112	0	0

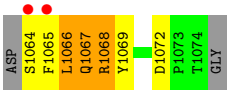
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: 13-meric peptide from Epidermal growth factor receptor

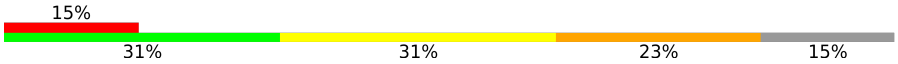
Chain A:

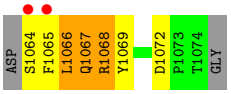




• Molecule 1: 13-meric peptide from Epidermal growth factor receptor

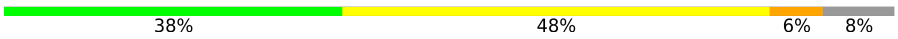
Chain C:

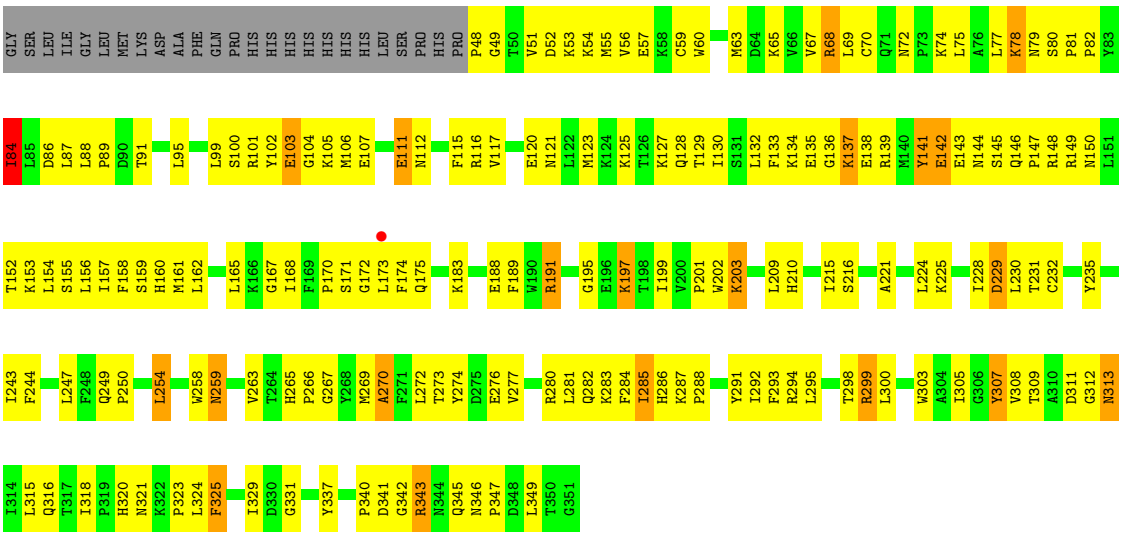




• Molecule 2: E3 ubiquitin-protein ligase CBL

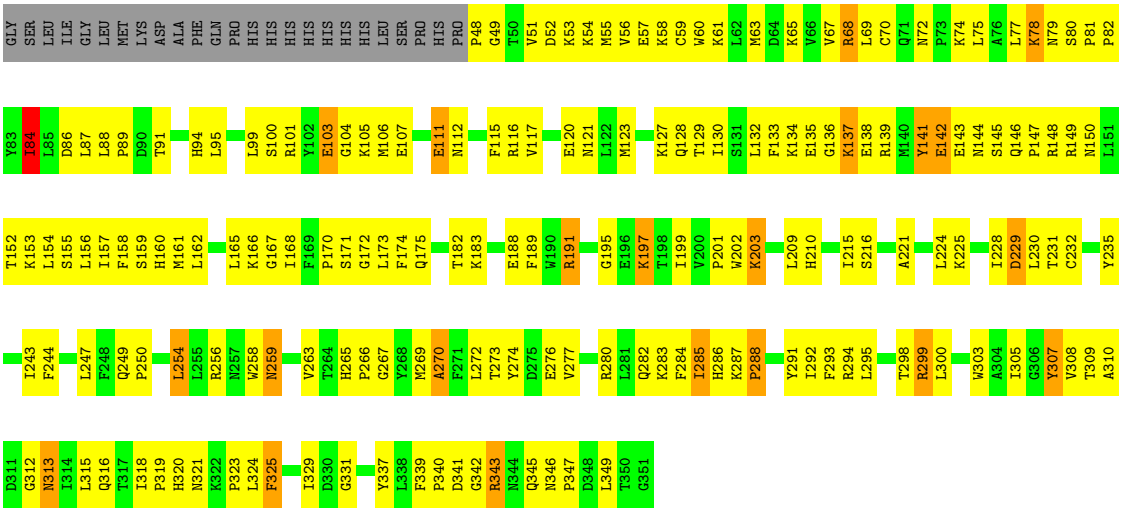
Chain B:





• Molecule 2: E3 ubiquitin-protein ligase CBL

Chain D:


GLY SER LEU ILE GLY LEU MET LYS ASP ALA PHE GLN PRO HIS HIS HIS HIS HIS HIS HIS HIS LEU SER PRO HIS PRO P48 G49 T50 V51 D52 K53 K54 M55 V56 E57 K58 C59 W60 K61 L62 M63 D64 K65 V66 V67 R68 L69 C70 Q71 N72 P73 K74 L75 A76 L77 K78 N79 S80 P81 P82
Y83 I84 L85 D86 L87 L88 P89 D90 T91 H94 L95 L99 S100 R101 Y102 E103 G104 K105 M106 E107 E111 N112 F115 R116 V117 E120 N121 L122 M123 K127 Q128 T129 I130 S131 L132 F133 K134 E135 G136 K137 E138 R139 M140 Y141 E142 E143 N144 S145 Q146 P147 R148 R149 N150 L151
T152 K153 L154 S155 L156 I157 F158 S159 H160 M161 L162 L165 K166 G167 I168 F169 P170 S171 G172 L173 F174 Q175 T182 K183 E188 F189 W190 R191 G195 E196 K197 T198 I199 V200 P201 W202 K203 L209 H210 I215 S216 A221 L224 K225 I228 D229 L230 T231 C232 Y235
I243 F244 L247 F248 Q249 P250 L254 L255 R256 N257 W258 N259 V263 T264 H265 P266 G267 Y268 M269 A270 F271 L272 T273 Y274 D275 E276 V277 R280 L281 Q282 K283 F284 I285 H286 K287 P288 Y291 I292 F293 R294 L295 T298 R299 L300 W303 A304 I305 G306 Y307 V308 T309 A310
D311 G312 N313 I314 L315 Q316 T317 I318 P319 H320 N321 K322 P323 L324 F325 I329 D330 G331 Y337 L338 F339 P340 D341 G342 R343 N344 Q345 N346 P347 D348 L349 T350 G351

