



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:52 PM UTC

PDB ID : 1TKZ / pdb_00001tkz
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN
COMPLEX WITH GW429576
Authors : Hopkins, A.L.; Ren, J.; Stuart, D.I.; Stammers, D.K.
Deposited on : 2004-06-09
Resolution : 2.81 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

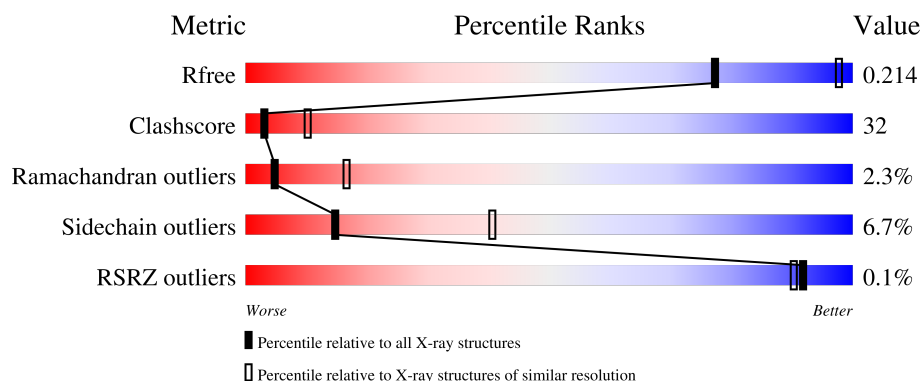
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

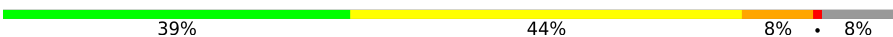
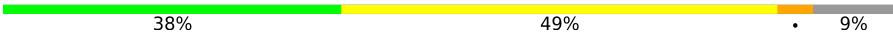
The reported resolution of this entry is 2.81 Å.

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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	560	
2	B	440	

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
3	PO4	A	1302	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7612 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 Pol polyprotein, Reverse transcriptase, Chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			4247	2754	701	784	8			

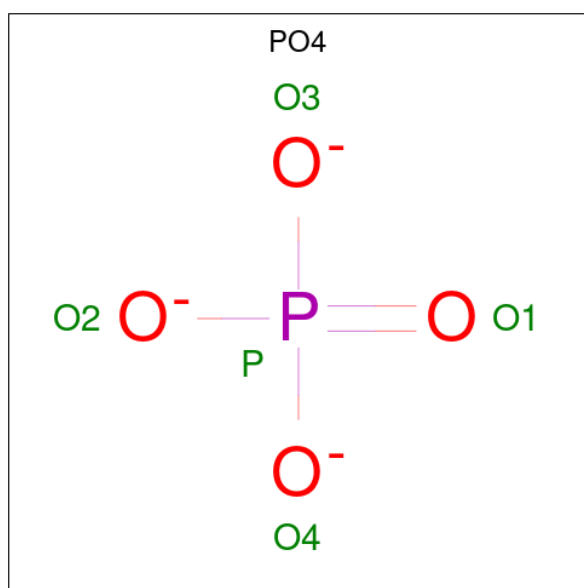
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	modified residue	UNP P04585

- Molecule 2 is a protein called Pol polyprotein, Reverse transcriptase, Chain B.

