



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:34 AM UTC

PDB ID : 2PG8 / pdb_00002pg8
Title : Crystal structure of R254K mutant of DpgC with bound substrate analog
Authors : Fielding, E.N.
Deposited on : 2007-04-09
Resolution : 3.00 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)
Xtrriage (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

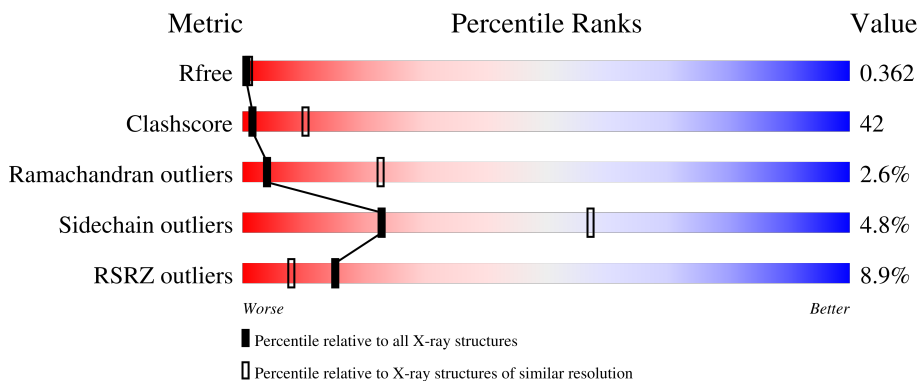
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	417	
1	B	417	
1	C	417	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9923 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.

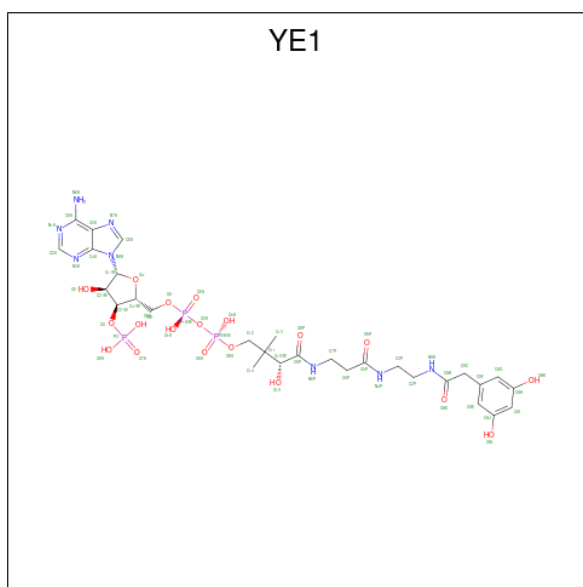
- Molecule 1 is a protein called DpgC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	417	3186	2003	588	585	10	0	0	0
1	B	417	3232	2029	600	593	10	0	0	0
1	C	415	3201	2010	594	587	10	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

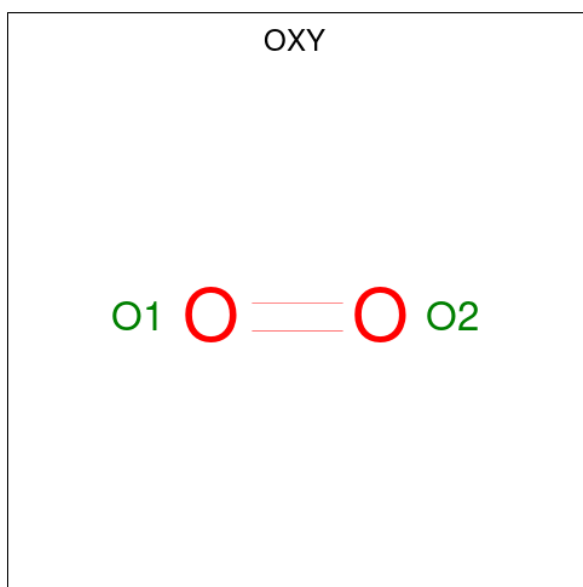
Chain	Residue	Modelled	Actual	Comment	Reference
A	254	LYS	ARG	engineered mutation	UNP Q8KCLK7
B	254	LYS	ARG	engineered mutation	UNP Q8KCLK7
C	254	LYS	ARG	engineered mutation	UNP Q8KCLK7

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-4-HYDROXY-3-(PHOSPHONOXY)TETRAHYDROFURAN-2-YL]METHYL (3R)-4-({3-[(2-{[(3,5-DIHYDROXYPHENYL)ACETYL]AMINO}ETHYL)AMINO]-3-OXOPROPYL}AMINO)-3-HYDROXY-2,2-DIMETHYL-4-OXOBUTYL DIHYDROGEN DIPHOSPHATE (CCD ID: YE1) (formula: C₂₉H₄₃N₈O₁₉P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	59	29	8	19	3	0	0
2	B	1	59	29	8	19	3	0	0
2	C	1	59	29	8	19	3	0	0

- Molecule 3 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	1	2	2	0	0

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

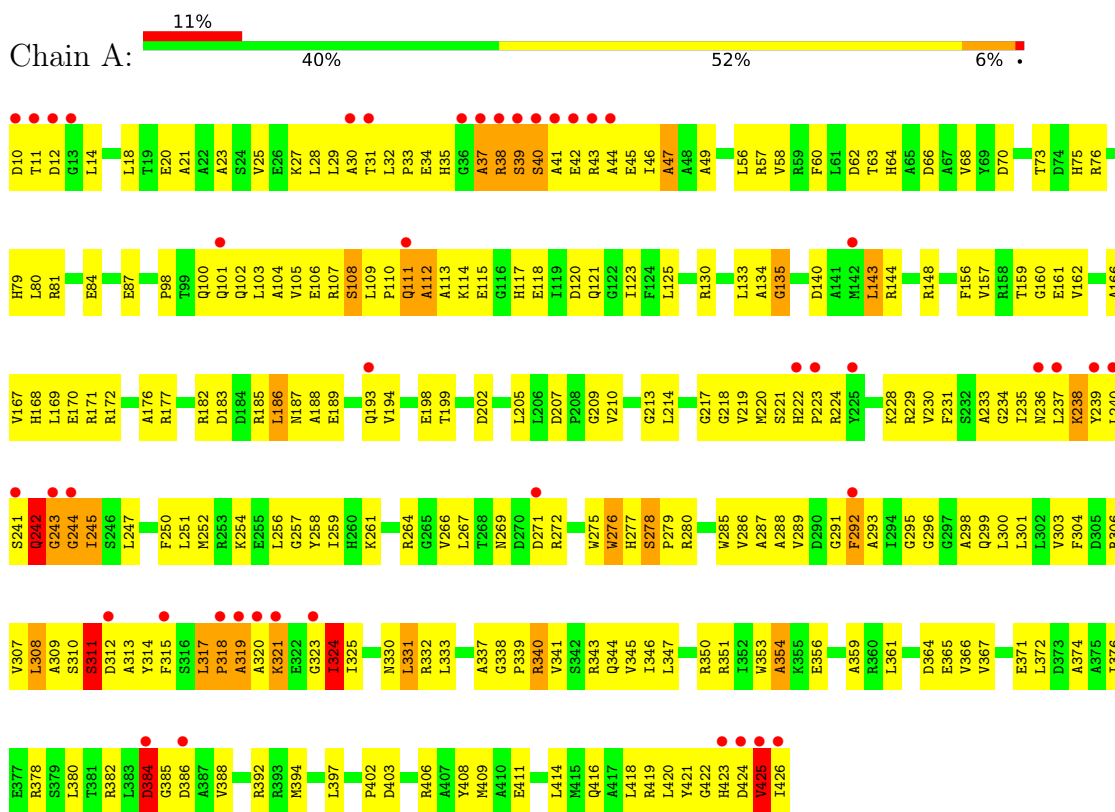
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	0	0
4	B	43	Total O 43 43	0	0
4	C	36	Total O 36 36	0	0

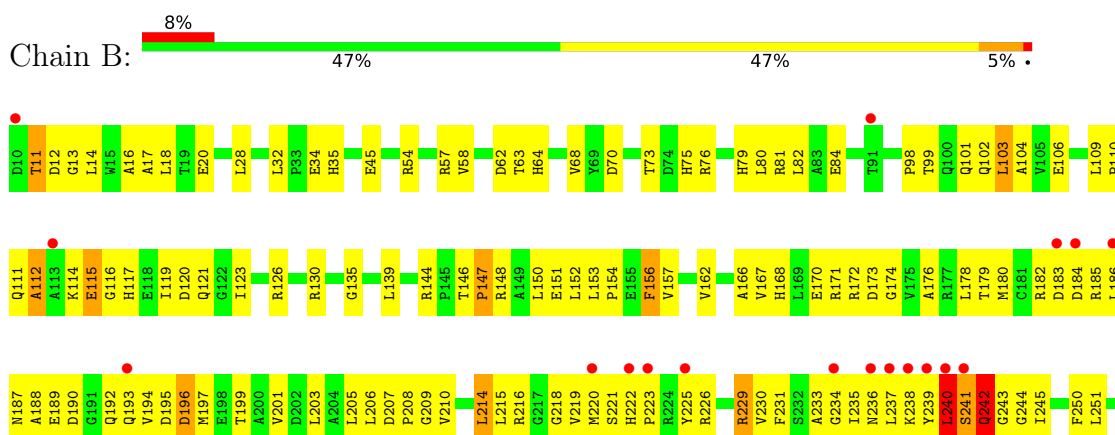
3 Residue-property plots i

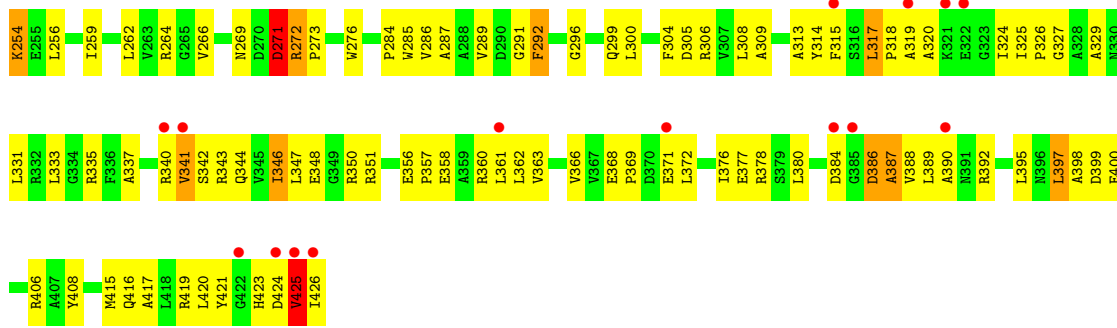
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DpgC

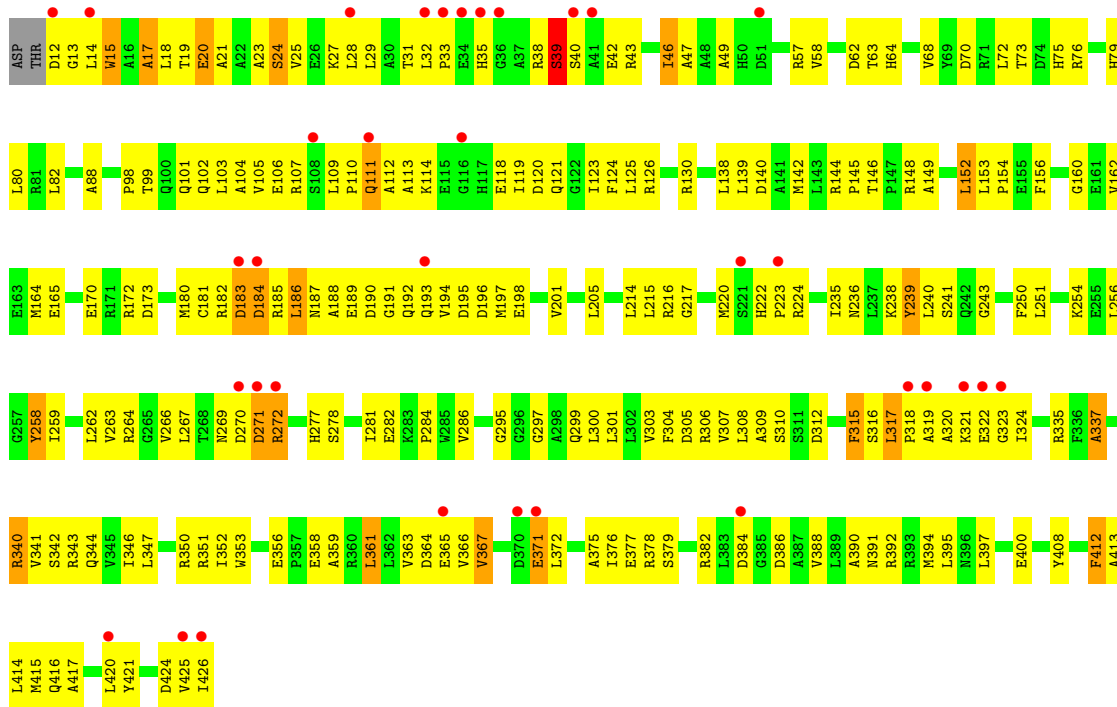


• Molecule 1: DpgC





• Molecule 1: DpgC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.05Å 155.31Å 169.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	61.2 (50.00-3.00) 93.5 (50.00-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 3.01Å)	Xtrriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.331 , 0.367 0.330 , 0.362	Depositor DCC
R_{free} test set	7438 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtrriage
Anisotropy	0.730	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	9923	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.94 % 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 6.3135e-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: OXY, YE1

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	0.58	0/3245	0.98	9/4403 (0.2%)
1	B	0.59	0/3292	1.05	24/4462 (0.5%)
1	C	0.58	0/3261	1.01	19/4419 (0.4%)
All	All	0.58	0/9798	1.01	52/13284 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	2
1	C	0	4
All	All	0	15

