Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 03:48 PM JST

PDB ID	:	5ZLF
Title	:	CRYSTAL STRUCTURE OF OCTAPRENYL PYROPHOSPHATE SYNTHASE FROM ESCHERICHIA COLI WITH ligand BPH-629
Authors	:	Han, X.; Liu, W.D.; Zheng, Y.Y.; Ko, T.P.; Chen, C.C.; Guo, R.T.
Deposited on	:	2018-03-27
Resolution	:	2.85 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:

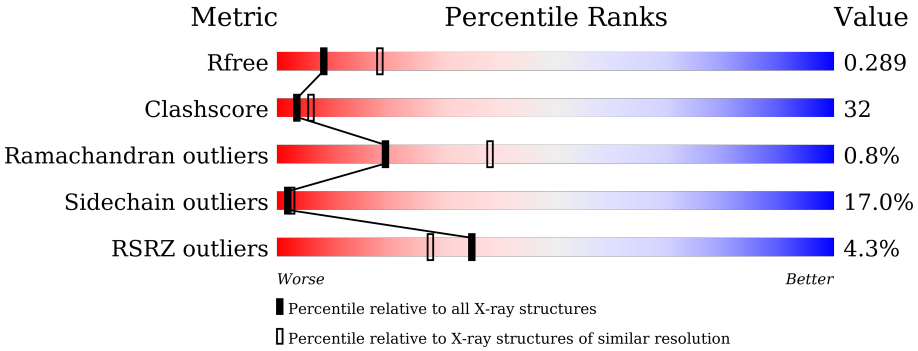
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.85 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	323	4%; 54%, 31%, 6%, 9%
1	B	323	3%; 41%, 32%, 7%, 20%
1	C	323	2%; 50%, 28%, 10%, 11%
1	D	323	6%; 53%, 27%, 8%, •, 11%

2 Entry composition (i)

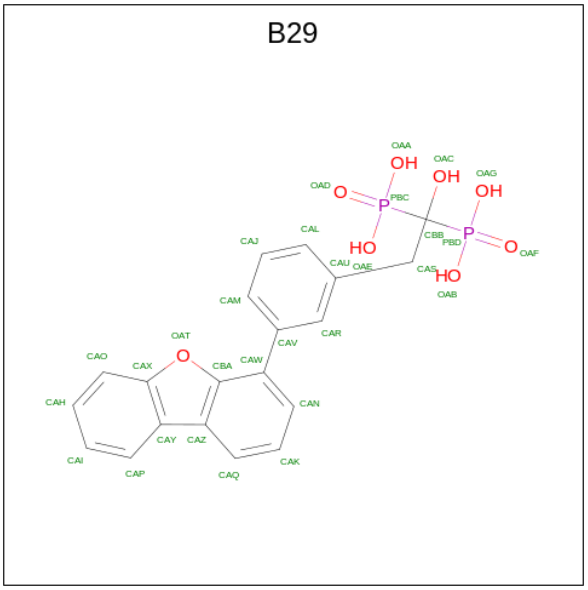
There are 4 unique types of molecules in this entry. The entry contains 8664 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Octaprenyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	2244	1409	387	436	12	0	0	0
1	B	259	1987	1256	336	383	12	0	0	0
1	C	286	2185	1376	372	424	13	0	0	0
1	D	289	2210	1388	380	431	11	0	0	0

- Molecule 2 is [2-(3-DIBENZOFURAN-4-YL-PHENYL)-1-HYDROXY-1-PHOSPHONO-ETHYL]-PHOSPHONIC ACID (three-letter code: B29) (formula: $C_{20}H_{18}O_8P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	30	20	8	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
			Total	Mg		
3	D	1	1	1	0	0

- Molecule 4 is water.

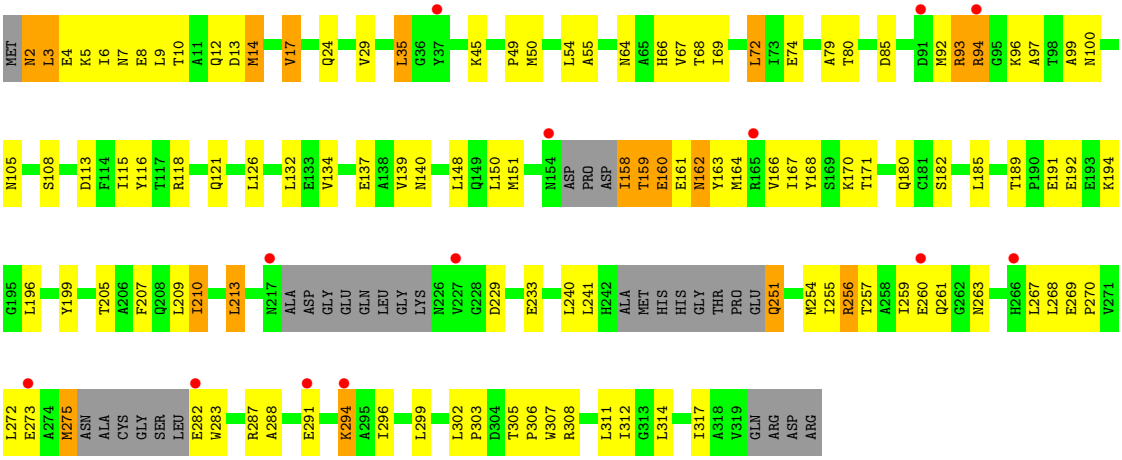
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	2	2	2	0	0
			Total	O		
4	C	3	3	3	0	0
			Total	O		
4	D	1	1	1	0	0

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.

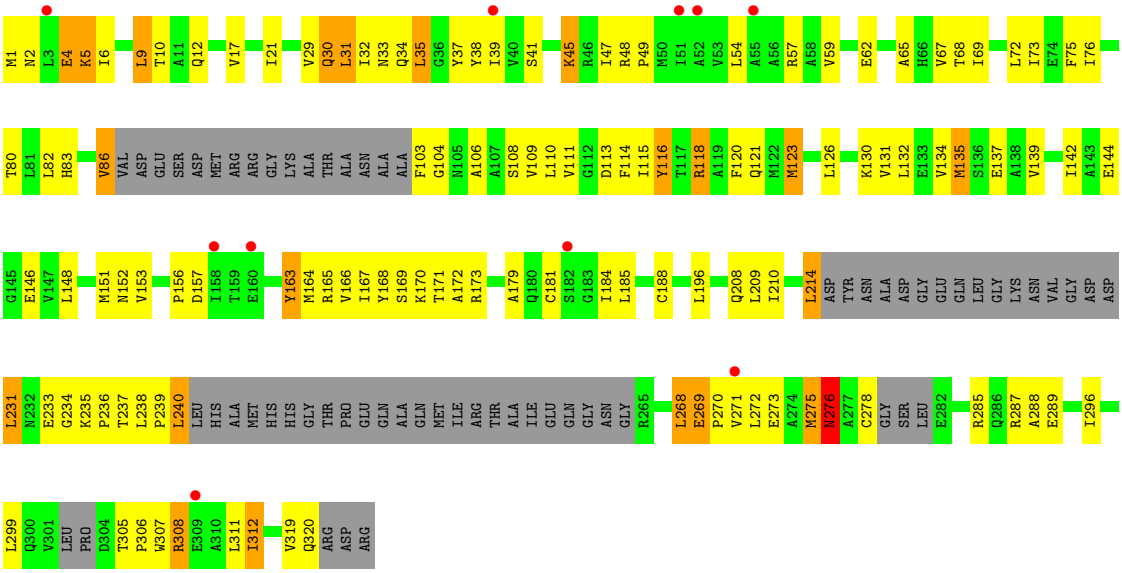
• Molecule 1: Octaprenyl diphosphate synthase

Chain A: 4% 54% 31% 6% 9%



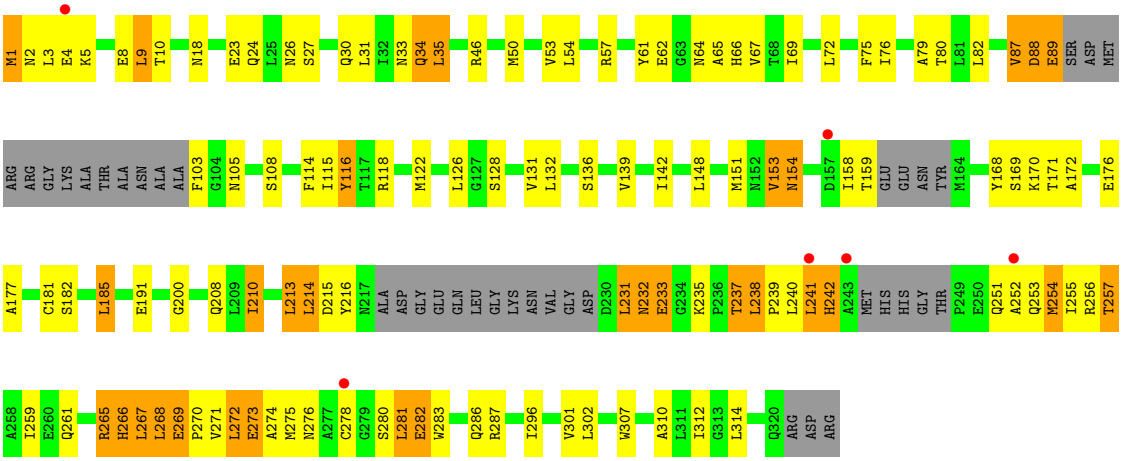
• Molecule 1: Octaprenyl diphosphate synthase

