



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:26 am BST

PDB ID : 4GDN
Title : Structure of FmtA-like protein
Authors : Cougnoux, A.; Gibold, L.; Delmas, J.; Robin, F.; Dalmaso, G.; Bonnet, R.
Deposited on : 2012-08-01
Resolution : 3.20 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

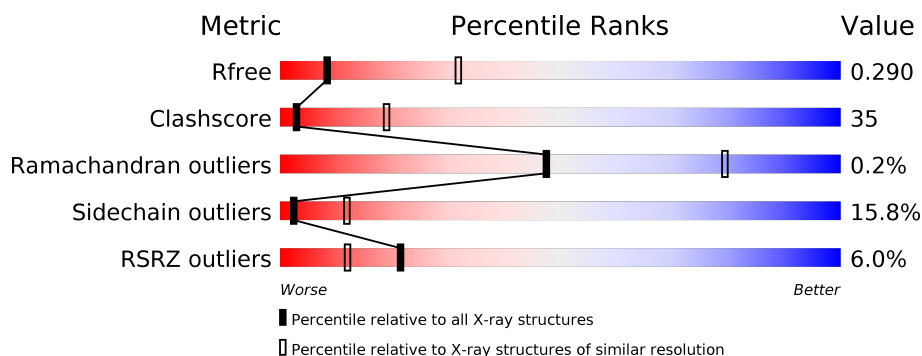
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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 $\leq 5\%$. 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	342	<div> <div>4%</div> <div> <div></div> <div>48%</div> <div>39%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	342	<div> <div>2%</div> <div> <div></div> <div>48%</div> <div>39%</div> <div>11%</div> <div>.</div> </div> </div>
1	C	342	<div> <div>10%</div> <div> <div></div> <div>52%</div> <div>35%</div> <div>10%</div> <div>.</div> </div> </div>
1	D	342	<div> <div>7%</div> <div> <div></div> <div>50%</div> <div>39%</div> <div>8%</div> <div>.</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10649 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.

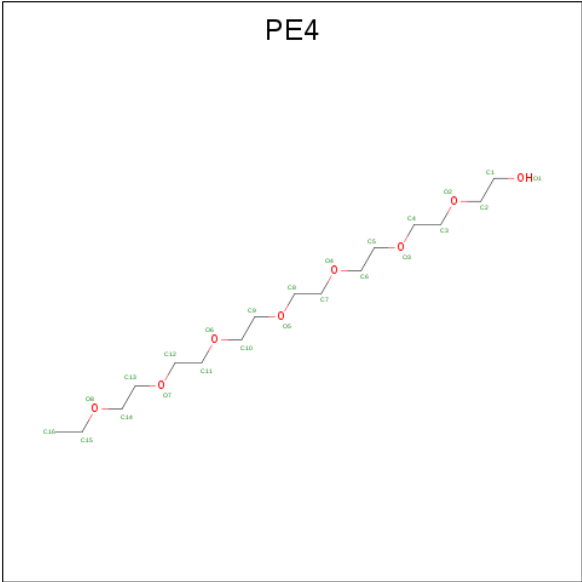
- Molecule 1 is a protein called Protein flp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2674	1692	458	518	6			
1	B	336	Total	C	N	O	S	0	0	0
			2658	1684	456	512	6			
1	C	329	Total	C	N	O	S	0	0	0
			2616	1658	447	505	6			
1	D	333	Total	C	N	O	S	0	0	0
			2642	1673	454	509	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MET	-	INITIATING METHIONINE	UNP Q7A3Q5
B	29	MET	-	INITIATING METHIONINE	UNP Q7A3Q5
C	29	MET	-	INITIATING METHIONINE	UNP Q7A3Q5
D	29	MET	-	INITIATING METHIONINE	UNP Q7A3Q5

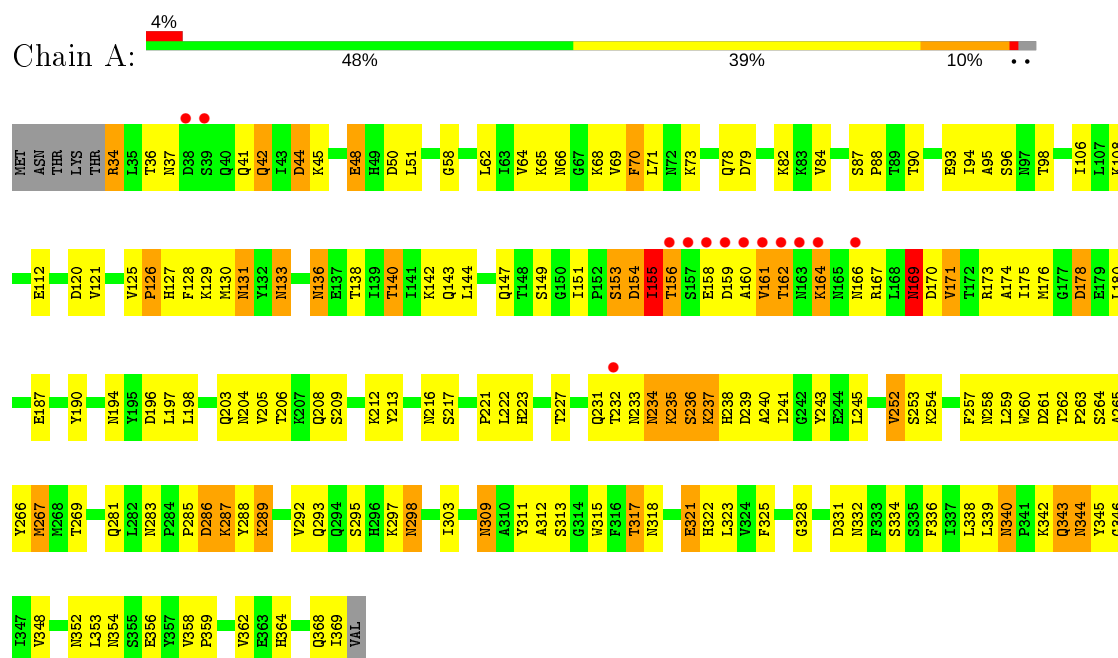
- Molecule 2 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



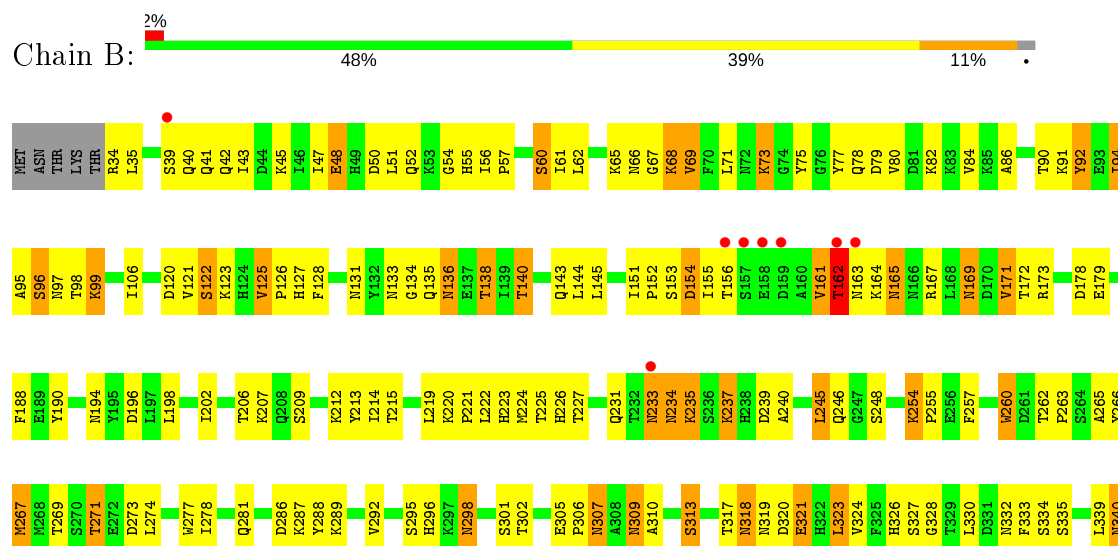
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Protein flp

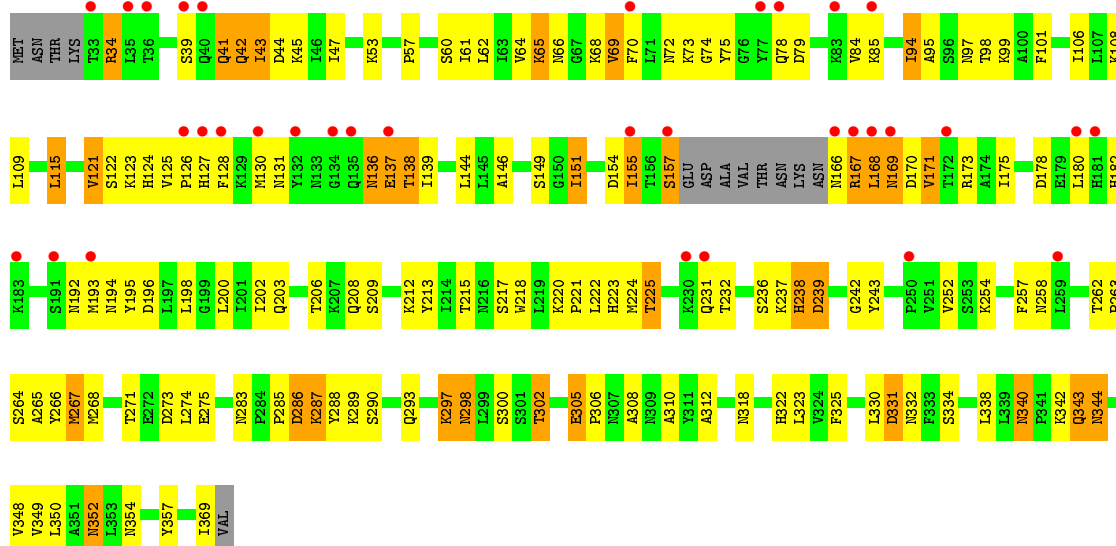


• Molecule 1: Protein flp

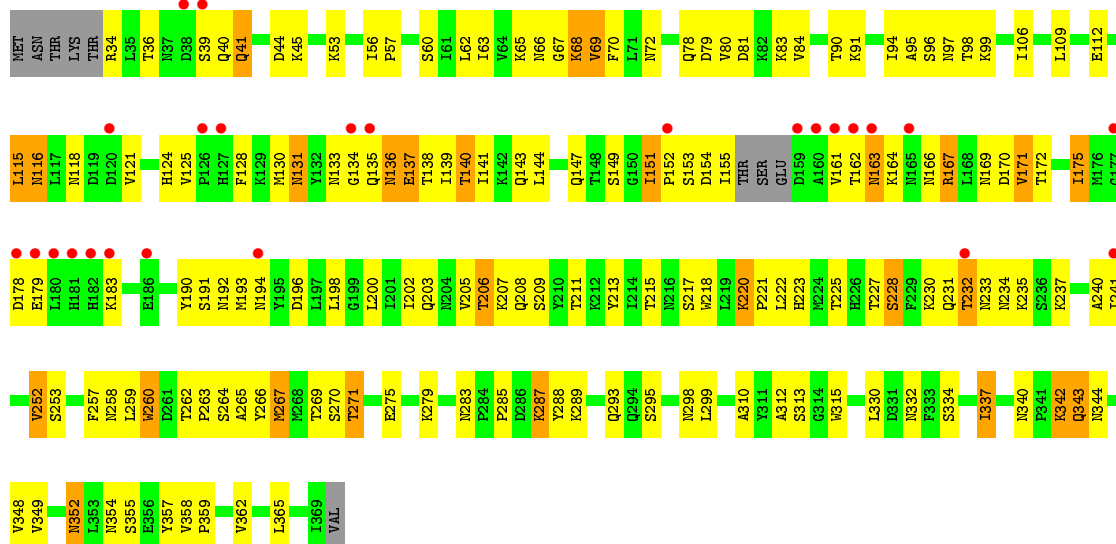




• Molecule 1: Protein flp



• Molecule 1: Protein flp



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	179.71Å 179.71Å 287.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.73 – 3.20 85.76 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.4 (85.73-3.20) 96.4 (85.76-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.257 , 0.295 0.257 , 0.290	Depositor DCC
R_{free} test set	2217 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10649	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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, 0.333 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: PE4