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.86Å 110.17Å 55.82Å 90.00° 89.94° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 39.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	51.8 (20.00-2.60) 91.3 (39.29-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.278 0.249 , 0.257	Depositor DCC
R_{free} test set	2860 reflections (13.04%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 28.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.458 for -h,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5405	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: PTR

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	0.68	0/79	0.96	0/104
1	C	0.65	0/79	0.95	0/104
2	B	0.52	0/2556	0.65	0/3449
2	D	0.51	0/2556	0.65	0/3449
All	All	0.52	0/5270	0.66	0/7106

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	95	0	80	16	0
1	C	95	0	80	19	0
2	B	2490	0	2499	232	0
2	D	2490	0	2499	232	0
3	A	6	0	0	0	0
3	B	111	0	0	16	0
3	C	6	0	0	1	0
3	D	112	0	0	18	0
All	All	5405	0	5158	478	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 46.

All (478) 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)
2:D:82:PRO:HG3	2:D:156:LEU:HD12	1.33	1.09
2:D:277:VAL:HG13	2:D:292:ILE:HD11	1.37	1.05
2:B:82:PRO:HG3	2:B:156:LEU:HD12	1.33	1.04
2:B:282:GLN:HE22	2:B:285:ILE:HD12	1.23	1.00
2:D:282:GLN:HE22	2:D:285:ILE:HD12	1.22	1.00
2:B:277:VAL:HG13	2:B:292:ILE:HD11	1.40	0.99
2:B:156:LEU:HD11	2:B:273:THR:HG22	1.46	0.98
2:D:156:LEU:HD11	2:D:273:THR:HG22	1.47	0.96
2:B:82:PRO:HG3	2:B:156:LEU:CD1	2.01	0.91
1:C:1068:ARG:HB3	2:D:274:TYR:CE2	2.06	0.90
2:B:331:GLY:HA3	2:B:337:TYR:CD2	2.06	0.90
2:D:331:GLY:HA3	2:D:337:TYR:CD2	2.06	0.90
1:A:1068:ARG:HB3	2:B:274:TYR:CE2	2.07	0.90
2:D:82:PRO:HG3	2:D:156:LEU:CD1	2.00	0.89
2:B:188:GLU:HA	2:B:191:ARG:NH1	1.92	0.84
1:A:1066:LEU:HD21	2:B:298:THR:HG21	1.59	0.84
2:D:188:GLU:HA	2:D:191:ARG:NH1	1.93	0.83
1:C:1066:LEU:O	1:C:1067:GLN:HG3	1.79	0.83
2:D:273:THR:O	2:D:277:VAL:HG23	1.77	0.82
2:D:277:VAL:HG13	2:D:292:ILE:CD1	2.09	0.82
2:B:149:ARG:HG3	2:B:149:ARG:HH11	1.45	0.81
2:B:273:THR:O	2:B:277:VAL:HG23	1.80	0.81
1:C:1066:LEU:HD21	2:D:298:THR:HG21	1.61	0.81
2:D:149:ARG:HG3	2:D:149:ARG:HH11	1.45	0.80
2:D:269:MET:HB3	2:D:272:LEU:HD12	1.62	0.80
1:A:1066:LEU:O	1:A:1067:GLN:HG3	1.81	0.80
2:B:153:LYS:HA	3:B:448:HOH:O	1.82	0.80
2:B:77:LEU:HA	2:B:78:LYS:NZ	1.98	0.79
2:B:272:LEU:HB2	3:B:373:HOH:O	1.81	0.79
2:B:202:TRP:HB3	2:B:203:LYS:HZ3	1.47	0.79
2:D:77:LEU:HA	2:D:78:LYS:NZ	1.97	0.79
2:B:269:MET:HB3	2:B:272:LEU:HD12	1.64	0.79
2:B:203:LYS:CD	2:B:203:LYS:H	1.96	0.79
1:C:1066:LEU:HA	3:C:17:HOH:O	1.82	0.79
2:B:149:ARG:HB3	3:B:359:HOH:O	1.81	0.79
2:B:283:LYS:HE2	2:B:284:PHE:CZ	2.19	0.78
2:D:202:TRP:HB3	2:D:203:LYS:HZ3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:LYS:CD	2:D:203:LYS:H	1.97	0.78
2:B:340:PRO:HD3	2:B:346:ASN:ND2	1.99	0.77
2:D:283:LYS:HE2	2:D:284:PHE:CZ	2.18	0.77
2:D:49:GLY:O	2:D:116:ARG:HD2	1.85	0.77
2:B:277:VAL:HG13	2:B:292:ILE:CD1	2.13	0.77
2:B:49:GLY:O	2:B:116:ARG:HD2	1.85	0.76
2:D:91:THR:OG1	2:D:162:LEU:HD13	1.86	0.76
2:B:320:HIS:HA	3:B:406:HOH:O	1.86	0.75
2:D:229:ASP:OD1	2:D:232:CYS:HA	1.86	0.75
2:B:307:TYR:CE1	2:B:315:LEU:HB2	2.21	0.75
2:D:307:TYR:CE1	2:D:315:LEU:HB2	2.22	0.74
2:D:340:PRO:HD3	2:D:346:ASN:ND2	2.02	0.73
2:D:134:LYS:HA	3:D:397:HOH:O	1.88	0.73
2:B:229:ASP:OD1	2:B:232:CYS:HA	1.89	0.73
2:B:129:THR:OG1	2:B:154:LEU:HD23	1.89	0.72
2:B:228:ILE:HG12	2:B:244:PHE:CD1	2.24	0.72
2:D:188:GLU:HA	2:D:191:ARG:HH11	1.54	0.72
2:D:282:GLN:HE22	2:D:285:ILE:CD1	2.01	0.72
2:B:161:MET:HG2	2:B:231:THR:HG22	1.69	0.72
2:D:203:LYS:H	2:D:203:LYS:CE	2.03	0.72
2:D:129:THR:OG1	2:D:154:LEU:HD23	1.89	0.72
2:D:228:ILE:HG12	2:D:244:PHE:CD1	2.24	0.72
2:B:203:LYS:H	2:B:203:LYS:CE	2.02	0.72
2:D:78:LYS:NZ	2:D:78:LYS:H	1.88	0.71
2:D:86:ASP:O	2:D:89:PRO:HD2	1.90	0.71
2:B:282:GLN:HE22	2:B:285:ILE:CD1	2.00	0.71
1:C:1065:PHE:CD2	1:C:1066:LEU:N	2.57	0.71
2:D:225:LYS:HG2	3:D:417:HOH:O	1.89	0.71
2:B:78:LYS:NZ	2:B:78:LYS:H	1.89	0.71
2:D:68:ARG:HG3	2:D:69:LEU:H	1.56	0.71
2:B:84:ILE:HD13	2:B:84:ILE:C	2.11	0.70
2:B:340:PRO:HD3	2:B:346:ASN:HD22	1.53	0.70
2:D:65:LYS:HE2	2:D:69:LEU:HD11	1.72	0.70
1:A:1065:PHE:CD2	1:A:1066:LEU:N	2.58	0.70
2:D:84:ILE:HD13	2:D:84:ILE:C	2.12	0.70
2:B:88:LEU:HB2	2:B:89:PRO:HD3	1.73	0.70
2:D:161:MET:HG2	2:D:231:THR:HG22	1.72	0.70
2:D:199:ILE:HD11	2:D:235:TYR:HB3	1.72	0.70