Chain B: 3% 41% 32% 7% 20%



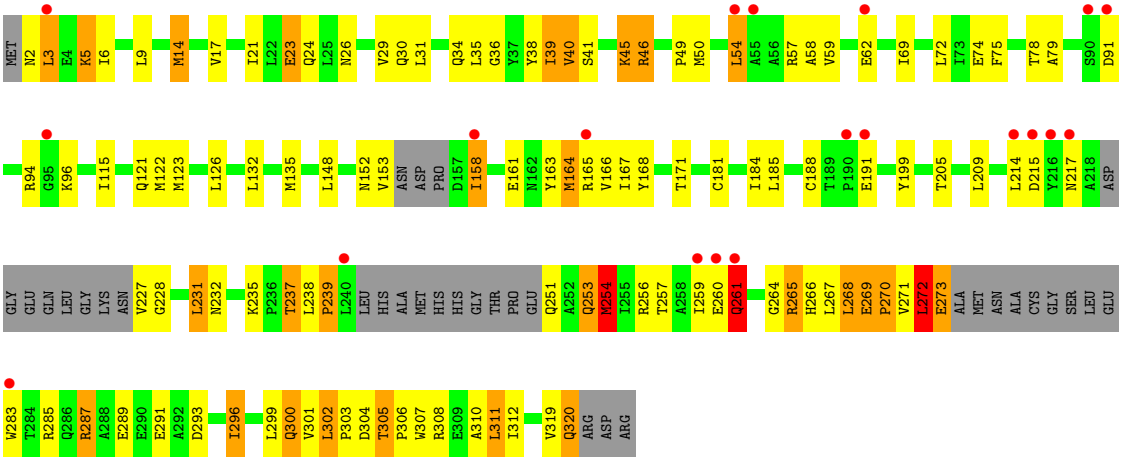
• Molecule 1: Octaprenyl diphosphate synthase

Chain C:



• Molecule 1: Octaprenyl diphosphate synthase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	149.34Å 46.65Å 215.74Å 90.00° 101.08° 90.00°	Depositor
Resolution (Å)	24.87 – 2.85 24.87 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.7 (24.87-2.85) 98.7 (24.87-2.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 2.84Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.241 , 0.299 0.250 , 0.289	Depositor DCC
R_{free} test set	1730 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	77.8	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 71.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8664	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.34% 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: MG, B29

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	0.29	0/2271	0.49	0/3074
1	B	0.26	0/2011	0.44	0/2722
1	C	0.28	0/2213	0.49	0/2998
1	D	0.28	0/2236	0.50	0/3027
All	All	0.28	0/8731	0.48	0/11821

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	2244	0	2234	139	0
1	B	1987	0	1988	148	0
1	C	2185	0	2181	145	0
1	D	2210	0	2201	147	0
2	A	30	0	14	2	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
All	All	8664	0	8618	551	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 32.

