



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:53 AM UTC

PDB ID : 8H1R / pdb_00008h1r
Title : Crystal structure of LptDE-YifL complex
Authors : Luo, Q.; Huang, Y.
Deposited on : 2022-10-03
Resolution : 2.98 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

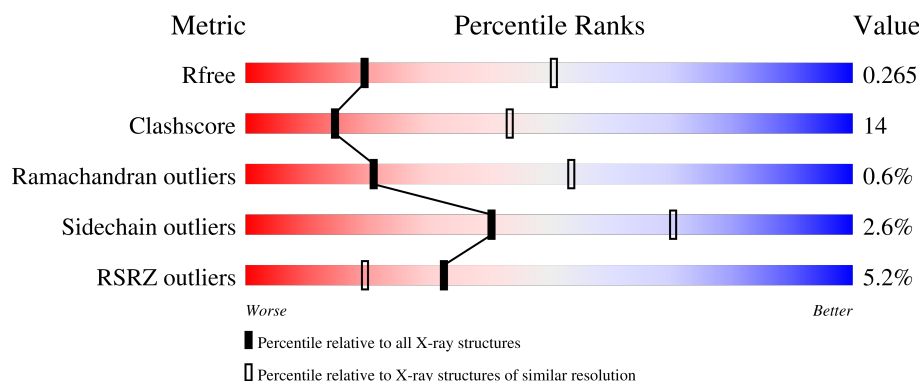
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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 $\leq 5\%$. 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	924	5% 56% 23% • 20%
1	D	924	5% 58% 26% • 15%
2	B	207	% 65% 17% • 17%
2	E	207	% 62% 21% • 17%
3	C	67	% 13% • 82%

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Mol	Chain	Length	Quality of chain
3	F	67	3% 13% 82%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PCJ	A	1001	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15559 atoms, of which 210 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 LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	736	Total	C	N	O	S	0	0	0
			5976	3778	1035	1148	15			
1	D	789	Total	C	N	O	S	0	0	0
			6387	4041	1106	1223	17			

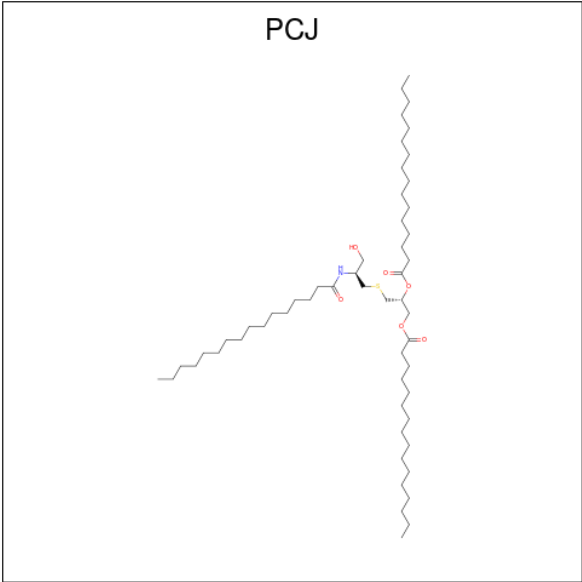
- Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1341	818	247	272	4			
2	E	172	Total	C	N	O	S	0	0	0
			1341	818	247	272	4			

- Molecule 3 is a protein called Uncharacterized lipoprotein YifL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	0	0	0
			90	62	13	15			
3	F	12	Total	C	N	O	0	0	0
			90	62	13	15			

- Molecule 4 is (2R)-3-{[(2S)-3-HYDROXY-2-(PALMITOYLAMINO)PROPYL]THIO}PROPANE-1,2-DIYL DIHEXADECANOATE (CCD ID: PCJ) (formula: C₅₄H₁₀₅NO₆S) (labeled as "Ligand of Interest" by depositor).

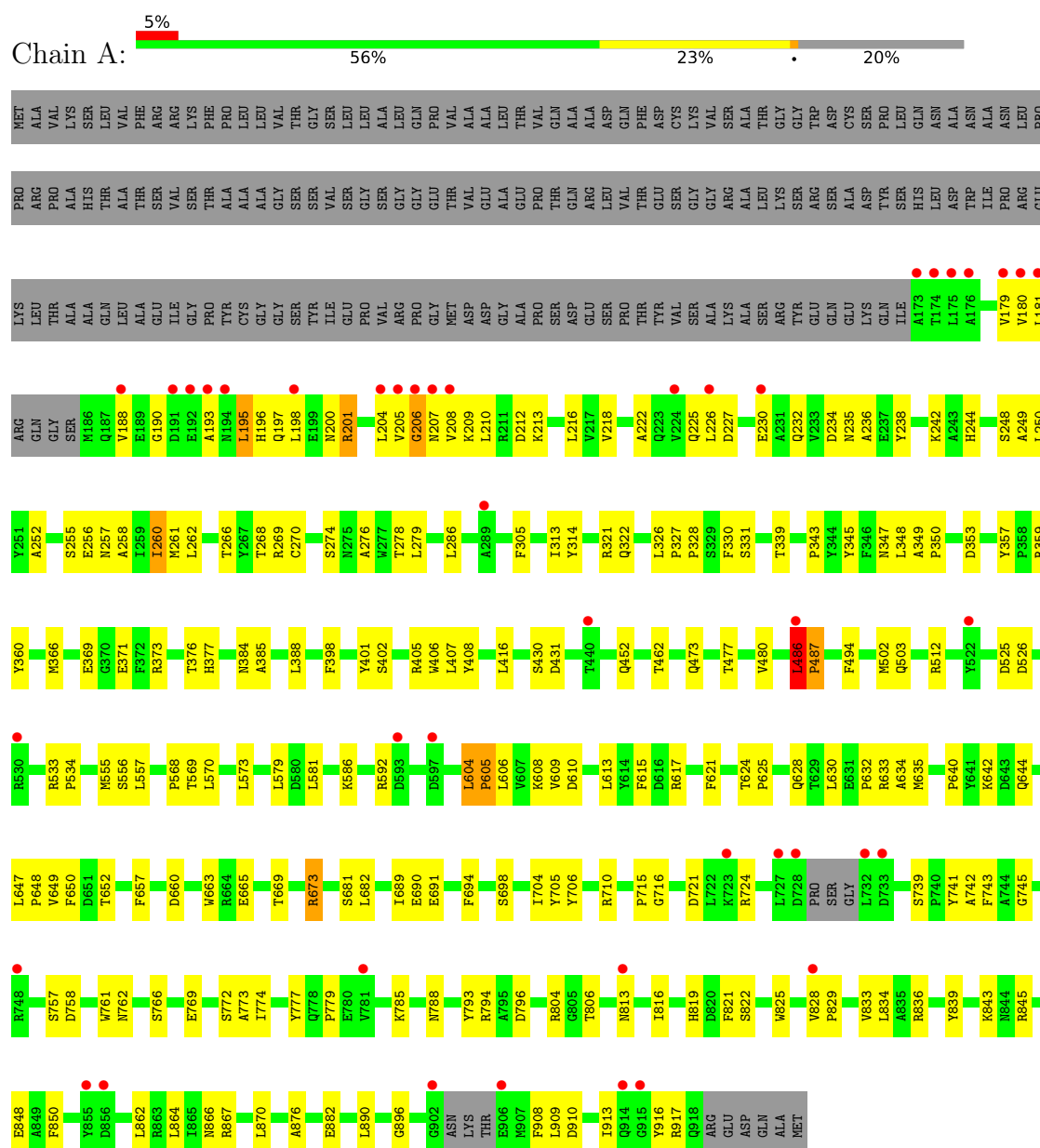


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	0	0
			167	54	105	1	6	1		
4	D	1	Total	C	H	N	O	S	0	0
			167	54	105	1	6	1		

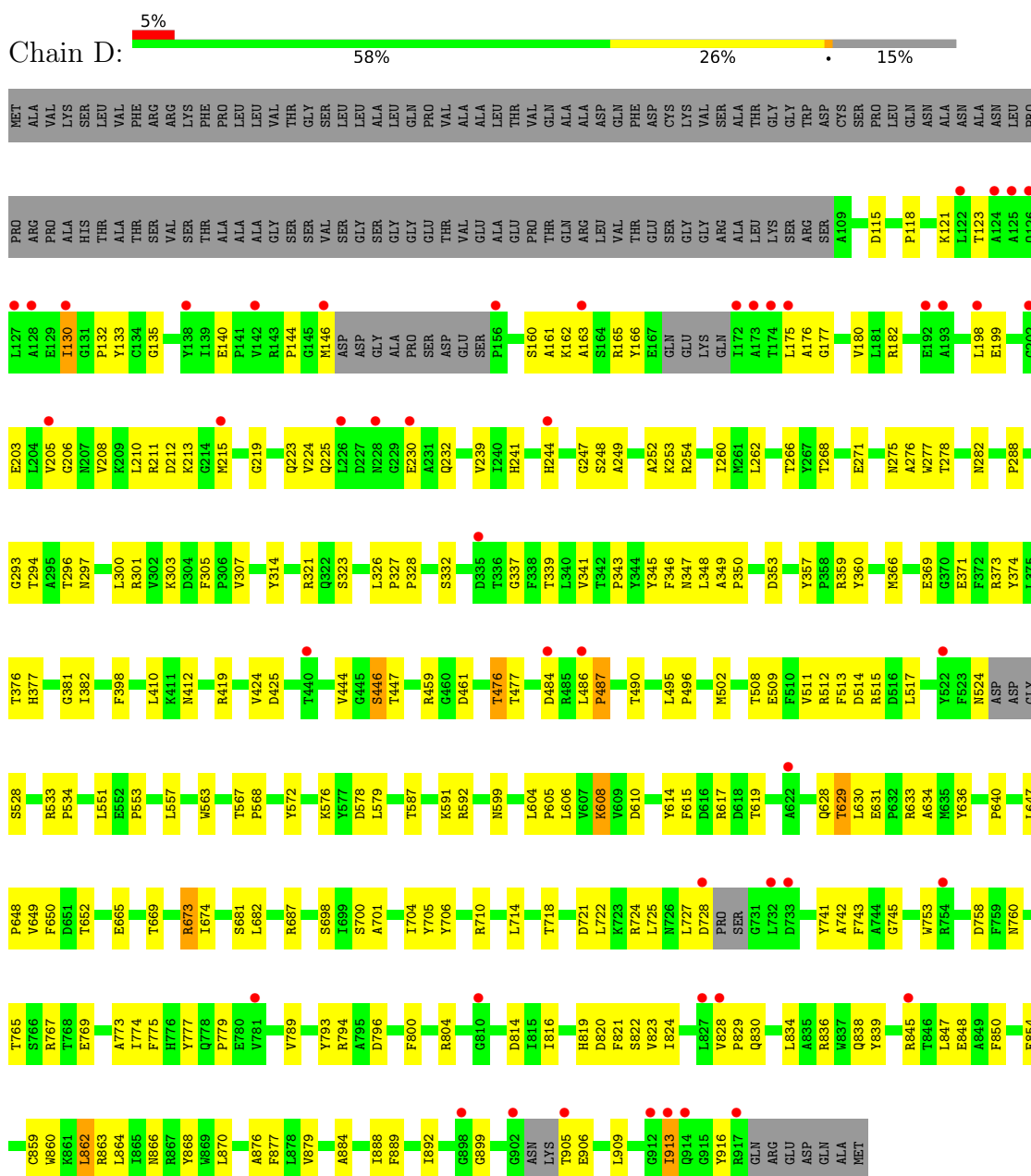
3 Residue-property plots [i](#)