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	0.53	0/2734	0.77	3/3709 (0.1%)
1	B	0.53	0/2718	0.77	2/3689 (0.1%)
1	C	0.50	0/2675	0.73	1/3629 (0.0%)
1	D	0.48	0/2701	0.70	0/3664
All	All	0.51	0/10828	0.75	6/14691 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	VAL	CB-CA-C	-5.40	101.14	111.40
1	A	126	PRO	N-CD-CG	-5.34	95.19	103.20
1	B	162	THR	N-CA-CB	5.33	120.43	110.30
1	A	159	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	238	HIS	CB-CA-C	-5.10	100.20	110.40
1	A	126	PRO	N-CA-CB	-5.04	97.06	102.60

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	2674	0	2628	183	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2658	0	2605	235	0
1	C	2616	0	2567	165	0
1	D	2642	0	2587	163	0
2	D	24	0	34	0	0
3	A	7	0	0	0	0
3	B	15	0	0	1	0
3	C	6	0	0	1	0
3	D	7	0	0	1	0
All	All	10649	0	10421	731	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 35.

All (731) 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:B:122:SER:O	1:B:123:LYS:HG2	1.34	1.25
1:B:68:LYS:HB2	1:B:68:LYS:NZ	1.37	1.17
1:A:356:GLU:O	1:A:359:PRO:HD2	1.44	1.15
1:A:130:MET:HG2	1:A:180:LEU:HD21	1.30	1.11
1:C:137:GLU:HA	1:C:137:GLU:OE1	1.45	1.11
1:B:306:PRO:HA	3:B:408:HOH:O	1.50	1.10
1:B:125:VAL:HG11	1:B:128:PHE:HB2	1.31	1.10
1:B:323:LEU:H	1:B:323:LEU:HD12	1.04	1.09
1:D:125:VAL:HG11	1:D:128:PHE:HB2	1.33	1.09
1:B:318:ASN:C	1:B:318:ASN:HD22	1.54	1.06
1:B:323:LEU:HD12	1:B:323:LEU:N	1.67	1.05
1:C:125:VAL:HG11	1:C:128:PHE:HB2	1.34	1.05
1:B:356:GLU:O	1:B:359:PRO:HD2	1.56	1.05
1:C:94:ILE:HG23	1:C:97:ASN:HB2	1.39	1.04
1:D:125:VAL:CG1	1:D:128:PHE:HB2	1.87	1.04
1:B:94:ILE:HG23	1:B:97:ASN:HB2	1.39	1.01
1:B:122:SER:O	1:B:123:LYS:CG	2.08	1.00
1:B:125:VAL:HG13	1:B:126:PRO:HD2	1.41	1.00
1:B:298:ASN:HD21	1:B:317:THR:HG21	1.29	0.98
1:B:106:ILE:HD12	1:B:198:LEU:HD22	1.45	0.97
1:C:98:THR:OG1	1:C:267:MET:HB3	1.64	0.97
1:C:298:ASN:ND2	1:C:298:ASN:H	1.51	0.97
1:B:68:LYS:HB2	1:B:68:LYS:HZ3	1.16	0.97
1:A:334:SER:HB2	1:A:354:ASN:HA	1.46	0.96
1:C:171:VAL:CG2	1:C:175:ILE:HG13	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:ASN:HA	1:C:312:ALA:HB2	1.47	0.95
1:B:68:LYS:NZ	1:B:68:LYS:CB	2.30	0.95
1:A:289:LYS:NZ	1:A:289:LYS:HB3	1.81	0.95
1:D:130:MET:CE	1:D:175:ILE:HB	1.96	0.94
1:C:151:ILE:HD11	1:C:193:MET:HB2	1.47	0.94
1:B:131:ASN:HB3	1:B:136:ASN:HA	1.50	0.93
1:B:68:LYS:HB2	1:B:68:LYS:HZ2	1.21	0.93
1:B:235:LYS:HB2	1:B:239:ASP:HB2	1.47	0.93
1:A:289:LYS:HZ3	1:A:289:LYS:HB3	1.31	0.92
1:A:233:ASN:HD21	1:A:254:LYS:HB2	1.32	0.92
1:B:255:PRO:HD3	1:B:332:ASN:HD21	1.32	0.92
1:B:255:PRO:HD3	1:B:332:ASN:ND2	1.84	0.91
1:D:130:MET:HE2	1:D:175:ILE:HB	1.48	0.90
1:D:140:THR:HG23	1:D:143:GLN:HG3	1.53	0.90
1:C:34:ARG:H	1:C:34:ARG:HD2	1.36	0.90
1:B:41:GLN:HB3	1:B:43:ILE:HD13	1.52	0.90
1:C:65:LYS:HG3	1:C:369:ILE:CG2	2.02	0.89
1:C:215:THR:O	1:C:220:LYS:HG2	1.72	0.89
1:D:83:LYS:O	1:D:83:LYS:HD3	1.73	0.88
1:C:121:VAL:HG11	1:C:128:PHE:CD2	2.09	0.88
1:A:127:HIS:O	1:B:207:LYS:HE3	1.74	0.87
1:C:217:SER:O	1:C:221:PRO:HG2	1.74	0.87
1:A:298:ASN:HA	1:A:312:ALA:HB2	1.54	0.87
1:B:155:ILE:O	1:B:155:ILE:HG22	1.72	0.87
1:B:156:THR:HB	1:B:178:ASP:OD2	1.76	0.86
1:D:206:THR:HG21	1:D:213:TYR:HB2	1.56	0.86
1:B:334:SER:OG	1:B:354:ASN:HA	1.75	0.86
1:C:298:ASN:H	1:C:298:ASN:HD22	1.23	0.86
1:D:97:ASN:HD21	1:D:337:ILE:HB	1.38	0.86
1:D:202:ILE:O	1:D:206:THR:HB	1.76	0.85
1:A:171:VAL:HG22	1:A:171:VAL:O	1.76	0.85
1:A:166:ASN:HD21	1:A:173:ARG:NH2	1.75	0.85
1:A:154:ASP:OD1	1:A:155:ILE:HB	1.77	0.84
1:B:318:ASN:C	1:B:318:ASN:ND2	2.30	0.84
1:C:65:LYS:HB3	1:C:70:PHE:CD2	2.12	0.84
1:D:206:THR:HG22	1:D:208:GLN:HG2	1.57	0.84
1:A:206:THR:HG22	1:A:208:GLN:HG2	1.58	0.83
1:D:241:ILE:HG21	1:D:252:VAL:CG2	2.09	0.83
1:B:125:VAL:HG13	1:B:126:PRO:CD	2.08	0.83
1:A:166:ASN:ND2	1:A:173:ARG:NH2	2.27	0.82
1:A:297:LYS:O	1:A:312:ALA:HB1	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:GLU:HG3	1:C:306:PRO:HD2	1.62	0.82
1:C:65:LYS:HG3	1:C:369:ILE:HG21	1.59	0.82
1:A:130:MET:CG	1:A:180:LEU:HD21	2.10	0.82
1:C:171:VAL:HG23	1:C:171:VAL:O	1.79	0.81
1:B:95:ALA:HA	1:B:265:ALA:O	1.80	0.81
1:B:342:LYS:O	1:B:343:GLN:HB2	1.79	0.80
1:C:171:VAL:HG23	1:C:175:ILE:HG13	1.61	0.80
1:D:206:THR:CG2	1:D:208:GLN:HG2	2.10	0.80
1:A:151:ILE:HD12	1:A:194:ASN:ND2	1.97	0.80
1:C:298:ASN:ND2	1:C:298:ASN:N	2.28	0.80
1:B:106:ILE:CD1	1:B:198:LEU:HD22	2.12	0.79
1:A:171:VAL:CG2	1:A:171:VAL:O	2.30	0.79
1:B:323:LEU:CD1	1:B:323:LEU:N	2.44	0.79
1:A:161:VAL:HG13	1:A:162:THR:N	1.98	0.79
1:A:289:LYS:NZ	1:A:289:LYS:CB	2.45	0.79
1:C:169:ASN:HD22	1:C:169:ASN:C	1.87	0.79
1:A:166:ASN:HD21	1:A:173:ARG:HH22	1.29	0.78
1:B:235:LYS:HB2	1:B:239:ASP:CB	2.12	0.78
1:C:171:VAL:CG2	1:C:171:VAL:O	2.30	0.78
1:B:318:ASN:ND2	1:B:321:GLU:H	1.81	0.78
1:D:259:LEU:O	1:D:262:THR:HG22	1.82	0.78
1:B:206:THR:HG21	1:B:213:TYR:CD1	2.18	0.78
1:A:169:ASN:O	1:A:171:VAL:HG12	1.83	0.78
1:A:79:ASP:HB3	1:A:84:VAL:HG12	1.65	0.78
1:D:241:ILE:CG2	1:D:252:VAL:HG22	2.14	0.78
1:B:323:LEU:CD1	1:B:323:LEU:H	1.93	0.77
1:B:92:TYR:HB3	1:B:333:PHE:CE2	2.19	0.77
1:A:36:THR:HG23	1:A:36:THR:O	1.83	0.77
1:C:151:ILE:HD11	1:C:193:MET:CB	2.13	0.77
1:B:96:SER:HB2	1:B:328:GLY:HA2	1.67	0.77
1:B:133:ASN:CG	1:B:134:GLY:H	1.87	0.76
1:B:309:ASN:HD22	1:B:309:ASN:H	1.30	0.76
1:B:198:LEU:O	1:B:202:ILE:HD12	1.86	0.76
1:D:171:VAL:CG1	1:D:260:TRP:HB2	2.15	0.76
1:C:69:VAL:O	1:C:69:VAL:CG2	2.34	0.76
1:B:162:THR:HG23	1:B:163:ASN:CB	2.16	0.76
1:A:205:VAL:HA	1:B:127:HIS:CD2	2.21	0.75
1:D:161:VAL:HB	1:D:164:LYS:O	1.85	0.75
1:B:60:SER:HB3	1:B:271:THR:OG1	1.86	0.75
1:A:154:ASP:O	1:A:155:ILE:HG22	1.87	0.74
1:A:233:ASN:ND2	1:A:254:LYS:HB2	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:VAL:CG1	1:B:128:PHE:HB2	2.15	0.74
1:A:171:VAL:HB	1:A:260:TRP:CD2	2.23	0.74
1:D:155:ILE:HD13	1:D:193:MET:CE	2.17	0.73
1:D:116:ASN:HD22	1:D:118:ASN:H	1.36	0.73
1:D:334:SER:HB2	1:D:354:ASN:HA	1.69	0.73
1:C:298:ASN:N	1:C:298:ASN:HD22	1.86	0.73
1:D:40:GLN:O	1:D:41:GLN:NE2	2.21	0.73
1:B:79:ASP:HB3	1:B:84:VAL:HG12	1.70	0.73
1:A:205:VAL:HG22	1:B:127:HIS:NE2	2.04	0.73
1:B:318:ASN:HD21	1:B:321:GLU:H	1.34	0.73
1:B:298:ASN:ND2	1:B:317:THR:HG21	2.03	0.72
1:B:234:ASN:C	1:B:234:ASN:HD22	1.92	0.72
1:B:171:VAL:CG2	1:B:171:VAL:O	2.37	0.72
1:C:257:PHE:HB2	1:C:266:TYR:OH	1.89	0.72
1:A:254:LYS:HD2	1:A:254:LYS:O	1.90	0.72
1:A:309:ASN:H	1:A:309:ASN:HD22	1.33	0.72
1:B:122:SER:O	1:B:123:LYS:CB	2.38	0.71
1:A:151:ILE:HD12	1:A:194:ASN:HD21	1.55	0.71
1:A:212:LYS:HE2	1:A:216:ASN:HD21	1.56	0.71
1:C:289:LYS:O	1:C:293:GLN:HG3	1.90	0.71
1:A:285:PRO:HG2	1:A:288:TYR:HD2	1.54	0.71
1:A:297:LYS:O	1:A:312:ALA:CB	2.38	0.71