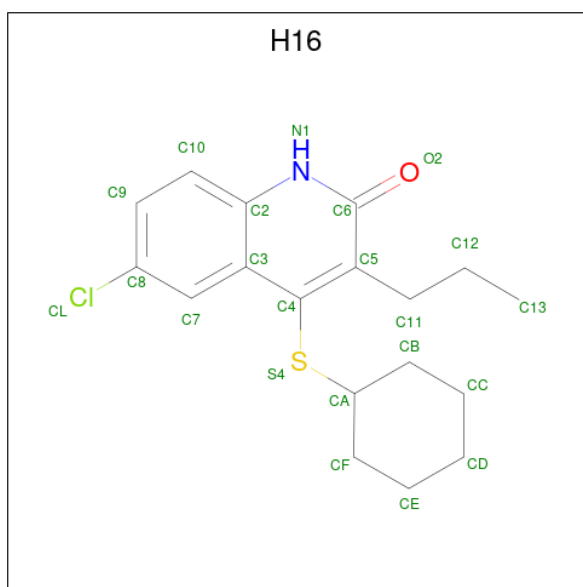
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3328	2173	548	600	7			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 6-CHLORO-4-(CYCLOHEXYLSULFANYL)-3-PROPYLQUINOLIN-2(1H)-ONE (CCD ID: H16) (formula: C₁₈H₂₂ClNOS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			22	18	1	1	1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.80Å 115.20Å 65.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 2.81 29.81 – 2.81	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.81-2.81) 93.8 (29.81-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.283 0.199 , 0.214	Depositor DCC
R_{free} test set	1169 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 86.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7612	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, PO4, H16