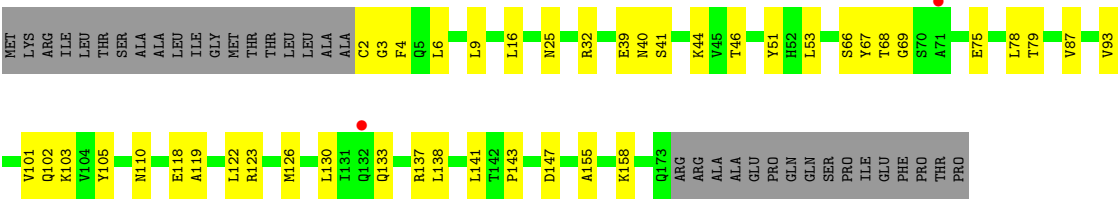
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: LPS-assembly protein LptD

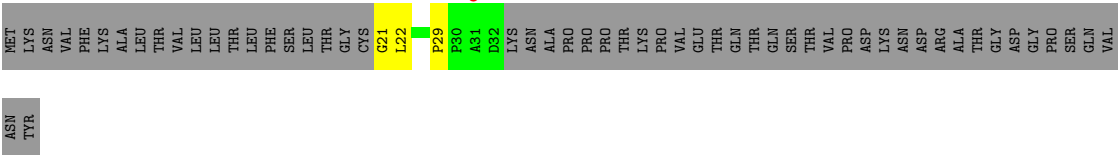


• Molecule 1: LPS-assembly protein LptD

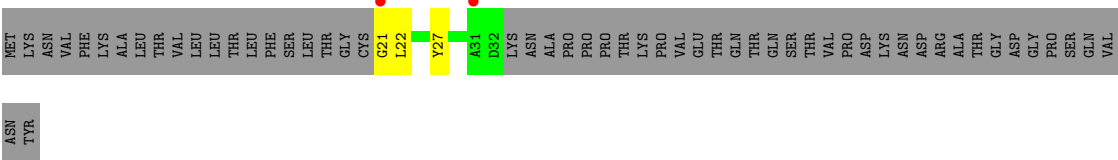




● Molecule 3: Uncharacterized lipoprotein YifL



● Molecule 3: Uncharacterized lipoprotein YifL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.85Å 140.47Å 133.18Å 90.00° 104.39° 90.00°	Depositor
Resolution (Å)	43.25 – 2.98 43.25 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.25-2.98) 97.2 (43.25-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.234 , 0.264 0.237 , 0.265	Depositor DCC
R_{free} test set	3322 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	72.3	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15559	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3420e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PCJ

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	0.48	0/6127	0.70	2/8307 (0.0%)
1	D	0.46	0/6549	0.65	0/8878
2	B	0.45	0/1353	0.69	0/1826
2	E	0.44	0/1353	0.62	0/1826
3	C	0.64	0/94	0.67	0/128
3	F	0.56	0/94	0.69	0/128
All	All	0.47	0/15570	0.67	2/21093 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	LEU	CA-C-N	-6.59	111.61	119.84
1	A	486	LEU	C-N-CA	-6.59	111.61	119.84