1:A:93:GLU:OE2	1:A:235:LYS:NZ	2.23	0.71
1:A:166:ASN:CG	1:A:173:ARG:HH21	1.94	0.71
1:D:94:ILE:CD1	1:D:267:MET:HG2	2.21	0.71
1:C:121:VAL:CG1	1:C:128:PHE:CD2	2.74	0.70
1:D:97:ASN:ND2	1:D:337:ILE:HB	2.05	0.70
1:B:162:THR:HG23	1:B:163:ASN:HB2	1.73	0.70
1:D:171:VAL:HG11	1:D:260:TRP:HB2	1.72	0.70
1:A:154:ASP:OD1	1:A:154:ASP:C	2.30	0.70
1:C:283:ASN:HD21	1:C:344:ASN:HD21	1.38	0.70
1:D:79:ASP:HB3	1:D:84:VAL:HG12	1.72	0.70
1:B:65:LYS:O	1:B:67:GLY:N	2.22	0.69
1:A:298:ASN:HD21	1:A:317:THR:HG21	1.56	0.69
1:A:79:ASP:HB3	1:A:84:VAL:CG1	2.22	0.69
1:B:62:LEU:HB2	1:B:271:THR:HG22	1.75	0.69
1:B:79:ASP:HB3	1:B:84:VAL:CG1	2.22	0.69
1:D:79:ASP:HB3	1:D:84:VAL:CG1	2.22	0.69
1:A:283:ASN:HD21	1:A:344:ASN:HD21	1.41	0.69
1:D:136:ASN:ND2	1:D:136:ASN:C	2.43	0.69
1:A:283:ASN:ND2	1:A:344:ASN:HD21	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:GLN:HG3	1:D:209:SER:HA	1.74	0.68
1:A:125:VAL:CG1	1:A:128:PHE:HB2	2.22	0.68
1:A:161:VAL:CG1	1:A:162:THR:N	2.56	0.68
1:B:136:ASN:ND2	1:B:136:ASN:C	2.47	0.68
1:B:169:ASN:O	1:B:171:VAL:HG12	1.94	0.68
1:A:206:THR:HG21	1:A:213:TYR:CD1	2.28	0.68
1:B:69:VAL:CG2	1:B:69:VAL:O	2.42	0.68
1:D:151:ILE:HD11	1:D:193:MET:HB3	1.74	0.68
1:D:241:ILE:CG2	1:D:252:VAL:CG2	2.70	0.68
1:B:43:ILE:N	1:B:43:ILE:HD12	2.09	0.68
1:B:224:MET:HE2	1:B:277:TRP:HB2	1.75	0.68
1:D:125:VAL:HG12	1:D:128:PHE:HB2	1.75	0.68
1:D:65:LYS:HE2	1:D:70:PHE:CE1	2.28	0.68
1:C:34:ARG:HD2	1:C:34:ARG:N	2.08	0.67
1:C:65:LYS:HD2	1:C:70:PHE:HE2	1.58	0.67
1:B:334:SER:HG	1:B:354:ASN:HA	1.57	0.67
1:B:156:THR:CB	1:B:178:ASP:OD2	2.43	0.67
1:B:97:ASN:ND2	1:B:335:SER:HB2	2.10	0.67
1:C:297:LYS:O	1:C:297:LYS:HG3	1.94	0.66
1:D:67:GLY:O	1:D:279:LYS:NZ	2.27	0.66
1:A:153:SER:HB3	1:A:190:TYR:O	1.94	0.66
1:A:96:SER:HB3	1:A:328:GLY:HA2	1.77	0.66
1:D:66:ASN:O	1:D:68:LYS:HD2	1.96	0.66
1:B:92:TYR:HB3	1:B:333:PHE:HE2	1.59	0.66
1:D:155:ILE:HD13	1:D:193:MET:HE3	1.77	0.66
1:B:233:ASN:C	1:B:233:ASN:HD22	1.99	0.66
1:B:131:ASN:HB3	1:B:136:ASN:CA	2.23	0.66
1:C:130:MET:HE1	1:C:175:ILE:HG22	1.78	0.66
1:C:94:ILE:HG23	1:C:97:ASN:CB	2.20	0.66
1:A:356:GLU:O	1:A:359:PRO:CD	2.35	0.66
1:B:136:ASN:ND2	1:B:136:ASN:O	2.29	0.66
1:D:91:LYS:NZ	1:D:228:SER:OG	2.29	0.66
1:B:68:LYS:CB	1:B:68:LYS:HZ3	2.00	0.66
1:A:98:THR:HG23	1:A:267:MET:HE3	1.77	0.66
1:A:235:LYS:HB3	1:A:239:ASP:HB2	1.78	0.65
1:C:125:VAL:CG1	1:C:128:PHE:HB2	2.21	0.65
1:D:196:ASP:HA	1:D:263:PRO:HG2	1.78	0.65
1:A:136:ASN:ND2	1:A:136:ASN:O	2.29	0.65
1:C:99:LYS:HE2	1:C:195:TYR:HB2	1.78	0.65
1:C:41:GLN:O	1:C:41:GLN:NE2	2.30	0.65
1:B:340:ASN:ND2	1:B:342:LYS:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ASN:O	1:B:165:ASN:ND2	2.30	0.65
1:B:94:ILE:HG13	1:B:269:THR:HG22	1.79	0.65
1:A:222:LEU:O	1:A:223:HIS:HB2	1.97	0.65
1:C:208:GLN:HE21	1:C:212:LYS:HD3	1.62	0.65
1:B:234:ASN:O	1:B:234:ASN:ND2	2.30	0.65
1:B:43:ILE:H	1:B:43:ILE:HD12	1.61	0.65
1:D:151:ILE:HD11	1:D:193:MET:CB	2.27	0.65
1:A:243:TYR:O	1:A:353:LEU:HD12	1.97	0.64
1:C:169:ASN:ND2	1:C:169:ASN:O	2.30	0.64
1:A:106:ILE:CD1	1:A:198:LEU:HD22	2.27	0.64
1:A:298:ASN:HD22	1:A:298:ASN:N	1.94	0.64
1:B:235:LYS:CB	1:B:239:ASP:CB	2.75	0.64
1:C:167:ARG:HD2	1:C:258:ASN:HA	1.79	0.64
1:A:253:SER:HB3	1:A:332:ASN:HB3	1.80	0.64
1:C:151:ILE:CD1	1:C:193:MET:HB2	2.26	0.64
1:D:136:ASN:ND2	1:D:136:ASN:O	2.30	0.64
1:D:233:ASN:ND2	1:D:233:ASN:O	2.30	0.64
1:B:222:LEU:HD13	1:B:224:MET:HE3	1.79	0.64
1:C:65:LYS:HB3	1:C:70:PHE:CE2	2.32	0.64
1:B:106:ILE:HG13	1:B:202:ILE:HD11	1.80	0.64
1:B:257:PHE:HB2	1:B:266:TYR:OH	1.98	0.64
1:B:255:PRO:CD	1:B:332:ASN:HD21	2.08	0.64
1:C:94:ILE:CG2	1:C:97:ASN:HB2	2.23	0.64
1:C:137:GLU:CA	1:C:137:GLU:OE1	2.30	0.63
1:D:171:VAL:HG12	1:D:260:TRP:CB	2.28	0.63
1:A:166:ASN:CG	1:A:173:ARG:NH2	2.52	0.63
1:A:166:ASN:OD1	1:A:173:ARG:NH2	2.25	0.63
1:C:136:ASN:ND2	1:C:136:ASN:O	2.30	0.63
1:C:125:VAL:HG13	1:C:126:PRO:HD2	1.80	0.63
1:A:292:VAL:O	1:A:295:SER:HB3	1.99	0.63
1:D:169:ASN:O	1:D:171:VAL:HG13	1.99	0.63
1:A:127:HIS:HB2	1:B:207:LYS:HE2	1.80	0.63
1:C:131:ASN:HB3	1:C:136:ASN:HA	1.80	0.63
1:B:125:VAL:HG12	1:B:128:PHE:H	1.63	0.62
1:B:138:THR:O	1:B:138:THR:HG22	1.99	0.62
1:B:292:VAL:O	1:B:295:SER:HB3	1.99	0.62
1:A:131:ASN:HB3	1:A:136:ASN:HA	1.81	0.62
1:C:286:ASP:N	1:C:286:ASP:OD2	2.32	0.62
1:D:287:LYS:HE2	1:D:288:TYR:CE2	2.34	0.62
1:C:131:ASN:HA	1:C:136:ASN:HA	1.81	0.62
1:C:169:ASN:O	1:C:171:VAL:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:LEU:HD22	1:C:338:LEU:HD11	1.79	0.62
1:C:95:ALA:HA	1:C:265:ALA:O	1.99	0.62
1:A:125:VAL:HG11	1:A:128:PHE:HB2	1.82	0.62
1:B:133:ASN:OD1	1:B:134:GLY:N	2.33	0.62
1:A:227:THR:HG23	1:A:269:THR:HB	1.82	0.62
1:B:321:GLU:HB3	1:B:323:LEU:HD11	1.81	0.62
1:C:98:THR:HG22	1:C:263:PRO:O	2.00	0.62
1:D:147:GLN:OE1	1:D:190:TYR:HA	2.00	0.62
1:B:220:LYS:HB2	1:B:221:PRO:HD3	1.82	0.62
1:C:65:LYS:CG	1:C:369:ILE:HG21	2.29	0.61
1:C:78:GLN:HE22	1:C:238:HIS:HA	1.64	0.61
1:A:217:SER:O	1:A:221:PRO:HG2	2.00	0.61
1:B:140:THR:HG23	1:B:143:GLN:CD	2.19	0.61
1:C:65:LYS:HG3	1:C:369:ILE:HG23	1.82	0.61
1:C:298:ASN:HB3	1:C:310:ALA:HB1	1.83	0.61
1:D:137:GLU:OE2	1:D:183:LYS:HE3	2.01	0.61
1:C:257:PHE:CB	1:C:266:TYR:OH	2.48	0.61
1:A:262:THR:N	1:A:263:PRO:HD2	2.15	0.61
1:A:36:THR:O	1:A:36:THR:CG2	2.48	0.61
1:D:137:GLU:OE1	1:D:137:GLU:HA	2.00	0.61
1:D:167:ARG:HB3	1:D:258:ASN:HD22	1.66	0.61
1:B:224:MET:CE	1:B:277:TRP:HB2	2.31	0.60
1:B:47:ILE:HG21	1:B:75:TYR:CD1	2.36	0.60
1:D:202:ILE:CG2	1:D:213:TYR:HD2	2.14	0.60
1:D:90:THR:CG2	1:D:240:ALA:HB2	2.31	0.60
1:B:171:VAL:HG22	1:B:171:VAL:O	2.02	0.60
1:D:213:TYR:CE1	1:D:217:SER:CB	2.84	0.60
1:D:232:THR:O	1:D:233:ASN:HB3	2.01	0.60
1:A:173:ARG:CD	1:B:207:LYS:O	2.48	0.60
1:B:55:HIS:CD2	1:B:248:SER:HB3	2.37	0.60
1:C:101:PHE:CD2	1:C:267:MET:HE1	2.37	0.60
1:D:171:VAL:HG23	1:D:175:ILE:HD11	1.83	0.60
1:B:55:HIS:HD2	1:B:248:SER:HB3	1.66	0.60
1:C:47:ILE:HG21	1:C:75:TYR:CD2	2.37	0.60
1:C:130:MET:HG2	1:C:180:LEU:HD21	1.83	0.60
1:B:155:ILE:CG2	1:B:155:ILE:O	2.46	0.60
1:B:245:LEU:HD22	1:B:353:LEU:HD11	1.84	0.59
1:D:222:LEU:O	1:D:223:HIS:HB2	2.01	0.59
1:A:286:ASP:HA	1:A:289:LYS:HG3	1.84	0.59
1:B:154:ASP:OD1	1:B:155:ILE:HG13	2.02	0.59
1:B:56:ILE:HG12	1:B:353:LEU:HD23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:VAL:HB	1:B:260:TRP:CD2	2.37	0.59
1:D:98:THR:HG23	1:D:267:MET:HE3	1.84	0.59
1:A:231:GLN:O	1:A:232:THR:HB	2.03	0.59
1:D:109:LEU:HB3	1:D:115:LEU:HD23	1.82	0.59
1:D:155:ILE:HD13	1:D:193:MET:HE2	1.83	0.59
1:D:65:LYS:HE2	1:D:70:PHE:CD1	2.38	0.59
1:A:34:ARG:HD2	1:A:34:ARG:N	2.17	0.59
1:C:331:ASP:N	1:C:331:ASP:OD2	2.30	0.59
1:B:234:ASN:C	1:B:234:ASN:ND2	2.55	0.59
1:B:96:SER:O	1:B:99:LYS:HG3	2.02	0.59