All (551) 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:305:THR:CG2	1:D:306:PRO:HD2	1.55	1.36
1:B:269:GLU:OE2	1:B:270:PRO:HD3	1.25	1.35
1:D:305:THR:HG22	1:D:306:PRO:CD	1.57	1.33
1:B:171:THR:HG21	1:B:208:GLN:OE1	1.35	1.19
1:D:36:GLY:O	1:D:40:VAL:HG23	1.44	1.16
1:C:69:ILE:HD11	1:C:185:LEU:CD2	1.77	1.14
1:B:156:PRO:CD	1:B:268:LEU:HD12	1.77	1.13
1:C:253:GLN:O	1:C:257:THR:HG22	1.49	1.11
1:D:9:LEU:HD21	1:D:307:TRP:CZ3	1.84	1.11
1:A:296:ILE:HD12	1:A:312:ILE:HG23	1.27	1.11
1:B:142:ILE:HA	1:B:169:SER:O	1.52	1.07
1:D:254:MET:HE3	1:D:254:MET:HA	1.36	1.06
1:B:156:PRO:HD3	1:B:268:LEU:CD1	1.86	1.05
1:C:69:ILE:HD11	1:C:185:LEU:HD23	1.36	1.05
1:D:3:LEU:HD23	1:D:3:LEU:H	1.16	1.05
1:A:9:LEU:HD21	1:A:307:TRP:CZ3	1.90	1.05
1:A:9:LEU:CD2	1:A:307:TRP:CZ3	2.40	1.05
1:C:240:LEU:CD2	1:C:259:ILE:HD11	1.87	1.04
1:C:191:GLU:HG2	1:C:301:VAL:HG21	1.37	1.04
1:B:123:MET:SD	1:B:135:MET:CG	2.46	1.03
1:C:233:GLU:OE2	1:C:265:ARG:HG2	1.58	1.03
1:C:9:LEU:HD11	1:C:307:TRP:CZ3	1.94	1.03
1:D:45:LYS:HE2	1:D:45:LYS:HA	1.40	1.02
1:C:69:ILE:CD1	1:C:185:LEU:HD23	1.91	1.00
1:B:269:GLU:OE2	1:B:270:PRO:CD	2.08	0.99
1:A:296:ILE:CD1	1:A:312:ILE:HG23	1.92	0.99
1:D:9:LEU:CD2	1:D:307:TRP:CZ3	2.45	0.98
1:D:285:ARG:HH22	1:D:320:GLN:CB	1.74	0.98
1:B:214:LEU:HD22	1:B:214:LEU:H	1.26	0.98
1:B:156:PRO:HD3	1:B:268:LEU:HD12	0.99	0.97
1:B:156:PRO:CD	1:B:268:LEU:CD1	2.42	0.97
1:A:158:ILE:CG2	1:A:241:LEU:CD2	2.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ASN:O	1:B:6:ILE:HD12	1.63	0.96
1:A:6:ILE:HG21	1:A:50:MET:HE1	1.47	0.96
1:C:216:TYR:CD2	1:C:275:MET:CE	2.47	0.96
1:C:254:MET:HE3	1:C:270:PRO:HB2	1.48	0.95
1:C:240:LEU:HD21	1:C:259:ILE:HD11	1.46	0.94
1:B:123:MET:SD	1:B:135:MET:HB3	2.08	0.94
1:D:58:ALA:O	1:D:303:PRO:HG3	1.68	0.94
1:B:156:PRO:HB3	1:B:268:LEU:HD11	1.50	0.93
1:B:156:PRO:CB	1:B:268:LEU:HD11	2.00	0.92
1:B:308:ARG:HG2	1:B:308:ARG:HH21	1.36	0.89
1:A:167:ILE:HG23	1:A:171:THR:OG1	1.70	0.89
1:B:123:MET:SD	1:B:135:MET:HG3	2.11	0.89
1:B:10:THR:HG22	1:B:54:LEU:HD21	1.52	0.89
1:A:68:THR:O	1:A:72:LEU:HD23	1.73	0.89
1:C:254:MET:CE	1:C:270:PRO:CB	2.51	0.89
1:B:296:ILE:HG23	1:B:312:ILE:HD13	1.54	0.88
1:D:9:LEU:HD21	1:D:307:TRP:CE3	2.09	0.88
1:D:302:LEU:HB3	1:D:303:PRO:HD2	1.55	0.88
1:D:285:ARG:NH2	1:D:320:GLN:HB3	1.89	0.88
1:C:216:TYR:CD2	1:C:275:MET:HE2	2.09	0.87
1:A:140:ASN:ND2	1:B:118:ARG:HE	1.72	0.87
1:B:123:MET:SD	1:B:135:MET:CB	2.63	0.87
1:C:216:TYR:CE2	1:C:275:MET:HE1	2.10	0.87
1:C:254:MET:CE	1:C:270:PRO:HB3	2.05	0.86
1:A:116:TYR:HE2	1:B:120:PHE:CE2	1.93	0.86
1:B:111:VAL:O	1:B:115:ILE:HD13	1.74	0.86
1:C:69:ILE:HD11	1:C:185:LEU:HD21	1.55	0.86
1:B:45:LYS:O	1:B:45:LYS:HD3	1.77	0.85
1:B:171:THR:CG2	1:B:208:GLN:OE1	2.24	0.85
1:D:251:GLN:NE2	1:D:271:VAL:HG11	1.91	0.85
1:C:216:TYR:CD2	1:C:275:MET:HE1	2.11	0.84
1:B:238:LEU:HD12	1:B:238:LEU:O	1.76	0.84
1:A:158:ILE:CG2	1:A:241:LEU:HD21	2.05	0.83
1:D:285:ARG:NH2	1:D:320:GLN:CB	2.42	0.83
1:A:151:MET:SD	1:B:31:LEU:HD22	2.19	0.83
1:D:285:ARG:HH22	1:D:320:GLN:HB2	1.41	0.83
1:C:9:LEU:O	1:C:9:LEU:HD12	1.80	0.82
1:D:285:ARG:HH22	1:D:320:GLN:HB3	1.44	0.82
1:D:305:THR:CB	1:D:306:PRO:HD2	2.10	0.82
1:A:240:LEU:CD2	1:A:259:ILE:HD11	2.10	0.81
1:A:9:LEU:HD21	1:A:307:TRP:CE3	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:TYR:HD2	1:C:275:MET:CE	1.89	0.81
1:A:92:MET:HG2	1:A:97:ALA:HA	1.62	0.81
1:B:276:ASN:O	1:B:276:ASN:ND2	2.14	0.81
1:C:216:TYR:CE2	1:C:275:MET:CE	2.64	0.81
1:A:140:ASN:HD21	1:B:118:ARG:HE	1.30	0.80
1:D:215:ASP:O	1:D:228:GLY:HA2	1.82	0.80
1:B:45:LYS:HE2	1:B:45:LYS:HA	1.64	0.80
1:C:254:MET:SD	1:C:267:LEU:HD11	2.22	0.79
1:B:275:MET:SD	1:B:275:MET:N	2.56	0.79
1:C:278:CYS:SG	1:C:280:SER:HB2	2.23	0.79
1:D:36:GLY:O	1:D:40:VAL:CG2	2.29	0.79
1:C:254:MET:HE1	1:C:270:PRO:HB3	1.62	0.78
1:D:35:LEU:O	1:D:39:ILE:HG22	1.82	0.78
1:D:305:THR:HG22	1:D:306:PRO:HD2	0.81	0.78
1:B:305:THR:OG1	1:B:306:PRO:HD2	1.83	0.78
1:C:69:ILE:CD1	1:C:185:LEU:CD2	2.54	0.77
1:D:199:TYR:CE2	1:D:311:LEU:HD23	2.19	0.77
1:B:308:ARG:HG2	1:B:308:ARG:NH2	1.97	0.76
1:A:189:THR:HG23	1:A:192:GLU:H	1.51	0.76
1:D:191:GLU:OE1	1:D:301:VAL:HG11	1.87	0.75
1:A:35:LEU:HD21	1:A:99:ALA:HB1	1.67	0.75
1:C:216:TYR:HD2	1:C:275:MET:HE2	1.45	0.75
1:C:254:MET:CE	1:C:270:PRO:HB2	2.14	0.75
1:A:9:LEU:HD23	1:A:307:TRP:CZ3	2.23	0.74
1:C:269:GLU:HB2	1:C:270:PRO:HD3	1.67	0.74
1:D:273:GLU:OE1	1:D:273:GLU:HA	1.85	0.74
1:A:126:LEU:HD13	1:A:185:LEU:HD21	1.70	0.74
1:B:9:LEU:O	1:B:9:LEU:HG	1.86	0.74
1:D:3:LEU:H	1:D:3:LEU:CD2	1.95	0.74
1:A:49:PRO:HG3	1:A:74:GLU:HB2	1.68	0.74
1:D:302:LEU:CB	1:D:303:PRO:HD2	2.16	0.74
1:D:57:ARG:HH12	1:D:62:GLU:HA	1.53	0.73
1:D:265:ARG:HG3	1:D:265:ARG:HH11	1.52	0.73
1:A:305:THR:HG23	1:A:308:ARG:H	1.53	0.73
1:A:69:ILE:HA	1:A:72:LEU:HD21	1.70	0.73
1:A:272:LEU:HD23	1:A:272:LEU:N	2.02	0.73
1:B:76:ILE:HD12	1:B:139:VAL:HG11	1.69	0.73
1:C:114:PHE:HD2	1:C:115:ILE:HD12	1.54	0.73
1:D:302:LEU:CB	1:D:303:PRO:CD	2.66	0.72
1:D:5:LYS:HD3	1:D:5:LYS:C	2.08	0.72
1:A:158:ILE:HG23	1:A:241:LEU:HD22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:LEU:HD12	1:D:272:LEU:O	1.88	0.72
1:A:150:LEU:HD23	1:A:151:MET:SD	2.29	0.72
1:A:158:ILE:HG22	1:A:241:LEU:CD2	2.20	0.72
1:A:158:ILE:HG23	1:A:241:LEU:CD2	2.20	0.72
1:C:254:MET:HE1	1:C:270:PRO:CB	2.19	0.72
1:A:3:LEU:HD12	1:A:3:LEU:O	1.88	0.72
1:A:3:LEU:HD13	1:A:317:ILE:HD13	1.72	0.71
1:C:191:GLU:HG2	1:C:301:VAL:CG2	2.17	0.71
1:B:305:THR:OG1	1:B:306:PRO:CD	2.38	0.71
1:D:2:ASN:HB3	1:D:5:LYS:HB3	1.71	0.71
1:D:49:PRO:HG3	1:D:74:GLU:HB2	1.73	0.71
1:A:116:TYR:CE2	1:B:120:PHE:CE2	2.78	0.71
1:A:140:ASN:HD21	1:B:118:ARG:HH21	1.38	0.71
1:A:151:MET:SD	1:B:31:LEU:CD2	2.79	0.71
1:C:238:LEU:HB3	1:C:239:PRO:HD3	1.72	0.71
1:D:299:LEU:HD22	1:D:302:LEU:HD22	1.72	0.70
1:B:10:THR:CG2	1:B:54:LEU:HD21	2.22	0.70
1:C:30:GLN:CD	1:C:30:GLN:H	1.94	0.70
1:C:72:LEU:HB3	1:C:122:MET:HE2	1.72	0.70
1:C:240:LEU:HD21	1:C:259:ILE:CD1	2.19	0.70
1:C:9:LEU:HD11	1:C:307:TRP:CE3	2.26	0.70
1:D:45:LYS:HA	1:D:45:LYS:CE	2.09	0.69
1:D:267:LEU:O	1:D:267:LEU:HD23	1.93	0.69
1:A:9:LEU:CD2	1:A:307:TRP:CE3	2.74	0.69
1:D:302:LEU:HB3	1:D:303:PRO:CD	2.21	0.69
1:A:213:LEU:HD12	1:A:213:LEU:C	2.14	0.68