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	5976	0	5674	179	0
1	D	6387	0	6078	178	0
2	B	1341	0	1319	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1341	0	1319	35	0
3	C	90	0	88	6	0
3	F	90	0	88	3	0
4	A	62	105	105	26	0
4	D	62	105	105	4	0
All	All	15349	210	14776	419	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (419) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:THR:HG22	1:D:687:ARG:H	1.34	0.93
1:D:487:PRO:HD2	1:D:512:ARG:HB3	1.50	0.92
4:A:1001:PCJ:HN	3:C:21:GLY:N	1.69	0.89
1:A:613:LEU:O	1:A:632:PRO:HD2	1.77	0.85
1:A:487:PRO:HD2	1:A:512:ARG:HB3	1.59	0.85
1:D:376:THR:HG22	1:D:377:HIS:H	1.41	0.84
1:A:350:PRO:HG2	3:C:29:PRO:HG3	1.58	0.84
1:D:533:ARG:HD3	1:D:534:PRO:HD2	1.61	0.83
1:D:162:LYS:HG2	1:D:177:GLY:HA3	1.62	0.81
1:A:313:ILE:HD11	4:A:1001:PCJ:CB	2.12	0.79
1:D:326:LEU:HB2	1:D:343:PRO:HG2	1.63	0.79
1:A:376:THR:HG22	1:A:377:HIS:H	1.48	0.79
1:A:570:LEU:HD11	1:D:502:MET:HE1	1.64	0.78
1:A:864:LEU:HD13	1:A:890:LEU:HD13	1.65	0.78
1:D:553:PRO:HD2	1:D:572:TYR:O	1.82	0.78
1:A:773:ALA:O	1:A:774:ILE:HD13	1.84	0.77
1:A:260:ILE:HD11	1:A:286:LEU:HD12	1.68	0.76
2:B:68:THR:HG22	2:B:69:GLY:H	1.51	0.75
1:A:836:ARG:NH1	1:A:848:GLU:OE1	2.21	0.73
1:A:313:ILE:HD11	4:A:1001:PCJ:HB2	1.70	0.73
1:D:649:VAL:HG13	1:D:652:THR:HB	1.70	0.73
1:A:398:PHE:CE1	1:A:876:ALA:HB2	2.24	0.72
1:A:357:TYR:HB2	1:A:369:GLU:HB2	1.70	0.72
1:A:328:PRO:HG3	4:A:1001:PCJ:O3	1.89	0.71
1:A:870:LEU:HD13	1:A:882:GLU:HG3	1.72	0.71
1:A:867:ARG:HD2	1:A:908:PHE:CE2	2.25	0.71
2:B:82:ILE:HG13	2:B:130:LEU:HD13	1.71	0.71
1:A:819:HIS:CD2	1:A:839:TYR:HB3	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LEU:HB2	1:A:343:PRO:HG2	1.73	0.70
1:D:203:GLU:HG2	1:D:223:GLN:HG2	1.73	0.70
1:A:608:LYS:HE3	1:A:635:MET:HE2	1.71	0.70
1:A:793:TYR:HA	1:A:816:ILE:O	1.91	0.70
1:A:845:ARG:NH1	1:A:882:GLU:OE2	2.24	0.70
1:A:314:TYR:CE1	4:A:1001:PCJ:H642	2.27	0.69
1:A:649:VAL:HG13	1:A:652:THR:HB	1.72	0.69
1:D:615:PHE:HB2	1:D:630:LEU:HB3	1.75	0.69
1:A:305:PHE:HD2	4:A:1001:PCJ:H312	1.55	0.69
1:D:863:ARG:NH2	1:D:906:GLU:OE2	2.24	0.68
1:D:376:THR:HG22	1:D:377:HIS:N	2.09	0.68
1:A:353:ASP:OD2	1:A:373:ARG:NH1	2.26	0.68
2:E:9:LEU:HD12	2:E:9:LEU:H	1.58	0.67
1:A:828:VAL:HG13	1:A:829:PRO:HD2	1.77	0.67
1:D:371:GLU:OE2	1:D:373:ARG:HD2	1.95	0.67
2:E:2:CYS:SG	2:E:3:GLY:N	2.67	0.67
1:D:793:TYR:HA	1:D:816:ILE:O	1.94	0.67
1:A:328:PRO:HD3	4:A:1001:PCJ:H452	1.77	0.66
2:E:123:ARG:HA	2:E:126:MET:HE3	1.76	0.66
1:A:249:ALA:HB2	1:A:262:LEU:HB3	1.77	0.66
1:D:212:ASP:OD2	1:D:254:ARG:NH1	2.27	0.66
1:D:819:HIS:CD2	1:D:839:TYR:HB3	2.30	0.66
1:D:647:LEU:O	1:D:673:ARG:NH2	2.29	0.66
1:A:615:PHE:CE1	2:B:6:LEU:CD2	2.79	0.65
1:A:610:ASP:CG	1:A:633:ARG:HH21	2.05	0.64
1:A:250:LEU:O	1:A:250:LEU:HD23	1.97	0.64
4:A:1001:PCJ:C1	4:A:1001:PCJ:H1	2.25	0.64
1:D:490:THR:HG22	1:D:509:GLU:HG3	1.79	0.64
1:D:822:SER:HB3	1:D:836:ARG:HG3	1.78	0.64
1:D:868:TYR:CE1	1:D:884:ALA:HB1	2.33	0.64
1:A:195:LEU:O	1:A:196:HIS:ND1	2.30	0.64
1:D:215:MET:HG2	1:D:254:ARG:HH21	1.64	0.62
1:A:556:SER:HB3	1:A:569:THR:HG23	1.82	0.62
1:A:681:SER:OG	1:A:704:ILE:HG12	1.99	0.62
1:D:300:LEU:O	1:D:307:VAL:HG12	2.00	0.62
1:A:208:VAL:HG21	1:A:222:ALA:HB2	1.82	0.61
1:A:376:THR:HG22	1:A:377:HIS:N	2.15	0.61
1:A:660:ASP:OD2	2:B:103:LYS:HE3	2.00	0.61
1:D:144:PRO:HB2	1:D:182:ARG:HH22	1.64	0.61
1:D:850:PHE:CE2	1:D:913:ILE:HD13	2.36	0.61
1:D:819:HIS:CE1	1:D:821:PHE:CE2	2.89	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:617:ARG:NH2	1:D:628:GLN:OE1	2.31	0.61
1:A:305:PHE:HD2	4:A:1001:PCJ:C31	2.14	0.60
1:D:789:VAL:HG13	1:D:821:PHE:CD1	2.36	0.60
1:D:819:HIS:ND1	1:D:821:PHE:CE2	2.69	0.60
1:A:328:PRO:CD	4:A:1001:PCJ:H452	2.31	0.60
1:D:332:SER:HA	1:D:337:GLY:O	2.01	0.60
1:A:615:PHE:CE1	2:B:6:LEU:HD23	2.37	0.60
1:D:341:VAL:HG22	1:D:359:ARG:HG2	1.84	0.60
1:A:314:TYR:CD1	4:A:1001:PCJ:H642	2.37	0.60
1:D:353:ASP:OD1	1:D:373:ARG:HD3	2.00	0.60
1:D:461:ASP:O	2:E:32:ARG:HD2	2.01	0.60
1:A:359:ARG:NE	1:A:369:GLU:OE2	2.28	0.59
1:A:502:MET:HG2	1:A:503:GLN:N	2.17	0.59
1:A:642:LYS:O	1:A:644:GLN:HG3	2.01	0.59
1:D:301:ARG:HA	1:D:305:PHE:O	2.02	0.59
1:A:407:LEU:C	1:A:407:LEU:HD23	2.27	0.59
1:A:321:ARG:NH1	1:A:345:TYR:OH	2.35	0.59
2:B:68:THR:HG22	2:B:69:GLY:N	2.17	0.59
1:D:629:THR:HG22	1:D:687:ARG:N	2.14	0.59
1:A:606:LEU:HD11	1:A:665:GLU:HB2	1.85	0.58
1:D:877:PHE:O	1:D:879:VAL:HG23	2.03	0.58
1:D:130:ILE:H	1:D:130:ILE:HD12	1.68	0.58
1:A:249:ALA:CB	1:A:262:LEU:HB3	2.34	0.58
1:A:828:VAL:CG1	1:A:829:PRO:HD2	2.34	0.57
1:D:769:GLU:HG3	1:D:796:ASP:HB3	1.86	0.57
1:D:669:THR:HG21	2:E:118:GLU:HA	1.86	0.57
1:D:789:VAL:HG13	1:D:821:PHE:CE1	2.39	0.57
4:D:1001:PCJ:C	3:F:21:GLY:HA2	2.34	0.57
1:A:321:ARG:HH21	1:A:350:PRO:HA	1.69	0.57
1:A:557:LEU:O	1:A:568:PRO:HD2	2.05	0.57
1:D:328:PRO:HD3	4:D:1001:PCJ:C45	2.35	0.57
1:D:828:VAL:HG13	1:D:829:PRO:HD2	1.85	0.57
1:D:165:ARG:HG2	1:D:166:TYR:H	1.69	0.57
1:D:909:LEU:HA	1:D:913:ILE:HD12	1.86	0.56
2:B:53:LEU:HD22	2:B:138:LEU:HD11	1.86	0.56
1:D:294:THR:HG22	1:D:314:TYR:HB3	1.86	0.56
2:E:68:THR:HG22	2:E:69:GLY:H	1.70	0.56
2:E:79:THR:HG23	2:E:102:GLN:HG2	1.86	0.56
1:A:179:VAL:HG11	1:A:193:ALA:HB2	1.87	0.56
1:D:868:TYR:HE1	1:D:884:ALA:HB1	1.68	0.56
1:A:250:LEU:HD23	1:A:250:LEU:C	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:850:PHE:CZ	1:D:913:ILE:HD13	2.41	0.56
1:D:410:LEU:HD23	1:D:424:VAL:HG11	1.88	0.55
3:C:22:LEU:C	3:C:22:LEU:HD23	2.31	0.55
1:D:446:SER:OG	1:D:447:THR:N	2.27	0.55
1:A:579:LEU:HD11	1:A:648:PRO:HD3	1.89	0.55
1:A:648:PRO:HG2	1:A:650:PHE:CE2	2.42	0.55
1:D:459:ARG:NH1	2:E:25:ASN:OD1	2.30	0.55
1:D:579:LEU:HD11	1:D:648:PRO:HD3	1.88	0.55
1:A:773:ALA:C	1:A:774:ILE:HD13	2.32	0.55
1:A:819:HIS:CE1	1:A:821:PHE:CE2	2.94	0.55
1:A:610:ASP:OD2	1:A:633:ARG:NH2	2.40	0.54
1:D:210:LEU:HD23	1:D:211:ARG:N	2.22	0.54
1:A:609:VAL:O	1:A:635:MET:HA	2.07	0.54
2:B:123:ARG:HA	2:B:126:MET:HE3	1.88	0.54
1:D:350:PRO:HB3	3:F:27:TYR:CZ	2.42	0.54
1:D:486:LEU:HB2	1:D:487:PRO:HD3	1.88	0.54
1:D:133:TYR:CD2	1:D:830:GLN:HG2	2.43	0.54
1:D:864:LEU:HD11	1:D:888:ILE:HD11	1.90	0.54
1:A:706:TYR:CG	1:A:710:ARG:NH1	2.76	0.54
2:B:2:CYS:SG	2:B:3:GLY:N	2.80	0.54
1:D:135:GLY:N	1:D:271:GLU:OE2	2.35	0.54
1:D:212:ASP:OD1	1:D:213:LYS:N	2.37	0.54
1:A:398:PHE:CD1	1:A:876:ALA:HB2	2.42	0.54
1:D:328:PRO:HD3	4:D:1001:PCJ:H451	1.90	0.54
1:D:864:LEU:HD12	1:D:889:PHE:O	2.06	0.54
1:A:794:ARG:HD2	2:B:75:GLU:OE2	2.07	0.54
2:E:105:TYR:CZ	2:E:119:ALA:HB2	2.43	0.54
1:D:353:ASP:OD2	1:D:373:ARG:NH1	2.42	0.53
1:D:794:ARG:HD2	2:E:75:GLU:OE2	2.08	0.53
1:A:819:HIS:NE2	1:A:839:TYR:HB3	2.22	0.53
1:D:652:THR:HA	1:D:669:THR:O	2.09	0.53
1:D:829:PRO:O	1:D:830:GLN:HB2	2.08	0.53
1:A:777:TYR:CE1	1:A:779:PRO:HG3	2.44	0.53
4:A:1001:PCJ:N	3:C:21:GLY:N	2.49	0.53
1:D:718:THR:HG23	1:D:721:ASP:H	1.74	0.53
1:A:321:ARG:NH2	1:A:350:PRO:HA	2.23	0.53
1:A:822:SER:HB3	1:A:836:ARG:HG3	1.89	0.53
1:A:502:MET:HE1	1:A:555:MET:SD	2.48	0.53
1:D:144:PRO:HD2	1:D:182:ARG:HH12	1.72	0.53
1:A:617:ARG:NH2	1:A:628:GLN:OE1	2.39	0.53
1:A:270:CYS:HB3	1:A:274:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:MET:HE3	1:A:555:MET:HB3	1.91	0.53
1:A:909:LEU:HD23	1:A:916:TYR:CE2	2.44	0.52
1:D:133:TYR:CE2	1:D:830:GLN:HG2	2.44	0.52
1:A:212:ASP:OD1	1:A:213:LYS:N	2.34	0.52
1:A:657:PHE:HE2	1:A:742:ALA:HB2	1.74	0.52
1:A:533:ARG:HD3	1:A:534:PRO:HD2	1.90	0.52
1:D:357:TYR:HB2	1:D:369:GLU:HB2	1.92	0.52
1:A:180:VAL:C	1:A:181:LEU:HD12	2.35	0.52
1:A:360:TYR:HB2	1:A:366:MET:HE1	1.91	0.52
1:A:698:SER:O	1:A:745:GLY:HA2	2.10	0.52
2:E:39:GLU:C	2:E:41:SER:H	2.18	0.52
1:D:374:TYR:CZ	1:D:381:GLY:HA3	2.44	0.52
1:D:524:ASN:N	1:D:528:SER:O	2.37	0.52
1:D:819:HIS:NE2	1:D:839:TYR:HB3	2.25	0.52
1:A:305:PHE:CD2	4:A:1001:PCJ:H312	2.42	0.51
1:A:682:LEU:HD12	1:A:705:TYR:CE2	2.45	0.51
1:A:704:ILE:HB	1:A:739:SER:HB3	1.91	0.51
1:D:777:TYR:CE1	1:D:779:PRO:HD3	2.45	0.51
1:A:850:PHE:CD1	1:A:850:PHE:C	2.88	0.51
1:D:341:VAL:HG21	1:D:359:ARG:NH1	2.25	0.51
1:D:199:GLU:OE2	1:D:225:GLN:NE2	2.43	0.51
2:B:101:VAL:HG12	2:B:130:LEU:HD21	1.91	0.51
1:A:385:ALA:HA	1:A:407:LEU:O	2.10	0.51
1:A:605:PRO:HD2	1:A:640:PRO:CG	2.40	0.51
1:A:669:THR:HG21	2:B:118:GLU:HA	1.93	0.51
1:A:682:LEU:HD12	1:A:705:TYR:HE2	1.76	0.51
1:D:487:PRO:CD	1:D:512:ARG:HB3	2.30	0.51
4:A:1001:PCJ:H1	4:A:1001:PCJ:H2	1.92	0.51
2:E:101:VAL:HG12	2:E:130:LEU:HD21	1.92	0.51
1:A:269:ARG:HD3	1:A:896:GLY:HA3	1.93	0.50
2:E:66:SER:HB2	2:E:75:GLU:HB2	1.92	0.50
1:D:339:THR:HA	1:D:360:TYR:O	2.11	0.50
1:D:614:TYR:HD1	1:D:631:GLU:HG2	1.76	0.50
1:A:819:HIS:ND1	1:A:821:PHE:CE2	2.80	0.50
1:D:248:SER:H	1:D:266:THR:HB	1.76	0.50
2:B:21:VAL:HG23	2:B:45:VAL:HG13	1.93	0.50
1:A:788:ASN:HB2	1:A:822:SER:OG	2.12	0.50
1:A:910:ASP:OD2	1:A:917:ARG:NH1	2.36	0.49
1:D:838:GLN:NE2	2:E:67:TYR:HE2	2.10	0.49
1:D:576:LYS:NZ	1:D:599:ASN:HB3	2.28	0.49
1:D:476:THR:OG1	1:D:477:THR:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:SER:HB3	1:D:180:VAL:CG2	2.42	0.49
2:E:87:VAL:HG22	2:E:93:VAL:HG12	1.94	0.49
1:A:348:LEU:O	1:A:349:ALA:HB2	2.13	0.49
1:A:462:THR:HG22	1:A:494:PHE:CZ	2.47	0.49
1:D:321:ARG:HH12	1:D:350:PRO:HA	1.78	0.49
2:B:32:ARG:NH1	2:B:36:GLU:OE2	2.46	0.49
1:D:144:PRO:HD2	1:D:182:ARG:NH1	2.28	0.48
1:D:617:ARG:HG2	1:D:619:THR:HG23	1.95	0.48
1:A:625:PRO:HD2	1:A:691:GLU:OE2	2.12	0.48
1:A:486:LEU:CB	1:A:487:PRO:HD3	2.43	0.48
1:A:615:PHE:HB2	1:A:630:LEU:HB3	1.94	0.48
1:A:633:ARG:HG3	1:A:663:TRP:CH2	2.49	0.48
1:A:769:GLU:HG3	1:A:796:ASP:HB3	1.94	0.48
4:A:1001:PCJ:C65	4:A:1001:PCJ:HB1	2.42	0.48
1:D:208:VAL:HG12	1:D:219:GLY:O	2.13	0.48
1:D:486:LEU:CB	1:D:487:PRO:HD3	2.43	0.48
1:A:909:LEU:HD23	1:A:916:TYR:HE2	1.79	0.48
1:D:360:TYR:HB2	1:D:366:MET:HE1	1.96	0.48
1:A:657:PHE:CE2	1:A:742:ALA:HB2	2.49	0.48