1:C:136:ASN:ND2	1:C:136:ASN:C	2.55	0.59
1:A:171:VAL:HB	1:A:260:TRP:CE3	2.37	0.59
1:B:235:LYS:CB	1:B:239:ASP:HB3	2.32	0.59
1:D:213:TYR:CE1	1:D:217:SER:HB2	2.37	0.59
1:A:204:ASN:HB3	1:B:126:PRO:HB2	1.85	0.59
1:C:123:LYS:HG3	1:C:124:HIS:CD2	2.37	0.59
1:B:131:ASN:CB	1:B:136:ASN:HA	2.27	0.59
1:B:161:VAL:HG13	1:B:161:VAL:O	2.03	0.58
1:C:155:ILE:HD11	1:C:157:SER:OG	2.03	0.58
1:B:305:GLU:HA	1:B:305:GLU:OE1	2.02	0.58
1:B:133:ASN:CG	1:B:134:GLY:N	2.52	0.58
1:D:136:ASN:C	1:D:136:ASN:HD22	2.05	0.58
1:A:161:VAL:HG13	1:A:162:THR:H	1.69	0.58
1:A:318:ASN:ND2	1:A:321:GLU:HB2	2.17	0.58
1:C:283:ASN:ND2	1:C:344:ASN:HD21	2.00	0.58
1:D:62:LEU:HB2	1:D:271:THR:HG22	1.85	0.58
1:B:262:THR:HA	1:B:266:TYR:HB2	1.85	0.58
1:C:65:LYS:CB	1:C:70:PHE:HD2	2.16	0.58
1:C:98:THR:OG1	1:C:267:MET:CB	2.48	0.58
1:B:43:ILE:H	1:B:43:ILE:CD1	2.16	0.58
1:A:232:THR:O	1:A:233:ASN:HB3	2.04	0.58
1:A:323:LEU:HD22	1:A:338:LEU:HD11	1.86	0.58
1:B:120:ASP:OD1	1:B:121:VAL:N	2.37	0.58
1:D:130:MET:HE1	1:D:175:ILE:HB	1.81	0.58
1:A:241:ILE:CG2	1:A:252:VAL:HG23	2.34	0.57
1:C:69:VAL:HG23	1:C:69:VAL:O	2.03	0.57
1:B:90:THR:CG2	1:B:240:ALA:HB2	2.34	0.57
1:C:167:ARG:O	1:C:167:ARG:HG3	2.04	0.57
1:D:106:ILE:CD1	1:D:198:LEU:HD22	2.34	0.57
1:A:94:ILE:CD1	1:A:267:MET:HG2	2.34	0.57
1:B:131:ASN:O	1:B:179:GLU:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:THR:HG23	1:D:143:GLN:CG	2.32	0.57
1:A:130:MET:HG2	1:A:180:LEU:CD2	2.20	0.57
1:D:315:TRP:HZ3	1:D:337:ILE:CG2	2.18	0.57
1:A:90:THR:CG2	1:A:240:ALA:HB2	2.35	0.57
1:A:125:VAL:HG13	1:A:126:PRO:HD2	1.85	0.57
1:B:163:ASN:CG	1:B:164:LYS:H	2.08	0.57
1:B:145:LEU:HD22	1:B:313:SER:HB3	1.86	0.56
1:D:153:SER:HA	1:D:191:SER:HB2	1.87	0.56
1:D:234:ASN:OD1	1:D:234:ASN:C	2.43	0.56
1:D:289:LYS:O	1:D:293:GLN:HG3	2.05	0.56
1:D:171:VAL:CG1	1:D:260:TRP:CB	2.82	0.56
1:C:257:PHE:HB2	1:C:266:TYR:CZ	2.41	0.56
1:C:262:THR:HA	1:C:266:TYR:HB2	1.87	0.56
1:B:154:ASP:C	1:B:154:ASP:OD1	2.44	0.56
1:A:289:LYS:HZ2	1:A:289:LYS:CB	2.18	0.56
1:A:106:ILE:HD12	1:A:198:LEU:HD22	1.87	0.56
1:A:175:ILE:CD1	1:A:197:LEU:HD13	2.36	0.56
1:A:95:ALA:O	1:A:265:ALA:HA	2.06	0.56
1:A:281:GLN:HG2	1:A:339:LEU:CD1	2.36	0.56
1:A:136:ASN:ND2	1:A:136:ASN:C	2.59	0.56
1:A:233:ASN:HD21	1:A:254:LYS:CB	2.14	0.56
1:C:68:LYS:CD	1:C:69:VAL:H	2.18	0.56
1:D:94:ILE:HD11	1:D:267:MET:HG2	1.87	0.55
1:C:342:LYS:O	1:C:343:GLN:HB2	2.04	0.55
1:A:171:VAL:HB	1:A:260:TRP:CG	2.41	0.55
1:C:130:MET:HE1	1:C:175:ILE:CG2	2.37	0.55
1:A:257:PHE:HB2	1:A:266:TYR:OH	2.07	0.55
1:A:309:ASN:H	1:A:309:ASN:ND2	2.04	0.55
1:A:62:LEU:HB3	1:A:348:VAL:HB	1.89	0.55
1:A:262:THR:HA	1:A:266:TYR:HB2	1.87	0.55
1:B:162:THR:HG23	1:B:163:ASN:N	2.22	0.55
1:B:60:SER:CB	1:B:92:TYR:OH	2.54	0.55
1:D:285:PRO:HG2	1:D:288:TYR:HD2	1.72	0.55
1:C:69:VAL:HG22	1:C:69:VAL:O	2.05	0.55
1:D:206:THR:HG21	1:D:213:TYR:CB	2.34	0.54
1:C:155:ILE:HG13	1:C:157:SER:N	2.22	0.54
1:A:140:THR:HG23	1:A:143:GLN:CG	2.38	0.54
1:C:151:ILE:CD1	1:C:193:MET:CB	2.85	0.54
1:B:140:THR:HG23	1:B:143:GLN:CG	2.38	0.54
1:C:121:VAL:HG11	1:C:128:PHE:CE2	2.42	0.54
1:C:198:LEU:O	1:C:202:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:SER:O	1:A:313:SER:HB2	2.07	0.54
1:B:222:LEU:CD1	1:B:224:MET:HE3	2.37	0.54
1:D:137:GLU:CA	1:D:137:GLU:OE1	2.55	0.54
1:A:140:THR:HG23	1:A:143:GLN:HG3	1.89	0.54
1:A:37:ASN:N	1:A:70:PHE:O	2.36	0.54
1:B:78:GLN:NE2	1:B:90:THR:OG1	2.40	0.54
1:B:94:ILE:HG13	1:B:269:THR:CG2	2.37	0.54
1:C:262:THR:N	1:C:263:PRO:CD	2.71	0.54
1:D:220:LYS:N	1:D:221:PRO:CD	2.70	0.54
1:B:305:GLU:CD	1:B:306:PRO:HD2	2.28	0.53
1:B:56:ILE:HA	1:B:353:LEU:CD2	2.39	0.53
1:A:286:ASP:HA	1:A:289:LYS:CG	2.37	0.53
1:A:64:VAL:O	1:A:345:TYR:HA	2.09	0.53
1:B:40:GLN:O	1:B:41:GLN:NE2	2.41	0.53
1:B:94:ILE:CG2	1:B:97:ASN:HB2	2.27	0.53
1:C:203:GLN:HG3	1:C:209:SER:HA	1.90	0.53
1:B:97:ASN:HD22	1:B:335:SER:HB2	1.72	0.53
1:C:169:ASN:ND2	1:C:169:ASN:C	2.54	0.53
1:D:67:GLY:N	1:D:344:ASN:OD1	2.41	0.53
1:A:321:GLU:O	1:A:322:HIS:HB2	2.08	0.53
1:C:65:LYS:CG	1:C:369:ILE:CG2	2.82	0.53
1:B:318:ASN:HD22	1:B:319:ASN:N	2.03	0.53
1:A:289:LYS:O	1:A:293:GLN:HG3	2.09	0.53
1:B:222:LEU:O	1:B:223:HIS:HB2	2.09	0.53
1:B:222:LEU:HD13	1:B:224:MET:CE	2.38	0.53
1:C:334:SER:HB3	1:C:354:ASN:HA	1.91	0.53
1:C:65:LYS:CB	1:C:70:PHE:CD2	2.85	0.53
1:D:83:LYS:CD	1:D:83:LYS:O	2.52	0.53
1:A:65:LYS:HG2	1:A:70:PHE:CD1	2.44	0.53
1:B:164:LYS:O	1:B:164:LYS:CG	2.58	0.52
1:B:98:THR:OG1	1:B:267:MET:HB3	2.09	0.52
1:B:94:ILE:HD13	1:B:97:ASN:HB3	1.91	0.52
1:D:167:ARG:HB2	1:D:259:LEU:H	1.74	0.52
1:D:60:SER:HB3	1:D:271:THR:OG1	2.09	0.52
1:A:140:THR:HG23	1:A:143:GLN:CD	2.30	0.52
1:B:140:THR:HG23	1:B:143:GLN:HG3	1.90	0.52
1:D:144:LEU:HB2	1:D:198:LEU:HD21	1.92	0.52
1:A:42:GLN:O	1:A:45:LYS:HG2	2.10	0.52
1:C:101:PHE:CD2	1:C:267:MET:CE	2.93	0.52
1:C:297:LYS:O	1:C:297:LYS:CG	2.58	0.52
1:D:230:LYS:HE2	1:D:257:PHE:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ASN:C	1:B:169:ASN:HD22	2.12	0.52
1:D:62:LEU:HB3	1:D:348:VAL:HB	1.91	0.52
1:C:242:GLY:HA3	1:C:332:ASN:HB2	1.91	0.52
1:D:298:ASN:OD1	1:D:310:ALA:HB3	2.10	0.52
1:B:246:GLN:OE1	1:B:246:GLN:HA	2.09	0.52
1:C:106:ILE:HG12	1:C:202:ILE:HD11	1.92	0.52
1:C:64:VAL:HA	1:C:69:VAL:HA	1.91	0.52
1:D:109:LEU:HB2	1:D:115:LEU:HD21	1.91	0.52
1:A:149:SER:OG	1:A:151:ILE:HD12	2.09	0.52
1:B:309:ASN:H	1:B:309:ASN:ND2	2.05	0.52
1:B:237:LYS:HD3	1:B:237:LYS:N	2.22	0.52
1:C:61:ILE:HG13	1:C:349:VAL:HG22	1.91	0.51
1:D:218:TRP:C	1:D:221:PRO:HD2	2.31	0.51
1:B:47:ILE:O	1:B:51:LEU:HG	2.09	0.51
1:B:164:LYS:HG3	1:B:164:LYS:O	2.09	0.51
1:B:257:PHE:HD2	1:B:266:TYR:CE2	2.28	0.51
1:B:361:LEU:O	1:B:361:LEU:HD12	2.11	0.51
1:C:283:ASN:HD21	1:C:344:ASN:ND2	2.05	0.51
1:C:79:ASP:HB3	1:C:84:VAL:HG12	1.91	0.51
1:A:147:GLN:HE21	1:A:311:TYR:HE2	1.57	0.51
1:B:153:SER:HB2	1:B:190:TYR:O	2.10	0.51
1:B:39:SER:OG	1:B:40:GLN:N	2.42	0.51
1:C:139:ILE:HG21	1:C:144:LEU:CD2	2.40	0.51
1:A:58:GLY:CA	1:A:352:ASN:HD21	2.23	0.51
1:A:356:GLU:C	1:A:359:PRO:HD2	2.25	0.51
1:D:109:LEU:CB	1:D:115:LEU:CD2	2.89	0.51
1:D:230:LYS:HE2	1:D:257:PHE:CE1	2.46	0.51
1:A:160:ALA:O	1:A:161:VAL:HG23	2.10	0.51
1:B:68:LYS:CB	1:B:68:LYS:HZ2	2.07	0.51
1:C:131:ASN:CA	1:C:136:ASN:HA	2.40	0.51
1:C:218:TRP:C	1:C:221:PRO:HD2	2.31	0.51
1:A:71:LEU:HD11	1:A:73:LYS:CB	2.41	0.51
1:C:285:PRO:HG2	1:C:288:TYR:HD2	1.76	0.51
1:B:60:SER:HB2	1:B:92:TYR:OH	2.11	0.50
1:C:239:ASP:OD1	1:C:239:ASP:N	2.44	0.50
1:C:308:ALA:HB2	1:C:325:PHE:CZ	2.46	0.50
1:D:162:THR:CG2	1:D:163:ASN:N	2.74	0.50
1:A:196:ASP:HA	1:A:263:PRO:HG2	1.92	0.50
1:C:206:THR:HG22	1:C:208:GLN:HB3	1.93	0.50
1:C:68:LYS:HD3	1:C:69:VAL:HG13	1.94	0.50