2:B:188:GLU:HA	2:B:191:ARG:HH11	1.53	0.70
2:D:305:ILE:HG21	2:D:337:TYR:CE1	2.27	0.70
2:D:88:LEU:HB2	2:D:89:PRO:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:ARG:HG3	2:B:69:LEU:H	1.57	0.69
2:B:91:THR:OG1	2:B:162:LEU:HD13	1.93	0.69
2:B:305:ILE:HG21	2:B:337:TYR:CE1	2.28	0.69
1:C:1068:ARG:HB3	2:D:274:TYR:CZ	2.27	0.69
2:D:52:ASP:OD2	2:D:54:LYS:HB2	1.93	0.69
1:A:1068:ARG:HB3	2:B:274:TYR:CZ	2.27	0.68
2:B:101:ARG:HD3	2:B:173:LEU:CD1	2.23	0.68
2:D:101:ARG:HD3	2:D:173:LEU:CD1	2.23	0.68
2:B:52:ASP:OD2	2:B:54:LYS:HB2	1.93	0.68
2:B:144:ASN:HB3	2:B:149:ARG:HH21	1.59	0.68
2:D:272:LEU:HD22	2:D:276:GLU:HB3	1.76	0.68
2:B:56:VAL:HG12	2:B:60:TRP:NE1	2.09	0.67
2:B:86:ASP:O	2:B:89:PRO:HD2	1.94	0.67
2:B:199:ILE:HD11	2:B:235:TYR:HB3	1.75	0.67
1:A:1064:SER:HB3	2:B:79:ASN:ND2	2.09	0.67
2:B:282:GLN:NE2	2:B:285:ILE:HD12	2.05	0.67
2:D:203:LYS:H	2:D:203:LYS:HD3	1.59	0.67
2:B:203:LYS:H	2:B:203:LYS:HD3	1.58	0.67
2:D:144:ASN:HB3	2:D:149:ARG:HH21	1.59	0.67
2:D:340:PRO:HD3	2:D:346:ASN:HD22	1.56	0.67
1:C:1064:SER:HB3	2:D:79:ASN:ND2	2.10	0.66
2:B:68:ARG:HG3	2:B:69:LEU:N	2.10	0.66
2:B:272:LEU:HD22	2:B:276:GLU:HB3	1.77	0.66
2:D:280:ARG:HH21	2:D:341:ASP:CG	1.99	0.66
2:D:56:VAL:HG12	2:D:60:TRP:NE1	2.09	0.66
2:D:100:SER:O	2:D:103:GLU:HB2	1.96	0.65
2:B:65:LYS:HE2	2:B:69:LEU:HD11	1.76	0.65
2:D:123:MET:HG2	2:D:127:LYS:HE3	1.79	0.65
2:B:280:ARG:HH21	2:B:341:ASP:CG	2.00	0.65
2:D:68:ARG:HG3	2:D:69:LEU:N	2.10	0.65
2:B:132:LEU:HD21	2:B:147:PRO:O	1.96	0.64
2:B:188:GLU:HA	2:B:191:ARG:HD3	1.78	0.64
2:D:282:GLN:NE2	2:D:285:ILE:HD12	2.04	0.64
2:B:123:MET:HG2	2:B:127:LYS:HE3	1.79	0.64
2:B:243:ILE:HD13	2:B:300:LEU:HD22	1.79	0.63
1:C:1068:ARG:NH2	2:D:274:TYR:HB3	2.13	0.63
2:D:188:GLU:HA	2:D:191:ARG:HD3	1.79	0.63
2:D:132:LEU:HD21	2:D:147:PRO:O	1.99	0.63
2:B:72:ASN:HD21	2:B:74:LYS:HB2	1.63	0.63
2:B:188:GLU:CA	2:B:191:ARG:NH1	2.61	0.63
2:B:152:THR:HG21	2:B:276:GLU:CD	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:319:PRO:HA	3:D:367:HOH:O	1.98	0.63
2:D:152:THR:HG21	2:D:276:GLU:CD	2.20	0.62
2:D:188:GLU:CA	2:D:191:ARG:NH1	2.62	0.62
2:B:100:SER:O	2:B:103:GLU:HB2	2.00	0.62
2:D:191:ARG:O	2:D:195:GLY:HA2	1.99	0.62
2:D:282:GLN:O	2:D:285:ILE:HB	2.00	0.62
2:B:191:ARG:O	2:B:195:GLY:HA2	1.98	0.61
2:B:282:GLN:O	2:B:285:ILE:HB	2.00	0.61
1:A:1068:ARG:NH2	2:B:274:TYR:HB3	2.16	0.61
2:D:149:ARG:HG3	2:D:149:ARG:NH1	2.14	0.61
1:A:1068:ARG:NH2	2:B:80:SER:HB2	2.15	0.61
2:B:63:MET:O	2:B:67:VAL:HG23	2.01	0.61
2:B:149:ARG:HG3	2:B:149:ARG:NH1	2.15	0.60
2:D:269:MET:HE2	2:D:272:LEU:HD11	1.82	0.60
2:D:72:ASN:HD21	2:D:74:LYS:HB2	1.65	0.60
2:B:244:PHE:CE2	2:B:254:LEU:HD11	2.37	0.60
2:D:63:MET:O	2:D:67:VAL:HG23	2.02	0.60
2:B:346:ASN:ND2	2:B:347:PRO:HD2	2.16	0.59
2:D:303:TRP:CD2	2:D:324:LEU:HD22	2.37	0.59
2:D:144:ASN:HA	2:D:149:ARG:HE	1.68	0.59
2:D:244:PHE:CE2	2:D:254:LEU:HD11	2.38	0.59
2:B:81:PRO:HA	2:B:82:PRO:C	2.23	0.59
2:D:346:ASN:ND2	2:D:347:PRO:HD2	2.16	0.59
2:B:144:ASN:HA	2:B:149:ARG:HE	1.67	0.59
2:B:259:ASN:HA	2:B:263:VAL:CG2	2.32	0.59
2:D:57:GLU:HA	3:D:356:HOH:O	2.03	0.59
2:B:87:LEU:HD22	2:B:159:SER:HA	1.84	0.59
2:D:56:VAL:HG21	2:D:99:LEU:HD11	1.85	0.58
2:D:243:ILE:HD13	2:D:300:LEU:HD22	1.84	0.58
2:D:87:LEU:HD22	2:D:159:SER:HA	1.85	0.58
2:B:84:ILE:HG22	3:B:442:HOH:O	2.03	0.58
2:B:65:LYS:HD3	2:B:130:ILE:HD12	1.85	0.58
2:B:303:TRP:CD2	2:B:324:LEU:HD22	2.39	0.58
1:C:1068:ARG:NH1	2:D:81:PRO:HD2	2.18	0.58
2:D:259:ASN:HA	2:D:263:VAL:CG2	2.34	0.58
2:B:203:LYS:H	2:B:203:LYS:HE2	1.68	0.58
2:B:203:LYS:HD3	2:B:203:LYS:N	2.19	0.58
2:B:48:PRO:HB3	2:B:120:GLU:OE1	2.03	0.57
2:D:81:PRO:HA	2:D:82:PRO:C	2.23	0.57
2:D:229:ASP:OD1	2:D:232:CYS:CA	2.51	0.57
2:B:56:VAL:HG21	2:B:99:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:ASN:O	2:D:154:LEU:HD13	2.04	0.57
1:C:1068:ARG:NH2	2:D:80:SER:HB2	2.18	0.57
2:D:277:VAL:CG1	2:D:292:ILE:HD11	2.22	0.57
2:B:56:VAL:HG12	2:B:60:TRP:CE2	2.40	0.57
2:B:340:PRO:CD	2:B:346:ASN:HD22	2.18	0.57
2:B:52:ASP:O	2:B:55:MET:HB3	2.05	0.56
2:B:139:ARG:HA	2:B:142:GLU:OE2	2.04	0.56
2:B:343:ARG:NE	3:B:391:HOH:O	2.29	0.56
2:D:78:LYS:H	2:D:78:LYS:HZ3	1.52	0.56
2:D:139:ARG:HA	2:D:142:GLU:OE2	2.05	0.56
2:B:229:ASP:OD1	2:B:232:CYS:CA	2.53	0.56
2:D:56:VAL:HG12	2:D:60:TRP:CE2	2.40	0.56
2:D:104:GLY:C	2:D:106:MET:H	2.08	0.56
2:D:288:PRO:HG2	3:D:384:HOH:O	2.05	0.56
2:D:86:ASP:C	2:D:89:PRO:HD2	2.26	0.56
1:A:1066:LEU:N	1:A:1066:LEU:HD12	2.20	0.56