2:B:93:VAL:HG23	2:B:93:VAL:O	2.13	0.48
1:D:862:LEU:HD13	1:D:892:ILE:HG13	1.95	0.48
1:A:314:TYR:CE1	4:A:1001:PCJ:C64	2.96	0.48
2:B:82:ILE:HG13	2:B:130:LEU:CD1	2.43	0.48
1:D:161:ALA:HB1	1:D:176:ALA:O	2.14	0.48
1:A:238:TYR:CE2	1:A:262:LEU:HD13	2.49	0.48
1:D:587:THR:O	1:D:591:LYS:HB2	2.14	0.48
1:D:682:LEU:HD12	1:D:705:TYR:CE2	2.48	0.48
2:E:78:LEU:HB3	2:E:126:MET:HE1	1.95	0.48
2:E:78:LEU:CB	2:E:126:MET:HE1	2.43	0.48
1:D:118:PRO:O	1:D:123:THR:OG1	2.21	0.47
1:A:234:ASP:O	1:A:235:ASN:C	2.57	0.47
2:B:56:VAL:HG22	2:B:83:ASN:O	2.14	0.47
1:D:230:GLU:HA	1:D:254:ARG:O	2.14	0.47
1:A:502:MET:CG	1:A:503:GLN:N	2.77	0.47
1:A:762:ASN:HB2	1:A:769:GLU:OE1	2.13	0.47
4:A:1001:PCJ:H332	4:A:1001:PCJ:H361	1.51	0.47
1:D:605:PRO:HD2	1:D:640:PRO:CG	2.45	0.47
1:D:682:LEU:HD12	1:D:705:TYR:HE2	1.79	0.47
1:A:270:CYS:SG	1:A:276:ALA:HB3	2.54	0.47
2:B:122:LEU:HD12	2:B:122:LEU:HA	1.55	0.47
2:E:68:THR:HG22	2:E:69:GLY:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:SER:H	1:A:266:THR:HB	1.79	0.47
1:D:247:GLY:HA3	1:D:266:THR:O	2.14	0.47
1:D:698:SER:O	1:D:745:GLY:HA2	2.15	0.47
2:E:53:LEU:HD22	2:E:138:LEU:HD11	1.96	0.47
1:A:647:LEU:O	1:A:673:ARG:NH2	2.47	0.46
1:D:282:ASN:HB2	1:D:297:ASN:HB2	1.97	0.46
1:D:741:TYR:O	1:D:760:ASN:HA	2.15	0.46
2:E:51:TYR:OH	2:E:147:ASP:OD1	2.32	0.46
2:B:137:ARG:O	2:B:141:LEU:HD13	2.14	0.46
1:D:215:MET:HE3	1:D:288:PRO:HG3	1.97	0.46
1:D:348:LEU:O	1:D:349:ALA:HB2	2.15	0.46
4:D:1001:PCJ:O	3:F:21:GLY:HA2	2.14	0.46
1:D:163:ALA:HB3	1:D:176:ALA:HB3	1.98	0.46
1:A:261:MET:O	1:A:262:LEU:HD23	2.15	0.46
1:A:260:ILE:CD1	1:A:262:LEU:HD21	2.45	0.46
1:A:621:PHE:O	1:A:624:THR:OG1	2.32	0.46
1:D:773:ALA:O	1:D:774:ILE:HD13	2.16	0.46
1:D:249:ALA:CB	1:D:262:LEU:HB3	2.45	0.46
1:D:514:ASP:OD1	1:D:515:ARG:N	2.48	0.46
1:D:909:LEU:HD23	1:D:916:TYR:CE2	2.51	0.46
1:A:314:TYR:O	4:A:1001:PCJ:H651	2.15	0.46
1:A:706:TYR:CD2	1:A:710:ARG:NH1	2.84	0.46
1:D:215:MET:CE	1:D:288:PRO:HG3	2.45	0.46
1:D:345:TYR:CE2	1:D:347:ASN:HB2	2.51	0.46
1:A:260:ILE:HD12	1:A:262:LEU:HD21	1.97	0.46
1:A:406:TRP:CE2	1:A:430:SER:HB3	2.51	0.46
1:D:557:LEU:O	1:D:568:PRO:HD2	2.15	0.46
1:A:328:PRO:HG3	4:A:1001:PCJ:C26	2.45	0.45
1:A:407:LEU:HD23	1:A:408:TYR:N	2.30	0.45
1:A:777:TYR:CZ	1:A:779:PRO:HG3	2.50	0.45
1:A:819:HIS:NE2	1:A:839:TYR:CB	2.79	0.45
1:D:576:LYS:HZ2	1:D:599:ASN:HB3	1.80	0.45
1:A:198:LEU:C	1:A:200:ASN:H	2.24	0.45
1:A:833:VAL:HG22	1:A:834:LEU:N	2.31	0.45
1:D:249:ALA:HB2	1:D:262:LEU:HB3	1.97	0.45
1:D:753:TRP:HB3	1:D:777:TYR:HD1	1.81	0.45
1:D:850:PHE:CD1	1:D:850:PHE:C	2.93	0.45
2:E:93:VAL:HG23	2:E:93:VAL:O	2.16	0.45
1:A:502:MET:CE	1:A:555:MET:SD	3.05	0.45
1:A:634:ALA:HA	1:A:681:SER:O	2.16	0.45
2:B:78:LEU:HB2	2:B:126:MET:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:TRP:HA	1:D:301:ARG:O	2.16	0.45
1:A:305:PHE:CD2	4:A:1001:PCJ:C31	2.98	0.45
1:D:224:VAL:HG12	1:D:225:GLN:H	1.81	0.45
1:D:823:VAL:HG22	1:D:824:ILE:N	2.30	0.45
2:B:33:GLU:HB2	2:B:131:ILE:HD11	1.97	0.45
1:A:209:LYS:HG2	1:A:218:VAL:HG12	1.99	0.45
1:A:405:ARG:HD3	1:A:431:ASP:OD1	2.17	0.45
1:A:487:PRO:HD2	1:A:512:ARG:CB	2.38	0.45
2:B:101:VAL:HG22	2:B:102:GLN:N	2.32	0.45
1:D:160:SER:HB3	1:D:180:VAL:HG22	1.99	0.45
1:A:205:VAL:HG12	1:A:206:GLY:N	2.32	0.45
1:A:190:GLY:HA2	1:A:207:ASN:O	2.16	0.44
1:A:581:LEU:HD23	1:A:586:LYS:HG2	1.99	0.44
1:D:215:MET:HG2	1:D:260:ILE:HD11	2.00	0.44
2:B:148:GLU:HG2	2:B:151:ARG:HH21	1.82	0.44
1:D:681:SER:OG	1:D:704:ILE:HG12	2.18	0.44
1:D:814:ASP:OD1	2:E:68:THR:HG22	2.16	0.44
1:A:345:TYR:CE2	1:A:347:ASN:HB2	2.52	0.44
4:A:1001:PCJ:H1	4:A:1001:PCJ:C2	2.47	0.44
4:A:1001:PCJ:HB1	4:A:1001:PCJ:H652	1.98	0.44
1:D:175:LEU:HD12	1:D:175:LEU:HA	1.82	0.44
1:A:822:SER:HB2	1:A:913:ILE:HG12	2.00	0.44
1:D:293:GLY:O	1:D:314:TYR:HA	2.17	0.44
3:C:22:LEU:C	3:C:22:LEU:CD2	2.91	0.44
1:D:847:LEU:HA	1:D:870:LEU:HD22	1.99	0.44
1:D:140:GLU:HG2	1:D:241:HIS:CE1	2.53	0.43
1:D:610:ASP:OD2	1:D:633:ARG:NH2	2.49	0.43
4:A:1001:PCJ:SG	4:A:1001:PCJ:O47	2.76	0.43
1:D:327:PRO:CD	1:D:899:GLY:HA2	2.48	0.43
2:E:16:LEU:HD12	2:E:143:PRO:HG3	2.01	0.43
1:A:785:LYS:HD3	1:A:825:TRP:CZ2	2.53	0.43
1:A:850:PHE:HB2	1:A:866:ASN:O	2.18	0.43
1:D:648:PRO:HG2	1:D:650:PHE:CE2	2.54	0.43
1:A:204:LEU:HB3	1:A:222:ALA:HB3	2.01	0.43
1:D:346:PHE:HB3	1:D:348:LEU:HD21	2.01	0.43
1:D:606:LEU:HD11	1:D:665:GLU:HB2	1.99	0.43
1:D:614:TYR:CD1	1:D:631:GLU:HG2	2.52	0.43
1:A:242:LYS:HA	1:A:242:LYS:HD3	1.80	0.43
1:A:480:VAL:HG22	2:B:110:ASN:HB3	2.01	0.43
1:D:634:ALA:HA	1:D:681:SER:O	2.18	0.43
1:A:201:ARG:H	1:A:201:ARG:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:LEU:CB	2:B:126:MET:HE1	2.49	0.43
1:D:800:PHE:HB3	2:E:110:ASN:HB2	1.99	0.43
1:A:689:ILE:HG22	1:A:690:GLU:O	2.19	0.43
1:A:210:LEU:O	1:A:216:LEU:HD12	2.19	0.43
1:D:608:LYS:HA	1:D:636:TYR:O	2.19	0.43
1:D:847:LEU:HD23	1:D:870:LEU:HD22	2.01	0.43
2:E:103:LYS:HD3	2:E:122:LEU:HD11	2.01	0.43
2:E:133:GLN:O	2:E:137:ARG:HG3	2.19	0.43
1:A:604:LEU:O	1:A:604:LEU:HD12	2.19	0.43
1:A:794:ARG:NH1	2:B:75:GLU:OE2	2.49	0.43
1:D:425:ASP:OD1	1:D:425:ASP:C	2.62	0.43
1:D:508:THR:HG22	1:D:551:LEU:HD22	2.00	0.43
1:D:563:TRP:HB2	2:E:6:LEU:HD22	1.99	0.43
1:A:321:ARG:HA	3:C:22:LEU:O	2.18	0.43
2:B:31:VAL:O	2:B:35:LYS:HG3	2.18	0.43
1:D:617:ARG:HB3	2:E:4:PHE:CE1	2.54	0.43
1:D:724:ARG:HG2	1:D:725:LEU:HD12	2.01	0.43
1:A:741:TYR:HB3	1:A:743:PHE:CE1	2.54	0.42
4:A:1001:PCJ:H1	4:A:1001:PCJ:H12	1.99	0.42
1:D:268:THR:HB	1:D:278:THR:HG22	2.01	0.42
1:D:495:LEU:O	1:D:496:PRO:C	2.60	0.42
1:A:321:ARG:O	1:A:322:GLN:HG3	2.19	0.42
1:D:275:ASN:O	1:D:303:LYS:HA	2.19	0.42
1:D:605:PRO:HD2	1:D:640:PRO:HG3	2.01	0.42
1:D:823:VAL:CG2	1:D:824:ILE:N	2.83	0.42
1:D:276:ALA:O	1:D:303:LYS:N	2.35	0.42
1:D:398:PHE:CE1	1:D:876:ALA:HB2	2.53	0.42
1:D:652:THR:HG22	1:D:714:LEU:HD21	2.00	0.42
1:D:836:ARG:NH1	1:D:848:GLU:OE1	2.48	0.42
2:E:101:VAL:HG22	2:E:102:GLN:N	2.35	0.42
1:A:804:ARG:HB3	1:A:806:THR:HG22	2.00	0.42
1:A:828:VAL:CG1	1:A:829:PRO:CD	2.97	0.42
1:A:910:ASP:C	1:A:910:ASP:OD1	2.62	0.42
1:A:757:SER:HA	1:A:772:SER:O	2.19	0.42
2:E:137:ARG:O	2:E:141:LEU:HD13	2.19	0.42
1:A:188:VAL:HG22	1:A:210:LEU:HD13	2.02	0.42
1:A:269:ARG:HD3	1:A:896:GLY:CA	2.49	0.42
1:D:327:PRO:CG	1:D:899:GLY:HA2	2.50	0.42
1:D:834:LEU:HD12	1:D:834:LEU:O	2.19	0.42
2:E:155:ALA:HA	2:E:158:LYS:HE3	2.02	0.42
2:B:101:VAL:HG12	2:B:130:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:820:ASP:OD2	1:D:836:ARG:NH2	2.53	0.42
1:A:331:SER:OG	1:A:339:THR:HB	2.20	0.42
1:A:477:THR:HG22	1:A:533:ARG:HH22	1.85	0.42
1:D:224:VAL:HG12	1:D:225:GLN:N	2.34	0.42
1:D:282:ASN:N	1:D:296:THR:O	2.45	0.42
1:D:576:LYS:HE3	1:D:578:ASP:OD1	2.19	0.42
1:D:819:HIS:CE1	1:D:821:PHE:CD2	3.07	0.42
1:A:487:PRO:CD	1:A:512:ARG:HB3	2.40	0.42
1:A:328:PRO:HD3	4:A:1001:PCJ:C45	2.48	0.41
1:A:452:GLN:NE2	1:A:473:GLN:HB2	2.35	0.41
2:E:44:LYS:HD3	2:E:44:LYS:HA	1.95	0.41
1:A:694:PHE:CD1	1:A:694:PHE:N	2.89	0.41
2:B:101:VAL:CG2	2:B:102:GLN:N	2.84	0.41
1:A:330:PHE:CD1	1:A:330:PHE:N	2.87	0.41
1:A:371:GLU:OE2	1:A:373:ARG:HD2	2.21	0.41
1:A:691:GLU:H	1:A:691:GLU:CD	2.29	0.41
1:D:617:ARG:HB3	2:E:4:PHE:CD1	2.56	0.41
1:D:727:LEU:HD21	1:D:804:ARG:HH12	1.85	0.41
1:D:775:PHE:CZ	1:D:777:TYR:HB2	2.54	0.41
1:A:255:SER:HB3	1:A:256:GLU:H	1.72	0.41
1:A:268:THR:HB	1:A:278:THR:HG22	2.02	0.41
1:A:326:LEU:HB3	1:A:327:PRO:CD	2.50	0.41
1:A:761:TRP:CZ2	1:A:766:SER:HA	2.55	0.41
1:D:115:ASP:CG	1:D:211:ARG:HH22	2.28	0.41
1:D:232:GLN:HA	1:D:252:ALA:O	2.20	0.41
2:E:122:LEU:HD12	2:E:122:LEU:HA	1.76	0.41
1:A:715:PRO:O	1:A:806:THR:OG1	2.38	0.41
1:D:673:ARG:O	1:D:674:ILE:HD13	2.21	0.41
1:D:859:CYS:O	1:D:860:TRP:HB3	2.21	0.41
2:E:39:GLU:C	2:E:41:SER:N	2.78	0.41
1:D:706:TYR:CG	1:D:710:ARG:NH1	2.89	0.41
1:D:769:GLU:HG3	1:D:796:ASP:CB	2.51	0.41
1:A:592:ARG:NH1	1:A:724:ARG:HD2	2.36	0.41
1:A:716:GLY:HA2	1:A:721:ASP:HB3	2.02	0.41
1:D:327:PRO:HA	1:D:328:PRO:HD3	2.01	0.41
1:D:765:THR:O	1:D:767:ARG:HG2	2.21	0.41
1:D:854:GLU:OE2	1:D:916:TYR:OH	2.38	0.41
1:A:196:HIS:HB3	1:A:197:GLN:H	1.67	0.41
1:A:401:TYR:CG	1:A:402:SER:N	2.89	0.41
2:B:62:GLN:NE2	2:B:76:PHE:CD2	2.89	0.41
1:D:232:GLN:OE1	1:D:253:LYS:NZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:592:ARG:HD2	1:D:724:ARG:HE	1.86	0.41
1:D:722:LEU:HD13	1:D:728:ASP:OD2	2.21	0.41
1:A:188:VAL:CG1	1:A:204:LEU:HD13	2.51	0.40
1:A:279:LEU:HA	1:A:279:LEU:HD12	1.88	0.40
1:A:232:GLN:HA	1:A:252:ALA:O	2.21	0.40
1:A:592:ARG:O	1:A:592:ARG:HG2	2.21	0.40
1:A:813:ASN:HB2	1:A:843:LYS:NZ	2.36	0.40
1:D:701:ALA:HA	1:D:742:ALA:O	2.21	0.40
1:A:384:ASN:O	1:A:408:TYR:HA	2.22	0.40
1:A:721:ASP:OD1	1:A:721:ASP:N	2.53	0.40
1:D:511:VAL:HG13	1:D:513:PHE:CE2	2.56	0.40
1:A:179:VAL:HG11	1:A:193:ALA:CB	2.51	0.40
1:A:225:GLN:HB3	1:A:230:GLU:HB3	2.04	0.40
1:A:225:GLN:HG2	1:A:226:LEU:CD1	2.51	0.40
4:A:1001:PCJ:O3	4:A:1001:PCJ:H452	2.21	0.40
1:D:205:VAL:HG12	1:D:206:GLY:N	2.36	0.40
1:D:567:THR:O	1:D:567:THR:HG22	2.21	0.40
1:D:700:SER:O	1:D:743:PHE:HA	2.21	0.40
1:D:789:VAL:HG13	1:D:821:PHE:HD1	1.86	0.40
1:D:850:PHE:HB2	1:D:866:ASN:O	2.21	0.40
1:A:218:VAL:O	1:A:236:ALA:HA	2.22	0.40
1:A:256:GLU:C	1:A:258:ALA:H	2.29	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	728/924 (79%)	679 (93%)	44 (6%)	5 (1%)	18	50
1	D	777/924 (84%)	719 (92%)	53 (7%)	5 (1%)	21	53
2	B	170/207 (82%)	164 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	170/207 (82%)	164 (96%)	5 (3%)	1 (1%)	21	53
3	C	10/67 (15%)	10 (100%)	0	0	100	100
3	F	10/67 (15%)	10 (100%)	0	0	100	100
All	All	1865/2396 (78%)	1746 (94%)	108 (6%)	11 (1%)	21	53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	487	PRO
1	D	121	LYS
1	A	487	PRO
1	D	198	LEU
2	E	40	ASN
1	A	206	GLY
1	A	526	ASP
1	A	195	LEU
1	A	257	ASN
1	D	132	PRO
1	D	913	ILE