1:A:50:MET:SD	1:A:314:LEU:HD11	2.34	0.68
1:B:163:TYR:CE1	1:B:238:LEU:HB2	2.28	0.68
1:A:159:THR:HG23	1:A:162:ASN:HB2	1.76	0.67
1:D:254:MET:HA	1:D:254:MET:CE	2.20	0.67
1:B:209:LEU:CD2	1:B:238:LEU:HD23	2.25	0.67
1:A:126:LEU:HD13	1:A:185:LEU:CD2	2.25	0.66
1:B:214:LEU:HD22	1:B:214:LEU:N	2.02	0.66
1:A:3:LEU:HD12	1:A:3:LEU:C	2.16	0.66
1:A:93:ARG:HG3	1:A:93:ARG:O	1.94	0.66
1:D:153:VAL:HG12	1:D:260:GLU:HA	1.77	0.66
1:B:131:VAL:O	1:B:135:MET:HB2	1.95	0.66
1:D:199:TYR:CZ	1:D:311:LEU:HD23	2.30	0.66
1:C:9:LEU:HD12	1:C:9:LEU:C	2.14	0.66
1:B:240:LEU:C	1:B:240:LEU:HD23	2.16	0.65
1:D:199:TYR:CE2	1:D:311:LEU:CD2	2.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:MET:HE3	1:D:254:MET:CA	2.19	0.65
1:D:302:LEU:HG	1:D:303:PRO:CD	2.25	0.65
1:B:45:LYS:HA	1:B:45:LYS:CE	2.22	0.65
1:B:238:LEU:HD12	1:B:238:LEU:C	2.16	0.65
1:B:137:GLU:OE2	1:B:173:ARG:NH2	2.30	0.65
1:D:6:ILE:HD13	1:D:310:ALA:O	1.96	0.65
1:C:238:LEU:O	1:C:238:LEU:HD12	1.97	0.65
1:B:123:MET:SD	1:B:135:MET:HG2	2.36	0.65
1:A:4:GLU:O	1:A:4:GLU:HG2	1.97	0.65
1:C:281:LEU:CD2	1:C:281:LEU:H	2.09	0.65
1:D:231:LEU:H	1:D:231:LEU:CD2	2.10	0.65
1:B:114:PHE:HD1	1:B:115:ILE:HD12	1.62	0.64
1:D:305:THR:HG22	1:D:306:PRO:HD3	1.72	0.64
1:C:27:SER:O	1:C:33:ASN:ND2	2.31	0.64
1:C:266:HIS:CE1	1:C:267:LEU:HD22	2.33	0.64
1:D:148:LEU:HD12	1:D:152:ASN:HD22	1.63	0.64
1:A:140:ASN:HD21	1:B:118:ARG:NE	1.93	0.64
1:B:57:ARG:HH12	1:B:62:GLU:HA	1.63	0.64
1:A:13:ASP:OD2	1:A:66:HIS:NE2	2.28	0.64
1:C:254:MET:HE3	1:C:270:PRO:CB	2.17	0.63
1:A:6:ILE:HG21	1:A:50:MET:CE	2.26	0.63
1:C:240:LEU:HD22	1:C:259:ILE:HD11	1.75	0.63
1:C:240:LEU:O	1:C:240:LEU:HD23	1.99	0.63
1:D:260:GLU:HG2	1:D:260:GLU:O	1.99	0.63
1:A:54:LEU:HD23	1:A:311:LEU:HD23	1.80	0.63
1:C:57:ARG:NH1	1:C:61:TYR:O	2.31	0.63
1:A:167:ILE:HA	1:A:171:THR:HG23	1.81	0.63
1:B:238:LEU:N	1:B:239:PRO:HD2	2.14	0.63
1:D:285:ARG:NH2	1:D:320:GLN:HB2	2.12	0.63
1:A:302:LEU:HB2	1:A:303:PRO:HD2	1.80	0.62
1:A:116:TYR:CE2	1:B:120:PHE:HE2	2.17	0.62
1:C:66:HIS:HA	1:C:69:ILE:HD13	1.81	0.62
1:A:137:GLU:HA	1:B:121:GLN:NE2	2.15	0.62
1:A:69:ILE:HA	1:A:72:LEU:CD2	2.28	0.62
1:A:303:PRO:O	1:A:308:ARG:HD3	2.00	0.62
1:B:39:ILE:O	1:B:39:ILE:HG22	2.00	0.62
1:C:2:ASN:HD21	1:C:4:GLU:HB3	1.65	0.62
1:A:158:ILE:HG22	1:A:241:LEU:HD21	1.78	0.62
1:C:253:GLN:O	1:C:257:THR:CG2	2.39	0.62
1:C:254:MET:SD	1:C:267:LEU:CD1	2.87	0.62
1:A:168:TYR:CE1	1:A:205:THR:HG21	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:THR:OG1	1:A:306:PRO:HD2	2.00	0.62
1:D:265:ARG:HH11	1:D:265:ARG:CG	2.13	0.61
1:A:140:ASN:ND2	1:B:121:GLN:OE1	2.33	0.61
1:A:140:ASN:HD21	1:B:118:ARG:NH2	1.97	0.61
1:B:65:ALA:HB3	1:B:185:LEU:HD21	1.81	0.61
1:D:9:LEU:C	1:D:9:LEU:HD23	2.20	0.61
1:D:215:ASP:O	1:D:228:GLY:CA	2.49	0.61
1:B:130:LYS:O	1:B:134:VAL:HG23	2.01	0.61
1:B:296:ILE:HG23	1:B:312:ILE:CD1	2.30	0.61
1:A:134:VAL:HG11	1:A:180:GLN:NE2	2.16	0.61
1:B:4:GLU:OE1	1:B:4:GLU:N	2.33	0.61
1:D:126:LEU:HD13	1:D:185:LEU:HD21	1.81	0.61
1:D:269:GLU:N	1:D:270:PRO:HD3	2.16	0.61
1:D:6:ILE:HG23	1:D:310:ALA:HB1	1.83	0.60
1:A:240:LEU:HD21	1:A:259:ILE:HD11	1.81	0.60
1:C:9:LEU:CD1	1:C:307:TRP:CZ3	2.79	0.60
1:C:24:GLN:HG3	1:C:122:MET:SD	2.41	0.60
1:D:58:ALA:O	1:D:303:PRO:CG	2.47	0.60
1:D:302:LEU:HG	1:D:303:PRO:HD3	1.83	0.60
1:A:160:GLU:N	1:A:160:GLU:OE2	2.34	0.60
1:D:165:ARG:O	1:D:168:TYR:N	2.34	0.60
1:B:54:LEU:HB2	1:B:311:LEU:HD21	1.83	0.60
1:B:76:ILE:HD12	1:B:139:VAL:CG1	2.31	0.60
1:C:231:LEU:HB3	1:C:265:ARG:HH11	1.66	0.60
1:D:191:GLU:OE1	1:D:301:VAL:CG1	2.50	0.60
1:B:142:ILE:CA	1:B:169:SER:O	2.40	0.60
1:D:214:LEU:HD12	1:D:217:ASN:HB3	1.84	0.60
1:C:281:LEU:H	1:C:281:LEU:HD23	1.67	0.60
1:C:88:ASP:OD1	1:C:88:ASP:N	2.29	0.60
1:A:251:GLN:HE21	1:A:251:GLN:C	2.05	0.59
1:A:299:LEU:HD23	1:A:312:ILE:HG13	1.83	0.59
1:D:268:LEU:HD23	1:D:268:LEU:O	2.01	0.59
1:D:271:VAL:HG12	1:D:271:VAL:O	2.01	0.59
1:B:156:PRO:CG	1:B:268:LEU:CD1	2.79	0.59
1:B:270:PRO:O	1:B:271:VAL:CG2	2.50	0.59
1:C:89:GLU:HA	1:C:89:GLU:OE1	2.03	0.59
1:C:281:LEU:HD23	1:C:281:LEU:N	2.17	0.59
1:D:164:MET:HE3	1:D:205:THR:HG21	1.85	0.59
1:D:261:GLN:O	1:D:261:GLN:NE2	2.33	0.59
1:D:158:ILE:O	1:D:158:ILE:HG22	2.03	0.59
1:B:308:ARG:HH21	1:B:308:ARG:CG	2.12	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:VAL:CG1	1:D:260:GLU:HA	2.31	0.59
1:B:296:ILE:HD13	1:B:312:ILE:HG23	1.85	0.58
1:C:142:ILE:HA	1:C:169:SER:O	2.03	0.58
1:B:30:GLN:O	1:B:34:GLN:HG2	2.02	0.58
1:B:120:PHE:HA	1:B:123:MET:HE2	1.86	0.58
1:A:66:HIS:HA	1:A:69:ILE:HG22	1.85	0.58
1:D:251:GLN:HE21	1:D:271:VAL:HG11	1.64	0.58
1:C:233:GLU:OE2	1:C:265:ARG:CG	2.42	0.58
1:C:283:TRP:O	1:C:286:GLN:N	2.36	0.58
1:A:299:LEU:HD21	1:A:311:LEU:HB3	1.86	0.58
1:B:156:PRO:N	1:B:268:LEU:CD1	2.66	0.58
1:C:191:GLU:CG	1:C:301:VAL:HG21	2.23	0.58
1:A:6:ILE:CG2	1:A:50:MET:HE1	2.30	0.58
1:B:59:VAL:HG11	1:B:188:CYS:HB2	1.85	0.58
1:D:163:TYR:CE2	1:D:237:THR:O	2.57	0.57
1:A:9:LEU:HD23	1:A:307:TRP:HZ3	1.66	0.57
1:A:14:MET:O	1:A:17:VAL:HG13	2.03	0.57
1:D:41:SER:O	1:D:41:SER:OG	2.22	0.57
1:A:167:ILE:CG2	1:A:171:THR:OG1	2.47	0.57
1:D:300:GLN:OE1	1:D:300:GLN:HA	2.04	0.57
1:B:296:ILE:HD13	1:B:312:ILE:CG2	2.34	0.57
1:C:266:HIS:HE1	1:C:267:LEU:HD22	1.67	0.57
1:D:164:MET:CE	1:D:205:THR:CG2	2.82	0.57
1:C:271:VAL:HA	1:C:274:ALA:HB3	1.87	0.57
1:C:65:ALA:O	1:C:69:ILE:HD12	2.05	0.57
1:D:231:LEU:N	1:D:231:LEU:HD23	2.19	0.57
1:D:9:LEU:CD2	1:D:307:TRP:CE3	2.84	0.56
1:C:273:GLU:HG3	1:C:274:ALA:N	2.19	0.56
1:B:156:PRO:CD	1:B:268:LEU:HD11	2.32	0.56
1:B:285:ARG:NH2	1:B:320:GLN:O	2.39	0.56
1:C:272:LEU:O	1:C:276:ASN:ND2	2.30	0.56
1:D:3:LEU:HD23	1:D:3:LEU:N	2.02	0.56
1:C:238:LEU:HD12	1:C:238:LEU:C	2.25	0.56
1:C:231:LEU:N	1:C:231:LEU:HD23	2.20	0.56
1:C:216:TYR:CE2	1:C:275:MET:HE2	2.38	0.56
1:B:209:LEU:HD22	1:B:238:LEU:HD23	1.86	0.56
1:A:14:MET:HE3	1:A:17:VAL:HG11	1.87	0.55
1:B:156:PRO:CG	1:B:268:LEU:HD11	2.36	0.55
1:B:305:THR:HG23	1:B:307:TRP:H	1.72	0.55
1:D:302:LEU:HG	1:D:303:PRO:HD2	1.88	0.55
1:A:3:LEU:HD13	1:A:317:ILE:CD1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLN:HA	1:A:24:GLN:OE1	2.06	0.55
1:D:305:THR:CG2	1:D:306:PRO:CD	2.42	0.55
1:A:80:THR:HG23	2:A:901:B29:CBA	2.37	0.55