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	ASP	N-CA-C	-9.03	102.41	113.97
1	B	14	LEU	N-CA-C	-7.65	103.40	112.89
1	C	384	ASP	N-CA-C	7.59	119.34	111.14
1	B	386	ASP	N-CA-C	-7.53	104.22	113.41
1	B	387	ALA	N-CA-C	-7.46	103.23	111.36
1	A	338	GLY	CA-C-N	7.30	127.31	119.28
1	A	338	GLY	C-N-CA	7.30	127.31	119.28
1	C	258	TYR	N-CA-C	7.20	119.13	111.28
1	C	346	ILE	N-CA-C	6.55	118.14	111.00
1	B	115	GLU	N-CA-C	-6.41	105.44	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	317	LEU	CA-C-N	6.38	127.81	119.84
1	B	317	LEU	C-N-CA	6.38	127.81	119.84
1	A	108	SER	N-CA-CB	-6.38	102.07	111.51
1	C	361	LEU	N-CA-C	-6.35	105.36	113.23
1	C	19	THR	N-CA-C	6.34	117.85	111.07
1	B	135	GLY	CA-C-N	6.33	126.02	119.56
1	B	135	GLY	C-N-CA	6.33	126.02	119.56
1	A	160	GLY	N-CA-C	-6.30	106.55	115.43
1	C	121	GLN	N-CA-C	-6.25	104.58	111.82
1	A	346	ILE	N-CA-C	6.19	116.37	110.74
1	C	375	ALA	N-CA-C	-6.18	104.54	111.28
1	B	346	ILE	N-CA-C	6.09	117.64	111.00
1	C	160	GLY	N-CA-C	-5.99	107.05	115.32
1	B	17	ALA	N-CA-C	-5.97	104.68	111.07
1	C	386	ASP	N-CA-C	-5.96	106.01	113.28
1	B	242	GLN	O-C-N	-5.91	114.57	122.49
1	C	181	CYS	N-CA-C	5.89	116.85	108.54
1	B	417	ALA	N-CA-C	-5.89	104.86	111.28
1	B	156	PHE	N-CA-C	-5.85	104.82	111.14
1	B	289	VAL	N-CA-C	5.84	116.52	107.99
1	B	371	GLU	N-CA-C	5.71	120.24	112.88
1	C	412	PHE	N-CA-C	-5.62	104.85	110.97
1	B	240	LEU	N-CA-C	-5.57	105.29	111.36
1	B	229	ARG	N-CA-C	-5.48	103.30	110.53
1	B	241	SER	N-CA-C	-5.45	105.42	111.36
1	C	337	ALA	N-CA-C	5.45	117.42	110.61
1	C	46	ILE	N-CA-C	-5.43	105.20	110.42
1	A	354	ALA	N-CA-C	5.34	117.79	111.33
1	B	146	THR	CA-C-N	5.28	125.34	119.32
1	B	146	THR	C-N-CA	5.28	125.34	119.32
1	C	320	ALA	N-CA-C	5.23	119.42	112.72
1	C	424	ASP	N-CA-C	5.18	116.93	111.28
1	B	103	LEU	N-CA-C	-5.18	105.64	111.28
1	B	292	PHE	N-CA-C	5.17	115.87	108.74
1	C	138	LEU	N-CA-C	-5.13	105.87	111.82
1	C	17	ALA	N-CA-C	-5.10	104.80	111.02
1	C	20	GLU	N-CA-C	-5.09	105.85	111.71
1	A	278	SER	N-CA-C	5.08	117.88	108.94
1	B	356	GLU	CA-C-N	5.08	126.19	119.84
1	B	356	GLU	C-N-CA	5.08	126.19	119.84
1	A	321	LYS	N-CA-C	5.07	116.88	111.36
1	C	297	GLY	N-CA-C	-5.07	106.62	112.50

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	GLN	Peptide
1	A	243	GLY	Peptide
1	A	292	PHE	Peptide
1	A	317	LEU	Peptide
1	A	37	ALA	Peptide
1	A	384	ASP	Peptide
1	A	39	SER	Peptide
1	A	40	SER	Peptide
1	A	41	ALA	Peptide
1	B	241	SER	Mainchain
1	B	242	GLN	Mainchain
1	C	184	ASP	Peptide
1	C	317	LEU	Peptide
1	C	39	SER	Peptide
1	C	40	SER	Peptide

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	3186	0	3176	334	0
1	B	3232	0	3244	258	0
1	C	3201	0	3201	235	0
2	A	59	0	37	20	0
2	B	59	0	37	12	0
2	C	59	0	37	11	0
3	A	2	0	0	1	0
3	C	2	0	0	0	0
4	A	44	0	0	4	0
4	B	43	0	0	2	0
4	C	36	0	0	2	0
All	All	9923	0	9732	817	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 42.