1:D:342:LYS:O	1:D:343:GLN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:VAL:HB	1:A:359:PRO:HD3	1.93	0.50
1:A:78:GLN:HG2	1:A:84:VAL:HG13	1.94	0.50
1:B:202:ILE:O	1:B:206:THR:HB	2.12	0.50
1:B:206:THR:CG2	1:B:213:TYR:CD1	2.92	0.50
1:C:68:LYS:HD2	1:C:69:VAL:H	1.76	0.50
1:D:154:ASP:OD1	1:D:154:ASP:O	2.30	0.50
1:D:349:VAL:CG1	1:D:358:VAL:HG13	2.42	0.50
1:A:298:ASN:ND2	1:A:317:THR:HG21	2.26	0.50
1:B:209:SER:OG	1:B:212:LYS:HB2	2.11	0.50
1:D:315:TRP:HZ3	1:D:337:ILE:HG21	1.76	0.50
1:C:271:THR:HG23	1:C:350:LEU:HD12	1.94	0.50
1:B:227:THR:HG23	1:B:269:THR:HB	1.94	0.50
1:C:62:LEU:HB3	1:C:348:VAL:HB	1.94	0.50
1:D:344:ASN:OD1	1:D:344:ASN:O	2.30	0.50
1:A:94:ILE:HD11	1:A:267:MET:HG2	1.94	0.50
1:B:334:SER:HB2	1:B:358:VAL:HG21	1.94	0.50
1:C:138:THR:O	1:C:138:THR:HG22	2.12	0.50
1:D:162:THR:HG23	1:D:163:ASN:N	2.27	0.50
1:A:125:VAL:HG12	1:A:128:PHE:HB2	1.91	0.49
1:A:167:ARG:O	1:A:259:LEU:HB2	2.12	0.49
1:A:206:THR:HG22	1:A:208:GLN:CG	2.36	0.49
1:B:298:ASN:HD22	1:B:298:ASN:N	2.10	0.49
1:C:154:ASP:O	1:C:154:ASP:OD1	2.30	0.49
1:B:128:PHE:HD1	1:B:172:THR:HG23	1.76	0.49
1:B:307:ASN:O	1:B:307:ASN:ND2	2.30	0.49
1:C:95:ALA:HB2	1:C:330:LEU:HG	1.94	0.49
1:B:125:VAL:CG1	1:B:126:PRO:HD2	2.28	0.49
1:D:95:ALA:HB2	1:D:330:LEU:HG	1.94	0.49
1:C:267:MET:HG3	1:C:268:MET:N	2.27	0.49
1:B:97:ASN:ND2	1:B:335:SER:CB	2.75	0.49
1:D:130:MET:HE1	1:D:175:ILE:CG2	2.43	0.49
1:B:171:VAL:O	1:B:171:VAL:HG23	2.12	0.49
1:B:281:GLN:HG2	1:B:339:LEU:HD13	1.95	0.49
1:D:128:PHE:CZ	1:D:130:MET:HG3	2.47	0.49
1:D:194:ASN:O	1:D:198:LEU:HG	2.12	0.49
1:D:213:TYR:CD1	1:D:217:SER:HB2	2.48	0.49
1:C:149:SER:OG	1:C:194:ASN:ND2	2.42	0.49
1:D:359:PRO:O	1:D:362:VAL:HG22	2.12	0.49
1:B:226:HIS:HD2	1:B:273:ASP:OD1	1.95	0.48
1:C:139:ILE:CG2	1:C:144:LEU:CD2	2.91	0.48
1:C:155:ILE:HG13	1:C:157:SER:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:THR:CG2	1:B:178:ASP:OD2	2.61	0.48
1:B:55:HIS:CD2	1:B:248:SER:CB	2.96	0.48
1:C:131:ASN:CB	1:C:136:ASN:HA	2.43	0.48
1:A:203:GLN:HG3	1:A:209:SER:HA	1.94	0.48
1:B:235:LYS:HB3	1:B:239:ASP:HB3	1.95	0.48
1:B:43:ILE:N	1:B:43:ILE:CD1	2.74	0.48
1:B:342:LYS:O	1:B:343:GLN:CB	2.55	0.48
1:B:62:LEU:HB3	1:B:348:VAL:HB	1.95	0.48
1:B:69:VAL:HG23	1:B:69:VAL:O	2.12	0.48
1:D:149:SER:HB2	1:D:151:ILE:HG22	1.94	0.48
1:D:352:ASN:HD22	1:D:352:ASN:C	2.16	0.48
1:B:153:SER:CB	1:B:190:TYR:O	2.62	0.48
1:A:173:ARG:HD2	1:B:207:LYS:O	2.13	0.48
1:B:171:VAL:HB	1:B:260:TRP:CE3	2.49	0.48
1:A:196:ASP:HA	1:A:263:PRO:CG	2.43	0.48
1:B:287:LYS:HG3	1:B:288:TYR:CD2	2.49	0.48
1:B:94:ILE:HD13	1:B:97:ASN:CB	2.44	0.48
1:C:322:HIS:O	1:C:340:ASN:ND2	2.46	0.48
1:D:222:LEU:O	1:D:223:HIS:CB	2.60	0.48
1:B:48:GLU:O	1:B:52:GLN:HG3	2.13	0.48
1:D:262:THR:HG23	1:D:263:PRO:HD3	1.96	0.48
1:B:69:VAL:O	1:B:69:VAL:HG22	2.12	0.48
1:C:222:LEU:O	1:C:223:HIS:HB2	2.14	0.48
1:C:72:ASN:ND2	1:C:275:GLU:OE2	2.47	0.48
1:A:162:THR:HB	1:A:164:LYS:O	2.13	0.47
1:B:342:LYS:HD2	1:B:342:LYS:HA	1.67	0.47
1:C:274:LEU:O	1:C:275:GLU:C	2.53	0.47
1:A:232:THR:HG22	1:A:234:ASN:H	1.77	0.47
1:A:281:GLN:HG2	1:A:339:LEU:HD13	1.95	0.47
1:A:205:VAL:CG2	1:B:127:HIS:NE2	2.75	0.47
1:A:209:SER:H	1:B:164:LYS:NZ	2.12	0.47
1:D:109:LEU:HB2	1:D:115:LEU:CD2	2.44	0.47
1:A:359:PRO:O	1:A:362:VAL:HG22	2.14	0.47
1:D:202:ILE:CG2	1:D:213:TYR:CD2	2.96	0.47
1:A:311:TYR:CD1	1:A:315:TRP:O	2.67	0.47
1:B:301:SER:HA	1:B:310:ALA:HA	1.97	0.47
1:D:287:LYS:CE	1:D:288:TYR:CE2	2.96	0.47
1:B:125:VAL:CG1	1:B:128:PHE:H	2.27	0.47
1:D:56:ILE:HD11	1:D:355:SER:HB3	1.96	0.47
1:B:92:TYR:N	1:B:92:TYR:CD1	2.82	0.47
1:C:79:ASP:HB3	1:C:84:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:THR:N	1:D:263:PRO:HD2	2.29	0.47
1:A:127:HIS:O	1:B:207:LYS:CE	2.55	0.47
1:D:298:ASN:HA	1:D:312:ALA:HB2	1.96	0.47
1:B:94:ILE:HG22	1:B:95:ALA:N	2.29	0.47
1:D:63:ILE:HD11	1:D:365:LEU:HD22	1.96	0.47
1:A:287:LYS:HE2	1:A:287:LYS:HB2	1.64	0.47
1:D:115:LEU:CD1	1:D:141:ILE:HD13	2.45	0.47
1:C:42:GLN:HB2	1:C:45:LYS:HD3	1.97	0.46
1:A:169:ASN:O	1:A:171:VAL:N	2.47	0.46
1:B:134:GLY:HA3	1:C:344:ASN:HB2	1.96	0.46
1:B:262:THR:HG22	1:B:266:TYR:HB2	1.97	0.46
1:B:48:GLU:OE1	1:B:75:TYR:CD2	2.68	0.46
1:C:243:TYR:CE1	1:C:252:VAL:HG12	2.50	0.46
1:C:42:GLN:NE2	1:C:42:GLN:H	2.13	0.46
1:D:265:ALA:O	1:D:266:TYR:HB2	2.15	0.46
1:D:287:LYS:HE3	1:D:287:LYS:HB2	1.47	0.46
1:B:162:THR:HG23	1:B:163:ASN:HB3	1.95	0.46
1:D:267:MET:HE2	1:D:267:MET:HB2	1.83	0.46
1:D:72:ASN:ND2	1:D:275:GLU:OE2	2.48	0.46
1:B:125:VAL:CG1	1:B:126:PRO:N	2.79	0.46
1:C:65:LYS:CD	1:C:70:PHE:HE2	2.25	0.46
1:D:171:VAL:HG12	1:D:260:TRP:HB3	1.97	0.46
1:A:147:GLN:HG3	1:A:311:TYR:CD2	2.50	0.46
1:B:226:HIS:HB2	1:B:273:ASP:OD2	2.15	0.46
1:D:41:GLN:HA	1:D:41:GLN:NE2	2.29	0.46
1:D:96:SER:O	1:D:99:LYS:HG3	2.15	0.46
1:C:41:GLN:H	1:C:41:GLN:HE21	1.64	0.46
1:C:42:GLN:OE1	1:C:43:ILE:N	2.49	0.46
1:D:109:LEU:CB	1:D:115:LEU:HD23	2.44	0.46
1:D:315:TRP:CZ3	1:D:337:ILE:HG21	2.50	0.46
1:D:91:LYS:HG2	1:D:270:SER:HB3	1.97	0.46
1:D:62:LEU:CD1	1:D:69:VAL:HG12	2.46	0.46
1:A:336:PHE:CD1	1:A:362:VAL:HG11	2.51	0.46
1:C:146:ALA:HB1	1:C:300:SER:HB3	1.99	0.46
1:D:109:LEU:HB3	1:D:115:LEU:CD2	2.44	0.46
1:A:155:ILE:HG23	1:A:155:ILE:O	2.16	0.45
1:A:236:SER:OG	1:A:237:LYS:N	2.49	0.45
1:C:171:VAL:CG2	1:C:175:ILE:CG1	2.83	0.45
1:C:60:SER:HA	1:C:74:GLY:HA2	1.98	0.45
1:C:99:LYS:HE2	1:C:195:TYR:CB	2.46	0.45
1:A:120:ASP:HB3	1:A:138:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:GLN:HE21	1:D:231:GLN:HB3	1.62	0.45
1:A:166:ASN:O	1:A:260:TRP:CZ3	2.70	0.45
1:A:241:ILE:CG2	1:A:252:VAL:CG2	2.94	0.45
1:A:340:ASN:ND2	1:A:342:LYS:O	2.49	0.45
1:C:131:ASN:HB3	1:C:136:ASN:CA	2.46	0.45
1:C:68:LYS:CD	1:C:69:VAL:HG13	2.47	0.45
1:D:220:LYS:HB2	1:D:221:PRO:HD3	1.97	0.45
1:D:167:ARG:HD2	1:D:258:ASN:HA	1.97	0.45
1:B:309:ASN:ND2	1:B:317:THR:O	2.50	0.45
1:C:308:ALA:HB2	1:C:325:PHE:HZ	1.81	0.45
1:B:54:GLY:O	1:B:55:HIS:HB2	2.17	0.45
1:C:123:LYS:HB2	1:C:123:LYS:HE3	1.68	0.45
1:D:206:THR:CG2	1:D:208:GLN:CG	2.89	0.45
1:B:56:ILE:HA	1:B:353:LEU:HD23	1.98	0.45
1:D:45:LYS:HB2	1:D:45:LYS:HE3	1.69	0.45
1:B:215:THR:HA	1:B:219:LEU:HB2	1.98	0.45
1:B:194:ASN:O	1:B:198:LEU:HG	2.18	0.44
1:C:168:LEU:HD13	1:C:168:LEU:HA	1.63	0.44
1:B:98:THR:O	1:B:98:THR:HG22	2.17	0.44
1:B:356:GLU:C	1:B:359:PRO:HD2	2.34	0.44
1:C:213:TYR:CE1	1:C:217:SER:OG	2.69	0.44
1:D:130:MET:HE1	1:D:175:ILE:CB	2.47	0.44
1:D:337:ILE:HD12	1:D:348:VAL:HG13	1.99	0.44
1:A:175:ILE:HD12	1:A:197:LEU:HD13	1.99	0.44
1:A:50:ASP:OD2	1:A:364:HIS:HD2	2.00	0.44
1:B:125:VAL:CG1	1:B:126:PRO:CD	2.90	0.44
1:C:57:PRO:HB2	1:C:352:ASN:OD1	2.18	0.44
1:D:137:GLU:OE1	1:D:138:THR:N	2.50	0.44
1:A:258:ASN:HD22	1:A:258:ASN:N	2.14	0.44
1:C:99:LYS:HE2	1:C:195:TYR:CG	2.53	0.44