1:B:152:ASN:O	1:B:236:PRO:HG2	2.06	0.55
1:C:237:THR:HB	1:C:239:PRO:HD2	1.88	0.55
2:A:901:B29:HAP	1:B:113:ASP:OD2	2.07	0.55
1:C:282:GLU:HA	1:C:282:GLU:OE2	2.06	0.55
1:A:210:ILE:HD13	1:A:213:LEU:HD21	1.89	0.54
1:D:6:ILE:CD1	1:D:310:ALA:O	2.54	0.54
1:D:231:LEU:H	1:D:231:LEU:HD23	1.72	0.54
1:B:69:ILE:HA	1:B:72:LEU:HG	1.90	0.54
1:B:231:LEU:HD12	1:B:231:LEU:O	2.07	0.54
1:A:14:MET:HE3	1:A:14:MET:HA	1.90	0.54
1:A:3:LEU:HA	1:A:317:ILE:HD11	1.90	0.54
1:A:288:ALA:HA	1:A:291:GLU:OE1	2.08	0.54
1:D:261:GLN:NE2	1:D:261:GLN:HA	2.23	0.54
1:D:302:LEU:CG	1:D:303:PRO:HD2	2.37	0.54
1:D:164:MET:HE1	1:D:205:THR:CG2	2.38	0.53
1:B:168:TYR:OH	1:B:173:ARG:NH1	2.42	0.53
1:A:291:GLU:HA	1:A:294:LYS:HB2	1.91	0.53
1:A:299:LEU:HD12	1:A:302:LEU:HD21	1.88	0.53
1:B:181:CYS:HA	1:B:184:ILE:HG22	1.91	0.53
1:A:14:MET:HE3	1:A:17:VAL:CG1	2.38	0.53
1:D:45:LYS:O	1:D:45:LYS:HD3	2.09	0.53
1:B:270:PRO:C	1:B:271:VAL:HG23	2.29	0.53
1:B:179:ALA:HB1	1:B:196:LEU:HB3	1.91	0.53
1:A:14:MET:HE3	1:A:14:MET:CA	2.38	0.52
1:A:14:MET:HA	1:A:17:VAL:CG1	2.38	0.52
1:A:116:TYR:HE2	1:B:120:PHE:CD2	2.26	0.52
1:A:158:ILE:HG21	1:A:241:LEU:HD21	1.89	0.52
1:D:50:MET:O	1:D:54:LEU:HB2	2.10	0.52
1:A:35:LEU:HD21	1:A:99:ALA:CB	2.38	0.52
1:C:82:LEU:O	1:C:108:SER:HB3	2.10	0.52
1:B:156:PRO:CA	1:B:268:LEU:HD11	2.40	0.52
1:C:283:TRP:O	1:C:286:GLN:HB2	2.09	0.52
1:D:269:GLU:N	1:D:270:PRO:CD	2.74	0.51
1:B:115:ILE:CD1	1:B:115:ILE:N	2.73	0.51
1:C:64:ASN:O	1:C:67:VAL:HG22	2.10	0.51
1:D:289:GLU:HG2	1:D:319:VAL:HG21	1.91	0.51
1:A:105:ASN:HD22	1:B:103:PHE:N	2.09	0.51
1:D:293:ASP:HA	1:D:296:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:LEU:HD12	1:C:270:PRO:HG2	1.92	0.51
1:D:254:MET:SD	1:D:267:LEU:HD11	2.50	0.51
1:C:18:ASN:OD1	1:C:46:ARG:NH2	2.40	0.51
1:A:113:ASP:OD2	1:B:83:HIS:ND1	2.32	0.51
1:C:153:VAL:HG13	1:C:154:ASN:OD1	2.10	0.51
1:D:261:GLN:NE2	1:D:261:GLN:CA	2.73	0.51
1:D:302:LEU:CG	1:D:303:PRO:CD	2.88	0.51
1:B:80:THR:HG22	1:B:116:TYR:OH	2.11	0.51
1:D:231:LEU:CD2	1:D:231:LEU:N	2.73	0.51
1:D:254:MET:CE	1:D:254:MET:CA	2.86	0.51
1:A:164:MET:HE1	1:A:167:ILE:HD12	1.93	0.51
1:C:69:ILE:HD13	1:C:185:LEU:HD23	1.89	0.51
1:B:72:LEU:O	1:B:76:ILE:HG12	2.11	0.50
1:C:151:MET:SD	1:D:31:LEU:HB2	2.51	0.50
1:C:281:LEU:CD2	1:C:281:LEU:N	2.73	0.50
1:C:301:VAL:HG13	1:C:302:LEU:HD12	1.93	0.50
1:A:140:ASN:HD21	1:B:118:ARG:CZ	2.23	0.50
1:C:65:ALA:O	1:C:69:ILE:CD1	2.59	0.50
1:D:209:LEU:HD22	1:D:238:LEU:HD22	1.92	0.50
1:A:305:THR:HG22	1:A:308:ARG:HB2	1.93	0.50
1:B:148:LEU:HG	1:B:166:VAL:CG2	2.42	0.50
1:B:76:ILE:O	1:B:80:THR:HG23	2.12	0.50
1:C:80:THR:HG22	1:C:116:TYR:OH	2.10	0.50
1:A:79:ALA:HB2	1:A:115:ILE:HG22	1.93	0.50
1:A:151:MET:CE	1:B:31:LEU:HD22	2.42	0.50
1:C:153:VAL:HG13	1:C:154:ASN:CG	2.32	0.50
1:D:164:MET:CE	1:D:205:THR:HG21	2.42	0.50
1:B:37:TYR:CD1	1:B:37:TYR:C	2.86	0.49
1:D:54:LEU:HD13	1:D:311:LEU:HG	1.94	0.49
1:D:163:TYR:CZ	1:D:237:THR:O	2.65	0.49
1:A:150:LEU:HD13	1:B:110:LEU:HD12	1.93	0.49
1:B:59:VAL:HG11	1:B:188:CYS:CB	2.42	0.49
1:B:73:ILE:HD11	1:B:135:MET:CE	2.42	0.49
1:B:275:MET:SD	1:B:276:ASN:N	2.85	0.49
1:C:216:TYR:N	1:C:216:TYR:CD1	2.75	0.49
1:B:269:GLU:OE2	1:B:269:GLU:HA	2.11	0.49
1:C:69:ILE:HD12	1:C:69:ILE:H	1.76	0.49
1:D:9:LEU:CD2	1:D:307:TRP:HZ3	2.20	0.49
1:A:2:ASN:N	1:A:2:ASN:ND2	2.60	0.49
1:B:115:ILE:HD12	1:B:115:ILE:N	2.27	0.49
1:C:171:THR:HG21	1:C:208:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:THR:OG1	1:B:126:LEU:HD21	2.13	0.49
1:B:156:PRO:N	1:B:268:LEU:HD11	2.27	0.49
1:A:132:LEU:HD13	1:B:132:LEU:HD13	1.94	0.49
1:C:153:VAL:HG23	1:C:235:LYS:HD3	1.95	0.49
1:C:310:ALA:O	1:C:314:LEU:HG	2.12	0.49
1:C:231:LEU:CB	1:C:265:ARG:HH11	2.26	0.49
1:B:163:TYR:CZ	1:B:238:LEU:HB2	2.48	0.48
1:B:164:MET:HA	1:B:167:ILE:HG12	1.95	0.48
1:C:254:MET:CE	1:C:267:LEU:HD12	2.43	0.48
1:C:176:GLU:HA	1:C:200:GLY:HA3	1.95	0.48
1:A:166:VAL:HG22	1:A:170:LYS:NZ	2.28	0.48
1:A:269:GLU:N	1:A:270:PRO:CD	2.76	0.48
1:A:168:TYR:HE1	1:A:205:THR:HG21	1.78	0.48
1:C:131:VAL:HG23	1:C:181:CYS:SG	2.53	0.48
1:C:132:LEU:HD13	1:D:132:LEU:HD13	1.96	0.48
1:D:21:ILE:HG21	1:D:40:VAL:HG11	1.96	0.48
1:B:146:GLU:OE2	1:B:170:LYS:CD	2.61	0.48
1:C:213:LEU:C	1:C:213:LEU:HD23	2.33	0.48
1:C:139:VAL:HA	1:C:142:ILE:HD12	1.96	0.48
1:A:269:GLU:HB2	1:A:270:PRO:HD3	1.96	0.47
1:B:29:VAL:HB	1:B:32:ILE:HD12	1.96	0.47
1:B:168:TYR:HA	1:B:172:ALA:HB3	1.96	0.47
1:C:216:TYR:HE2	1:C:275:MET:CE	2.24	0.47
1:D:253:GLN:O	1:D:253:GLN:HG2	2.13	0.47
1:D:38:TYR:CD1	1:D:38:TYR:C	2.87	0.47
1:A:7:ASN:H	1:A:7:ASN:ND2	2.12	0.47
1:C:159:THR:HA	1:C:241:LEU:HD12	1.96	0.47
1:D:235:LYS:HG3	1:D:237:THR:HG23	1.95	0.47
1:B:54:LEU:CB	1:B:311:LEU:HD21	2.43	0.47
1:A:251:GLN:OE1	1:A:273:GLU:OE1	2.32	0.47
1:C:1:MET:SD	1:C:5:LYS:HE3	2.55	0.47
1:C:31:LEU:HD21	1:C:103:PHE:CE1	2.49	0.47
1:D:9:LEU:HD23	1:D:307:TRP:CZ3	2.45	0.47
1:A:6:ILE:CG2	1:A:50:MET:CE	2.89	0.47
1:A:64:ASN:O	1:A:67:VAL:HG22	2.14	0.47
1:C:88:ASP:HB2	1:C:89:GLU:H	1.55	0.47
1:D:238:LEU:N	1:D:239:PRO:HD3	2.30	0.47
1:B:289:GLU:HA	1:B:319:VAL:HG11	1.97	0.47
1:B:305:THR:HG23	1:B:307:TRP:N	2.29	0.47
1:D:39:ILE:HG12	1:D:78:THR:HG23	1.97	0.47
1:D:165:ARG:O	1:D:166:VAL:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HG12	1:A:163:TYR:HB2	1.97	0.47
1:C:148:LEU:HD13	1:D:29:VAL:HG22	1.97	0.47
1:C:76:ILE:O	1:C:80:THR:HG23	2.15	0.46
1:D:21:ILE:HD13	1:D:74:GLU:HG2	1.97	0.46
1:C:241:LEU:HA	1:C:241:LEU:HD22	1.66	0.46
1:D:289:GLU:HA	1:D:319:VAL:HG11	1.97	0.46
1:D:299:LEU:HD12	1:D:312:ILE:HG12	1.98	0.46
1:A:275:MET:SD	1:A:275:MET:C	2.94	0.46
1:C:254:MET:CE	1:C:267:LEU:CD1	2.94	0.46
1:A:100:ASN:OD1	1:A:100:ASN:N	2.48	0.46
1:A:116:TYR:OH	1:A:139:VAL:HG21	2.15	0.46
1:B:86:VAL:HB	1:B:104:GLY:HA3	1.97	0.46
1:B:214:LEU:N	1:B:214:LEU:HD13	2.31	0.46
1:C:79:ALA:HB2	1:C:115:ILE:HG22	1.97	0.46
1:C:170:LYS:HG3	1:C:171:THR:N	2.30	0.45
1:A:272:LEU:HD13	1:A:275:MET:CE	2.47	0.45
1:D:168:TYR:OH	1:D:291:GLU:OE1	2.28	0.45
1:A:113:ASP:OD1	1:B:83:HIS:CE1	2.69	0.45
1:B:270:PRO:O	1:B:271:VAL:HG22	2.16	0.45
1:B:296:ILE:HG23	1:B:312:ILE:HG23	1.97	0.45
1:C:31:LEU:HD21	1:C:103:PHE:HE1	1.81	0.45
1:C:126:LEU:HD13	1:C:185:LEU:HD21	1.99	0.45
1:C:268:LEU:HD22	1:C:272:LEU:CD1	2.46	0.45