All (817) 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:A:230:VAL:HG11	1:A:292:PHE:CE2	1.49	1.47
1:B:183:ASP:HA	1:B:220:MET:SD	1.55	1.45
1:B:337:ALA:CB	1:B:341:VAL:HG11	1.51	1.37
1:A:230:VAL:CG1	1:A:292:PHE:CE2	2.24	1.18
1:C:266:VAL:HG23	1:C:281:ILE:HG22	1.24	1.16
1:B:337:ALA:HB1	1:B:341:VAL:HG11	1.23	1.14
1:C:99:THR:HG23	1:C:102:GLN:HE21	0.96	1.12
1:C:99:THR:HG23	1:C:102:GLN:NE2	1.66	1.10
1:C:182:ARG:HH11	1:C:185:ARG:HD2	1.02	1.09
1:A:230:VAL:HG11	1:A:292:PHE:CZ	1.89	1.08
1:A:111:GLN:HA	1:A:114:LYS:HD2	1.18	1.07
1:C:111:GLN:HG2	1:C:243:GLY:HA2	1.37	1.07
1:B:337:ALA:CB	1:B:341:VAL:CG1	2.32	1.06
1:A:384:ASP:HB2	1:C:321:LYS:HZ1	1.16	1.05
1:A:38:ARG:HH11	1:A:38:ARG:CG	1.67	1.05
1:B:337:ALA:HB1	1:B:341:VAL:CG1	1.85	1.05
1:C:266:VAL:CG2	1:C:281:ILE:CG2	2.35	1.03
1:B:139:LEU:CD2	1:B:256:LEU:HD22	1.87	1.03
1:B:183:ASP:CA	1:B:220:MET:SD	2.49	1.00
1:C:182:ARG:NH1	1:C:185:ARG:HD2	1.77	0.99
1:C:186:LEU:CD1	1:C:220:MET:HE2	1.94	0.97
1:C:266:VAL:HG23	1:C:281:ILE:CG2	1.93	0.97
1:C:266:VAL:CG2	1:C:281:ILE:HG22	1.96	0.94
1:A:110:PRO:HG2	1:A:113:ALA:HB3	1.48	0.94
1:A:425:VAL:O	1:A:426:ILE:HG13	1.65	0.94
1:A:143:LEU:HD13	1:A:280:ARG:CD	1.97	0.94
1:C:191:GLY:HA2	1:C:250:PHE:HD1	1.33	0.93
1:A:12:ASP:OD2	1:A:14:LEU:HB2	1.69	0.93
1:A:183:ASP:HA	1:A:220:MET:SD	2.09	0.92
1:A:308:LEU:HD13	1:A:365:GLU:HB2	1.52	0.92
1:C:286:VAL:HG22	1:C:306:ARG:HB3	1.49	0.91
1:B:254:LYS:NZ	1:B:259:ILE:HD11	1.86	0.91
1:A:308:LEU:N	1:A:308:LEU:HD22	1.85	0.90
1:C:186:LEU:H	1:C:220:MET:HE1	1.35	0.90
1:B:194:VAL:HG21	1:B:250:PHE:CD1	2.06	0.90
1:A:38:ARG:HH11	1:A:38:ARG:HG3	1.36	0.90
1:B:254:LYS:HZ3	1:B:259:ILE:HD11	1.38	0.89
1:B:183:ASP:HB2	1:B:221:SER:N	1.87	0.89
1:C:186:LEU:HD12	1:C:220:MET:HE2	1.51	0.89
1:A:308:LEU:N	1:A:308:LEU:CD2	2.35	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:HA	1:B:220:MET:HE3	1.54	0.88
1:B:337:ALA:HB1	1:B:341:VAL:CB	2.02	0.88
1:C:308:LEU:HD23	1:C:365:GLU:HB3	1.55	0.88
1:B:337:ALA:HB3	1:B:341:VAL:HG11	1.54	0.88
1:B:423:HIS:HD2	4:B:1027:HOH:O	1.58	0.87
1:C:254:LYS:HE3	2:C:999:YE1:OAL	1.72	0.87
1:B:99:THR:H	1:B:102:GLN:HE21	1.19	0.87
1:A:112:ALA:HB2	1:A:426:ILE:HG21	1.55	0.87
1:B:214:LEU:HD12	1:B:380:LEU:HD21	1.54	0.87
1:B:176:ALA:HB2	1:B:210:VAL:HG11	1.55	0.86
1:B:337:ALA:HB1	1:B:341:VAL:HG21	1.55	0.86
1:C:20:GLU:O	1:C:23:ALA:HB3	1.74	0.86
1:A:238:LYS:O	1:A:242:GLN:HG2	1.76	0.86
1:A:143:LEU:CD1	1:A:280:ARG:HD3	2.05	0.85
1:C:39:SER:H	1:C:42:GLU:HB2	1.41	0.85
1:A:38:ARG:O	1:A:40:SER:HA	1.76	0.85
1:A:337:ALA:HB1	1:A:341:VAL:HG11	1.54	0.85
1:A:319:ALA:HB1	1:A:323:GLY:HA3	1.57	0.85
1:A:183:ASP:HB2	1:A:221:SER:N	1.92	0.84
1:A:254:LYS:HE2	2:A:997:YE1:HAI	1.57	0.84
1:A:38:ARG:HH11	1:A:38:ARG:HG2	1.43	0.83
1:B:235:ILE:HD11	1:B:245:ILE:HD12	1.60	0.83
1:A:40:SER:N	1:A:42:GLU:H	1.76	0.83
1:A:143:LEU:HD13	1:A:280:ARG:HD2	1.58	0.83
1:A:307:VAL:C	1:A:308:LEU:HD22	2.03	0.83
1:C:99:THR:OG1	1:C:102:GLN:HG3	1.79	0.83
1:A:111:GLN:CA	1:A:114:LYS:HD2	2.07	0.83
1:B:337:ALA:HB1	1:B:341:VAL:CG2	2.09	0.82
1:A:108:SER:O	1:A:109:LEU:HD23	1.81	0.81
1:B:214:LEU:C	1:B:214:LEU:HD23	2.06	0.81
1:A:337:ALA:CB	1:A:341:VAL:HG11	2.11	0.81
1:B:286:VAL:HG22	1:B:306:ARG:HB3	1.63	0.80
1:C:39:SER:N	1:C:42:GLU:HB2	1.95	0.80
1:A:183:ASP:HB2	1:A:221:SER:H	1.45	0.80
1:A:39:SER:C	1:A:42:GLU:H	1.90	0.80
1:C:39:SER:H	1:C:42:GLU:CB	1.94	0.80
1:A:230:VAL:CG1	1:A:292:PHE:CZ	2.58	0.80
1:A:287:ALA:HB2	1:A:304:PHE:CE1	2.17	0.80
1:B:236:ASN:HA	2:B:998:YE1:N1A	1.97	0.79
1:B:139:LEU:HD21	1:B:256:LEU:HD22	1.63	0.79
1:A:106:GLU:OE1	1:A:114:LYS:HB3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ARG:HH11	1:B:272:ARG:CG	1.95	0.79
1:C:186:LEU:H	1:C:220:MET:CE	1.95	0.79
1:C:99:THR:CG2	1:C:102:GLN:HE21	1.87	0.78
1:B:147:PRO:O	1:B:151:GLU:HG3	1.82	0.78
1:A:426:ILE:HG22	1:A:426:ILE:O	1.84	0.78
1:A:143:LEU:CD1	1:A:280:ARG:CD	2.61	0.78
1:A:189:GLU:HB2	1:A:235:ILE:HA	1.66	0.78
1:B:167:VAL:HG12	1:B:168:HIS:N	1.99	0.78
1:A:286:VAL:HG22	1:A:306:ARG:HB3	1.65	0.77
1:A:337:ALA:O	1:A:341:VAL:CG2	2.33	0.77
1:B:139:LEU:CD1	1:B:406:ARG:HG3	2.16	0.76
1:B:388:VAL:HG12	1:B:388:VAL:O	1.84	0.76
1:A:112:ALA:CA	1:A:426:ILE:HD13	2.15	0.76
1:B:139:LEU:HD11	1:B:406:ARG:HG3	1.65	0.76
1:A:29:LEU:HD11	1:A:115:GLU:HG3	1.67	0.76
1:A:109:LEU:HB3	1:A:110:PRO:HD2	1.67	0.76
1:C:28:LEU:N	1:C:28:LEU:HD12	2.01	0.76
1:B:337:ALA:HB3	1:B:341:VAL:CG1	2.12	0.76
1:B:111:GLN:O	1:B:112:ALA:CB	2.33	0.76
1:C:18:LEU:HD11	1:C:57:ARG:HG2	1.67	0.75
1:A:231:PHE:HB3	1:A:292:PHE:O	1.87	0.75
1:B:139:LEU:HD23	1:B:256:LEU:HD22	1.68	0.75
1:C:182:ARG:HH11	1:C:185:ARG:CD	1.92	0.75
1:C:266:VAL:HG22	1:C:281:ILE:CG2	2.15	0.75
1:A:337:ALA:O	1:A:341:VAL:HG21	1.87	0.75
1:B:126:ARG:O	1:B:130:ARG:HG3	1.87	0.74
1:A:425:VAL:O	1:A:426:ILE:CG1	2.36	0.74
1:A:353:TRP:O	1:A:356:GLU:HG2	1.87	0.74
1:C:322:GLU:O	1:C:425:VAL:HG22	1.87	0.74
1:A:46:ILE:HG23	1:A:47:ALA:H	1.52	0.74
1:B:82:LEU:HD11	1:B:256:LEU:HD12	1.68	0.74
1:B:361:LEU:O	1:B:362:LEU:HD23	1.88	0.74
1:C:186:LEU:HD13	1:C:220:MET:HE2	1.68	0.74
1:B:167:VAL:HG12	1:B:168:HIS:H	1.52	0.73
1:B:423:HIS:CD2	4:B:1027:HOH:O	2.36	0.73
1:B:223:PRO:HA	1:B:226:ARG:HG3	1.69	0.73
1:B:419:ARG:O	1:B:425:VAL:HG21	1.87	0.73
1:B:291:GLY:O	1:B:313:ALA:HA	1.89	0.73
1:A:135:GLY:HA3	1:A:406:ARG:HD2	1.70	0.73
2:A:997:YE1:O9A	2:A:997:YE1:O2'	2.04	0.73
1:A:112:ALA:HB2	1:A:426:ILE:HD13	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LEU:O	1:C:21:ALA:HB3	1.89	0.73
1:C:12:ASP:CG	1:C:13:GLY:H	1.97	0.72
1:A:189:GLU:HB3	1:A:250:PHE:HZ	1.54	0.72
1:C:343:ARG:HG3	1:C:343:ARG:HH11	1.54	0.72
1:C:180:MET:HE2	1:C:215:LEU:HD11	1.72	0.72
1:B:222:HIS:O	1:B:226:ARG:HG2	1.89	0.72
1:B:324:ILE:HD11	2:B:998:YE1:HAC1	1.72	0.72
1:A:143:LEU:HD12	1:A:280:ARG:HD3	1.71	0.72
1:B:101:GLN:O	1:B:104:ALA:HB3	1.90	0.72
1:B:186:LEU:HD11	1:B:225:TYR:CD1	2.24	0.72
1:B:272:ARG:HB2	1:B:273:PRO:HD2	1.70	0.72
1:A:14:LEU:HD23	1:A:60:PHE:HA	1.70	0.72
1:B:237:LEU:O	1:B:240:LEU:N	2.20	0.72
1:B:189:GLU:OE2	1:B:254:LYS:HE3	1.90	0.71
1:A:254:LYS:HE2	2:A:997:YE1:CAI	2.20	0.71
1:A:261:LYS:HD3	1:A:266:VAL:HG12	1.69	0.71
1:A:98:PRO:CG	1:A:117:HIS:HB3	2.20	0.71
1:C:39:SER:H	1:C:42:GLU:CG	2.03	0.71
1:B:130:ARG:HG2	1:B:130:ARG:HH11	1.56	0.71
1:B:272:ARG:HH11	1:B:272:ARG:HG2	1.56	0.71
1:C:262:LEU:O	1:C:392:ARG:NH2	2.24	0.71
1:B:182:ARG:HB2	1:B:187:ASN:OD1	1.90	0.70
1:B:194:VAL:CG2	1:B:250:PHE:CE1	2.74	0.70
1:A:230:VAL:CG1	1:A:292:PHE:CD2	2.74	0.70
1:C:130:ARG:HG2	1:C:130:ARG:HH11	1.56	0.70
1:C:281:ILE:HG23	1:C:281:ILE:O	1.90	0.70
1:A:217:GLY:O	1:A:229:ARG:HD3	1.89	0.70
1:B:99:THR:N	1:B:102:GLN:HE21	1.89	0.70
2:B:998:YE1:O9A	2:B:998:YE1:O2'	2.08	0.70
1:A:111:GLN:HA	1:A:114:LYS:CD	2.11	0.70
1:C:182:ARG:O	1:C:184:ASP:N	2.22	0.70
1:A:110:PRO:O	1:A:111:GLN:C	2.35	0.69
1:B:139:LEU:HD21	1:B:256:LEU:CD2	2.21	0.69
1:A:257:GLY:O	1:A:261:LYS:HG3	1.91	0.69
1:A:422:GLY:O	1:A:425:VAL:HG12	1.93	0.69
1:B:296:GLY:O	1:B:299:GLN:HB2	1.92	0.69
1:A:46:ILE:HG23	1:A:47:ALA:N	2.06	0.69
1:B:194:VAL:CG2	1:B:250:PHE:CD1	2.76	0.69
1:C:57:ARG:HD2	1:C:120:ASP:OD1	1.93	0.69
1:C:182:ARG:HB2	1:C:187:ASN:HA	1.75	0.69
1:A:321:LYS:HZ2	1:B:384:ASP:HB2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ILE:CD1	1:B:250:PHE:HE2	2.05	0.69
1:B:337:ALA:O	1:B:341:VAL:CG2	2.40	0.69
1:A:73:THR:HG22	1:A:80:LEU:HD12	1.75	0.69
1:A:98:PRO:HG3	1:A:117:HIS:HB3	1.75	0.69
1:A:220:MET:HA	1:A:220:MET:HE2	1.76	0.68
1:A:425:VAL:O	1:A:425:VAL:HG13	1.93	0.68
1:A:343:ARG:O	1:A:347:LEU:HB2	1.93	0.68
1:B:99:THR:HG23	1:B:102:GLN:NE2	2.08	0.68
1:B:139:LEU:CD2	1:B:256:LEU:CD2	2.69	0.68
1:A:311:SER:O	1:A:354:ALA:HB3	1.92	0.68
1:C:39:SER:O	1:C:42:GLU:HG3	1.94	0.68
1:B:166:ALA:HB1	1:B:193:GLN:OE1	1.93	0.68
1:A:43:ARG:O	1:A:46:ILE:HG22	1.92	0.68
1:A:112:ALA:CB	1:A:426:ILE:HD13	2.24	0.68
1:A:87:GLU:OE2	1:A:100:GLN:HB2	1.94	0.68
1:B:317:LEU:HD12	1:B:346:ILE:HG12	1.76	0.68
1:C:182:ARG:HB3	1:C:185:ARG:HG2	1.76	0.68
1:B:99:THR:H	1:B:102:GLN:NE2	1.92	0.67
1:B:186:LEU:HA	1:B:220:MET:CE	2.25	0.67
1:B:325:ILE:O	2:B:998:YE1:HAG	1.94	0.67
1:A:169:LEU:HD12	1:A:170:GLU:H	1.59	0.67
1:B:73:THR:HG22	1:B:80:LEU:HD12	1.75	0.67
1:A:354:ALA:HB1	1:A:366:VAL:CG1	2.23	0.67
1:A:343:ARG:HG3	1:A:343:ARG:HH11	1.60	0.67
1:A:384:ASP:HB2	1:C:321:LYS:NZ	2.03	0.67
1:C:222:HIS:CE1	1:C:224:ARG:H	2.13	0.66
2:C:999:YE1:OAD	2:C:999:YE1:HAE	1.95	0.66
1:A:414:LEU:O	1:A:418:LEU:HG	1.96	0.66
1:B:194:VAL:HG23	1:B:250:PHE:CE1	2.30	0.66
1:A:38:ARG:HG2	1:A:38:ARG:NH1	2.06	0.66
1:B:254:LYS:NZ	1:B:259:ILE:CD1	2.58	0.66
2:A:997:YE1:OAD	2:A:997:YE1:HAE	1.95	0.66
1:C:371:GLU:HG3	1:C:371:GLU:O	1.95	0.66
1:C:282:GLU:OE1	1:C:392:ARG:NH1	2.29	0.66
1:B:337:ALA:HB2	1:B:341:VAL:HG11	1.72	0.66
1:A:39:SER:HA	1:A:40:SER:HB3	1.78	0.65
1:B:408:TYR:CE1	1:C:394:MET:HE3	2.30	0.65
1:B:183:ASP:OD2	1:B:221:SER:HB3	1.96	0.65
2:B:998:YE1:OAD	2:B:998:YE1:HAE	1.95	0.65
1:C:235:ILE:HB	2:C:999:YE1:HAE	1.78	0.65
1:B:170:GLU:OE1	1:B:172:ARG:HD3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:SER:O	1:A:42:GLU:N	2.30	0.65
1:A:185:ARG:O	1:A:186:LEU:HB2	1.95	0.65
1:A:304:PHE:O	1:C:340:ARG:NH2	2.29	0.65
1:B:166:ALA:HB1	1:B:193:GLN:CD	2.22	0.65
1:C:103:LEU:O	1:C:106:GLU:HB2	1.97	0.65
1:A:43:ARG:CA	1:A:46:ILE:HG22	2.27	0.65
1:C:216:ARG:HG2	1:C:217:GLY:H	1.62	0.65
1:A:106:GLU:CD	1:A:114:LYS:HB3	2.21	0.65
1:A:287:ALA:HB2	1:A:304:PHE:CD1	2.32	0.65
1:A:425:VAL:O	1:A:425:VAL:CG1	2.44	0.65
1:A:397:LEU:O	1:A:397:LEU:HD23	1.97	0.64
1:B:237:LEU:O	1:B:239:TYR:N	2.30	0.64
1:A:112:ALA:HA	1:A:426:ILE:CD1	2.28	0.64
1:B:172:ARG:O	1:B:173:ASP:HB2	1.97	0.64
1:A:267:LEU:HA	1:A:280:ARG:HG2	1.80	0.64
1:B:98:PRO:HG3	1:B:117:HIS:HB3	1.79	0.64
1:A:318:PRO:O	1:A:320:ALA:N	2.30	0.64
1:C:191:GLY:HA2	1:C:250:PHE:CD1	2.23	0.64
1:A:143:LEU:HD13	1:A:280:ARG:HD3	1.71	0.64
1:B:272:ARG:CG	1:B:272:ARG:NH1	2.59	0.64
1:C:111:GLN:HB2	1:C:241:SER:O	1.98	0.64
1:A:112:ALA:HA	1:A:426:ILE:HD13	1.80	0.64
1:A:310:SER:O	1:A:311:SER:C	2.41	0.64
1:B:176:ALA:HB2	1:B:210:VAL:CG1	2.27	0.64
1:A:239:TYR:O	1:A:244:GLY:N	2.31	0.63
1:A:367:VAL:CG1	1:A:372:LEU:HD13	2.28	0.63
1:C:35:HIS:CE1	1:C:113:ALA:HA	2.33	0.63
1:A:275:TRP:CD1	1:A:279:PRO:HA	2.33	0.63
1:C:28:LEU:HD12	1:C:28:LEU:H	1.62	0.63
1:B:11:THR:C	1:B:13:GLY:H	2.07	0.63
1:C:266:VAL:HG22	1:C:281:ILE:HG23	1.80	0.63
1:C:372:LEU:O	1:C:376:ILE:HG13	1.98	0.63
1:A:264:ARG:HG2	1:A:264:ARG:HH11	1.63	0.63
1:C:73:THR:HG22	1:C:80:LEU:HD12	1.81	0.63
1:A:111:GLN:HB2	1:A:243:GLY:CA	2.28	0.63
1:B:305:ASP:OD2	1:B:392:ARG:NH1	2.32	0.63
1:C:308:LEU:HD21	1:C:365:GLU:OE1	1.99	0.63
1:A:111:GLN:HB2	1:A:243:GLY:HA2	1.80	0.63
1:C:82:LEU:HB2	4:C:1007:HOH:O	1.97	0.63
1:A:118:GLU:HB2	1:A:421:TYR:HE2	1.63	0.63
1:A:254:LYS:HZ2	1:A:259:ILE:HD11	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:PRO:HA	1:B:360:ARG:NH1	2.14	0.62
1:A:46:ILE:CG2	1:A:47:ALA:H	2.12	0.62
1:B:309:ALA:HB3	1:B:363:VAL:HG11	1.80	0.62
1:A:38:ARG:CG	1:A:38:ARG:NH1	2.39	0.62
1:A:411:GLU:HG2	4:A:1020:HOH:O	2.00	0.62
1:C:186:LEU:HA	1:C:220:MET:HE2	1.80	0.62
1:A:254:LYS:NZ	1:A:259:ILE:HD11	2.15	0.62
1:A:319:ALA:CB	1:A:323:GLY:HA3	2.29	0.62
1:C:111:GLN:HG3	1:C:240:LEU:O	1.99	0.62
1:A:170:GLU:OE2	1:A:172:ARG:HD3	2.00	0.62
1:A:312:ASP:CG	1:A:312:ASP:O	2.42	0.62
1:B:99:THR:HG23	1:B:102:GLN:HE21	1.63	0.61
1:A:354:ALA:HB1	1:A:366:VAL:HG13	1.82	0.61
1:B:337:ALA:CB	1:B:341:VAL:CB	2.72	0.61
1:B:372:LEU:O	1:B:376:ILE:HG13	2.00	0.61
1:A:314:TYR:CG	1:A:351:ARG:HD2	2.35	0.61
2:A:997:YE1:HC8	2:A:997:YE1:O10	2.01	0.61
1:A:374:ALA:HB1	1:A:378:ARG:HH12	1.66	0.61
1:B:176:ALA:CB	1:B:210:VAL:HG11	2.30	0.61
1:C:182:ARG:C	1:C:184:ASP:H	2.07	0.61
2:C:999:YE1:O10	2:C:999:YE1:HC8	2.01	0.61
1:A:235:ILE:H	2:A:997:YE1:HC22	1.66	0.60
1:A:27:LYS:O	1:A:30:ALA:N	2.34	0.60
1:A:296:GLY:O	1:A:299:GLN:HB2	2.00	0.60
1:A:343:ARG:HB3	1:A:347:LEU:HD12	1.83	0.60
1:C:222:HIS:CG	1:C:223:PRO:HD2	2.36	0.60