1:A:325:PHE:HB3	1:A:338:LEU:HD12	1.99	0.44
1:A:44:ASP:O	1:A:48:GLU:HB2	2.18	0.44
1:C:42:GLN:C	1:C:42:GLN:CD	2.76	0.44
1:D:283:ASN:ND2	1:D:344:ASN:HD21	2.16	0.44
1:A:204:ASN:OD1	1:B:126:PRO:HB3	2.17	0.44
1:D:80:VAL:HG12	1:D:81:ASP:N	2.33	0.44
1:C:175:ILE:HG12	1:C:193:MET:HE3	2.00	0.44
1:C:302:THR:HG22	1:C:302:THR:O	2.18	0.43
1:D:166:ASN:HA	1:D:166:ASN:HD22	1.63	0.43
1:A:241:ILE:HG21	1:A:252:VAL:HG23	1.99	0.43
1:B:274:LEU:O	1:B:278:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:PHE:HB3	1:C:338:LEU:HD12	1.99	0.43
1:A:131:ASN:HB3	1:A:136:ASN:CA	2.48	0.43
1:A:222:LEU:O	1:A:223:HIS:CB	2.65	0.43
1:D:233:ASN:O	1:D:233:ASN:CG	2.56	0.43
1:A:281:GLN:HG2	1:A:339:LEU:HD11	2.00	0.43
1:B:57:PRO:HD3	1:B:353:LEU:HD22	2.00	0.43
1:C:305:GLU:HG3	1:C:306:PRO:CD	2.41	0.43
1:C:167:ARG:HB3	3:C:402:HOH:O	2.18	0.43
1:C:236:SER:O	1:C:237:LYS:HB2	2.18	0.43
1:D:192:ASN:O	1:D:264:SER:OG	2.37	0.43
1:D:283:ASN:HD21	1:D:344:ASN:HD21	1.66	0.43
1:B:125:VAL:HG13	1:B:126:PRO:N	2.33	0.43
1:B:214:ILE:HG22	1:B:219:LEU:HG	2.00	0.43
1:B:318:ASN:ND2	1:B:320:ASP:N	2.66	0.43
1:B:358:VAL:HB	1:B:359:PRO:HD3	2.01	0.43
1:C:130:MET:CE	1:C:175:ILE:HG22	2.47	0.43
1:D:234:ASN:OD1	1:D:235:LYS:N	2.52	0.43
1:C:298:ASN:OD1	1:C:310:ALA:HB3	2.18	0.43
1:D:206:THR:HG22	1:D:208:GLN:CG	2.38	0.43
1:D:262:THR:N	1:D:263:PRO:CD	2.81	0.43
1:A:196:ASP:OD1	1:A:263:PRO:HG2	2.18	0.43
1:A:336:PHE:CE1	1:A:362:VAL:HG21	2.53	0.43
1:A:261:ASP:C	1:A:263:PRO:HD2	2.40	0.43
1:A:286:ASP:OD2	1:A:286:ASP:N	2.32	0.43
1:B:169:ASN:O	1:B:169:ASN:ND2	2.30	0.43
1:C:130:MET:HE3	1:C:175:ILE:O	2.18	0.43
1:D:106:ILE:HD12	1:D:198:LEU:HD22	1.99	0.43
1:D:115:LEU:HD12	1:D:141:ILE:CD1	2.49	0.43
1:A:58:GLY:N	1:A:352:ASN:HD21	2.17	0.43
1:A:68:LYS:HD2	1:A:68:LYS:HA	1.85	0.43
1:B:144:LEU:HB2	1:B:198:LEU:HD21	2.01	0.43
1:B:233:ASN:ND2	1:B:233:ASN:C	2.70	0.43
1:A:342:LYS:O	1:A:343:GLN:HB2	2.19	0.42
1:A:71:LEU:HD11	1:A:73:LYS:HB3	2.00	0.42
1:B:309:ASN:ND2	1:B:318:ASN:HA	2.34	0.42
1:C:121:VAL:CG1	1:C:122:SER:N	2.80	0.42
1:C:252:VAL:HG23	1:C:252:VAL:O	2.19	0.42
1:A:262:THR:N	1:A:263:PRO:CD	2.81	0.42
1:B:71:LEU:HD11	1:B:73:LYS:HB2	2.00	0.42
1:C:131:ASN:OD1	1:C:131:ASN:N	2.52	0.42
1:D:153:SER:HA	1:D:191:SER:CB	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:MET:HE2	1:A:267:MET:HB2	1.55	0.42
1:A:71:LEU:HD11	1:A:73:LYS:HB2	2.00	0.42
1:B:62:LEU:HB2	1:B:271:THR:CG2	2.45	0.42
1:B:77:TYR:HB2	1:B:80:VAL:HG12	2.01	0.42
1:A:257:PHE:HB2	1:A:266:TYR:CZ	2.55	0.42
1:B:220:LYS:HB2	1:B:221:PRO:CD	2.47	0.42
1:B:254:LYS:HG3	1:B:254:LYS:O	2.19	0.42
1:D:164:LYS:HA	1:D:164:LYS:HD3	1.74	0.42
1:D:230:LYS:HB3	1:D:266:TYR:HB3	2.01	0.42
1:D:227:THR:HG23	1:D:269:THR:HB	2.02	0.42
1:A:156:THR:HG21	1:A:178:ASP:OD2	2.19	0.42
1:B:219:LEU:O	1:B:224:MET:N	2.51	0.42
1:C:166:ASN:O	1:C:167:ARG:HB3	2.20	0.42
1:D:78:GLN:HG3	1:D:240:ALA:HA	2.00	0.42
1:A:149:SER:OG	1:A:194:ASN:ND2	2.50	0.42
1:B:196:ASP:HA	1:B:263:PRO:HG2	2.01	0.42
1:B:92:TYR:HB3	1:B:333:PHE:CD2	2.53	0.42
1:C:106:ILE:HD13	1:C:202:ILE:HD13	2.01	0.42
1:C:109:LEU:CB	1:C:115:LEU:HD21	2.49	0.42
1:D:169:ASN:HB2	3:D:504:HOH:O	2.20	0.42
1:B:94:ILE:HG23	1:B:97:ASN:CB	2.29	0.42
1:D:53:LYS:HD3	1:D:357:TYR:CE1	2.55	0.42
1:B:281:GLN:HG2	1:B:339:LEU:CD1	2.50	0.42
1:B:56:ILE:HA	1:B:353:LEU:HD22	2.02	0.42
1:B:95:ALA:HB2	1:B:330:LEU:HD12	2.02	0.42
1:C:109:LEU:HB2	1:C:115:LEU:HD21	2.02	0.42
1:D:124:HIS:ND1	1:D:205:VAL:CG2	2.83	0.42
1:D:121:VAL:HG23	1:D:139:ILE:O	2.19	0.42
1:C:192:ASN:HD22	1:C:192:ASN:HA	1.72	0.42
1:C:196:ASP:OD1	1:C:264:SER:OG	2.38	0.42
1:A:58:GLY:O	1:A:352:ASN:ND2	2.53	0.41
1:B:219:LEU:HD13	1:B:227:THR:HB	2.02	0.41
1:D:133:ASN:HB3	1:D:134:GLY:H	1.55	0.41
1:D:299:LEU:HD12	1:D:313:SER:H	1.85	0.41
1:A:64:VAL:O	1:A:346:GLY:N	2.45	0.41
1:B:47:ILE:HG21	1:B:75:TYR:CE1	2.55	0.41
1:D:131:ASN:O	1:D:179:GLU:HG3	2.20	0.41
1:A:285:PRO:HG2	1:A:288:TYR:CD2	2.44	0.41
1:A:289:LYS:HZ2	1:A:289:LYS:HB2	1.86	0.41
1:A:133:ASN:HD22	1:A:133:ASN:HA	1.56	0.41
1:A:154:ASP:OD1	1:A:154:ASP:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ILE:HG13	1:A:303:ILE:O	2.21	0.41
1:A:87:SER:HB2	1:A:88:PRO:CD	2.51	0.41
1:B:151:ILE:HA	1:B:152:PRO:HD3	1.77	0.41
1:B:163:ASN:OD1	1:B:164:LYS:N	2.36	0.41
1:B:235:LYS:CB	1:B:239:ASP:HB2	2.31	0.41
1:A:131:ASN:HA	1:A:136:ASN:HA	2.03	0.41
1:A:368:GLN:C	1:A:369:ILE:HG13	2.41	0.41
1:B:287:LYS:HE3	1:D:112:GLU:OE2	2.20	0.41
1:C:223:HIS:O	1:C:225:THR:HG22	2.20	0.41
1:C:44:ASP:OD2	1:C:73:LYS:HE2	2.20	0.41
1:A:166:ASN:ND2	1:A:170:ASP:O	2.53	0.41
1:A:121:VAL:HG21	1:A:144:LEU:HD11	2.03	0.41
1:B:47:ILE:HD11	1:B:365:LEU:HD21	2.02	0.41
1:C:206:THR:HG22	1:C:208:GLN:CB	2.50	0.41
1:D:298:ASN:H	1:D:298:ASN:ND2	2.18	0.41
1:B:78:GLN:HB3	1:B:86:ALA:HA	2.03	0.41
1:A:94:ILE:HD11	1:A:267:MET:CG	2.51	0.41
1:C:53:LYS:HB3	1:C:357:TYR:CE2	2.56	0.41
1:A:170:ASP:N	1:A:170:ASP:OD1	2.52	0.41
1:B:188:PHE:C	1:B:188:PHE:CD1	2.94	0.41
1:B:296:HIS:CD2	1:B:324:VAL:HG11	2.56	0.41
1:B:42:GLN:CD	1:B:42:GLN:H	2.24	0.41
1:C:130:MET:CE	1:C:175:ILE:O	2.69	0.41
1:D:235:LYS:HD3	1:D:240:ALA:O	2.21	0.41
1:D:342:LYS:O	1:D:343:GLN:CB	2.68	0.41
1:B:318:ASN:HB3	1:B:323:LEU:HD13	2.02	0.40
1:D:151:ILE:HA	1:D:152:PRO:HD3	1.87	0.40
1:D:253:SER:HB3	1:D:332:ASN:HB3	2.03	0.40
1:A:142:LYS:HE3	1:A:142:LYS:HB2	1.93	0.40
1:B:318:ASN:ND2	1:B:318:ASN:O	2.49	0.40
1:B:326:HIS:HD2	1:B:327:SER:O	2.04	0.40
1:B:60:SER:HB2	1:B:92:TYR:CE1	2.57	0.40
1:C:287:LYS:HB2	1:C:287:LYS:HE2	1.75	0.40
1:D:241:ILE:HG22	1:D:252:VAL:HG22	1.98	0.40
1:A:108:LYS:NZ	1:A:112:GLU:OE2	2.55	0.40
1:A:342:LYS:O	1:A:343:GLN:CB	2.70	0.40
1:A:205:VAL:CA	1:B:127:HIS:CD2	2.99	0.40
1:B:235:LYS:HE3	1:B:235:LYS:HB3	1.85	0.40
1:B:289:LYS:HB2	1:B:289:LYS:HE3	1.63	0.40
1:B:60:SER:C	1:B:61:ILE:HD12	2.41	0.40
1:C:126:PRO:HG2	1:C:127:HIS:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:MET:HG2	1:C:273:ASP:HB3	2.04	0.40
1:D:198:LEU:O	1:D:202:ILE:HG13	2.20	0.40
1:A:34:ARG:CD	1:A:34:ARG:N	2.85	0.40
1:C:42:GLN:C	1:C:42:GLN:OE1	2.60	0.40
1:D:94:ILE:HG12	1:D:267:MET:HG2	2.02	0.40
1:A:171:VAL:HG23	1:A:174:ALA:HB3	2.02	0.40
1:A:173:ARG:HG2	1:B:207:LYS:O	2.21	0.40
1:D:215:THR:O	1:D:220:LYS:CG	2.70	0.40
1:D:57:PRO:HD2	1:D:352:ASN:ND2	2.37	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	334/342 (98%)	320 (96%)	12 (4%)	2 (1%)	25	64
1	B	334/342 (98%)	321 (96%)	12 (4%)	1 (0%)	41	74
1	C	325/342 (95%)	315 (97%)	10 (3%)	0	100	100
1	D	329/342 (96%)	320 (97%)	9 (3%)	0	100	100
All	All	1322/1368 (97%)	1276 (96%)	43 (3%)	3 (0%)	47	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ILE
1	B	66	ASN
1	A	169	ASN