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	636/784 (81%)	622 (98%)	14 (2%)	45	73
1	D	678/784 (86%)	657 (97%)	21 (3%)	35	66
2	B	141/169 (83%)	136 (96%)	5 (4%)	32	63
2	E	141/169 (83%)	140 (99%)	1 (1%)	76	87
3	C	9/58 (16%)	9 (100%)	0	100	100
3	F	9/58 (16%)	8 (89%)	1 (11%)	6	23
All	All	1614/2022 (80%)	1572 (97%)	42 (3%)	40	70

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	ARG
1	A	227	ASP
1	A	244	HIS
1	A	260	ILE
1	A	388	LEU
1	A	416	LEU
1	A	486	LEU
1	A	525	ASP
1	A	573	LEU
1	A	604	LEU
1	A	605	PRO
1	A	673	ARG
1	A	758	ASP
1	A	862	LEU
2	B	9	LEU
2	B	62	GLN
2	B	101	VAL
2	B	109	GLU
2	B	148	GLU
1	D	130	ILE
1	D	146	MET
1	D	239	VAL
1	D	244	HIS
1	D	323	SER
1	D	382	ILE
1	D	412	ASN
1	D	419	ARG
1	D	444	VAL
1	D	446	SER
1	D	476	THR
1	D	484	ASP
1	D	517	LEU
1	D	604	LEU
1	D	608	LYS
1	D	629	THR
1	D	673	ARG
1	D	758	ASP
1	D	845	ARG
1	D	862	LEU
1	D	905	THR
2	E	46	THR
3	F	22	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	ASN
1	A	451	ASN
1	A	734	ASN
1	A	762	ASN
1	A	838	GLN
2	B	62	GLN
2	B	98	GLN
1	D	297	ASN
1	D	347	ASN
1	D	412	ASN
1	D	451	ASN
1	D	468	ASN
1	D	713	GLN
1	D	764	ASN
1	D	838	GLN
1	D	880	GLN
2	E	98	GLN
2	E	121	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PCJ	A	1001	-	60,61,61	2.08	11 (18%)	60,65,65	2.96	20 (33%)
4	PCJ	D	1001	-	60,61,61	0.86	2 (3%)	60,65,65	1.46	9 (15%)