1:B:376:ILE:O	1:B:380:LEU:HG	2.01	0.60
1:B:167:VAL:CG1	1:B:168:HIS:H	2.14	0.60
1:A:10:ASP:O	1:A:12:ASP:N	2.34	0.59
1:A:109:LEU:HB3	1:A:110:PRO:CD	2.32	0.59
1:B:194:VAL:HG23	1:B:250:PHE:HE1	1.67	0.59
1:A:241:SER:O	1:A:243:GLY:N	2.34	0.59
1:B:109:LEU:HB3	1:B:110:PRO:HD2	1.84	0.59
1:B:111:GLN:O	1:B:112:ALA:HB2	2.01	0.59
1:C:397:LEU:HD23	1:C:397:LEU:O	2.02	0.59
1:B:157:VAL:HA	1:B:171:ARG:NH2	2.17	0.59
1:B:226:ARG:HG3	1:B:226:ARG:HH11	1.67	0.59
1:C:307:VAL:HG12	1:C:363:VAL:HG13	1.83	0.59
1:A:272:ARG:NH2	1:A:278:SER:O	2.35	0.59
1:B:343:ARG:HG3	1:B:343:ARG:HH11	1.66	0.59
1:A:29:LEU:HD21	1:A:115:GLU:CD	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:OE1	2:A:997:YE1:HAE	2.02	0.59
1:C:350:ARG:HG2	1:C:351:ARG:N	2.17	0.59
1:A:39:SER:O	1:A:42:GLU:CA	2.50	0.59
1:B:325:ILE:HD11	1:C:390:ALA:HB1	1.82	0.59
1:C:39:SER:H	1:C:42:GLU:CD	2.11	0.59
1:B:357:PRO:HA	1:B:360:ARG:HH11	1.67	0.59
1:A:12:ASP:OD2	1:A:14:LEU:CB	2.48	0.59
1:A:166:ALA:HB1	1:A:193:GLN:OE1	2.03	0.59
1:B:318:PRO:O	1:B:320:ALA:N	2.34	0.58
1:C:324:ILE:HB	1:C:416:GLN:HE22	1.67	0.58
1:A:364:ASP:OD2	1:C:340:ARG:NH1	2.35	0.58
1:C:235:ILE:H	2:C:999:YE1:HC22	1.69	0.58
1:B:16:ALA:O	1:B:20:GLU:HB2	2.03	0.58
1:B:340:ARG:NH2	1:C:301:LEU:O	2.36	0.58
1:A:27:LYS:O	1:A:28:LEU:C	2.45	0.58
1:A:183:ASP:HA	1:A:220:MET:CE	2.33	0.58
2:A:997:YE1:O10	2:A:997:YE1:C8A	2.51	0.58
1:C:263:VAL:CG2	1:C:303:VAL:HG13	2.34	0.58
1:A:222:HIS:CG	1:A:223:PRO:HD2	2.39	0.58
1:C:21:ALA:O	1:C:25:VAL:HG23	2.03	0.58
1:A:205:LEU:HD12	1:A:266:VAL:HG13	1.85	0.58
1:B:194:VAL:HG21	1:B:250:PHE:CE1	2.38	0.58
1:A:230:VAL:HG11	1:A:292:PHE:HE2	1.53	0.57
1:A:254:LYS:CE	2:A:997:YE1:HAI	2.32	0.57
1:C:186:LEU:N	1:C:220:MET:HE1	2.14	0.57
1:A:40:SER:N	1:A:42:GLU:N	2.50	0.57
1:A:236:ASN:OD1	1:A:238:LYS:CB	2.52	0.57
1:C:216:ARG:HG2	1:C:217:GLY:N	2.19	0.57
1:C:310:SER:HB3	1:C:372:LEU:HD22	1.86	0.57
1:A:35:HIS:HA	1:A:38:ARG:HG2	1.86	0.57
1:B:348:GLU:HG3	1:C:306:ARG:NH1	2.19	0.57
1:C:281:ILE:HD11	4:C:1023:HOH:O	2.04	0.57
1:B:235:ILE:HD11	1:B:250:PHE:CE2	2.39	0.57
1:C:14:LEU:O	1:C:17:ALA:HB3	2.04	0.57
1:A:421:TYR:O	1:A:422:GLY:C	2.48	0.57
1:C:269:ASN:HB2	1:C:271:ASP:OD2	2.05	0.57
1:C:343:ARG:HG3	1:C:343:ARG:NH1	2.20	0.57
1:A:254:LYS:HD2	4:A:1006:HOH:O	2.04	0.56
1:C:111:GLN:HA	1:C:114:LYS:HE3	1.87	0.56
1:A:125:LEU:CD1	1:A:252:MET:HG3	2.36	0.56
1:A:235:ILE:HB	2:A:997:YE1:CAB	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:TRP:O	1:A:276:TRP:C	2.48	0.56
1:A:308:LEU:CD1	1:A:365:GLU:HB2	2.31	0.56
1:C:27:LYS:C	1:C:29:LEU:H	2.13	0.56
1:C:28:LEU:H	1:C:28:LEU:CD1	2.18	0.56
1:C:222:HIS:CD2	2:C:999:YE1:H4'	2.40	0.56
1:A:222:HIS:CE1	1:A:224:ARG:H	2.23	0.56
1:B:206:LEU:O	1:B:208:PRO:HD3	2.06	0.56
1:A:46:ILE:CG2	1:A:47:ALA:N	2.68	0.56
2:A:997:YE1:C8A	2:A:997:YE1:HO10	2.18	0.56
1:B:28:LEU:O	1:B:32:LEU:HB2	2.05	0.56
1:C:146:THR:O	1:C:149:ALA:HB3	2.04	0.56
1:C:284:PRO:HA	1:C:305:ASP:OD2	2.06	0.56
2:C:999:YE1:O10	2:C:999:YE1:C8A	2.53	0.56
1:B:254:LYS:HZ2	1:B:259:ILE:CD1	2.19	0.56
1:B:327:GLY:C	1:B:329:ALA:H	2.14	0.56
1:A:35:HIS:HA	1:A:38:ARG:NH1	2.20	0.56
1:B:153:LEU:N	1:B:154:PRO:HD2	2.21	0.56
1:A:110:PRO:O	1:A:112:ALA:N	2.38	0.56
1:A:272:ARG:HG2	1:A:272:ARG:NH1	2.21	0.56
1:A:378:ARG:O	1:A:382:ARG:HG3	2.06	0.56
1:C:186:LEU:N	1:C:220:MET:CE	2.68	0.56
1:C:39:SER:N	1:C:42:GLU:OE1	2.38	0.55
1:A:108:SER:C	1:A:109:LEU:HD23	2.32	0.55
1:A:186:LEU:HD12	1:A:220:MET:HG3	1.87	0.55
1:B:314:TYR:CD2	1:B:351:ARG:HD2	2.41	0.55
1:B:424:ASP:CG	1:B:425:VAL:H	2.15	0.55
1:B:235:ILE:HD11	1:B:250:PHE:HE2	1.71	0.55
1:C:28:LEU:N	1:C:28:LEU:CD1	2.68	0.55
1:B:207:ASP:OD2	1:B:210:VAL:HG23	2.07	0.55
1:C:269:ASN:O	1:C:271:ASP:CG	2.50	0.55
1:A:222:HIS:CD2	2:A:997:YE1:H4'	2.42	0.55
1:A:272:ARG:HG2	1:A:272:ARG:HH11	1.71	0.55
1:B:269:ASN:C	1:B:271:ASP:OD1	2.50	0.55
1:A:110:PRO:O	1:A:113:ALA:N	2.39	0.55
1:A:230:VAL:HG13	1:A:292:PHE:CE2	2.33	0.55
1:A:123:ILE:HD11	1:B:276:TRP:CZ3	2.42	0.55
1:C:103:LEU:O	1:C:107:ARG:HG3	2.07	0.55
1:A:218:GLY:O	1:A:220:MET:HE3	2.06	0.55
1:A:207:ASP:C	1:A:209:GLY:H	2.15	0.54
1:A:18:LEU:HD11	1:A:57:ARG:HG2	1.89	0.54
1:C:189:GLU:HA	1:C:193:GLN:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:TYR:CD1	1:C:239:TYR:N	2.73	0.54
1:A:254:LYS:HE2	2:A:997:YE1:OAL	2.08	0.54
1:C:186:LEU:HA	1:C:220:MET:CE	2.38	0.54
1:A:169:LEU:HD12	1:A:170:GLU:N	2.23	0.54
1:A:425:VAL:O	1:A:426:ILE:CB	2.55	0.54
1:C:172:ARG:HG2	1:C:173:ASP:OD2	2.08	0.54
1:A:354:ALA:HB1	1:A:366:VAL:HG11	1.90	0.54
1:C:12:ASP:CG	1:C:13:GLY:N	2.65	0.54
1:C:182:ARG:NH1	1:C:185:ARG:CD	2.62	0.54
1:C:295:GLY:O	1:C:299:GLN:HG3	2.08	0.54
1:A:236:ASN:HA	2:A:997:YE1:N1A	2.23	0.53
1:C:317:LEU:O	1:C:319:ALA:N	2.42	0.53
2:B:998:YE1:O10	2:B:998:YE1:C8A	2.57	0.53
1:A:372:LEU:O	1:A:376:ILE:HG13	2.08	0.53
1:A:176:ALA:HB2	1:A:210:VAL:HG11	1.90	0.53
1:B:183:ASP:HB2	1:B:221:SER:CB	2.38	0.53
1:A:101:GLN:O	1:A:104:ALA:HB3	2.08	0.53
1:A:394:MET:HE3	1:C:408:TYR:CE1	2.43	0.53
1:A:219:VAL:HG13	1:A:228:LYS:O	2.09	0.53
1:C:281:ILE:CG2	1:C:281:ILE:O	2.57	0.53
1:A:238:LYS:O	1:A:242:GLN:CG	2.54	0.53
1:B:197:MET:O	1:B:201:VAL:HG23	2.08	0.53
1:B:226:ARG:HG3	1:B:226:ARG:NH1	2.24	0.53
1:B:239:TYR:HB3	1:B:244:GLY:HA3	1.90	0.53
1:A:222:HIS:CE1	1:A:223:PRO:HG2	2.44	0.53
1:A:343:ARG:NH2	1:B:399:ASP:OD2	2.30	0.53
1:B:214:LEU:HD23	1:B:214:LEU:O	2.08	0.53
1:A:231:PHE:CD2	1:A:293:ALA:HB2	2.44	0.53
1:B:139:LEU:HD12	1:B:406:ARG:HG3	1.91	0.52
1:A:230:VAL:HG13	1:A:292:PHE:CD2	2.44	0.52
1:A:237:LEU:O	1:A:238:LYS:C	2.52	0.52
1:A:321:LYS:NZ	1:B:384:ASP:HB2	2.24	0.52
2:B:998:YE1:O10	2:B:998:YE1:HC8	2.09	0.52
1:A:103:LEU:HD11	1:A:121:GLN:NE2	2.23	0.52
1:A:189:GLU:CB	1:A:235:ILE:HA	2.38	0.52
1:A:235:ILE:HD11	1:A:245:ILE:HG21	1.90	0.52
1:B:130:ARG:HG2	1:B:130:ARG:NH1	2.22	0.52
1:C:250:PHE:O	1:C:254:LYS:HB2	2.10	0.52
1:A:324:ILE:HG12	3:A:3:OXY:O1	2.10	0.52
1:B:54:ARG:NH1	1:B:119:ILE:HD12	2.25	0.52
1:B:388:VAL:O	1:B:388:VAL:CG1	2.54	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:SER:OG	1:C:318:PRO:HD3	2.10	0.52
1:B:196:ASP:OD1	1:B:196:ASP:N	2.42	0.52
1:B:234:GLY:HA3	2:B:998:YE1:HPN4	1.75	0.52
1:C:201:VAL:HG21	1:C:258:TYR:HB2	1.92	0.52
1:A:331:LEU:HD13	1:A:408:TYR:HB2	1.92	0.52
1:A:340:ARG:NH2	1:B:304:PHE:O	2.42	0.52
1:A:419:ARG:HH12	1:B:386:ASP:CB	2.23	0.52
1:B:180:MET:SD	1:B:215:LEU:HD11	2.50	0.52
1:B:185:ARG:HG3	1:B:188:ALA:H	1.75	0.52
1:C:12:ASP:O	1:C:13:GLY:C	2.52	0.52
1:A:337:ALA:HB1	1:A:341:VAL:CG1	2.35	0.52
1:C:148:ARG:O	1:C:152:LEU:HG	2.10	0.52
1:C:263:VAL:HG23	1:C:303:VAL:CG1	2.39	0.52
1:C:353:TRP:O	1:C:356:GLU:HG2	2.10	0.52
1:C:27:LYS:C	1:C:29:LEU:N	2.69	0.51
1:C:263:VAL:HG12	1:C:264:ARG:HG3	1.92	0.51
1:A:111:GLN:HE21	1:A:426:ILE:CG1	2.23	0.51
2:C:999:YE1:O9A	2:C:999:YE1:O2'	2.23	0.51
1:A:134:ALA:O	1:A:135:GLY:C	2.52	0.51
1:B:424:ASP:CG	1:B:425:VAL:N	2.66	0.51
1:C:186:LEU:CA	1:C:220:MET:HE2	2.41	0.51
1:C:190:ASP:O	1:C:192:GLN:N	2.43	0.51
1:C:272:ARG:O	1:C:272:ARG:HG2	2.08	0.51
1:C:340:ARG:O	1:C:344:GLN:HG3	2.11	0.51
1:C:417:ALA:O	1:C:420:LEU:HB2	2.10	0.51
1:A:106:GLU:OE2	1:A:114:LYS:HB3	2.10	0.51
1:A:275:TRP:O	1:A:277:HIS:N	2.44	0.51
1:B:178:LEU:HD13	1:B:285:TRP:HZ3	1.75	0.51
1:B:235:ILE:HD11	1:B:245:ILE:CD1	2.38	0.51
1:B:343:ARG:HG3	1:B:343:ARG:NH1	2.24	0.51
1:B:425:VAL:HG12	1:B:426:ILE:N	2.24	0.51
1:B:106:GLU:O	1:B:114:LYS:HE3	2.10	0.51
1:B:167:VAL:CG1	1:B:168:HIS:N	2.67	0.51
1:B:309:ALA:CB	1:B:363:VAL:HG11	2.40	0.51
1:B:333:LEU:CD2	1:B:342:SER:HA	2.41	0.51
1:B:335:ARG:NH2	1:B:400:GLU:OE1	2.38	0.51
1:C:82:LEU:HD11	1:C:256:LEU:HD12	1.92	0.51
1:B:189:GLU:O	1:B:236:ASN:HB2	2.11	0.51
1:C:214:LEU:HD12	1:C:286:VAL:O	2.11	0.51
1:B:223:PRO:HA	1:B:226:ARG:CG	2.39	0.51
1:B:235:ILE:CD1	1:B:250:PHE:CE2	2.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:PHE:CD1	1:C:162:VAL:HG23	2.46	0.51
1:C:191:GLY:CA	1:C:250:PHE:HD1	2.13	0.51
1:C:337:ALA:O	1:C:341:VAL:HB	2.11	0.51
1:A:275:TRP:NE1	1:A:279:PRO:HA	2.25	0.51
1:A:314:TYR:CD2	1:A:351:ARG:HD2	2.45	0.51
1:A:240:LEU:HA	1:A:245:ILE:HG12	1.93	0.51
1:B:219:VAL:HA	1:B:229:ARG:HA	1.93	0.51
1:B:377:GLU:HA	1:B:380:LEU:HD12	1.91	0.51
1:C:31:THR:OG1	1:C:32:LEU:HD13	2.10	0.51
1:C:139:LEU:HD21	1:C:256:LEU:HD22	1.93	0.51
1:C:266:VAL:CG2	1:C:281:ILE:HG21	2.34	0.51
1:A:241:SER:C	1:A:243:GLY:N	2.69	0.50
1:A:239:TYR:HA	1:A:242:GLN:HG3	1.93	0.50
1:B:220:MET:HE2	1:B:230:VAL:HB	1.93	0.50
1:B:419:ARG:HH22	1:B:424:ASP:CG	2.19	0.50
1:C:235:ILE:HB	2:C:999:YE1:CAE	2.41	0.50
1:C:303:VAL:HG12	1:C:303:VAL:O	2.10	0.50
1:C:416:GLN:O	1:C:417:ALA:C	2.54	0.50
1:A:186:LEU:HB3	1:A:233:ALA:HB2	1.93	0.50
1:B:186:LEU:HD12	1:B:230:VAL:HG11	1.94	0.50
1:C:263:VAL:HG23	1:C:303:VAL:HG13	1.94	0.50
1:C:70:ASP:OD1	1:C:75:HIS:HA	2.12	0.50
1:A:58:VAL:HG12	1:A:62:ASP:OD2	2.11	0.50
1:A:241:SER:C	1:A:243:GLY:H	2.19	0.50
1:C:15:TRP:O	1:C:18:LEU:HB3	2.12	0.50
1:A:39:SER:C	1:A:42:GLU:N	2.61	0.50
1:A:40:SER:CA	1:A:42:GLU:H	2.24	0.50
1:C:101:GLN:O	1:C:104:ALA:HB3	2.12	0.50
1:A:32:LEU:HB3	1:A:33:PRO:HD2	1.94	0.50
1:A:43:ARG:O	1:A:47:ALA:N	2.43	0.50
1:A:331:LEU:HD13	1:A:408:TYR:CB	2.42	0.50
1:C:58:VAL:HG22	1:C:123:ILE:HG23	1.93	0.50
1:C:58:VAL:HG12	1:C:62:ASP:OD2	2.11	0.50
1:C:106:GLU:OE1	1:C:114:LYS:HB3	2.12	0.50
1:C:111:GLN:CG	1:C:243:GLY:HA2	2.24	0.50
1:A:98:PRO:HG2	1:A:117:HIS:HB3	1.94	0.50
1:B:98:PRO:HD3	1:B:120:ASP:HB2	1.93	0.50
1:B:111:GLN:O	1:B:112:ALA:HB3	2.11	0.50
1:A:207:ASP:C	1:A:209:GLY:N	2.70	0.49
1:B:98:PRO:CG	1:B:117:HIS:HB3	2.42	0.49
1:C:46:ILE:O	1:C:49:ALA:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:PHE:O	1:C:413:ALA:C	2.55	0.49
1:A:331:LEU:HA	1:B:398:ALA:CB	2.43	0.49
1:B:222:HIS:C	1:B:226:ARG:HG2	2.37	0.49
1:C:315:PHE:CD1	1:C:315:PHE:N	2.80	0.49
1:A:213:GLY:HA3	1:A:285:TRP:CE3	2.47	0.49
1:B:239:TYR:O	1:B:243:GLY:N	2.36	0.49
1:B:264:ARG:HH11	1:B:264:ARG:HG2	1.77	0.49
1:B:272:ARG:HB2	1:B:273:PRO:CD	2.42	0.49
1:B:337:ALA:O	1:B:341:VAL:HG21	2.10	0.49
1:A:230:VAL:HG21	1:A:292:PHE:CZ	2.47	0.49
1:A:38:ARG:HG3	1:A:38:ARG:NH1	2.14	0.49
1:A:167:VAL:CG1	1:A:168:HIS:N	2.75	0.49
1:C:352:ILE:HG21	1:C:359:ALA:HA	1.93	0.49
1:B:272:ARG:NH1	1:B:272:ARG:HG3	2.27	0.49
1:C:197:MET:HE3	1:C:258:TYR:CE2	2.47	0.49
1:A:207:ASP:OD1	1:A:209:GLY:N	2.42	0.49
1:B:221:SER:O	1:B:226:ARG:NE	2.45	0.49
1:A:110:PRO:CG	1:A:113:ALA:HB3	2.32	0.49
1:A:106:GLU:C	1:A:108:SER:H	2.21	0.49
1:A:176:ALA:HB2	1:A:210:VAL:CG1	2.43	0.49
1:A:264:ARG:HG2	1:A:264:ARG:NH1	2.25	0.49
1:B:419:ARG:NH2	1:B:424:ASP:OD2	2.46	0.49
1:A:111:GLN:C	1:A:113:ALA:H	2.20	0.49
1:A:111:GLN:O	1:A:114:LYS:HG3	2.13	0.48
1:C:197:MET:O	1:C:201:VAL:HG23	2.13	0.48
1:A:66:ASP:OD1	1:A:133:LEU:HB2	2.14	0.48
1:B:284:PRO:HA	1:B:305:ASP:OD2	2.13	0.48
1:A:251:LEU:HD13	1:A:416:GLN:CG	2.44	0.48
1:B:183:ASP:HB2	1:B:221:SER:H	1.73	0.48
1:B:343:ARG:O	1:B:347:LEU:HB2	2.13	0.48
1:C:236:ASN:HA	2:C:999:YE1:N1A	2.27	0.48
1:A:29:LEU:CD1	1:A:115:GLU:HG3	2.41	0.48
1:A:198:GLU:HA	1:A:258:TYR:HB3	1.94	0.48
1:A:11:THR:O	1:A:12:ASP:C	2.57	0.48
1:A:235:ILE:HB	2:A:997:YE1:HAE	1.94	0.48
1:A:384:ASP:H	1:C:321:LYS:NZ	2.11	0.48
1:B:11:THR:C	1:B:13:GLY:N	2.66	0.48
1:C:46:ILE:HG23	1:C:47:ALA:N	2.28	0.48
1:A:308:LEU:N	1:A:308:LEU:HD23	2.25	0.48
1:C:79:HIS:CD2	1:C:144:ARG:HD2	2.49	0.48
1:A:43:ARG:C	1:A:46:ILE:HG22	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PRO:HD3	1:A:120:ASP:HB2	1.96	0.48
1:B:58:VAL:HG12	1:B:62:ASP:OD2	2.14	0.48
1:C:139:LEU:CD2	1:C:256:LEU:HD22	2.43	0.48
1:C:184:ASP:CG	1:C:185:ARG:HE	2.20	0.48
1:A:171:ARG:HG2	1:A:171:ARG:HH11	1.79	0.48
1:A:189:GLU:HB3	1:A:250:PHE:CZ	2.40	0.48
1:A:339:PRO:O	1:A:343:ARG:HG3	2.14	0.48
1:B:271:ASP:OD1	1:B:271:ASP:N	2.36	0.48
1:A:105:VAL:O	1:A:109:LEU:HG	2.14	0.48
1:A:251:LEU:HD13	1:A:416:GLN:HG2	1.96	0.48
1:B:182:ARG:HD2	1:B:184:ASP:OD1	2.13	0.48
1:B:415:MET:O	1:B:419:ARG:HG2	2.14	0.48
1:A:296:GLY:O	1:A:300:LEU:HD22	2.14	0.47
1:C:215:LEU:HD23	1:C:304:PHE:CZ	2.49	0.47