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	301/309 (97%)	253 (84%)	48 (16%)	2	12
1	B	297/309 (96%)	246 (83%)	51 (17%)	2	10
1	C	294/309 (95%)	247 (84%)	47 (16%)	2	11
1	D	295/309 (96%)	253 (86%)	42 (14%)	3	15
All	All	1187/1236 (96%)	999 (84%)	188 (16%)	2	12

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	41	GLN
1	A	42	GLN
1	A	44	ASP
1	A	48	GLU
1	A	51	LEU
1	A	66	ASN
1	A	69	VAL
1	A	70	PHE
1	A	82	LYS
1	A	129	LYS
1	A	131	ASN
1	A	133	ASN
1	A	136	ASN
1	A	140	THR
1	A	153	SER
1	A	154	ASP
1	A	155	ILE
1	A	156	THR
1	A	158	GLU
1	A	161	VAL
1	A	162	THR
1	A	164	LYS
1	A	169	ASN

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Mol	Chain	Res	Type
1	A	171	VAL
1	A	176	MET
1	A	178	ASP
1	A	187	GLU
1	A	234	ASN
1	A	235	LYS
1	A	236	SER
1	A	237	LYS
1	A	238	HIS
1	A	245	LEU
1	A	252	VAL
1	A	264	SER
1	A	267	MET
1	A	286	ASP
1	A	287	LYS
1	A	289	LYS
1	A	298	ASN
1	A	309	ASN
1	A	317	THR
1	A	321	GLU
1	A	331	ASP
1	A	340	ASN
1	A	343	GLN
1	A	344	ASN
1	B	34	ARG
1	B	35	LEU
1	B	45	LYS
1	B	48	GLU
1	B	50	ASP
1	B	60	SER
1	B	68	LYS
1	B	69	VAL
1	B	73	LYS
1	B	82	LYS
1	B	91	LYS
1	B	92	TYR
1	B	94	ILE
1	B	96	SER
1	B	99	LYS
1	B	122	SER
1	B	125	VAL
1	B	135	GLN