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
4	PCJ	A	1001	-	-	40/66/66/66	-
4	PCJ	D	1001	-	-	37/66/66/66	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	PCJ	C66-N	8.74	1.52	1.34
4	A	1001	PCJ	O3-C26	6.75	1.53	1.33
4	D	1001	PCJ	O3-C26	4.05	1.45	1.33
4	A	1001	PCJ	CA-N	3.86	1.54	1.46
4	D	1001	PCJ	O2-C46	3.84	1.45	1.34
4	A	1001	PCJ	O2-C46	3.49	1.44	1.34
4	A	1001	PCJ	C25-C26	3.15	1.59	1.50
4	A	1001	PCJ	O28-C26	2.94	1.31	1.22
4	A	1001	PCJ	O3-C3	2.68	1.51	1.45
4	A	1001	PCJ	C45-C46	2.67	1.58	1.50
4	A	1001	PCJ	CB-SG	2.17	1.89	1.81
4	A	1001	PCJ	C65-C66	2.13	1.55	1.51
4	A	1001	PCJ	C24-C25	2.09	1.59	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	PCJ	C2-O2-C46	-11.69	89.82	117.80
4	A	1001	PCJ	C3-O3-C26	-9.70	81.66	117.12
4	D	1001	PCJ	CA-N-C66	5.64	131.21	122.88
4	A	1001	PCJ	O2-C46-C45	5.55	123.49	111.48
4	A	1001	PCJ	C-CA-CB	-5.41	90.11	113.64
4	D	1001	PCJ	C65-C66-N	5.04	124.74	115.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	PCJ	C44-C45-C46	-4.88	95.81	113.69
4	A	1001	PCJ	O2-C46-O47	-4.86	112.35	123.70
4	A	1001	PCJ	C63-C64-C65	-4.61	96.18	113.13
4	A	1001	PCJ	O3-C3-C2	4.28	120.72	108.40
4	A	1001	PCJ	C62-C61-C60	-4.03	93.98	114.37
4	A	1001	PCJ	C64-C65-C66	-3.62	103.15	113.19
4	A	1001	PCJ	C17-C16-C15	-3.58	96.27	114.37
4	D	1001	PCJ	O2-C46-C45	3.43	118.91	111.48
4	A	1001	PCJ	C65-C66-N	3.40	121.86	115.86
4	D	1001	PCJ	O67-C66-N	-3.30	117.36	122.95
4	D	1001	PCJ	C2-O2-C46	-2.82	111.05	117.80
4	A	1001	PCJ	C15-C14-C13	-2.78	100.31	114.37
4	A	1001	PCJ	O28-C26-C25	-2.70	113.23	123.78
4	A	1001	PCJ	C19-C18-C17	-2.62	101.14	114.37
4	A	1001	PCJ	O3-C26-C25	2.55	119.60	111.83
4	A	1001	PCJ	C11-C12-C13	-2.55	96.17	113.36
4	A	1001	PCJ	C-CA-N	2.43	114.81	109.63
4	D	1001	PCJ	O3-C26-C25	2.31	118.89	111.83
4	A	1001	PCJ	C60-C59-C58	-2.31	102.70	114.37
4	D	1001	PCJ	C1-SG-CB	2.28	106.02	101.94
4	D	1001	PCJ	O67-C66-C65	-2.27	117.91	122.02
4	D	1001	PCJ	C-CA-N	-2.20	104.94	109.63
4	A	1001	PCJ	O67-C66-C65	-2.16	118.11	122.02

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	PCJ	C-CA-CB-SG
4	A	1001	PCJ	N-CA-CB-SG
4	A	1001	PCJ	CB-CA-N-C66
4	D	1001	PCJ	C-CA-CB-SG
4	D	1001	PCJ	N-CA-CB-SG
4	D	1001	PCJ	SG-C1-C2-O2
4	D	1001	PCJ	SG-C1-C2-C3
4	D	1001	PCJ	C45-C46-O2-C2
4	D	1001	PCJ	O28-C26-O3-C3
4	A	1001	PCJ	O47-C46-O2-C2
4	D	1001	PCJ	O47-C46-O2-C2
4	D	1001	PCJ	C25-C26-O3-C3
4	A	1001	PCJ	C45-C46-O2-C2
4	D	1001	PCJ	C65-C66-N-CA