2:D:54:LYS:O	2:D:57:GLU:HB2	2.06	0.56
2:B:286:HIS:CD2	2:B:312:GLY:HA3	2.41	0.56
2:D:65:LYS:HD3	2:D:130:ILE:HD12	1.88	0.56
2:D:303:TRP:CD1	2:D:324:LEU:HB2	2.41	0.56
2:B:104:GLY:C	2:B:106:MET:H	2.09	0.56
2:B:294:ARG:HB2	3:B:364:HOH:O	2.07	0.55
2:D:325:PHE:O	2:D:329:ILE:HG12	2.06	0.55
2:D:48:PRO:HB3	2:D:120:GLU:OE1	2.07	0.55
2:D:203:LYS:HD3	2:D:203:LYS:N	2.21	0.55
2:B:54:LYS:O	2:B:57:GLU:HB2	2.06	0.55
2:B:101:ARG:HD3	2:B:173:LEU:HD13	1.87	0.55
2:D:202:TRP:CZ2	2:D:225:LYS:HB2	2.42	0.55
2:B:78:LYS:H	2:B:78:LYS:HZ3	1.54	0.55
2:D:228:ILE:O	2:D:230:LEU:HD13	2.07	0.55
2:B:277:VAL:CG1	2:B:292:ILE:HD11	2.26	0.55
2:D:286:HIS:CD2	2:D:312:GLY:HA3	2.42	0.55
1:A:1068:ARG:NH1	2:B:81:PRO:HD2	2.22	0.55
2:D:269:MET:O	2:D:270:ALA:O	2.25	0.55
2:B:86:ASP:C	2:B:89:PRO:HD2	2.27	0.55
2:B:303:TRP:CD1	2:B:324:LEU:HB2	2.42	0.55
2:D:52:ASP:O	2:D:55:MET:HB3	2.06	0.55
2:D:101:ARG:HD3	2:D:173:LEU:HD13	1.87	0.55
2:B:117:VAL:HG21	2:B:199:ILE:HD13	1.88	0.54
2:D:203:LYS:H	2:D:203:LYS:HE2	1.69	0.54
2:B:228:ILE:O	2:B:230:LEU:HD13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:117:VAL:HG21	2:D:199:ILE:HD13	1.87	0.54
2:D:101:ARG:NH1	2:D:173:LEU:HD11	2.23	0.54
2:D:136:GLY:O	2:D:139:ARG:HB2	2.07	0.54
2:D:199:ILE:HD11	2:D:235:TYR:CB	2.38	0.54
2:B:210:HIS:CD2	2:B:215:ILE:H	2.26	0.54
2:B:138:GLU:HA	2:B:141:TYR:CE2	2.42	0.54
2:B:101:ARG:NH1	2:B:173:LEU:HD11	2.23	0.54
2:B:202:TRP:CZ2	2:B:225:LYS:HB2	2.42	0.54
1:C:1066:LEU:N	1:C:1066:LEU:HD12	2.24	0.53
2:D:138:GLU:HA	2:D:141:TYR:CE2	2.43	0.53
2:B:269:MET:O	2:B:270:ALA:O	2.26	0.53
2:D:294:ARG:NH1	3:D:357:HOH:O	2.41	0.53
2:B:60:TRP:HD1	2:B:63:MET:HE3	1.74	0.53
2:B:136:GLY:O	2:B:139:ARG:HB2	2.08	0.53
2:D:210:HIS:CD2	2:D:215:ILE:H	2.27	0.53
2:B:188:GLU:HA	2:B:191:ARG:CD	2.39	0.53
1:C:1072:ASP:HB2	3:D:367:HOH:O	2.09	0.52
2:B:269:MET:HE2	2:B:272:LEU:HD11	1.92	0.52
2:D:77:LEU:HA	2:D:78:LYS:HZ3	1.75	0.52
2:B:215:ILE:HG21	2:B:221:ALA:HB2	1.91	0.52
2:B:188:GLU:CA	2:B:191:ARG:HH11	2.22	0.52
2:D:224:LEU:HA	2:D:258:TRP:CZ2	2.45	0.52
2:D:60:TRP:HD1	2:D:63:MET:HE3	1.75	0.52
2:D:152:THR:O	2:D:155:SER:HB2	2.10	0.51
2:B:325:PHE:O	2:B:329:ILE:HG12	2.10	0.51
2:D:188:GLU:HA	2:D:191:ARG:CD	2.40	0.51
2:D:68:ARG:HH11	2:D:68:ARG:HG2	1.75	0.51
2:B:68:ARG:HG2	2:B:68:ARG:HH11	1.76	0.51
2:B:145:SER:O	2:B:146:GLN:C	2.49	0.51
2:D:329:ILE:HD11	2:D:349:LEU:HB2	1.92	0.51
2:B:188:GLU:HA	2:B:191:ARG:CZ	2.41	0.51
2:D:51:VAL:HG11	2:D:115:PHE:CE2	2.46	0.51
2:D:244:PHE:HE2	2:D:254:LEU:HD11	1.76	0.51
2:D:259:ASN:HB3	3:D:383:HOH:O	2.09	0.51
2:B:277:VAL:HG21	2:B:294:ARG:HD3	1.92	0.51
2:B:84:ILE:HD13	2:B:84:ILE:O	2.11	0.50
2:D:84:ILE:HD13	2:D:84:ILE:O	2.10	0.50
2:B:244:PHE:HE2	2:B:254:LEU:HD11	1.75	0.50
2:B:87:LEU:HD13	2:B:159:SER:N	2.26	0.50
2:B:145:SER:O	2:B:148:ARG:N	2.44	0.50
2:B:259:ASN:HA	2:B:263:VAL:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:ASN:HA	2:B:149:ARG:NE	2.27	0.50
2:B:150:ASN:O	2:B:154:LEU:HD13	2.11	0.50
2:D:277:VAL:HG21	2:D:294:ARG:HD3	1.93	0.50
2:D:285:ILE:HG12	2:D:285:ILE:O	2.10	0.50
2:B:199:ILE:HD11	2:B:235:TYR:CB	2.42	0.49
2:B:269:MET:HE1	3:B:452:HOH:O	2.11	0.49
2:B:152:THR:O	2:B:155:SER:HB2	2.12	0.49
2:B:51:VAL:HG11	2:B:115:PHE:CE2	2.47	0.49
2:B:197:LYS:HB3	2:B:197:LYS:HZ2	1.77	0.49
2:B:183:LYS:NZ	3:B:374:HOH:O	2.44	0.49
2:D:101:ARG:HD3	2:D:173:LEU:HD11	1.94	0.49
2:B:285:ILE:HG12	2:B:285:ILE:O	2.12	0.49
2:D:87:LEU:HD13	2:D:159:SER:N	2.28	0.49
2:D:215:ILE:HG21	2:D:221:ALA:HB2	1.95	0.49
2:D:247:LEU:HD13	2:D:295:LEU:HD11	1.95	0.49
2:D:65:LYS:HG2	2:D:69:LEU:HD13	1.95	0.49
2:D:145:SER:O	2:D:148:ARG:N	2.46	0.49
2:B:65:LYS:HG2	2:B:69:LEU:HD13	1.95	0.48
2:D:188:GLU:HA	2:D:191:ARG:CZ	2.42	0.48
2:D:340:PRO:CD	2:D:346:ASN:HD22	2.23	0.48
2:B:101:ARG:HD3	2:B:173:LEU:HD11	1.94	0.48
2:D:144:ASN:HA	2:D:149:ARG:NE	2.28	0.48
1:A:1068:ARG:CZ	2:B:80:SER:HB2	2.43	0.48
2:D:104:GLY:O	2:D:106:MET:N	2.42	0.48
2:D:143:GLU:HG3	2:D:144:ASN:CG	2.33	0.48
2:B:329:ILE:HD11	2:B:349:LEU:HB2	1.95	0.48
2:B:143:GLU:HG3	2:B:144:ASN:CG	2.33	0.48
2:D:168:ILE:HG22	2:D:168:ILE:O	2.13	0.48
2:D:197:LYS:HB3	2:D:197:LYS:HZ2	1.78	0.48
2:B:104:GLY:O	2:B:106:MET:N	2.45	0.48
2:D:145:SER:O	2:D:146:GLN:C	2.49	0.48
2:D:188:GLU:CA	2:D:191:ARG:HH11	2.23	0.48
2:D:308:VAL:HA	2:D:313:ASN:O	2.13	0.48
2:D:51:VAL:HG11	2:D:115:PHE:HE2	1.79	0.47
2:B:143:GLU:HG3	2:B:144:ASN:OD1	2.14	0.47
2:B:134:LYS:HG3	2:B:135:GLU:HG3	1.96	0.47
2:B:84:ILE:C	2:B:84:ILE:CD1	2.82	0.47