1:A:256:LEU:CD2	1:A:409:MET:HE2	2.43	0.47
1:B:179:THR:HA	1:B:216:ARG:O	2.13	0.47
1:B:238:LYS:O	1:B:242:GLN:HG3	2.14	0.47
1:C:39:SER:O	1:C:42:GLU:N	2.30	0.47
1:B:157:VAL:HA	1:B:171:ARG:HH22	1.79	0.47
1:B:333:LEU:HD23	1:B:342:SER:HA	1.97	0.47
1:B:343:ARG:HG2	1:C:395:LEU:HD13	1.96	0.47
1:A:114:LYS:HD3	1:A:421:TYR:HE1	1.79	0.47
1:C:376:ILE:O	1:C:379:SER:HB3	2.15	0.47
1:A:25:VAL:HG22	1:A:49:ALA:HB1	1.95	0.47
1:A:66:ASP:CG	1:A:133:LEU:HD12	2.40	0.47
1:A:318:PRO:O	1:A:319:ALA:C	2.57	0.47
1:A:424:ASP:CG	1:A:425:VAL:N	2.73	0.47
1:A:31:THR:OG1	1:A:32:LEU:N	2.47	0.47
1:A:130:ARG:HG2	1:A:130:ARG:HH11	1.79	0.47
1:B:262:LEU:O	1:B:392:ARG:NH2	2.42	0.47
1:B:287:ALA:HB2	1:B:304:PHE:CE2	2.50	0.47
1:B:309:ALA:O	1:B:366:VAL:HA	2.15	0.47
1:B:315:PHE:CZ	1:B:363:VAL:HG21	2.49	0.47
1:C:43:ARG:O	1:C:46:ILE:HG22	2.14	0.47
1:C:182:ARG:C	1:C:184:ASP:N	2.70	0.47
1:C:184:ASP:OD2	1:C:185:ARG:NE	2.43	0.47
1:C:236:ASN:OD1	1:C:238:LYS:HB2	2.15	0.47
1:C:335:ARG:NH2	1:C:400:GLU:HB2	2.30	0.47
1:A:231:PHE:HD2	1:A:293:ALA:HB2	1.79	0.47
1:B:57:ARG:HD2	1:B:120:ASP:OD1	2.15	0.47
1:B:116:GLY:HA2	1:B:421:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:CB	1:A:110:PRO:CD	2.93	0.47
1:A:343:ARG:HG2	1:B:395:LEU:HD13	1.96	0.47
1:B:269:ASN:O	1:B:271:ASP:OD1	2.31	0.47
1:A:156:PHE:CE1	1:A:169:LEU:HG	2.50	0.46
1:A:287:ALA:HB2	1:A:304:PHE:CZ	2.50	0.46
1:C:343:ARG:HB3	1:C:347:LEU:HD12	1.96	0.46
1:C:352:ILE:N	1:C:352:ILE:HD12	2.29	0.46
1:A:43:ARG:C	1:A:45:GLU:N	2.73	0.46
1:C:180:MET:HE2	1:C:215:LEU:CD1	2.42	0.46
1:C:310:SER:OG	1:C:312:ASP:OD1	2.27	0.46
1:C:126:ARG:O	1:C:130:ARG:HG3	2.16	0.46
1:A:75:HIS:O	1:A:76:ARG:C	2.59	0.46
1:B:285:TRP:O	1:B:305:ASP:HB2	2.15	0.46
1:B:347:LEU:HD22	1:C:388:VAL:HG13	1.97	0.46
1:C:112:ALA:HA	1:C:426:ILE:HG21	1.96	0.46
2:A:997:YE1:OAD	2:A:997:YE1:CAE	2.62	0.46
1:A:367:VAL:HG22	1:A:371:GLU:HB2	1.97	0.46
1:A:388:VAL:O	1:A:392:ARG:HB2	2.16	0.46
1:B:397:LEU:HD23	1:B:397:LEU:O	2.16	0.46
1:C:130:ARG:HH11	1:C:130:ARG:CG	2.28	0.46
1:A:38:ARG:HA	1:A:38:ARG:HD3	1.53	0.46
1:A:240:LEU:HB2	1:A:245:ILE:CG1	2.46	0.46
1:A:311:SER:HA	1:A:366:VAL:CG1	2.46	0.46
1:B:70:ASP:OD1	1:B:75:HIS:HA	2.15	0.46
1:B:264:ARG:HG2	1:B:264:ARG:NH1	2.31	0.46
1:A:159:THR:HG22	1:A:161:GLU:N	2.31	0.46
1:A:324:ILE:HB	1:A:325:ILE:H	1.56	0.46
1:B:192:GLN:NE2	1:B:195:ASP:HB3	2.31	0.46
1:B:214:LEU:C	1:B:214:LEU:CD2	2.80	0.46
1:A:419:ARG:NH1	1:B:386:ASP:HB3	2.31	0.46
1:B:64:HIS:O	1:B:68:VAL:HG23	2.16	0.45
1:B:214:LEU:HD12	1:B:380:LEU:CD2	2.36	0.45
1:B:286:VAL:HG13	1:B:308:LEU:HD23	1.98	0.45
1:A:254:LYS:HE2	2:A:997:YE1:CAJ	2.45	0.45
1:A:298:ALA:HA	1:A:301:LEU:HG	1.99	0.45
1:A:341:VAL:O	1:A:344:GLN:HB2	2.17	0.45
4:A:1011:HOH:O	1:C:415:MET:HE1	2.16	0.45
1:C:38:ARG:HB3	1:C:42:GLU:HB3	1.98	0.45
1:C:164:MET:HE1	1:C:196:ASP:O	2.17	0.45
1:C:239:TYR:N	1:C:239:TYR:HD1	2.14	0.45
1:C:308:LEU:CD2	1:C:365:GLU:OE1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:GLU:C	1:C:379:SER:N	2.71	0.45
1:C:414:LEU:O	1:C:415:MET:C	2.57	0.45
1:A:156:PHE:O	1:A:171:ARG:NH2	2.49	0.45
1:A:157:VAL:HA	1:A:171:ARG:HH21	1.82	0.45
1:A:303:VAL:O	1:A:303:VAL:CG1	2.65	0.45
1:B:178:LEU:HD13	1:B:285:TRP:CZ3	2.51	0.45
1:C:153:LEU:HB3	1:C:154:PRO:CD	2.46	0.45
1:A:222:HIS:CD2	1:A:223:PRO:HD2	2.50	0.45
1:C:118:GLU:HB2	1:C:421:TYR:HE2	1.81	0.45
1:C:222:HIS:CE1	1:C:223:PRO:HG2	2.52	0.45
1:B:111:GLN:HB3	1:B:426:ILE:HD11	1.97	0.45
1:B:183:ASP:OD2	1:B:221:SER:CB	2.62	0.45
1:C:75:HIS:O	1:C:76:ARG:C	2.59	0.45
1:A:291:GLY:O	1:A:313:ALA:CB	2.65	0.45
1:A:295:GLY:HA3	2:A:997:YE1:HC21	1.98	0.45
1:A:319:ALA:HB3	4:A:1028:HOH:O	2.15	0.45
1:C:110:PRO:O	1:C:112:ALA:N	2.50	0.45
1:C:187:ASN:O	1:C:188:ALA:C	2.60	0.45
1:A:172:ARG:HB3	1:A:177:ARG:HE	1.82	0.45
1:A:189:GLU:HG3	1:A:234:GLY:O	2.17	0.45
1:A:289:VAL:HB	1:A:309:ALA:CB	2.47	0.45
1:B:387:ALA:C	1:B:389:LEU:H	2.23	0.45
1:A:40:SER:O	1:A:40:SER:OG	2.32	0.45
1:A:167:VAL:HG12	1:A:168:HIS:N	2.30	0.45
1:B:11:THR:O	1:B:13:GLY:N	2.50	0.45
1:B:337:ALA:O	1:B:341:VAL:HG23	2.16	0.45
1:C:58:VAL:HG22	1:C:123:ILE:CG2	2.47	0.45
1:A:397:LEU:HD23	1:A:397:LEU:C	2.41	0.45
1:A:46:ILE:O	1:A:47:ALA:C	2.60	0.44
1:B:222:HIS:CD2	2:B:998:YE1:H4'	2.52	0.44
1:B:237:LEU:N	2:B:998:YE1:N1A	2.63	0.44
1:A:21:ALA:HB2	1:A:56:LEU:HD12	1.98	0.44
1:A:219:VAL:HA	1:A:229:ARG:HB3	1.99	0.44
1:A:318:PRO:HG2	1:A:319:ALA:H	1.81	0.44
1:B:34:GLU:O	1:B:35:HIS:C	2.59	0.44
1:B:350:ARG:NH2	1:B:358:GLU:OE1	2.46	0.44
1:C:194:VAL:O	1:C:194:VAL:HG12	2.16	0.44
1:C:337:ALA:CB	1:C:361:LEU:HD13	2.47	0.44
1:B:233:ALA:HB2	1:B:292:PHE:HE2	1.82	0.44
1:B:237:LEU:O	1:B:238:LYS:C	2.59	0.44
1:C:39:SER:C	1:C:42:GLU:HB2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:HIS:O	1:C:68:VAL:HG23	2.17	0.44
1:B:115:GLU:HB2	1:B:117:HIS:CE1	2.52	0.44
1:B:150:LEU:HD23	1:B:150:LEU:HA	1.85	0.44
1:B:387:ALA:C	1:B:389:LEU:N	2.76	0.44
1:A:125:LEU:HD13	1:A:252:MET:HG3	2.00	0.44
1:A:256:LEU:HD21	1:A:409:MET:HE2	1.99	0.44
1:B:16:ALA:O	1:B:20:GLU:CB	2.66	0.44
1:C:363:VAL:HG12	1:C:364:ASP:N	2.32	0.44
1:A:156:PHE:HD1	1:A:162:VAL:HG23	1.82	0.44
1:A:296:GLY:O	1:A:300:LEU:CD2	2.65	0.44
1:C:164:MET:O	1:C:165:GLU:C	2.61	0.44
1:C:319:ALA:HB1	1:C:323:GLY:HA3	2.00	0.44
1:A:70:ASP:OD1	1:A:75:HIS:HA	2.17	0.44
1:A:189:GLU:CG	1:A:235:ILE:HA	2.48	0.44
1:A:236:ASN:ND2	2:A:997:YE1:HC2	2.33	0.44
1:B:237:LEU:C	1:B:239:TYR:N	2.75	0.44
1:C:377:GLU:C	1:C:379:SER:H	2.26	0.44
1:C:139:LEU:O	1:C:140:ASP:C	2.60	0.44
1:C:343:ARG:O	1:C:347:LEU:HB2	2.17	0.43
1:A:337:ALA:CB	1:A:341:VAL:CG1	2.91	0.43
1:C:277:HIS:CE1	1:C:278:SER:HG	2.31	0.43
1:A:117:HIS:O	1:A:120:ASP:HB2	2.17	0.43
1:A:148:ARG:HD3	1:A:199:THR:OG1	2.18	0.43
2:B:998:YE1:OAD	2:B:998:YE1:CAE	2.62	0.43
1:C:130:ARG:HG2	1:C:130:ARG:NH1	2.29	0.43
1:A:20:GLU:O	1:A:23:ALA:HB3	2.19	0.43
1:A:416:GLN:OE1	1:A:416:GLN:HA	2.19	0.43
1:C:82:LEU:HD12	1:C:142:MET:HE2	1.99	0.43
1:C:124:PHE:O	1:C:126:ARG:N	2.52	0.43
1:A:194:VAL:HG23	1:A:250:PHE:CE1	2.53	0.43
1:A:64:HIS:O	1:A:68:VAL:HG23	2.18	0.43
1:A:242:GLN:HG2	1:A:242:GLN:H	1.41	0.43
1:A:419:ARG:NH1	1:B:386:ASP:C	2.77	0.43
1:B:192:GLN:O	1:B:193:GLN:C	2.61	0.43
1:C:259:ILE:HG12	1:C:300:LEU:HD23	2.01	0.43
1:A:367:VAL:HG12	1:A:372:LEU:HD13	1.98	0.43
1:B:236:ASN:CG	1:B:239:TYR:CE2	2.97	0.43
1:B:237:LEU:HD11	2:B:998:YE1:HC71	1.99	0.43
1:A:242:GLN:HB2	1:A:243:GLY:O	2.18	0.43
1:B:223:PRO:HA	1:B:226:ARG:NH1	2.34	0.43
1:A:185:ARG:HG3	1:A:188:ALA:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:THR:OG1	1:B:102:GLN:HG3	2.19	0.43
1:B:205:LEU:CD1	1:B:266:VAL:HG13	2.49	0.43
1:B:326:PRO:HD2	1:C:391:ASN:OD1	2.18	0.43
1:A:79:HIS:CD2	1:A:144:ARG:HD2	2.53	0.42
1:A:207:ASP:O	1:A:209:GLY:N	2.52	0.42
1:B:238:LYS:O	1:B:242:GLN:CG	2.67	0.42
1:B:250:PHE:O	1:B:254:LYS:HB3	2.18	0.42
1:B:331:LEU:HB2	1:B:408:TYR:CD1	2.53	0.42
2:C:999:YE1:OAD	2:C:999:YE1:CAE	2.62	0.42
1:A:219:VAL:O	1:A:220:MET:HE2	2.19	0.42
1:A:343:ARG:HG3	1:A:343:ARG:NH1	2.29	0.42
1:B:103:LEU:HD11	1:B:121:GLN:HE22	1.84	0.42
1:C:99:THR:HG1	1:C:102:GLN:HG3	1.80	0.42
1:C:106:GLU:OE1	1:C:106:GLU:HA	2.18	0.42
1:C:109:LEU:HB3	1:C:110:PRO:HD2	2.01	0.42
1:C:111:GLN:OE1	1:C:421:TYR:CE1	2.72	0.42
1:A:111:GLN:O	1:A:113:ALA:N	2.52	0.42
1:A:350:ARG:HG2	1:A:351:ARG:N	2.33	0.42
1:B:75:HIS:O	1:B:76:ARG:C	2.61	0.42
1:B:148:ARG:HD3	1:B:199:THR:HG21	1.99	0.42
1:B:314:TYR:C	1:B:315:PHE:CD2	2.98	0.42
1:A:81:ARG:HB2	1:A:84:GLU:OE1	2.19	0.42
1:A:177:ARG:HG2	1:A:214:LEU:HD23	2.00	0.42
1:A:374:ALA:HB1	1:A:378:ARG:NH1	2.32	0.42
1:B:174:GLY:HA2	1:B:209:GLY:O	2.19	0.42
1:C:316:SER:HB3	1:C:351:ARG:HB3	2.00	0.42
1:A:214:LEU:HD22	1:A:380:LEU:HD11	2.01	0.42
1:A:235:ILE:N	2:A:997:YE1:HC22	2.34	0.42
1:B:340:ARG:O	1:B:344:GLN:HG3	2.20	0.42
1:C:190:ASP:C	1:C:192:GLN:H	2.27	0.42
1:A:144:ARG:NH2	1:A:269:ASN:OD1	2.53	0.42
1:A:247:LEU:HB2	1:A:420:LEU:HD23	2.02	0.42
1:A:388:VAL:HG13	1:C:347:LEU:HD22	2.00	0.42
1:C:170:GLU:OE2	1:C:172:ARG:NH1	2.52	0.42
1:C:215:LEU:HD23	1:C:304:PHE:HZ	1.84	0.42
1:C:350:ARG:HH22	1:C:358:GLU:CD	2.28	0.42
1:A:331:LEU:HA	1:B:398:ALA:HB1	2.02	0.42
1:B:205:LEU:HD12	1:B:266:VAL:HG13	2.00	0.42
1:B:235:ILE:HD12	1:B:250:PHE:HE2	1.83	0.42
1:C:309:ALA:O	1:C:366:VAL:HA	2.19	0.42
1:A:35:HIS:C	1:A:37:ALA:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ARG:O	1:A:344:GLN:HG3	2.19	0.42
1:A:419:ARG:HD3	1:B:390:ALA:CB	2.49	0.42
1:A:240:LEU:HB2	1:A:245:ILE:HG13	2.02	0.42
1:A:311:SER:HA	1:A:366:VAL:HG12	2.01	0.42
1:B:416:GLN:O	1:B:420:LEU:HD13	2.20	0.42
1:A:330:ASN:HB2	1:A:408:TYR:OH	2.20	0.42
1:B:54:ARG:NH2	1:B:116:GLY:O	2.53	0.42
1:A:359:ALA:C	1:A:361:LEU:H	2.28	0.41
1:B:172:ARG:O	1:B:173:ASP:CB	2.64	0.41
1:C:378:ARG:HG2	1:C:382:ARG:NH1	2.35	0.41
1:A:18:LEU:CD1	1:A:57:ARG:HG2	2.49	0.41
1:B:254:LYS:HG3	1:B:259:ILE:CD1	2.50	0.41
1:A:332:ARG:O	1:A:333:LEU:C	2.63	0.41
1:B:269:ASN:C	1:B:271:ASP:H	2.27	0.41
1:C:23:ALA:O	1:C:24:SER:C	2.63	0.41
1:C:110:PRO:C	1:C:112:ALA:N	2.79	0.41
1:B:162:VAL:HG21	1:B:203:LEU:CD1	2.50	0.41
1:B:223:PRO:HD3	1:B:226:ARG:NH2	2.35	0.41
1:B:231:PHE:HB3	1:B:292:PHE:O	2.20	0.41
1:B:239:TYR:HB3	1:B:244:GLY:CA	2.50	0.41
1:B:377:GLU:O	1:B:380:LEU:N	2.52	0.41
1:B:425:VAL:HG12	1:B:426:ILE:HG13	2.02	0.41
1:C:27:LYS:O	1:C:29:LEU:N	2.54	0.41
1:C:378:ARG:HG2	1:C:382:ARG:HH12	1.85	0.41
1:A:43:ARG:O	1:A:44:ALA:C	2.63	0.41
1:A:58:VAL:HG22	1:A:123:ILE:HG23	2.01	0.41
1:B:156:PHE:CD1	1:B:162:VAL:HG23	2.56	0.41
1:B:326:PRO:HG3	1:B:346:ILE:HG23	2.02	0.41
1:C:119:ILE:HA	1:C:417:ALA:HB1	2.01	0.41
1:A:43:ARG:O	1:A:45:GLU:N	2.54	0.41
1:A:70:ASP:OD1	1:A:76:ARG:NH1	2.53	0.41
1:A:247:LEU:O	1:A:252:MET:HG2	2.20	0.41
1:A:337:ALA:HB1	1:A:341:VAL:HG21	2.02	0.41
1:A:341:VAL:O	1:A:345:VAL:HG23	2.21	0.41
1:B:79:HIS:HD2	1:B:144:ARG:CZ	2.33	0.41
1:C:35:HIS:ND1	1:C:113:ALA:HA	2.36	0.41
1:C:341:VAL:O	1:C:342:SER:C	2.63	0.41
1:A:111:GLN:HB2	1:A:243:GLY:N	2.35	0.41
1:A:202:ASP:CG	1:A:261:LYS:HZ2	2.29	0.41
1:B:111:GLN:HB3	1:B:111:GLN:HE21	1.64	0.41
1:B:153:LEU:N	1:B:154:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HD23	1:A:308:LEU:H	1.84	0.41
1:A:343:ARG:HH11	1:A:343:ARG:CG	2.31	0.41
1:B:152:LEU:C	1:B:154:PRO:HD2	2.46	0.41
1:B:368:GLU:O	1:B:369:PRO:C	2.64	0.41
1:C:111:GLN:HG2	1:C:243:GLY:CA	2.27	0.41
1:C:198:GLU:O	1:C:198:GLU:CG	2.68	0.41
1:A:182:ARG:HB2	1:A:187:ASN:HA	2.03	0.41
1:A:230:VAL:CG2	1:A:292:PHE:CZ	3.04	0.41
1:A:250:PHE:O	1:A:254:LYS:HB2	2.21	0.41
1:B:81:ARG:HB2	1:B:84:GLU:OE1	2.20	0.41
1:B:162:VAL:HG21	1:B:203:LEU:HD13	2.02	0.41
1:B:337:ALA:CB	1:B:341:VAL:HB	2.51	0.41
1:C:72:LEU:HD22	1:C:88:ALA:HB1	2.02	0.41
1:C:139:LEU:HD23	1:C:139:LEU:HA	1.93	0.41
1:C:205:LEU:HD12	1:C:266:VAL:HG13	2.02	0.41
1:C:308:LEU:HD13	1:C:376:ILE:HG12	2.03	0.41
1:B:18:LEU:HD11	1:B:57:ARG:HG2	2.03	0.41
1:C:124:PHE:C	1:C:126:ARG:N	2.79	0.41
1:C:310:SER:HA	1:C:367:VAL:O	2.21	0.41
1:C:119:ILE:O	1:C:123:ILE:HG13	2.21	0.40
1:C:186:LEU:CA	1:C:220:MET:CE	2.98	0.40
1:C:251:LEU:HD13	1:C:416:GLN:CG	2.51	0.40
1:C:317:LEU:N	1:C:318:PRO:HD3	2.36	0.40
1:A:111:GLN:HE21	1:A:426:ILE:HG12	1.86	0.40
1:A:288:ALA:HA	1:A:308:LEU:O	2.21	0.40
1:B:166:ALA:HB3	1:B:196:ASP:OD2	2.21	0.40
1:B:251:LEU:HA	1:B:251:LEU:HD23	1.83	0.40
1:C:145:PRO:HD2	1:C:267:LEU:O	2.20	0.40
1:C:191:GLY:CA	1:C:250:PHE:CD1	2.96	0.40
1:C:193:GLN:C	1:C:195:ASP:N	2.78	0.40
1:C:190:ASP:C	1:C:192:GLN:N	2.80	0.40
1:C:222:HIS:ND1	1:C:224:ARG:N	2.65	0.40
1:C:350:ARG:CG	1:C:351:ARG:N	2.84	0.40
1:A:111:GLN:HG2	1:A:426:ILE:HD11	2.03	0.40
1:A:140:ASP:O	1:A:144:ARG:HG3	2.20	0.40
1:B:119:ILE:O	1:B:123:ILE:HG13	2.22	0.40
1:C:216:ARG:CG	1:C:217:GLY:N	2.84	0.40
1:A:188:ALA:HB1	1:A:236:ASN:HB2	2.04	0.40
1:B:218:GLY:HA2	1:B:229:ARG:NH1	2.36	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	415/417 (100%)	350 (84%)	47 (11%)	18 (4%)	2	12
1	B	415/417 (100%)	363 (88%)	45 (11%)	7 (2%)	7	32
1	C	413/417 (99%)	339 (82%)	67 (16%)	7 (2%)	7	32
All	All	1243/1251 (99%)	1052 (85%)	159 (13%)	32 (3%)	4	23