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Mol	Chain	Res	Type	Atoms
4	A	1001	PCJ	C25-C26-O3-C3
4	A	1001	PCJ	O28-C26-O3-C3
4	D	1001	PCJ	O67-C66-N-CA
4	A	1001	PCJ	C65-C66-N-CA
4	A	1001	PCJ	O67-C66-N-CA
4	A	1001	PCJ	C35-C36-C37-C38
4	A	1001	PCJ	C33-C34-C35-C36
4	A	1001	PCJ	C43-C44-C45-C46
4	A	1001	PCJ	C23-C24-C25-C26
4	D	1001	PCJ	O-C-CA-N
4	A	1001	PCJ	C22-C23-C24-C25
4	A	1001	PCJ	C61-C62-C63-C64
4	A	1001	PCJ	C36-C37-C38-C39
4	A	1001	PCJ	C42-C43-C44-C45
4	A	1001	PCJ	C52-C53-C54-C55
4	A	1001	PCJ	C54-C55-C56-C57
4	D	1001	PCJ	C60-C61-C62-C63
4	A	1001	PCJ	C41-C42-C43-C44
4	D	1001	PCJ	C23-C24-C25-C26
4	D	1001	PCJ	C19-C20-C21-C22
4	D	1001	PCJ	C32-C33-C34-C35
4	A	1001	PCJ	C16-C17-C18-C19
4	A	1001	PCJ	C60-C61-C62-C63
4	A	1001	PCJ	C32-C33-C34-C35
4	A	1001	PCJ	C58-C59-C60-C61
4	D	1001	PCJ	C42-C43-C44-C45
4	A	1001	PCJ	C56-C57-C58-C59
4	D	1001	PCJ	C53-C54-C55-C56
4	D	1001	PCJ	C14-C15-C16-C17
4	A	1001	PCJ	C13-C14-C15-C16
4	A	1001	PCJ	C14-C15-C16-C17
4	D	1001	PCJ	C13-C14-C15-C16
4	D	1001	PCJ	C22-C23-C24-C25
4	A	1001	PCJ	C12-C13-C14-C15
4	D	1001	PCJ	C38-C39-C40-C41
4	A	1001	PCJ	C21-C22-C23-C24
4	D	1001	PCJ	C33-C34-C35-C36
4	A	1001	PCJ	C63-C64-C65-C66
4	D	1001	PCJ	C62-C63-C64-C65
4	A	1001	PCJ	C53-C54-C55-C56
4	D	1001	PCJ	C35-C36-C37-C38
4	A	1001	PCJ	C51-C52-C53-C54

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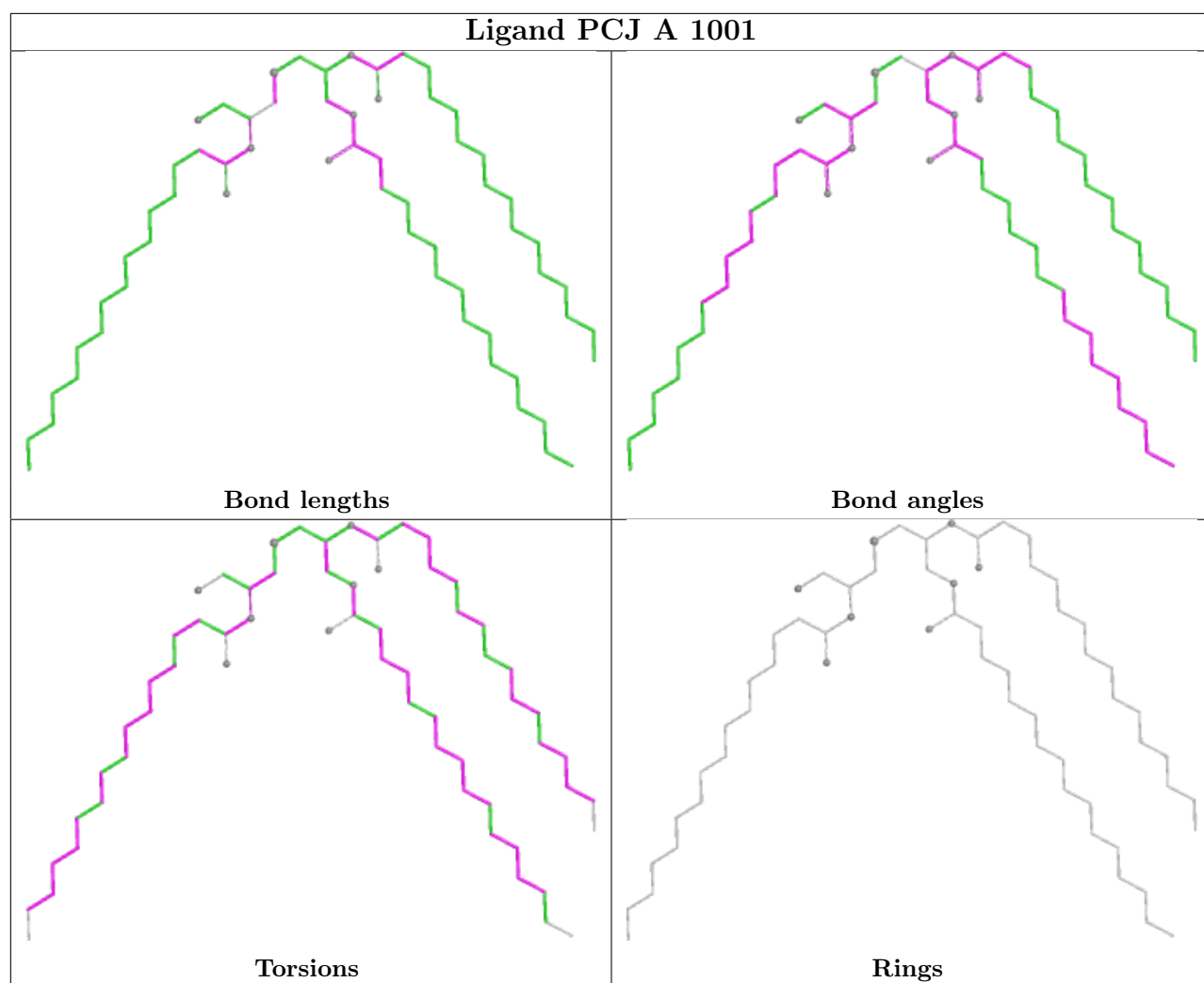
Mol	Chain	Res	Type	Atoms
4	A	1001	PCJ	C59-C60-C61-C62
4	D	1001	PCJ	C21-C22-C23-C24
4	D	1001	PCJ	C56-C57-C58-C59
4	A	1001	PCJ	C1-C2-C3-O3
4	A	1001	PCJ	C39-C40-C41-C42
4	D	1001	PCJ	C51-C52-C53-C54
4	A	1001	PCJ	C17-C18-C19-C20
4	A	1001	PCJ	O2-C2-C3-O3
4	D	1001	PCJ	C18-C19-C20-C21
4	D	1001	PCJ	C20-C21-C22-C23
4	D	1001	PCJ	CB-CA-N-C66
4	A	1001	PCJ	C18-C19-C20-C21
4	A	1001	PCJ	C19-C20-C21-C22
4	D	1001	PCJ	C41-C42-C43-C44
4	D	1001	PCJ	C57-C58-C59-C60
4	D	1001	PCJ	C54-C55-C56-C57
4	D	1001	PCJ	C44-C45-C46-O2
4	D	1001	PCJ	C34-C35-C36-C37
4	D	1001	PCJ	C40-C41-C42-C43
4	A	1001	PCJ	C31-C32-C33-C34
4	D	1001	PCJ	C44-C45-C46-O47

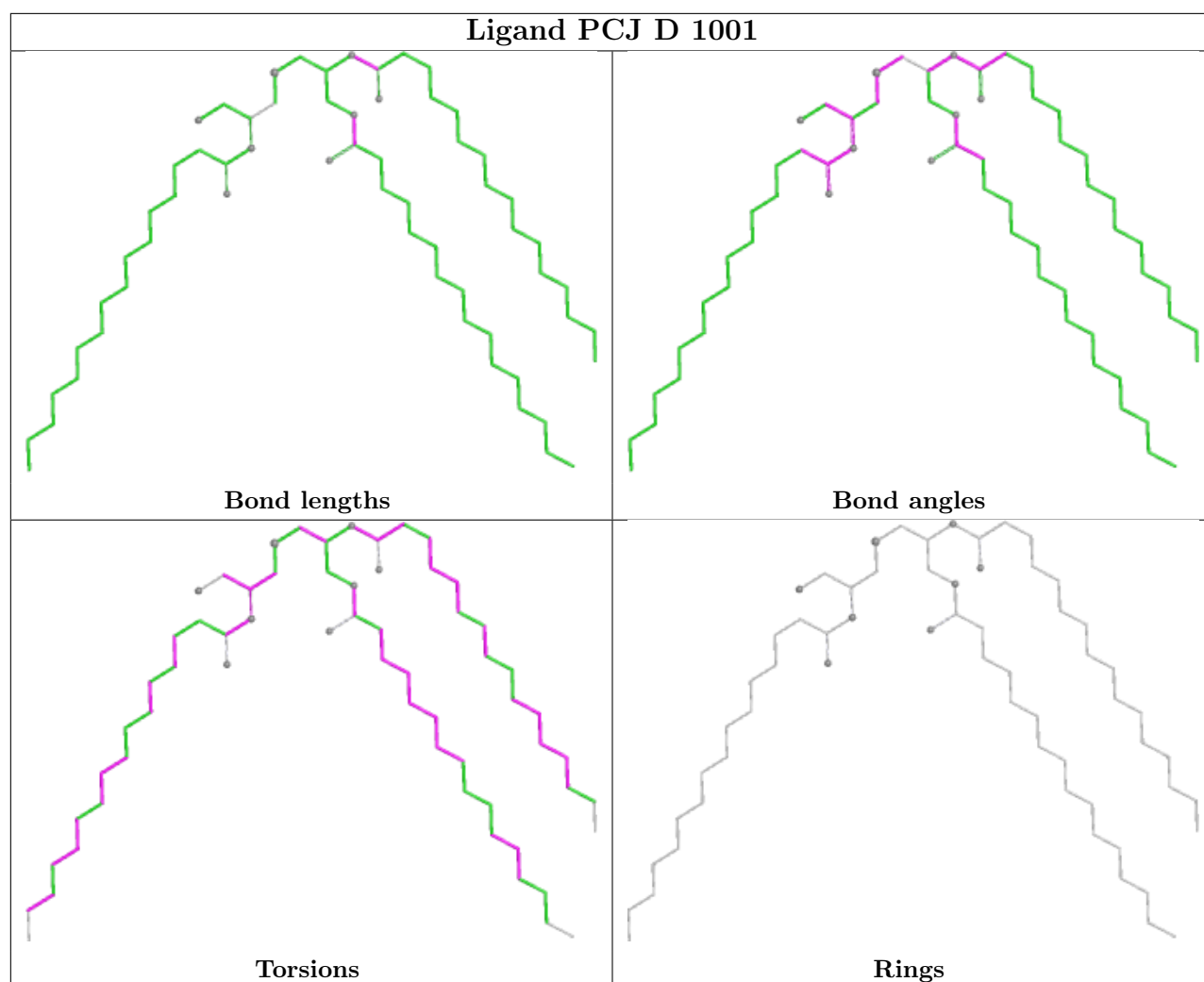
There are no ring outliers.