2:D:51:VAL:HG12	2:D:51:VAL:O	2.15	0.47
2:D:143:GLU:HG3	2:D:144:ASN:OD1	2.14	0.47
2:B:269:MET:HB2	3:B:373:HOH:O	2.14	0.47
1:C:1064:SER:CB	2:D:79:ASN:ND2	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:259:ASN:HA	2:D:263:VAL:HG23	1.95	0.47
2:B:89:PRO:HA	3:B:384:HOH:O	2.15	0.47
2:B:170:PRO:O	2:B:171:SER:HB2	2.15	0.47
2:D:167:GLY:O	2:D:170:PRO:HD3	2.13	0.47
2:D:170:PRO:O	2:D:171:SER:HB2	2.15	0.47
2:B:78:LYS:H	2:B:78:LYS:CD	2.28	0.47
2:B:167:GLY:O	2:B:170:PRO:HD3	2.15	0.47
2:B:168:ILE:O	2:B:168:ILE:HG22	2.15	0.47
2:D:65:LYS:HG2	2:D:69:LEU:CD1	2.45	0.47
2:D:303:TRP:O	2:D:318:ILE:HG23	2.15	0.47
2:D:343:ARG:NE	3:D:372:HOH:O	2.32	0.47
1:A:1065:PHE:HD2	1:A:1066:LEU:H	1.56	0.47
2:D:77:LEU:HD23	2:D:148:ARG:HH21	1.80	0.47
2:B:201:PRO:O	2:B:202:TRP:C	2.54	0.46
2:B:74:LYS:HB3	2:B:141:TYR:HB3	1.96	0.46
2:B:308:VAL:HA	2:B:313:ASN:O	2.15	0.46
2:D:101:ARG:HH11	2:D:173:LEU:HD11	1.80	0.46
2:D:201:PRO:O	2:D:202:TRP:C	2.53	0.46
1:A:1066:LEU:HD12	1:A:1066:LEU:H	1.80	0.46
2:B:158:PHE:HA	2:B:161:MET:CE	2.45	0.46
2:B:249:GLN:HB2	2:B:250:PRO:HA	1.97	0.46
2:D:158:PHE:HA	2:D:161:MET:CE	2.45	0.46
2:B:77:LEU:HA	2:B:78:LYS:HZ3	1.75	0.46
2:D:78:LYS:H	2:D:78:LYS:CD	2.27	0.46
2:D:202:TRP:N	2:D:203:LYS:NZ	2.64	0.46
2:B:65:LYS:HG2	2:B:69:LEU:CD1	2.45	0.46
2:B:77:LEU:HD23	2:B:148:ARG:HH21	1.80	0.46
2:B:224:LEU:HA	2:B:258:TRP:CZ2	2.50	0.46
2:D:154:LEU:HD12	2:D:154:LEU:N	2.30	0.46
2:D:291:TYR:CD1	2:D:337:TYR:HA	2.51	0.46
2:B:67:VAL:HG22	2:B:88:LEU:HD12	1.97	0.46
2:D:272:LEU:HD23	2:D:276:GLU:OE1	2.16	0.46
2:D:320:HIS:O	2:D:321:ASN:HB2	2.16	0.46
2:D:197:LYS:HA	2:D:197:LYS:HZ3	1.81	0.46
1:C:1068:ARG:CZ	2:D:80:SER:HB2	2.45	0.46
2:D:112:ASN:O	2:D:116:ARG:HG3	2.16	0.46
2:D:156:LEU:HD11	2:D:273:THR:CG2	2.32	0.46
2:D:249:GLN:HB2	2:D:250:PRO:HA	1.98	0.46
1:A:1064:SER:CB	2:B:79:ASN:ND2	2.76	0.46
2:B:323:PRO:HA	3:B:403:HOH:O	2.15	0.46
2:D:54:LYS:HB3	3:D:407:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:LYS:HB3	2:D:141:TYR:HB3	1.97	0.46
2:B:51:VAL:HG12	2:B:51:VAL:O	2.16	0.45
2:D:67:VAL:HG22	2:D:88:LEU:HD12	1.98	0.45
2:D:272:LEU:O	2:D:294:ARG:HD2	2.15	0.45
2:B:101:ARG:HH11	2:B:173:LEU:HD11	1.82	0.45
2:D:69:LEU:HD23	2:D:133:PHE:CD2	2.52	0.45
2:D:134:LYS:HG3	2:D:135:GLU:HG3	1.97	0.45
2:B:101:ARG:NE	2:B:173:LEU:HD21	2.32	0.45
2:B:189:PHE:CZ	2:B:209:LEU:HA	2.52	0.45
2:B:70:CYS:HA	2:B:75:LEU:CD1	2.47	0.45
2:B:107:GLU:O	2:B:111:GLU:HB2	2.17	0.45
2:D:89:PRO:HA	3:D:402:HOH:O	2.16	0.45
2:D:189:PHE:C	2:D:189:PHE:CD1	2.89	0.45
2:D:202:TRP:N	2:D:203:LYS:HZ1	2.15	0.45
2:B:272:LEU:O	2:B:294:ARG:HD2	2.16	0.45
2:B:272:LEU:HD23	2:B:276:GLU:OE1	2.17	0.45
2:B:284:PHE:O	2:B:286:HIS:N	2.50	0.45
2:B:293:PHE:CD1	2:B:293:PHE:N	2.84	0.45
2:B:305:ILE:O	2:B:316:GLN:HA	2.17	0.45
2:D:189:PHE:CZ	2:D:209:LEU:HA	2.52	0.45
2:D:299:ARG:HH11	2:D:299:ARG:CG	2.30	0.45
2:B:189:PHE:CD1	2:B:189:PHE:C	2.90	0.45
2:B:202:TRP:N	2:B:203:LYS:NZ	2.65	0.45
2:B:277:VAL:CG2	2:B:294:ARG:HD3	2.46	0.45
2:B:82:PRO:HD2	2:B:273:THR:HB	1.99	0.44
2:B:286:HIS:NE2	3:B:423:HOH:O	2.21	0.44
2:B:197:LYS:HZ3	2:B:197:LYS:HA	1.82	0.44
2:D:70:CYS:HA	2:D:75:LEU:CD1	2.47	0.44
2:B:320:HIS:O	2:B:321:ASN:HB2	2.17	0.44
2:B:51:VAL:HG11	2:B:115:PHE:HE2	1.82	0.44
2:B:65:LYS:HA	2:B:68:ARG:HG2	1.99	0.44
2:B:173:LEU:N	2:B:173:LEU:HD22	2.33	0.44
2:B:284:PHE:O	2:B:287:LYS:N	2.49	0.44
2:D:101:ARG:NE	2:D:173:LEU:HD21	2.32	0.44
2:D:61:LYS:NZ	3:D:381:HOH:O	2.50	0.44
2:B:267:GLY:HA3	2:B:293:PHE:CE1	2.53	0.44
2:B:291:TYR:CD1	2:B:337:TYR:HA	2.52	0.44
2:B:294:ARG:HB3	3:B:373:HOH:O	2.18	0.44
2:D:65:LYS:HA	2:D:68:ARG:HG2	1.99	0.44
2:D:154:LEU:H	2:D:154:LEU:CD1	2.30	0.44
2:D:265:HIS:CD2	2:D:347:PRO:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:305:ILE:O	2:D:316:GLN:HA	2.18	0.44
2:D:309:THR:O	2:D:312:GLY:N	2.49	0.44
2:B:156:LEU:HD11	2:B:273:THR:CG2	2.31	0.44
2:B:281:LEU:HD23	2:B:281:LEU:HA	1.80	0.44
2:B:299:ARG:HH11	2:B:299:ARG:CG	2.30	0.44
2:D:277:VAL:CG2	2:D:294:ARG:HD3	2.48	0.44
2:B:265:HIS:CD2	2:B:347:PRO:HG2	2.53	0.44
2:D:82:PRO:HD2	2:D:273:THR:HB	1.99	0.43
2:D:170:PRO:C	2:D:172:GLY:H	2.21	0.43
2:D:280:ARG:NH2	2:D:341:ASP:OD2	2.45	0.43
2:B:112:ASN:O	2:B:116:ARG:HG3	2.18	0.43
2:B:309:THR:O	2:B:312:GLY:N	2.51	0.43
2:B:154:LEU:O	2:B:155:SER:C	2.55	0.43
2:B:247:LEU:HD13	2:B:295:LEU:HD11	2.00	0.43
2:D:59:CYS:SG	2:D:123:MET:HB2	2.58	0.43
1:C:1065:PHE:HD2	1:C:1066:LEU:H	1.55	0.43