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ALA
1	A	319	ALA
1	B	112	ALA
1	B	271	ASP
1	C	183	ASP
1	A	107	ARG
1	A	111	GLN
1	A	112	ALA
1	A	135	GLY
1	C	111	GLN
1	C	125	LEU
1	A	34	GLU
1	A	238	LYS
1	A	242	GLN
1	A	276	TRP
1	A	311	SER
1	A	318	PRO
1	A	423	HIS
1	B	12	ASP
1	B	378	ARG
1	C	15	TRP
1	B	425	VAL
1	B	319	ALA
1	C	371	GLU

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Mol	Chain	Res	Type
1	A	385	GLY
1	B	341	VAL
1	C	270	ASP
1	A	425	VAL
1	A	244	GLY
1	A	245	ILE
1	A	324	ILE
1	C	98	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/328 (97%)	300 (94%)	18 (6%)	18	52
1	B	327/328 (100%)	313 (96%)	14 (4%)	26	60
1	C	322/328 (98%)	308 (96%)	14 (4%)	26	60
All	All	967/984 (98%)	921 (95%)	46 (5%)	23	57

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	63	THR
1	A	102	GLN
1	A	143	LEU
1	A	186	LEU
1	A	242	GLN
1	A	271	ASP
1	A	308	LEU
1	A	311	SER
1	A	315	PHE
1	A	317	LEU
1	A	324	ILE
1	A	331	LEU
1	A	340	ARG