1:A:14:MET:CE	1:A:17:VAL:HG11	2.46	0.45
1:B:299:LEU:O	1:B:308:ARG:NE	2.45	0.45
1:C:296:ILE:HG23	1:C:312:ILE:HG12	1.98	0.45
1:A:94:ARG:HH11	1:A:94:ARG:CG	2.29	0.45
1:D:251:GLN:HE22	1:D:271:VAL:HG11	1.77	0.45
1:B:106:ALA:O	1:B:109:VAL:HG22	2.17	0.45
1:B:269:GLU:HB3	1:B:270:PRO:HD2	1.99	0.45
1:C:30:GLN:O	1:C:34:GLN:HG3	2.16	0.45
1:D:238:LEU:HD12	1:D:238:LEU:HA	1.85	0.45
1:A:163:TYR:O	1:A:163:TYR:CD1	2.70	0.44
1:D:9:LEU:HD23	1:D:9:LEU:O	2.17	0.44
1:D:191:GLU:HG2	1:D:301:VAL:HG11	1.99	0.44
1:B:270:PRO:O	1:B:271:VAL:HG23	2.14	0.44
1:C:238:LEU:C	1:C:238:LEU:CD1	2.86	0.44
1:D:30:GLN:O	1:D:34:GLN:HG2	2.17	0.44
1:D:135:MET:HB2	1:D:135:MET:HE2	1.85	0.44
1:A:29:VAL:HG13	1:B:151:MET:SD	2.57	0.44
1:A:55:ALA:HB1	1:A:196:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LEU:HA	1:B:75:PHE:HB2	1.99	0.44
1:B:163:TYR:O	1:B:163:TYR:CG	2.71	0.44
1:A:10:THR:CG2	1:A:54:LEU:HD13	2.47	0.44
1:D:14:MET:HE3	1:D:14:MET:O	2.17	0.44
1:D:181:CYS:HA	1:D:184:ILE:HD12	2.00	0.44
1:D:283:TRP:O	1:D:283:TRP:CD2	2.70	0.44
1:B:214:LEU:O	1:B:214:LEU:HD23	2.17	0.44
1:A:164:MET:HE2	1:A:164:MET:HA	2.00	0.44
1:C:231:LEU:HB3	1:C:265:ARG:NH1	2.32	0.44
1:A:283:TRP:O	1:A:283:TRP:CG	2.70	0.44
1:B:48:ARG:CB	1:B:49:PRO:CD	2.96	0.44
1:D:21:ILE:CD1	1:D:74:GLU:HG2	2.47	0.44
1:D:231:LEU:O	1:D:264:GLY:HA3	2.18	0.44
1:A:168:TYR:HD1	1:A:205:THR:HG1	1.64	0.43
1:B:270:PRO:C	1:B:271:VAL:CG2	2.86	0.43
1:C:177:ALA:O	1:C:181:CYS:HB2	2.18	0.43
1:A:199:TYR:CE2	1:A:311:LEU:HD22	2.53	0.43
1:A:269:GLU:N	1:A:270:PRO:HD2	2.32	0.43
1:C:283:TRP:O	1:C:287:ARG:N	2.48	0.43
1:A:163:TYR:CD1	1:A:163:TYR:C	2.88	0.43
1:B:82:LEU:O	1:B:108:SER:HB3	2.18	0.43
1:B:118:ARG:HA	1:B:118:ARG:HD3	1.59	0.43
1:C:278:CYS:SG	1:C:280:SER:CB	3.00	0.43
1:D:79:ALA:HB2	1:D:115:ILE:HG22	2.00	0.43
1:D:167:ILE:HG23	1:D:171:THR:OG1	2.18	0.43
1:A:233:GLU:HG3	1:A:233:GLU:O	2.18	0.43
1:B:17:VAL:HG12	1:B:21:ILE:HD12	2.00	0.43
1:C:18:ASN:OD1	1:C:46:ARG:NH1	2.51	0.43
1:C:118:ARG:O	1:C:122:MET:HG3	2.19	0.43
1:D:9:LEU:CD2	1:D:9:LEU:C	2.85	0.43
1:D:75:PHE:CD1	1:D:115:ILE:HG23	2.54	0.43
1:D:261:GLN:HE21	1:D:261:GLN:C	2.20	0.43
1:A:134:VAL:CG1	1:A:180:GLN:NE2	2.80	0.43
1:A:167:ILE:HA	1:A:171:THR:CG2	2.47	0.43
1:C:136:SER:HB3	1:D:121:GLN:HG2	2.01	0.43
1:B:35:LEU:O	1:B:35:LEU:HD22	2.19	0.43
1:C:2:ASN:ND2	1:C:4:GLU:HB3	2.32	0.43
1:C:242:HIS:CB	1:C:280:SER:OG	2.67	0.43
1:A:272:LEU:HD23	1:A:272:LEU:H	1.79	0.43
1:C:87:VAL:O	1:C:105:ASN:ND2	2.42	0.43
1:C:252:ALA:O	1:C:255:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ILE:HA	1:D:72:LEU:HG	2.01	0.42
1:A:299:LEU:CD1	1:A:302:LEU:HD21	2.49	0.42
1:C:57:ARG:HH12	1:C:62:GLU:HA	1.84	0.42
1:D:296:ILE:HB	1:D:312:ILE:HD13	2.00	0.42
1:B:17:VAL:HA	1:B:67:VAL:HG13	2.01	0.42
1:B:296:ILE:CD1	1:B:312:ILE:HG23	2.49	0.42
1:C:23:GLU:O	1:C:26:ASN:ND2	2.52	0.42
1:D:191:GLU:HG2	1:D:191:GLU:O	2.19	0.42
1:C:242:HIS:HB3	1:C:280:SER:OG	2.18	0.42
1:C:266:HIS:ND1	1:C:266:HIS:C	2.73	0.42
1:D:23:GLU:O	1:D:26:ASN:ND2	2.53	0.42
1:D:265:ARG:CG	1:D:265:ARG:NH1	2.73	0.42
1:D:304:ASP:HA	1:D:308:ARG:NE	2.35	0.42
1:A:45:LYS:HD3	1:A:45:LYS:HA	1.76	0.42
1:A:251:GLN:O	1:A:251:GLN:NE2	2.53	0.42
1:B:73:ILE:HD11	1:B:135:MET:HE1	2.02	0.42
1:A:213:LEU:HD12	1:A:213:LEU:O	2.20	0.42
1:C:69:ILE:HD12	1:C:69:ILE:N	2.34	0.42
1:C:168:TYR:HA	1:C:172:ALA:HB3	2.01	0.42
1:D:46:ARG:HE	1:D:46:ARG:HB3	1.47	0.42
1:D:164:MET:HE1	1:D:205:THR:HG22	2.00	0.42
1:D:45:LYS:HE2	1:D:45:LYS:CA	2.30	0.41
1:D:287:ARG:O	1:D:287:ARG:HG3	2.18	0.41
1:A:162:ASN:HD22	1:A:162:ASN:HA	1.61	0.41
1:A:251:GLN:C	1:A:251:GLN:NE2	2.73	0.41
1:B:5:LYS:HA	1:B:5:LYS:HD2	1.82	0.41
1:C:185:LEU:HD12	1:C:185:LEU:HA	1.75	0.41
1:A:116:TYR:HE2	1:B:120:PHE:HE2	1.48	0.41
1:B:214:LEU:N	1:B:214:LEU:CD2	2.73	0.41
1:C:10:THR:HG22	1:C:54:LEU:HD21	2.01	0.41
1:C:139:VAL:HA	1:C:142:ILE:HB	2.02	0.41
1:C:154:ASN:HA	1:C:259:ILE:O	2.20	0.41
1:D:231:LEU:HD23	1:D:232:ASN:H	1.86	0.41
1:A:94:ARG:HH11	1:A:94:ARG:HG3	1.86	0.41
1:C:269:GLU:HB2	1:C:270:PRO:CD	2.44	0.41
1:C:269:GLU:N	1:C:270:PRO:CD	2.83	0.41
1:B:153:VAL:HG13	1:B:234:GLY:O	2.21	0.41
1:B:181:CYS:HA	1:B:184:ILE:CG2	2.51	0.41
1:C:128:SER:O	1:C:131:VAL:HG12	2.21	0.41
1:D:148:LEU:CD1	1:D:152:ASN:HD22	2.30	0.41
1:D:293:ASP:HA	1:D:296:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:LEU:HD12	1:D:302:LEU:HA	1.82	0.41
1:A:275:MET:SD	1:A:275:MET:O	2.79	0.41
1:B:210:ILE:HG12	1:B:288:ALA:CB	2.50	0.41
1:B:269:GLU:CB	1:B:270:PRO:CD	2.99	0.41
1:C:30:GLN:O	1:C:34:GLN:CG	2.69	0.41
1:C:69:ILE:CG1	1:C:185:LEU:CD2	2.99	0.41
1:C:213:LEU:HD23	1:C:214:LEU:N	2.36	0.41
1:D:54:LEU:HD23	1:D:54:LEU:HA	1.88	0.41
1:A:85:ASP:O	1:A:100:ASN:ND2	2.55	0.40
1:D:24:GLN:HG3	1:D:122:MET:HE1	2.04	0.40
1:A:256:ARG:HA	1:A:256:ARG:HD3	1.60	0.40
1:B:163:TYR:CD1	1:B:163:TYR:C	2.93	0.40
1:C:50:MET:HA	1:C:53:VAL:HG22	2.03	0.40
1:C:268:LEU:HD22	1:C:272:LEU:HD13	2.03	0.40
1:A:96:LYS:HA	1:A:96:LYS:HD2	1.93	0.40
1:A:140:ASN:ND2	1:B:118:ARG:HH21	2.11	0.40
1:A:151:MET:SD	1:B:31:LEU:HD23	2.60	0.40
1:A:311:LEU:HD23	1:A:311:LEU:HA	1.83	0.40
1:C:72:LEU:HA	1:C:75:PHE:HB2	2.03	0.40
1:C:215:ASP:OD2	1:C:232:ASN:HB2	2.21	0.40
1:C:231:LEU:N	1:C:231:LEU:CD2	2.83	0.40
1:A:118:ARG:HE	1:A:121:GLN:NE2	2.20	0.40
1:B:276:ASN:ND2	1:B:276:ASN:C	2.73	0.40
1:C:35:LEU:HD13	1:C:35:LEU:HA	1.73	0.40
1:C:210:ILE:HD13	1:C:210:ILE:HA	1.75	0.40
1:D:59:VAL:HG11	1:D:188:CYS:HB2	2.03	0.40
1:D:181:CYS:O	1:D:185:LEU:HD12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/323 (88%)	264 (93%)	19 (7%)	0	100	100
1	B	247/323 (76%)	227 (92%)	18 (7%)	2 (1%)	19	38
1	C	276/323 (85%)	265 (96%)	10 (4%)	1 (0%)	34	56
1	D	279/323 (86%)	245 (88%)	28 (10%)	6 (2%)	6	14
All	All	1085/1292 (84%)	1001 (92%)	75 (7%)	9 (1%)	19	38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	261	GLN
1	D	272	LEU
1	B	268	LEU
1	B	276	ASN
1	C	158	ILE
1	D	237	THR
1	D	254	MET
1	D	270	PRO
1	D	239	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	233/256 (91%)	193 (83%)	40 (17%)	2	2
1	B	208/256 (81%)	171 (82%)	37 (18%)	2	2
1	C	229/256 (90%)	191 (83%)	38 (17%)	2	3
1	D	229/256 (90%)	191 (83%)	38 (17%)	2	3
All	All	899/1024 (88%)	746 (83%)	153 (17%)	2	2