2:B:121:ASN:HA	3:B:397:HOH:O	2.17	0.43
2:B:134:LYS:O	2:B:137:LYS:HG3	2.18	0.43
2:B:265:HIS:HA	2:B:266:PRO:HD2	1.79	0.43
2:D:157:ILE:O	2:D:161:MET:HG3	2.18	0.43
2:D:182:THR:HG22	2:D:183:LYS:HD2	2.01	0.43
2:D:267:GLY:HA3	2:D:293:PHE:CE1	2.54	0.43
2:B:95:LEU:HD23	2:B:165:LEU:HD21	2.01	0.43
2:B:154:LEU:N	2:B:154:LEU:HD12	2.34	0.43
1:C:1072:ASP:OD1	1:C:1072:ASP:C	2.57	0.43
2:D:107:GLU:O	2:D:111:GLU:HB2	2.19	0.43
2:D:174:PHE:O	2:D:175:GLN:HG2	2.18	0.43
2:D:188:GLU:HG3	2:D:191:ARG:CZ	2.48	0.43
2:D:293:PHE:CD1	2:D:293:PHE:N	2.86	0.43
2:D:323:PRO:HA	3:D:354:HOH:O	2.19	0.43
1:A:1064:SER:CB	2:B:79:ASN:HD21	2.32	0.43
2:B:72:ASN:ND2	2:B:74:LYS:HB2	2.32	0.43
2:D:154:LEU:N	2:D:154:LEU:CD1	2.82	0.43
2:D:65:LYS:O	2:D:68:ARG:HG3	2.19	0.43
2:D:95:LEU:HD23	2:D:165:LEU:HD21	2.00	0.43
2:B:170:PRO:C	2:B:172:GLY:H	2.22	0.43
2:D:156:LEU:O	2:D:160:HIS:CD2	2.72	0.43
2:D:138:GLU:O	2:D:142:GLU:OE1	2.37	0.42
2:D:269:MET:HE2	2:D:272:LEU:CD1	2.49	0.42
2:D:340:PRO:O	2:D:343:ARG:HB2	2.19	0.42
2:B:340:PRO:O	2:B:343:ARG:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LYS:O	2:B:68:ARG:HG3	2.19	0.42
2:B:345:GLN:NE2	2:B:345:GLN:HA	2.34	0.42
2:B:59:CYS:SG	2:B:123:MET:HB2	2.59	0.42
2:B:266:PRO:HG2	2:B:340:PRO:HB2	2.00	0.42
2:D:133:PHE:O	2:D:137:LYS:N	2.53	0.42
2:B:69:LEU:HD23	2:B:133:PHE:CG	2.55	0.42
2:B:303:TRP:CE2	2:B:324:LEU:HD22	2.54	0.42
2:D:69:LEU:HD23	2:D:133:PHE:CG	2.54	0.42
2:D:154:LEU:O	2:D:155:SER:C	2.58	0.42
2:D:266:PRO:HG2	2:D:340:PRO:HB2	2.00	0.42
2:B:87:LEU:HD11	2:B:159:SER:HB2	2.01	0.42
2:B:280:ARG:NH2	2:B:341:ASP:OD2	2.46	0.42
2:D:173:LEU:N	2:D:173:LEU:HD22	2.34	0.42
2:D:303:TRP:CE2	2:D:324:LEU:HD22	2.54	0.42
2:B:127:LYS:O	2:B:128:GLN:C	2.58	0.42
2:B:210:HIS:O	2:B:210:HIS:ND1	2.53	0.42
2:B:133:PHE:O	2:B:137:LYS:N	2.52	0.42
1:C:1066:LEU:HD12	1:C:1066:LEU:H	1.83	0.42
2:D:127:LYS:O	2:D:128:GLN:C	2.57	0.42
2:D:173:LEU:O	2:D:175:GLN:HG3	2.19	0.42
2:B:272:LEU:HD22	2:B:276:GLU:CB	2.48	0.42
2:D:153:LYS:O	2:D:154:LEU:C	2.58	0.42
2:D:256:ARG:NH2	3:D:457:HOH:O	2.51	0.42
2:B:69:LEU:HD23	2:B:133:PHE:CD2	2.54	0.42
2:B:173:LEU:O	2:B:175:GLN:HG3	2.20	0.42
2:D:229:ASP:HB3	3:D:417:HOH:O	2.20	0.42
2:B:68:ARG:HG3	2:B:69:LEU:HD12	2.02	0.41
2:D:78:LYS:NZ	2:D:78:LYS:N	2.63	0.41
2:B:125:LYS:NZ	2:B:232:CYS:O	2.44	0.41
2:B:153:LYS:O	2:B:154:LEU:C	2.58	0.41
2:B:174:PHE:O	2:B:175:GLN:HG2	2.19	0.41
1:C:1064:SER:CB	2:D:79:ASN:HD21	2.33	0.41
1:C:1068:ARG:HH21	2:D:274:TYR:HB3	1.85	0.41
2:D:121:ASN:HA	3:D:386:HOH:O	2.20	0.41
2:B:303:TRP:O	2:B:318:ILE:HG23	2.20	0.41
2:D:303:TRP:CG	2:D:324:LEU:HD22	2.56	0.41
2:D:127:LYS:O	2:D:130:ILE:N	2.53	0.41
2:D:318:ILE:O	2:D:320:HIS:CD2	2.74	0.41
2:B:269:MET:HB3	2:B:269:MET:HE3	1.78	0.41
2:D:134:LYS:O	2:D:137:LYS:HG3	2.20	0.41
2:D:149:ARG:NH1	2:D:149:ARG:CG	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:HIS:CD2	2:D:166:LYS:HG2	2.56	0.41
2:D:288:PRO:HB3	2:D:310:ALA:HA	2.03	0.41
2:B:188:GLU:HG3	2:B:191:ARG:CZ	2.50	0.41
2:D:210:HIS:ND1	2:D:210:HIS:O	2.54	0.41
2:D:272:LEU:HD22	2:D:276:GLU:CB	2.47	0.41
2:D:284:PHE:O	2:D:287:LYS:N	2.53	0.41
2:B:138:GLU:O	2:B:142:GLU:OE1	2.39	0.41
2:D:58:LYS:HE2	3:D:442:HOH:O	2.20	0.41
2:D:158:PHE:HA	2:D:161:MET:HE2	2.03	0.41
1:A:1072:ASP:OD1	1:A:1072:ASP:C	2.59	0.40
2:B:95:LEU:CD2	2:B:165:LEU:HD21	2.51	0.40
2:B:154:LEU:CD1	2:B:154:LEU:H	2.34	0.40
2:B:157:ILE:O	2:B:161:MET:HG3	2.21	0.40
2:B:158:PHE:HA	2:B:161:MET:HE2	2.03	0.40
2:B:345:GLN:CA	2:B:345:GLN:HE21	2.34	0.40
2:D:72:ASN:ND2	2:D:74:LYS:HB2	2.34	0.40
2:B:78:LYS:NZ	2:B:78:LYS:N	2.63	0.40
2:B:188:GLU:CB	2:B:191:ARG:NH1	2.85	0.40
2:B:321:ASN:N	3:B:393:HOH:O	2.54	0.40
2:D:339:PHE:HB3	2:D:343:ARG:O	2.22	0.40
2:B:102:TYR:O	2:B:104:GLY:N	2.54	0.40
2:B:144:ASN:O	2:B:149:ARG:NH2	2.54	0.40
2:B:156:LEU:O	2:B:160:HIS:CD2	2.74	0.40
2:B:331:GLY:HA3	2:B:337:TYR:HD2	1.74	0.40
2:D:84:ILE:HG22	3:D:404:HOH:O	2.21	0.40
2:D:209:LEU:HD12	2:D:209:LEU:O	2.20	0.40
2:D:342:GLY:O	2:D:343:ARG:C	2.60	0.40
2:D:345:GLN:HA	2:D:345:GLN:NE2	2.36	0.40
2:B:154:LEU:N	2:B:154:LEU:CD1	2.84	0.40
2:B:342:GLY:O	2:B:343:ARG:C	2.60	0.40
2:D:339:PHE:HA	2:D:340:PRO:HD2	1.95	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	8/13 (62%)	4 (50%)	2 (25%)	2 (25%)	0	0
1	C	8/13 (62%)	4 (50%)	2 (25%)	2 (25%)	0	0
2	B	302/329 (92%)	248 (82%)	44 (15%)	10 (3%)	4	6
2	D	302/329 (92%)	248 (82%)	44 (15%)	10 (3%)	4	6
All	All	620/684 (91%)	504 (81%)	92 (15%)	24 (4%)	3	4