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Mol	Chain	Res	Type
1	A	384	ASP
1	A	402	PRO
1	A	403	ASP
1	A	425	VAL
1	B	11	THR
1	B	45	GLU
1	B	63	THR
1	B	147	PRO
1	B	190	ASP
1	B	196	ASP
1	B	214	LEU
1	B	240	LEU
1	B	254	LYS
1	B	271	ASP
1	B	272	ARG
1	B	300	LEU
1	B	397	LEU
1	B	425	VAL
1	C	24	SER
1	C	33	PRO
1	C	39	SER
1	C	63	THR
1	C	105	VAL
1	C	152	LEU
1	C	183	ASP
1	C	186	LEU
1	C	239	TYR
1	C	271	ASP
1	C	272	ARG
1	C	315	PHE
1	C	340	ARG
1	C	367	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	111	GLN
1	A	121	GLN
1	B	79	HIS
1	B	100	GLN
1	B	102	GLN

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Mol	Chain	Res	Type
1	B	111	GLN
1	B	121	GLN
1	B	168	HIS
1	B	260	HIS
1	B	423	HIS
1	C	102	GLN
1	C	299	GLN
1	C	416	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](#)

5 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	$\# Z > 2$
3	OXY	A	3	-	1,1,1	1.12	0	-		
2	YE1	B	998	-	60,62,62	1.99	11 (18%)	87,92,92	2.09	11 (12%)
3	OXY	C	2	-	1,1,1	1.13	0	-		
2	YE1	A	997	-	60,62,62	1.98	11 (18%)	87,92,92	2.09	11 (12%)
2	YE1	C	999	-	60,62,62	1.98	11 (18%)	87,92,92	2.09	11 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YE1	B	998	-	-	2/55/71/71	0/4/4/4
2	YE1	A	997	-	-	2/55/71/71	0/4/4/4
2	YE1	C	999	-	-	2/55/71/71	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	999	YE1	OAD-CAB	9.72	1.42	1.23
2	B	998	YE1	OAD-CAB	9.70	1.42	1.23
2	A	997	YE1	OAD-CAB	9.69	1.42	1.23
2	C	999	YE1	P1A-O3A	-5.34	1.53	1.59
2	B	998	YE1	P1A-O3A	-5.29	1.53	1.59
2	A	997	YE1	P1A-O3A	-5.24	1.53	1.59
2	C	999	YE1	C2P-NAA	-4.81	1.35	1.46
2	A	997	YE1	C2P-NAA	-4.78	1.35	1.46
2	B	998	YE1	C2P-NAA	-4.78	1.35	1.46
2	B	998	YE1	P3'-O3'	-3.55	1.53	1.59
2	A	997	YE1	P3'-O3'	-3.43	1.53	1.59
2	C	999	YE1	P3'-O3'	-3.42	1.53	1.59
2	A	997	YE1	CAB-NAA	3.00	1.40	1.33
2	B	998	YE1	CAB-NAA	3.00	1.40	1.33
2	C	999	YE1	CAB-NAA	2.99	1.40	1.33
2	C	999	YE1	C5P-N4P	2.98	1.40	1.33
2	B	998	YE1	C5P-N4P	2.93	1.40	1.33
2	B	998	YE1	C9P-N8P	2.93	1.40	1.33
2	A	997	YE1	C5P-N4P	2.92	1.40	1.33
2	C	999	YE1	C9P-N8P	2.90	1.40	1.33
2	A	997	YE1	C9P-N8P	2.88	1.40	1.33
2	B	998	YE1	P2A-O3A	2.72	1.62	1.59
2	A	997	YE1	P2A-O3A	2.64	1.62	1.59
2	C	999	YE1	P2A-O3A	2.63	1.62	1.59
2	B	998	YE1	C3P-N4P	-2.53	1.40	1.46
2	A	997	YE1	C3P-N4P	-2.49	1.40	1.46
2	C	999	YE1	C3P-N4P	-2.48	1.40	1.46
2	B	998	YE1	C2A-N1A	2.26	1.38	1.33
2	A	997	YE1	C2A-N1A	2.22	1.37	1.33
2	C	999	YE1	C2A-N1A	2.15	1.37	1.33
2	B	998	YE1	CAC-CAB	2.15	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	999	YE1	CAC-CAB	2.14	1.56	1.52
2	A	997	YE1	CAC-CAB	2.10	1.56	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	998	YE1	C2P-NAA-CAB	-7.38	109.09	122.82
2	C	999	YE1	C2P-NAA-CAB	-7.36	109.13	122.82
2	A	997	YE1	C2P-NAA-CAB	-7.32	109.19	122.82
2	B	998	YE1	C7P-N8P-C9P	-7.25	109.53	122.55
2	A	997	YE1	C7P-N8P-C9P	-7.24	109.55	122.55
2	C	999	YE1	C3P-N4P-C5P	-7.18	109.46	122.82
2	C	999	YE1	C7P-N8P-C9P	-7.17	109.66	122.55
2	B	998	YE1	C3P-N4P-C5P	-7.17	109.48	122.82
2	A	997	YE1	C3P-N4P-C5P	-7.15	109.51	122.82
2	B	998	YE1	C6P-C7P-N8P	-6.52	98.13	112.00
2	A	997	YE1	C6P-C7P-N8P	-6.51	98.15	112.00
2	C	999	YE1	C6P-C7P-N8P	-6.49	98.19	112.00
2	A	997	YE1	O6A-P2A-O5A	-6.27	84.08	108.94
2	B	998	YE1	O6A-P2A-O5A	-6.26	84.12	108.94
2	C	999	YE1	O6A-P2A-O5A	-6.24	84.20	108.94
2	A	997	YE1	P3'-O3'-C3'	-5.26	109.38	123.43
2	B	998	YE1	P3'-O3'-C3'	-5.25	109.41	123.43
2	C	999	YE1	P3'-O3'-C3'	-5.24	109.43	123.43
2	A	997	YE1	C7P-C6P-C5P	-4.69	104.58	112.39
2	B	998	YE1	C7P-C6P-C5P	-4.67	104.62	112.39
2	C	999	YE1	C7P-C6P-C5P	-4.65	104.65	112.39
2	A	997	YE1	C14-C11-C10	3.21	114.24	108.77
2	C	999	YE1	C14-C11-C10	3.21	114.23	108.77
2	B	998	YE1	C14-C11-C10	3.20	114.23	108.77
2	C	999	YE1	C2'-C1'-N9A	-2.87	106.18	113.30
2	B	998	YE1	C2'-C1'-N9A	-2.87	106.19	113.30
2	A	997	YE1	C2'-C1'-N9A	-2.86	106.19	113.30
2	C	999	YE1	O9P-C9P-N8P	-2.40	117.90	122.98
2	B	998	YE1	O9P-C9P-N8P	-2.38	117.95	122.98
2	A	997	YE1	O9P-C9P-N8P	-2.38	117.95	122.98
2	A	997	YE1	P2A-O6A-C12	-2.23	108.98	121.12
2	B	998	YE1	P2A-O6A-C12	-2.22	109.01	121.12
2	C	999	YE1	P2A-O6A-C12	-2.21	109.10	121.12

There are no chirality outliers.

All (6) torsion outliers are listed below:

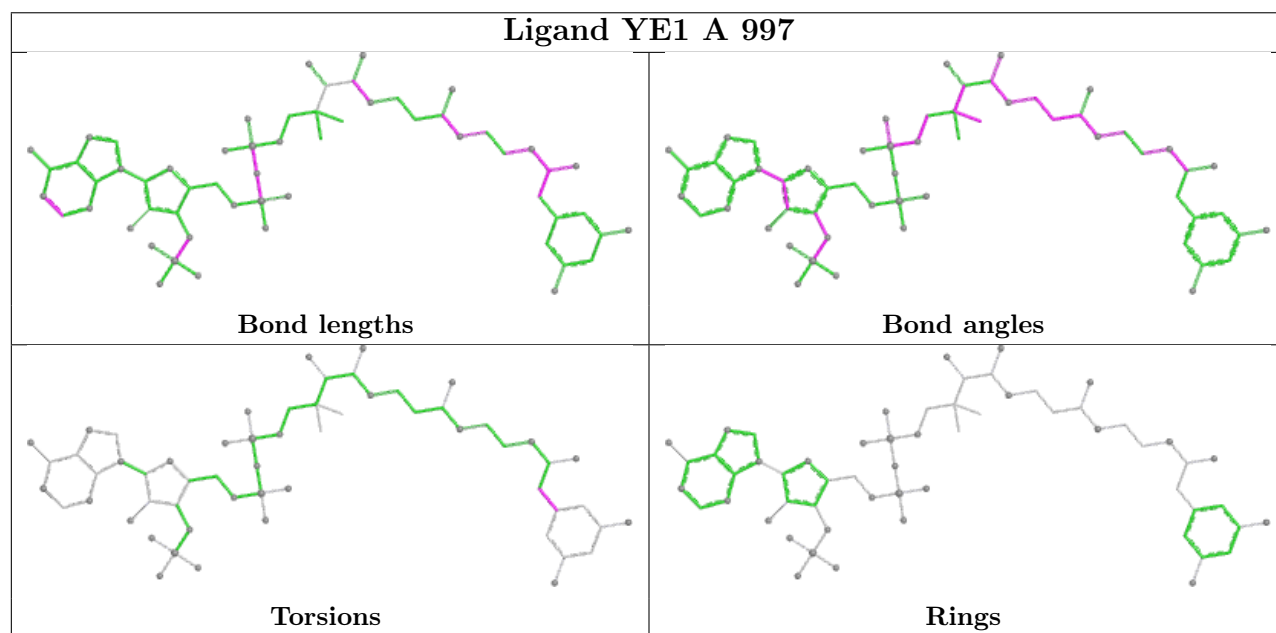
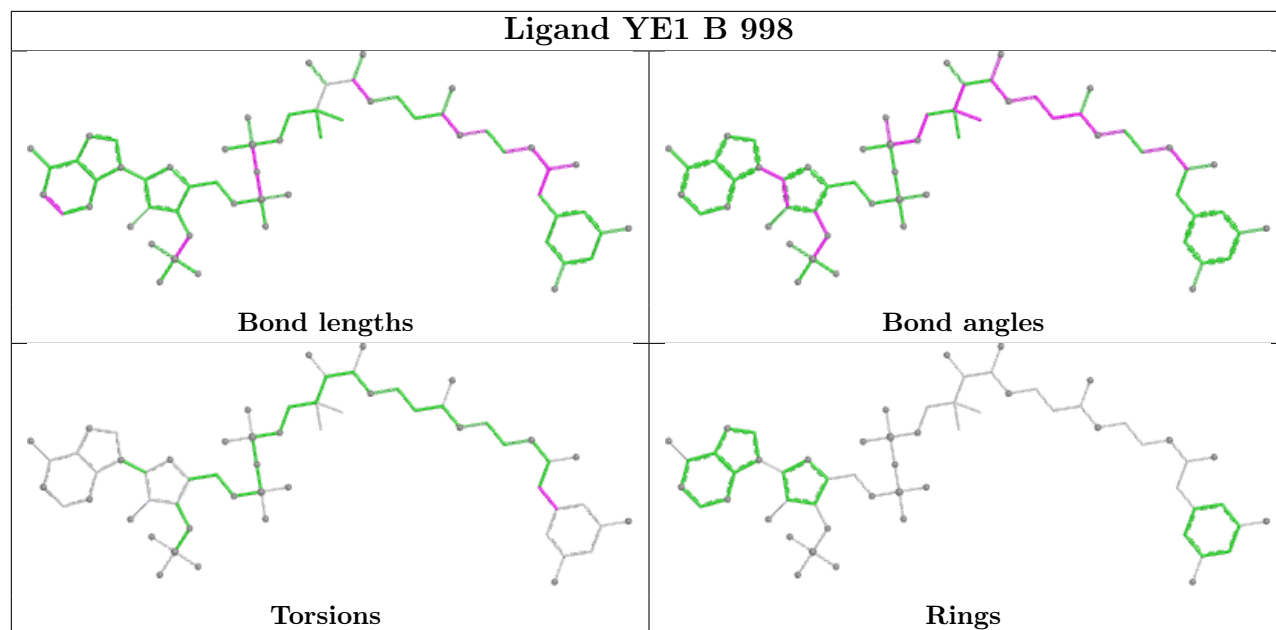
Mol	Chain	Res	Type	Atoms
2	A	997	YE1	CAB-CAC-CAF-CAE
2	B	998	YE1	CAB-CAC-CAF-CAE
2	C	999	YE1	CAB-CAC-CAF-CAE
2	A	997	YE1	CAB-CAC-CAF-CAG
2	B	998	YE1	CAB-CAC-CAF-CAG
2	C	999	YE1	CAB-CAC-CAF-CAG