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	3	LEU

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Mol	Chain	Res	Type
1	A	5	LYS
1	A	8	GLU
1	A	12	GLN
1	A	14	MET
1	A	17	VAL
1	A	35	LEU
1	A	72	LEU
1	A	93	ARG
1	A	94	ARG
1	A	108	SER
1	A	148	LEU
1	A	158	ILE
1	A	159	THR
1	A	160	GLU
1	A	161	GLU
1	A	162	ASN
1	A	182	SER
1	A	191	GLU
1	A	194	LYS
1	A	207	PHE
1	A	209	LEU
1	A	210	ILE
1	A	213	LEU
1	A	229	ASP
1	A	251	GLN
1	A	254	MET
1	A	255	ILE
1	A	256	ARG
1	A	257	THR
1	A	260	GLU
1	A	261	GLN
1	A	263	ASN
1	A	267	LEU
1	A	268	LEU
1	A	275	MET
1	A	282	GLU
1	A	287	ARG
1	A	294	LYS
1	B	1	MET
1	B	4	GLU
1	B	5	LYS
1	B	9	LEU

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Mol	Chain	Res	Type
1	B	12	GLN
1	B	30	GLN
1	B	31	LEU
1	B	33	ASN
1	B	35	LEU
1	B	38	TYR
1	B	41	SER
1	B	45	LYS
1	B	47	ILE
1	B	86	VAL
1	B	116	TYR
1	B	118	ARG
1	B	123	MET
1	B	135	MET
1	B	144	GLU
1	B	157	ASP
1	B	163	TYR
1	B	165	ARG
1	B	214	LEU
1	B	231	LEU
1	B	233	GLU
1	B	235	LYS
1	B	237	THR
1	B	240	LEU
1	B	269	GLU
1	B	272	LEU
1	B	273	GLU
1	B	275	MET
1	B	276	ASN
1	B	278	CYS
1	B	287	ARG
1	B	308	ARG
1	B	312	ILE
1	C	1	MET
1	C	3	LEU
1	C	8	GLU
1	C	9	LEU
1	C	34	GLN
1	C	35	LEU
1	C	87	VAL
1	C	88	ASP
1	C	89	GLU

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Mol	Chain	Res	Type
1	C	116	TYR
1	C	153	VAL
1	C	154	ASN
1	C	182	SER
1	C	185	LEU
1	C	210	ILE
1	C	213	LEU
1	C	214	LEU
1	C	231	LEU
1	C	232	ASN
1	C	233	GLU
1	C	237	THR
1	C	238	LEU
1	C	241	LEU
1	C	242	HIS
1	C	251	GLN
1	C	254	MET
1	C	256	ARG
1	C	257	THR
1	C	261	GLN
1	C	265	ARG
1	C	266	HIS
1	C	267	LEU
1	C	268	LEU
1	C	269	GLU
1	C	272	LEU
1	C	273	GLU
1	C	281	LEU
1	C	282	GLU
1	D	3	LEU
1	D	5	LYS
1	D	14	MET
1	D	17	VAL
1	D	23	GLU
1	D	39	ILE
1	D	40	VAL
1	D	45	LYS
1	D	46	ARG
1	D	54	LEU
1	D	91	ASP
1	D	94	ARG
1	D	96	LYS

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Mol	Chain	Res	Type
1	D	123	MET
1	D	158	ILE
1	D	161	GLU
1	D	164	MET
1	D	227	VAL
1	D	231	LEU
1	D	253	GLN
1	D	254	MET
1	D	256	ARG
1	D	257	THR
1	D	259	ILE
1	D	261	GLN
1	D	265	ARG
1	D	266	HIS
1	D	268	LEU
1	D	269	GLU
1	D	272	LEU
1	D	273	GLU
1	D	287	ARG
1	D	296	ILE
1	D	300	GLN
1	D	302	LEU
1	D	305	THR
1	D	311	LEU
1	D	320	GLN

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

Mol	Chain	Res	Type
1	A	2	ASN
1	A	7	ASN
1	A	12	GLN
1	A	121	GLN
1	A	140	ASN
1	A	162	ASN
1	A	180	GLN
1	A	251	GLN
1	A	263	ASN
1	B	30	GLN
1	B	33	ASN
1	B	121	GLN
1	B	140	ASN

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Mol	Chain	Res	Type
1	C	152	ASN
1	C	232	ASN
1	C	251	GLN
1	C	261	GLN
1	D	2	ASN
1	D	30	GLN
1	D	121	GLN
1	D	152	ASN
1	D	232	ASN
1	D	261	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	B29	A	901	3	29,33,33	1.53	5 (17%)	39,52,52	1.15	3 (7%)

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	B29	A	901	3	-	2/23/27/27	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	B29	OAC-CBB	-3.26	1.40	1.44
2	A	901	B29	CAY-CAX	-2.74	1.37	1.43
2	A	901	B29	CAZ-CBA	-2.56	1.38	1.43
2	A	901	B29	PBD-CBB	2.44	1.86	1.85
2	A	901	B29	PBC-CBB	2.37	1.86	1.85

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	B29	PBD-CBB-PBC	-3.01	107.42	112.81
2	A	901	B29	CAN-CAW-CBA	2.70	119.62	116.50
2	A	901	B29	OAG-PBD-CBB	2.16	111.02	106.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	B29	CBB-CAS-CAU-CAL
2	A	901	B29	CBB-CAS-CAU-CAR

There are no ring outliers.