2 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	PCJ	26	0
4	D	1001	PCJ	4	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 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	736/924 (79%)	0.36	43 (5%)	29 17	49, 74, 122, 161	0
1	D	789/924 (85%)	0.47	48 (6%)	27 16	51, 83, 121, 147	0
2	B	172/207 (83%)	0.13	3 (1%)	69 50	55, 71, 116, 132	0
2	E	172/207 (83%)	0.18	2 (1%)	76 59	58, 77, 116, 132	0
3	C	12/67 (17%)	0.99	1 (8%)	17 11	61, 67, 113, 120	0
3	F	12/67 (17%)	1.03	2 (16%)	4 3	65, 74, 116, 121	0
All	All	1893/2396 (79%)	0.38	99 (5%)	33 20	49, 77, 121, 161	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	THR	6.7
1	D	192	GLU	5.2
1	A	192	GLU	4.3
1	A	732	LEU	4.1
1	D	486	LEU	4.0
1	A	915	GLY	3.9
1	D	913	ILE	3.9
2	B	170	ALA	3.9
1	D	198	LEU	3.8
1	A	733	ASP	3.5
1	A	175	LEU	3.5
1	D	122	LEU	3.5
1	D	732	LEU	3.4
1	A	440	THR	3.4
1	A	191	ASP	3.3
1	A	914	GLN	3.3
1	A	194	ASN	3.2
1	D	440	THR	3.2
1	A	530	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	228	ASN	3.2
1	D	914	GLN	3.2
1	D	172	ILE	3.2
1	D	733	ASP	3.1
1	D	142	VAL	3.1
1	D	902	GLY	3.1
3	C	31	ALA	3.1
1	D	912	GLY	3.0
1	A	205	VAL	3.0
1	A	181	LEU	3.0
1	D	125	ALA	3.0
3	F	31	ALA	3.0
1	D	130	ILE	2.9
1	D	226	LEU	2.9
1	A	855	TYR	2.9
1	D	128	ALA	2.9
1	D	522	TYR	2.9
1	A	188	VAL	2.9
2	B	167	ALA	2.9
1	A	173	ALA	2.8
1	A	593	ASP	2.8
1	D	828	VAL	2.8
1	A	206	GLY	2.8
1	D	202	GLY	2.8
1	A	208	VAL	2.7
2	B	164	LEU	2.7
1	A	207	ASN	2.7
1	A	224	VAL	2.7
1	D	193	ALA	2.7
1	A	486	LEU	2.7
1	D	754	ARG	2.7
1	A	902	GLY	2.7
1	A	727	LEU	2.7
1	D	205	VAL	2.6
1	D	146	MET	2.6
1	D	124	ALA	2.6
1	A	723	LYS	2.6
1	A	828	VAL	2.6
1	D	484	ASP	2.6
1	D	845	ARG	2.5
1	D	156	PRO	2.5
1	D	917	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	175	LEU	2.5
1	A	226	LEU	2.5
1	A	180	VAL	2.5
1	D	905	THR	2.4
1	D	898	GLY	2.4
1	A	522	TYR	2.4
1	D	163	ALA	2.4
1	A	748	ARG	2.3
1	A	230	GLU	2.3
1	D	728	ASP	2.3
1	A	781	VAL	2.3
1	D	335	ASP	2.3
2	E	132	GLN	2.3
3	F	21	GLY	2.3
1	D	810	GLY	2.2
1	A	176	ALA	2.2
1	D	173	ALA	2.2
1	D	230	GLU	2.2
1	A	597	ASP	2.2
1	D	138	TYR	2.2
1	D	622	ALA	2.2
1	A	856	ASP	2.2
1	D	244	HIS	2.1
1	D	827	LEU	2.1
1	A	906	GLU	2.1
1	A	198	LEU	2.1
1	A	204	LEU	2.1
1	D	127	LEU	2.1
1	A	728	ASP	2.1
1	A	289	ALA	2.1
1	A	179	VAL	2.0
1	D	215	MET	2.0
1	D	126	GLN	2.0
1	A	813	ASN	2.0
1	A	193	ALA	2.0
1	D	174	THR	2.0
2	E	71	ALA	2.0
1	D	781	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

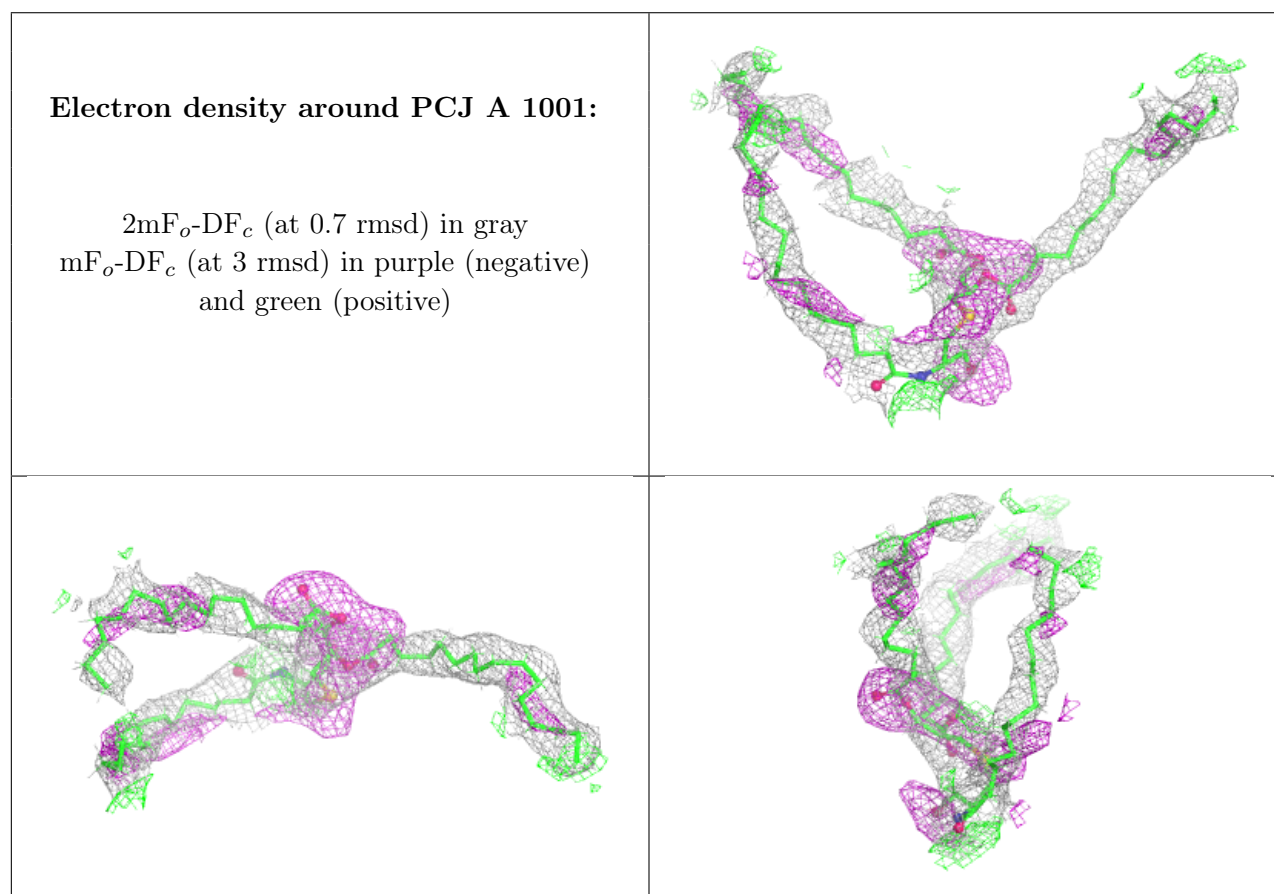
There are no oligosaccharides in this entry.

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.

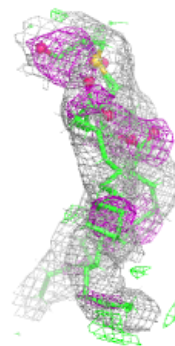
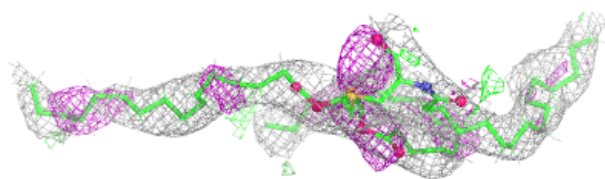
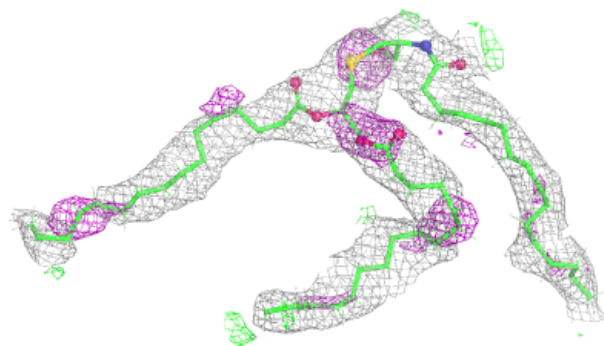
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PCJ	A	1001	62/62	0.70	0.16	44,60,69,99	0
4	PCJ	D	1001	62/62	0.75	0.14	41,60,72,80	0

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 PCJ D 1001:

$2mF_o-DF_c$ (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.