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	103	GLU
2	B	270	ALA
2	B	285	ILE
2	D	103	GLU
2	D	270	ALA
2	D	285	ILE
1	A	1067	GLN
1	A	1068	ARG
2	B	137	LYS
1	C	1067	GLN
1	C	1068	ARG
2	D	137	LYS
2	B	105	LYS
2	B	216	SER
2	D	105	LYS
2	D	216	SER
2	B	229	ASP
2	B	254	LEU
2	D	229	ASP
2	D	254	LEU
2	B	84	ILE
2	B	288	PRO
2	D	84	ILE
2	D	288	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	10/11 (91%)	9 (90%)	1 (10%)	7	14
1	C	10/11 (91%)	9 (90%)	1 (10%)	7	14
2	B	271/293 (92%)	254 (94%)	17 (6%)	18	36
2	D	271/293 (92%)	255 (94%)	16 (6%)	19	39
All	All	562/608 (92%)	527 (94%)	35 (6%)	18	37

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1066	LEU
2	B	53	LYS
2	B	68	ARG
2	B	78	LYS
2	B	84	ILE
2	B	111	GLU
2	B	141	TYR
2	B	142	GLU
2	B	191	ARG
2	B	197	LYS
2	B	203	LYS
2	B	259	ASN
2	B	299	ARG
2	B	307	TYR
2	B	311	ASP
2	B	313	ASN
2	B	325	PHE
2	B	343	ARG
1	C	1066	LEU
2	D	53	LYS
2	D	68	ARG
2	D	78	LYS
2	D	84	ILE
2	D	111	GLU
2	D	141	TYR
2	D	142	GLU
2	D	191	ARG
2	D	197	LYS
2	D	203	LYS
2	D	259	ASN