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Mol	Chain	Res	Type
1	B	136	ASN
1	B	138	THR
1	B	140	THR
1	B	154	ASP
1	B	162	THR
1	B	165	ASN
1	B	167	ARG
1	B	169	ASN
1	B	171	VAL
1	B	173	ARG
1	B	225	THR
1	B	231	GLN
1	B	233	ASN
1	B	234	ASN
1	B	235	LYS
1	B	237	LYS
1	B	245	LEU
1	B	254	LYS
1	B	260	TRP
1	B	267	MET
1	B	271	THR
1	B	286	ASP
1	B	298	ASN
1	B	302	THR
1	B	307	ASN
1	B	309	ASN
1	B	313	SER
1	B	318	ASN
1	B	321	GLU
1	B	323	LEU
1	B	340	ASN
1	B	342	LYS
1	B	343	GLN
1	C	34	ARG
1	C	39	SER
1	C	41	GLN
1	C	42	GLN
1	C	43	ILE
1	C	65	LYS
1	C	66	ASN
1	C	69	VAL
1	C	85	LYS

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Mol	Chain	Res	Type
1	C	94	ILE
1	C	108	LYS
1	C	115	LEU
1	C	121	VAL
1	C	136	ASN
1	C	137	GLU
1	C	138	THR
1	C	151	ILE
1	C	155	ILE
1	C	157	SER
1	C	167	ARG
1	C	168	LEU
1	C	169	ASN
1	C	170	ASP
1	C	171	VAL
1	C	173	ARG
1	C	178	ASP
1	C	182	HIS
1	C	200	LEU
1	C	225	THR
1	C	231	GLN
1	C	232	THR
1	C	239	ASP
1	C	254	LYS
1	C	267	MET
1	C	286	ASP
1	C	287	LYS
1	C	290	SER
1	C	297	LYS
1	C	298	ASN
1	C	302	THR
1	C	305	GLU
1	C	318	ASN
1	C	331	ASP
1	C	340	ASN
1	C	343	GLN
1	C	344	ASN
1	C	352	ASN
1	D	34	ARG
1	D	36	THR
1	D	39	SER
1	D	41	GLN

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Mol	Chain	Res	Type
1	D	44	ASP
1	D	68	LYS
1	D	69	VAL
1	D	115	LEU
1	D	116	ASN
1	D	131	ASN
1	D	135	GLN
1	D	136	ASN
1	D	137	GLU
1	D	140	THR
1	D	151	ILE
1	D	163	ASN
1	D	167	ARG
1	D	170	ASP
1	D	171	VAL
1	D	172	THR
1	D	175	ILE
1	D	178	ASP
1	D	200	LEU
1	D	206	THR
1	D	207	LYS
1	D	211	THR
1	D	220	LYS
1	D	225	THR
1	D	228	SER
1	D	232	THR
1	D	237	LYS
1	D	252	VAL
1	D	260	TRP
1	D	267	MET
1	D	271	THR
1	D	287	LYS
1	D	295	SER
1	D	337	ILE
1	D	340	ASN
1	D	342	LYS
1	D	343	GLN
1	D	352	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	66	ASN
1	A	97	ASN
1	A	124	HIS
1	A	133	ASN
1	A	136	ASN
1	A	192	ASN
1	A	194	ASN
1	A	204	ASN
1	A	208	GLN
1	A	216	ASN
1	A	226	HIS
1	A	258	ASN
1	A	283	ASN
1	A	294	GLN
1	A	298	ASN
1	A	309	ASN
1	A	319	ASN
1	A	322	HIS
1	A	340	ASN
1	A	352	ASN
1	A	354	ASN
1	A	364	HIS
1	A	366	ASN
1	A	368	GLN
1	B	78	GLN
1	B	97	ASN
1	B	127	HIS
1	B	165	ASN
1	B	166	ASN
1	B	192	ASN
1	B	194	ASN
1	B	204	ASN
1	B	226	HIS
1	B	231	GLN
1	B	234	ASN
1	B	238	HIS
1	B	294	GLN
1	B	298	ASN
1	B	309	ASN
1	B	318	ASN
1	B	319	ASN
1	B	326	HIS

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Mol	Chain	Res	Type
1	B	332	ASN
1	B	340	ASN
1	B	344	ASN
1	B	354	ASN
1	B	366	ASN
1	B	368	GLN
1	C	41	GLN
1	C	78	GLN
1	C	97	ASN
1	C	111	GLN
1	C	166	ASN
1	C	169	ASN
1	C	182	HIS
1	C	192	ASN
1	C	194	ASN
1	C	204	ASN
1	C	231	GLN
1	C	233	ASN
1	C	258	ASN
1	C	283	ASN
1	C	293	GLN
1	C	296	HIS
1	C	309	ASN
1	C	318	ASN
1	C	326	HIS
1	C	340	ASN
1	C	366	ASN
1	C	368	GLN
1	D	97	ASN
1	D	116	ASN
1	D	163	ASN
1	D	166	ASN
1	D	169	ASN
1	D	204	ASN
1	D	208	GLN
1	D	223	HIS
1	D	231	GLN
1	D	246	GLN
1	D	258	ASN
1	D	283	ASN
1	D	307	ASN
1	D	319	ASN

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Mol	Chain	Res	Type
1	D	322	HIS
1	D	340	ASN
1	D	352	ASN
1	D	366	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	PE4	D	401	-	23,23,23	0.66	0	22,22,22	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PE4	D	401	-	-	13/21/21/21	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

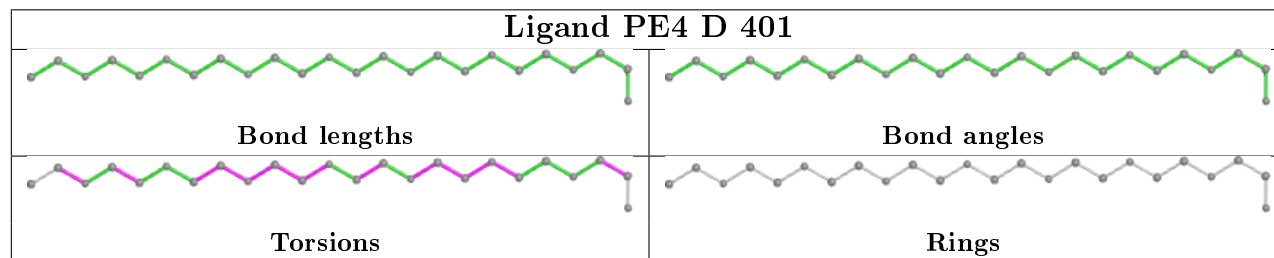
All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	PE4	O7-C13-C14-O8
2	D	401	PE4	O1-C1-C2-O2
2	D	401	PE4	O6-C10-C9-O5
2	D	401	PE4	O3-C5-C6-O4
2	D	401	PE4	O4-C7-C8-O5
2	D	401	PE4	C5-C6-O4-C7
2	D	401	PE4	C3-C4-O3-C5
2	D	401	PE4	O6-C11-C12-O7
2	D	401	PE4	C12-C11-O6-C10
2	D	401	PE4	C10-C9-O5-C8
2	D	401	PE4	C9-C10-O6-C11
2	D	401	PE4	C6-C5-O3-C4
2	D	401	PE4	C16-C15-O8-C14

There are no ring outliers.

No monomer is involved in short contacts.

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 than 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.



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	336/342 (98%)	0.39	13 (3%) 39 25	29, 47, 79, 98	0
1	B	336/342 (98%)	0.57	8 (2%) 59 44	31, 55, 86, 100	0
1	C	329/342 (96%)	0.83	34 (10%) 6 4	37, 60, 99, 116	0
1	D	333/342 (97%)	0.60	25 (7%) 14 8	36, 54, 93, 104	0
All	All	1334/1368 (97%)	0.59	80 (5%) 21 12	29, 53, 91, 116	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	THR	7.7
1	D	163	ASN	6.1
1	D	159	ASP	5.9
1	B	163	ASN	5.3
1	C	166	ASN	5.0
1	A	160	ALA	4.8
1	C	33	THR	4.3
1	D	39	SER	4.1
1	D	178	ASP	3.9
1	A	163	ASN	3.8
1	A	157	SER	3.7
1	C	126	PRO	3.7
1	D	232	THR	3.6
1	B	159	ASP	3.6
1	C	36	THR	3.6
1	C	35	LEU	3.5
1	D	182	HIS	3.5
1	A	162	THR	3.5
1	D	134	GLY	3.5
1	D	135	GLN	3.5
1	A	166	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	39	SER	3.5
1	C	85	LYS	3.5
1	B	156	THR	3.4
1	C	157	SER	3.4
1	A	159	ASP	3.4
1	C	169	ASN	3.2
1	C	193	MET	3.1
1	D	183	LYS	3.0
1	A	161	VAL	3.0
1	D	162	THR	3.0
1	A	156	THR	3.0
1	D	165	ASN	3.0
1	D	38	ASP	2.9
1	D	186	GLU	2.9
1	C	77	TYR	2.9
1	C	155	ILE	2.8
1	C	180	LEU	2.8
1	C	250	PRO	2.8
1	C	135	GLN	2.7
1	B	157	SER	2.7
1	A	38	ASP	2.7
1	B	233	ASN	2.7
1	C	168	LEU	2.6
1	B	158	GLU	2.6
1	D	177	GLY	2.5
1	C	128	PHE	2.5
1	C	191	SER	2.5
1	D	127	HIS	2.5
1	D	120	ASP	2.4
1	B	39	SER	2.4
1	C	259	LEU	2.4
1	D	179	GLU	2.3
1	D	160	ALA	2.3
1	C	230	LYS	2.3
1	D	126	PRO	2.3
1	C	134	GLY	2.3
1	C	39	SER	2.3
1	C	130	MET	2.3
1	D	181	HIS	2.3
1	C	40	GLN	2.2
1	C	137	GLU	2.2
1	C	172	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	127	HIS	2.2
1	A	164	LYS	2.2
1	C	132	TYR	2.1
1	C	183	LYS	2.1
1	D	152	PRO	2.1
1	C	181	HIS	2.1
1	C	83	LYS	2.1
1	D	241	ILE	2.1
1	D	180	LEU	2.1
1	C	78	GLN	2.1
1	D	161	VAL	2.1
1	A	158	GLU	2.1
1	A	232	THR	2.0
1	D	194	ASN	2.0
1	C	231	GLN	2.0
1	C	167	ARG	2.0
1	C	70	PHE	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](#)

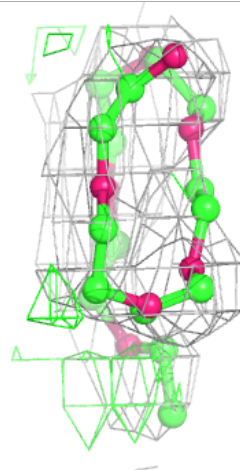
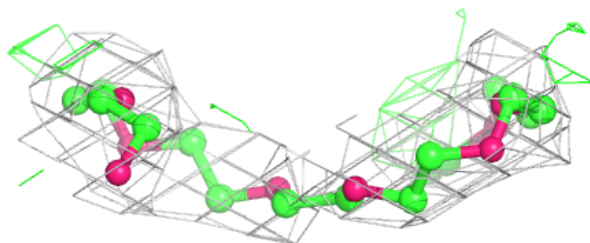
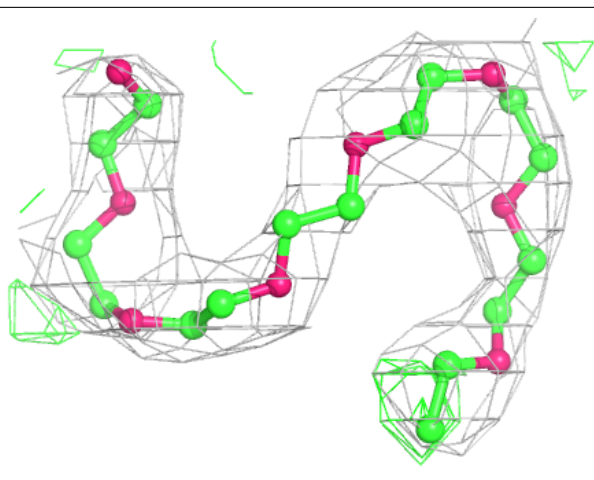
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PE4	D	401	24/24	0.76	0.29	94,98,99,99	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 PE4 D 401:

$2mF_o-DF_c$ (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.