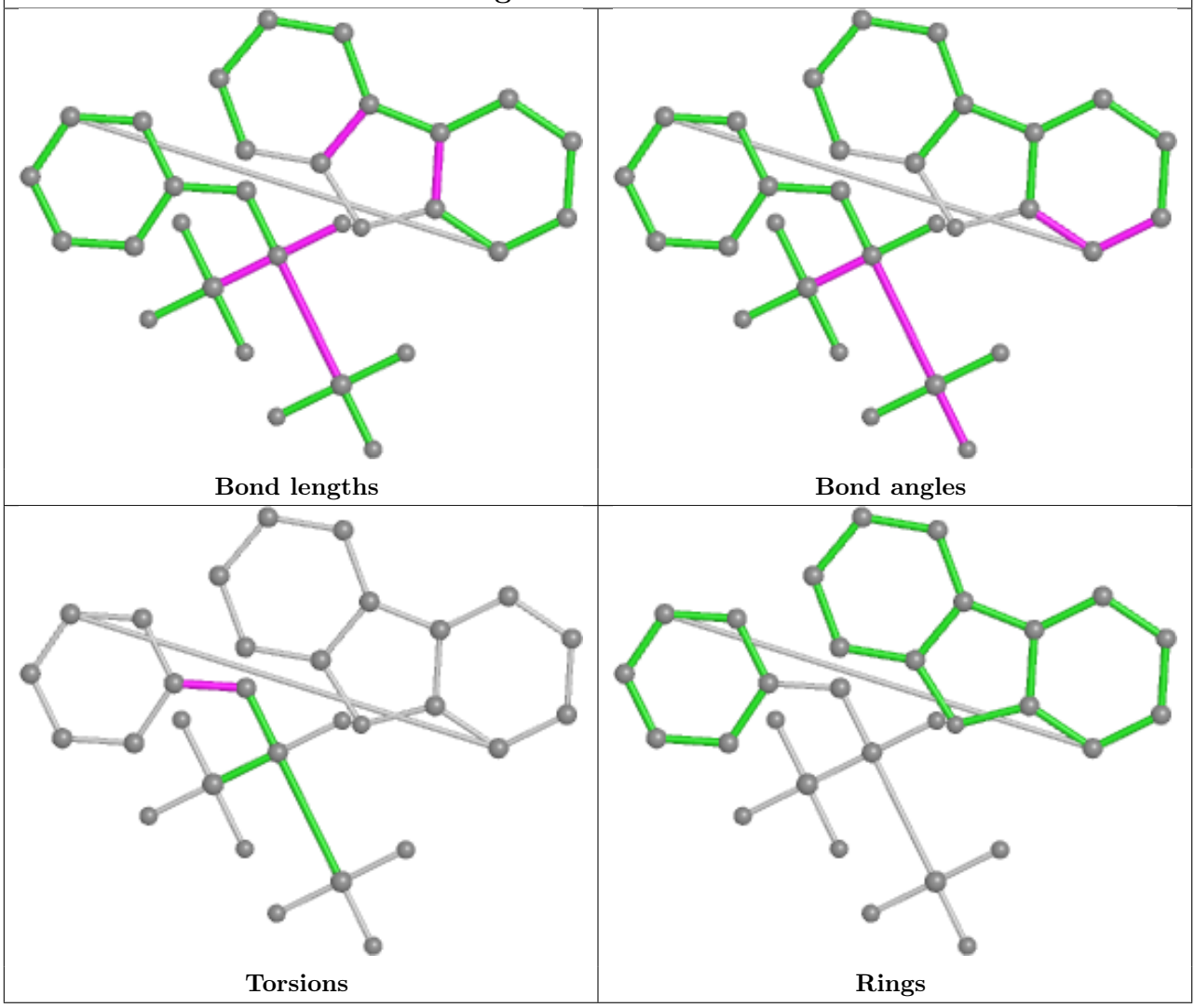
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	B29	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand B29 A 901



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	293/323 (90%)	0.12	13 (4%)	34	26	50, 96, 167, 225	0
1	B	259/323 (80%)	0.07	10 (3%)	39	31	50, 105, 170, 218	0
1	C	286/323 (88%)	-0.12	6 (2%)	63	58	39, 80, 162, 342	0
1	D	289/323 (89%)	0.08	20 (6%)	16	11	46, 104, 172, 239	0
All	All	1127/1292 (87%)	0.04	49 (4%)	35	27	39, 95, 170, 342	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	GLN	8.4
1	C	157	ASP	4.4
1	D	260	GLU	4.4
1	D	216	TYR	4.2
1	B	158	ILE	4.2
1	A	154	ASN	3.9
1	A	91	ASP	3.7
1	B	3	LEU	3.7
1	D	91	ASP	3.6
1	A	94	ARG	3.3
1	D	62	GLU	3.2
1	C	252	ALA	3.2
1	B	160	GLU	3.2
1	D	214	LEU	3.1
1	B	39	ILE	3.1
1	A	273	GLU	3.0
1	B	271	VAL	3.0
1	B	55	ALA	3.0
1	A	266	HIS	2.9
1	C	4	GLU	2.9
1	D	158	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	95	GLY	2.7
1	D	215	ASP	2.7
1	C	243	ALA	2.7
1	B	182	SER	2.6
1	D	90	SER	2.6
1	D	240	LEU	2.6
1	A	291	GLU	2.5
1	C	278	CYS	2.5
1	B	51	ILE	2.5
1	A	227	VAL	2.5
1	D	165	ARG	2.4
1	D	259	ILE	2.4
1	A	217	ASN	2.4
1	D	217	ASN	2.4
1	A	282	GLU	2.3
1	D	55	ALA	2.3
1	A	260	GLU	2.3
1	B	309	GLU	2.3
1	D	190	PRO	2.3
1	A	294	LYS	2.2
1	C	241	LEU	2.2
1	D	3	LEU	2.2
1	A	37	TYR	2.2
1	B	52	ALA	2.2
1	A	165	ARG	2.1
1	D	191	GLU	2.1
1	D	54	LEU	2.1
1	D	283	TRP	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 monosaccharides 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. The B-factors column lists the minimum,

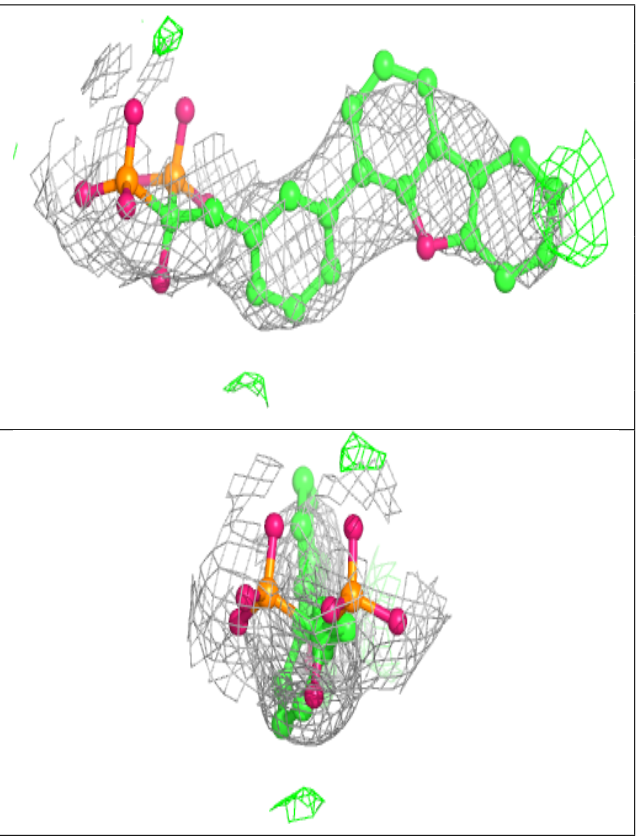
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	D	401	1/1	0.90	0.36	61,61,61,61	0
2	B29	A	901	30/30	0.91	0.19	106,125,132,134	0
3	MG	A	902	1/1	0.97	0.42	84,84,84,84	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around B29 A 901:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.