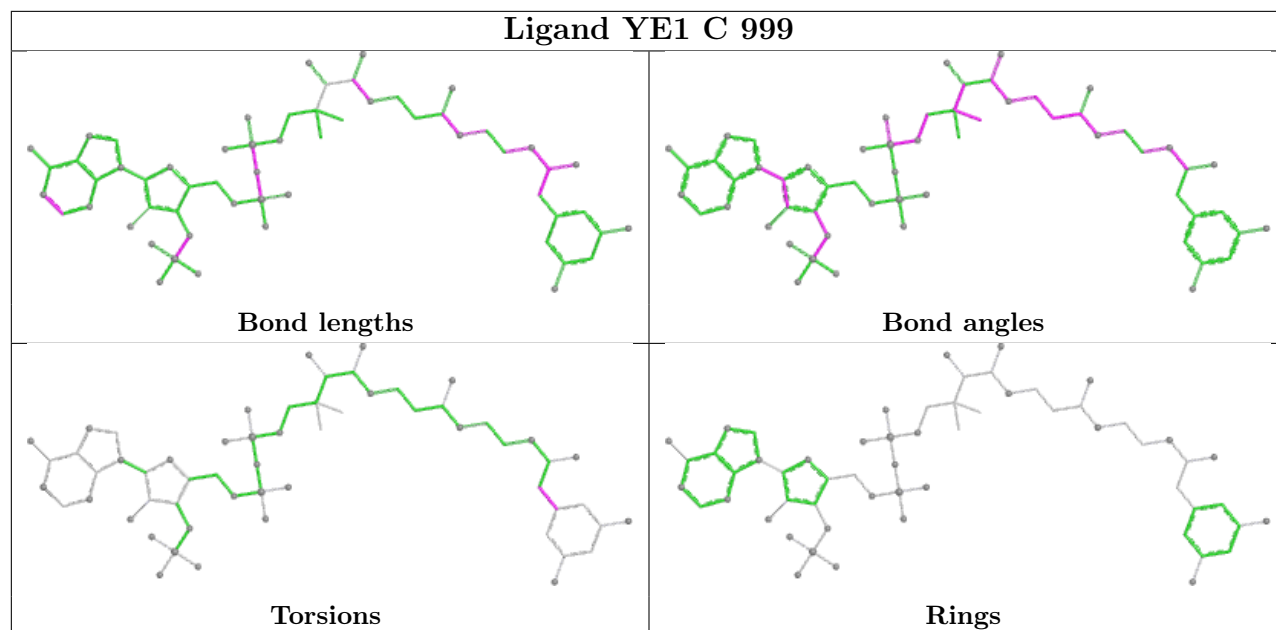
There are no ring outliers.

4 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3	OXY	1	0
2	B	998	YE1	12	0
2	A	997	YE1	20	0
2	C	999	YE1	11	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	417/417 (100%)	0.57	44 (10%) 11 6	20, 41, 68, 77	0
1	B	417/417 (100%)	0.47	33 (7%) 18 10	24, 42, 63, 72	0
1	C	415/417 (99%)	0.52	34 (8%) 17 9	21, 43, 63, 74	0
All	All	1249/1251 (99%)	0.52	111 (8%) 15 8	20, 42, 64, 77	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	319	ALA	7.4
1	B	321	LYS	5.7
1	B	193	GLN	5.6
1	C	183	ASP	5.5
1	A	425	VAL	5.4
1	A	39	SER	5.1
1	A	243	GLY	4.4
1	A	11	THR	4.4
1	B	220	MET	4.3
1	A	319	ALA	4.3
1	B	236	ASN	4.3
1	B	319	ALA	4.3
1	A	239	TYR	4.3
1	B	426	ILE	4.2
1	A	10	ASP	4.2
1	A	237	LEU	4.0
1	B	390	ALA	4.0
1	C	384	ASP	4.0
1	A	236	ASN	3.9
1	B	237	LEU	3.9
1	C	271	ASP	3.8
1	A	223	PRO	3.8
1	B	425	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	424	ASP	3.6
1	C	323	GLY	3.6
1	A	42	GLU	3.6
1	A	426	ILE	3.6
1	B	424	ASP	3.6
1	C	272	ARG	3.5
1	C	184	ASP	3.5
1	A	320	ALA	3.4
1	A	111	GLN	3.4
1	A	193	GLN	3.3
1	C	425	VAL	3.1
1	B	340	ARG	3.1
1	B	341	VAL	3.0
1	A	292	PHE	3.0
1	A	318	PRO	3.0
1	A	321	LYS	3.0
1	A	244	GLY	3.0
1	B	240	LEU	3.0
1	B	322	GLU	3.0
1	B	239	TYR	2.9
1	A	37	ALA	2.9
1	A	41	ALA	2.9
1	A	423	HIS	2.8
1	C	221	SER	2.8
1	C	51	ASP	2.8
1	C	426	ILE	2.8
1	B	238	LYS	2.8
1	B	91	THR	2.8
1	B	234	GLY	2.8
1	C	223	PRO	2.8
1	A	323	GLY	2.7
1	C	36	GLY	2.7
1	B	223	PRO	2.7
1	A	40	SER	2.7
1	B	184	ASP	2.7
1	B	241	SER	2.6
1	C	318	PRO	2.6
1	C	371	GLU	2.6
1	A	312	ASP	2.6
1	A	13	GLY	2.6
1	B	361	LEU	2.6
1	C	116	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	321	LYS	2.5
1	C	35	HIS	2.5
1	A	38	ARG	2.5
1	A	222	HIS	2.5
1	A	384	ASP	2.4
1	C	12	ASP	2.4
1	A	225	TYR	2.4
1	A	101	GLN	2.4
1	C	193	GLN	2.4
1	C	41	ALA	2.4
1	A	271	ASP	2.4
1	B	222	HIS	2.4
1	A	241	SER	2.4
1	C	40	SER	2.3
1	A	12	ASP	2.3
1	C	270	ASP	2.3
1	C	14	LEU	2.3
1	B	183	ASP	2.3
1	C	370	ASP	2.3
1	B	384	ASP	2.3
1	B	315	PHE	2.3
1	A	44	ALA	2.2
1	C	28	LEU	2.2
1	C	108	SER	2.2
1	A	386	ASP	2.2
1	A	31	THR	2.2
1	B	225	TYR	2.2
1	A	240	LEU	2.2
1	B	385	GLY	2.1
1	A	30	ALA	2.1
1	B	422	GLY	2.1
1	C	322	GLU	2.1
1	A	315	PHE	2.1
1	A	142	MET	2.1
1	C	420	LEU	2.1
1	B	113	ALA	2.1
1	A	36	GLY	2.1
1	B	186	LEU	2.1
1	B	371	GLU	2.1
1	C	33	PRO	2.1
1	C	34	GLU	2.1
1	C	365	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	32	LEU	2.0
1	C	111	GLN	2.0
1	B	10	ASP	2.0
1	A	43	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

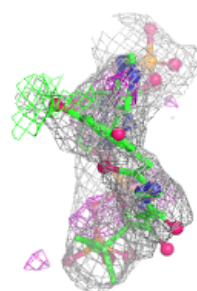
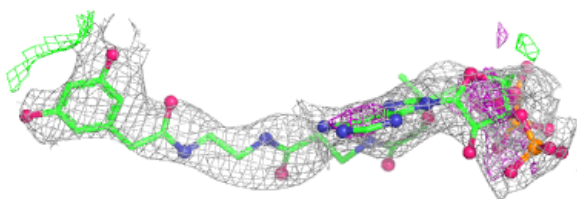
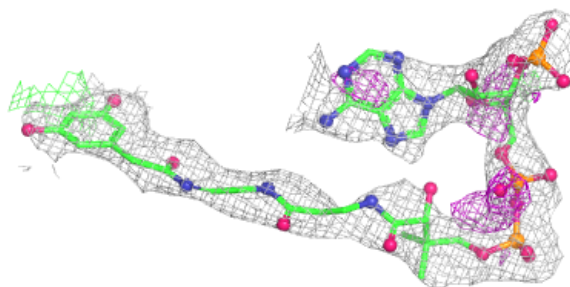
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	YE1	B	998	59/59	0.71	0.20	40,73,105,156	0
3	OXY	C	2	2/2	0.73	0.32	69,69,69,69	0
2	YE1	A	997	59/59	0.74	0.18	45,70,105,135	0
3	OXY	A	3	2/2	0.83	0.25	69,69,69,70	0
2	YE1	C	999	59/59	0.87	0.15	36,64,86,135	0

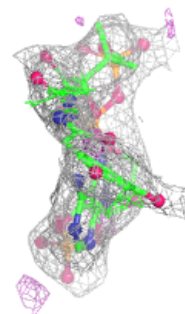
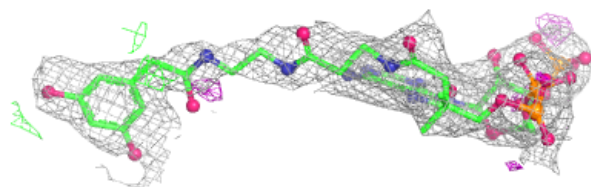
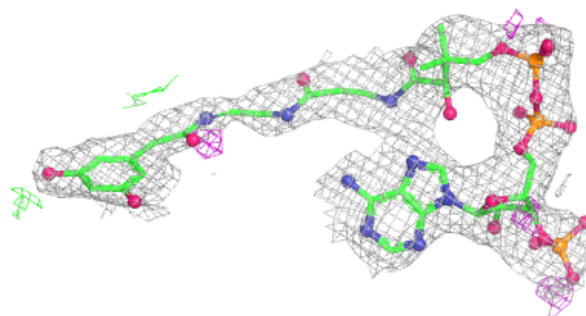
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

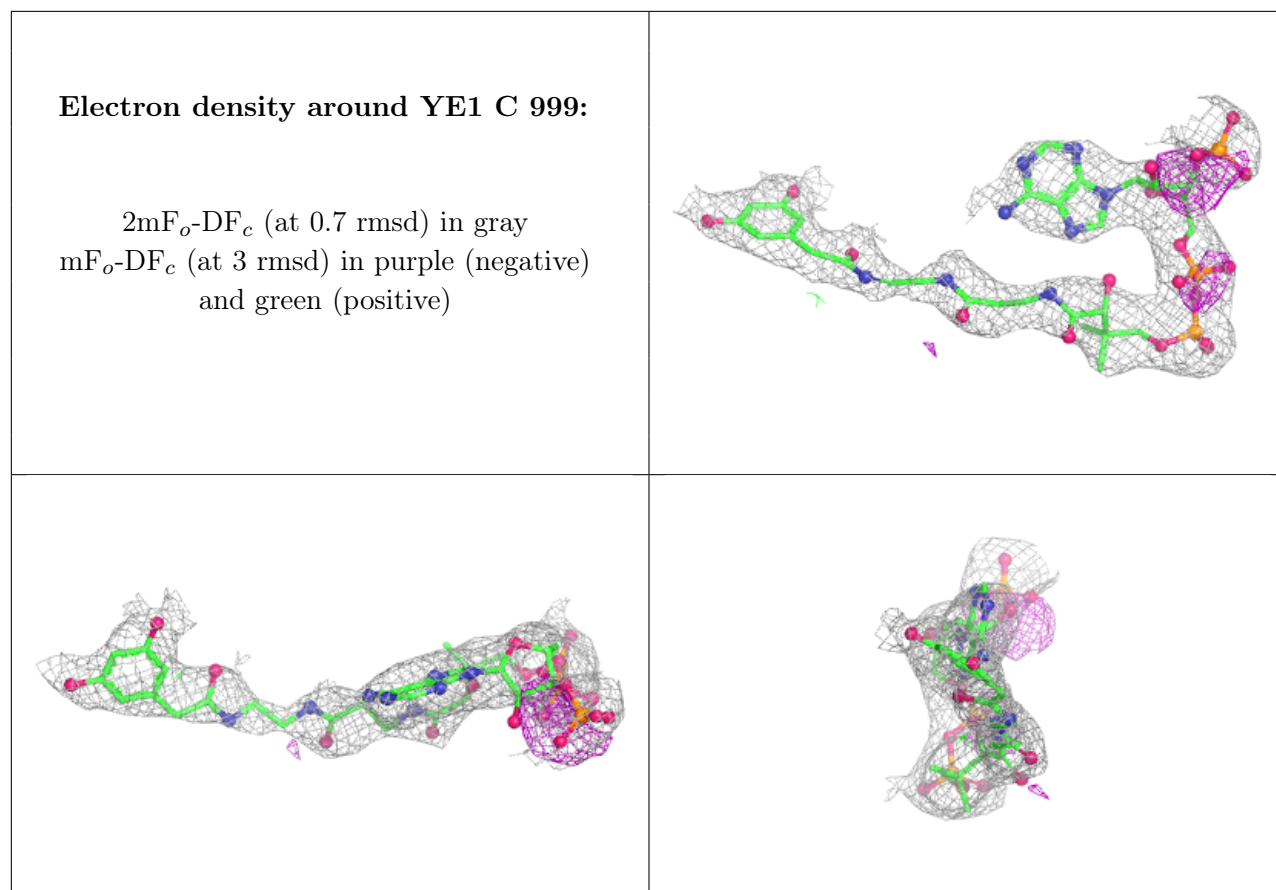
Electron density around YE1 B 998:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around YE1 A 997:**

$2mF_o-DF_c$ (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.