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Mol	Chain	Res	Type
2	D	299	ARG
2	D	307	TYR
2	D	313	ASN
2	D	325	PHE
2	D	343	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	79	ASN
2	B	94	HIS
2	B	160	HIS
2	B	213	HIS
2	B	282	GLN
2	B	313	ASN
2	B	316	GLN
2	B	321	ASN
2	B	344	ASN
2	B	345	GLN
2	B	346	ASN
2	D	79	ASN
2	D	94	HIS
2	D	160	HIS
2	D	213	HIS
2	D	257	ASN
2	D	282	GLN
2	D	286	HIS
2	D	316	GLN
2	D	321	ASN
2	D	344	ASN
2	D	345	GLN
2	D	346	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PTR	C	1069	1	15,16,17	1.47	1 (6%)	19,22,24	0.98	0
1	PTR	A	1069	1	15,16,17	1.48	2 (13%)	19,22,24	0.99	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
1	PTR	C	1069	1	-	1/10/11/13	0/1/1/1
1	PTR	A	1069	1	-	1/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1069	PTR	P-OH	3.43	1.64	1.59
1	C	1069	PTR	P-OH	3.37	1.64	1.59
1	A	1069	PTR	CE1-CD1	2.07	1.42	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1069	PTR	O-C-CA-CB
1	C	1069	PTR	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	10/13 (76%)	0.12	2 (20%)	1	0	22, 32, 48, 51	0
1	C	10/13 (76%)	0.10	2 (20%)	1	0	22, 32, 48, 51	0
2	B	304/329 (92%)	-0.43	1 (0%)	94	93	16, 32, 52, 71	0
2	D	304/329 (92%)	-0.43	0	100	100	16, 32, 52, 71	0
All	All	628/684 (91%)	-0.42	5 (0%)	86	84	16, 32, 52, 71	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1065	PHE	2.8
1	C	1064	SER	2.7
1	A	1064	SER	2.4
2	B	173	LEU	2.1
1	C	1065	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	B-factors(Å^2)	Q<0.9
1	PTR	C	1069	16/17	0.96	0.14	27,28,29,30	0
1	PTR	A	1069	16/17	0.97	0.13	27,28,29,30	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.