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	0/4352	1.10	28/5918 (0.5%)
2	B	0.57	0/3425	1.04	17/4652 (0.4%)
All	All	0.58	0/7777	1.07	45/10570 (0.4%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	TRP	N-CA-C	-10.95	93.54	109.96
1	A	349	LEU	N-CA-C	-9.92	101.31	113.41
1	A	250	ASP	N-CA-C	-9.17	101.99	113.55
1	A	89	GLU	N-CA-C	8.64	122.83	110.14
1	A	234	LEU	N-CA-C	7.79	121.78	107.99
1	A	139	THR	CA-C-N	7.42	127.38	120.03
1	A	139	THR	C-N-CA	7.42	127.38	120.03
2	B	96	HIS	N-CA-C	7.35	118.91	109.72
2	B	147	ASN	N-CA-C	-6.98	105.29	113.88
1	A	348	ASN	N-CA-C	6.88	119.71	110.35
2	B	343	GLN	N-CA-C	-6.60	105.24	113.55
1	A	320	ASP	CA-C-N	6.54	128.01	119.84
1	A	320	ASP	C-N-CA	6.54	128.01	119.84
2	B	69	THR	N-CA-C	-6.51	105.08	113.16
1	A	343	GLN	N-CA-C	-6.42	104.50	112.72
2	B	234	LEU	N-CA-C	-6.21	100.45	110.32
2	B	382	ILE	N-CA-C	6.14	116.30	110.53
1	A	136	ASN	N-CA-C	6.13	119.24	109.24
1	A	88	TRP	CA-C-N	-6.12	112.09	123.05
1	A	88	TRP	C-N-CA	-6.12	112.09	123.05
2	B	141	GLY	N-CA-C	-6.08	103.75	111.72
1	A	184	MET	CB-CA-C	-6.02	109.05	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	THR	N-CA-C	6.00	118.19	110.39
1	A	147	ASN	N-CA-C	-5.97	105.96	113.72
2	B	87	PHE	N-CA-C	5.80	118.18	108.02
2	B	233	GLU	N-CA-C	5.79	119.25	109.76
1	A	274	ILE	N-CA-C	-5.74	102.18	109.58
1	A	434	ILE	N-CA-C	5.73	117.00	108.23
1	A	142	ILE	N-CA-C	5.73	117.10	109.37
1	A	51	GLY	CA-C-N	5.69	125.78	119.87
1	A	51	GLY	C-N-CA	5.69	125.78	119.87
2	B	401	TRP	N-CA-C	5.67	120.47	113.50
2	B	413	GLU	N-CA-C	-5.63	101.30	110.20
2	B	231	GLY	N-CA-C	-5.56	107.30	115.30
1	A	201	LYS	N-CA-C	-5.49	104.68	111.33
2	B	139	THR	CA-C-N	5.43	125.51	119.32
2	B	139	THR	C-N-CA	5.43	125.51	119.32
1	A	382	ILE	N-CA-C	5.23	116.31	111.81
1	A	344	GLU	CA-C-N	5.20	126.34	119.84
1	A	344	GLU	C-N-CA	5.20	126.34	119.84
1	A	329	ILE	N-CA-C	5.20	115.96	108.48
1	A	500	GLN	N-CA-C	-5.13	105.77	111.36
2	B	391	LEU	N-CA-C	5.12	117.04	109.62
2	B	349	LEU	N-CA-C	-5.08	106.60	112.89
2	B	202	ILE	N-CA-C	-5.00	105.45	110.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4247	0	4275	284	0
2	B	3328	0	3353	220	0
3	A	15	0	0	4	0
4	A	22	0	22	2	0
All	All	7612	0	7650	481	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (481) 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:206:ARG:HH12	1:A:218:ASP:HA	1.28	0.98
2:B:227:PHE:HB3	2:B:231:GLY:HA2	1.49	0.95
1:A:195:ILE:HD13	1:A:195:ILE:H	1.33	0.94
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.50	0.93
2:B:66:LYS:HE3	2:B:230:MET:HG3	1.50	0.91
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.53	0.89
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.53	0.88
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.55	0.88
1:A:89:GLU:HG2	1:A:90:VAL:HG23	1.56	0.87
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.73	0.86
1:A:257:ILE:O	1:A:261:VAL:HG23	1.76	0.85
1:A:101:LYS:HD2	1:A:101:LYS:N	1.91	0.84
1:A:191:SER:HB3	1:A:198:HIS:ND1	1.93	0.84
1:A:206:ARG:NH1	1:A:218:ASP:HA	1.94	0.82
2:B:193:LEU:HD22	2:B:201:LYS:HD2	1.63	0.81
2:B:40:GLU:HG3	2:B:44:GLU:OE2	1.79	0.81
1:A:500:GLN:NE2	2:B:422:LEU:HD12	1.96	0.81
2:B:227:PHE:HB3	2:B:231:GLY:CA	2.12	0.80
2:B:242:GLN:HG2	2:B:353:LYS:HG2	1.65	0.78
2:B:362:THR:HG22	2:B:366:LYS:HD3	1.62	0.78
1:A:469:LEU:HD21	1:A:480:GLN:HG3	1.66	0.78
2:B:203:GLU:HG3	2:B:207:GLN:HE22	1.49	0.77
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.20	0.77
1:A:40:GLU:OE2	1:A:43:LYS:HD3	1.84	0.76
1:A:228:LEU:HA	1:A:232:TYR:O	1.86	0.76
2:B:295:LEU:N	2:B:295:LEU:HD12	2.02	0.75
2:B:297:GLU:O	2:B:301:LEU:HG	1.87	0.74
1:A:27:THR:HG23	1:A:30:LYS:HB2	1.69	0.73
2:B:266:TRP:O	2:B:269:GLN:HG2	1.88	0.73
2:B:330:GLN:HB2	2:B:338:THR:OG1	1.88	0.73
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.01	0.73
2:B:295:LEU:HD12	2:B:295:LEU:H	1.53	0.72
2:B:305:GLU:O	2:B:309:ILE:HG13	1.89	0.72
2:B:154:LYS:O	2:B:157:PRO:HD2	1.89	0.72
2:B:193:LEU:HD22	2:B:201:LYS:CD	2.20	0.72
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.19	0.71
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.26	0.71
1:A:476:LYS:HD2	1:A:476:LYS:O	1.90	0.71
2:B:234:LEU:HD21	2:B:377:THR:HG21	1.72	0.71
2:B:66:LYS:HG2	2:B:230:MET:HA	1.73	0.70
2:B:332:GLN:HA	2:B:424:LYS:HE3	1.74	0.70
1:A:125:ARG:HG2	1:A:146:TYR:O	1.92	0.70
1:A:89:GLU:CG	1:A:90:VAL:H	2.04	0.69
1:A:181:TYR:HE1	1:A:183:TYR:HB2	1.56	0.69
1:A:207:GLN:NE2	1:A:207:GLN:HA	2.06	0.69
1:A:253:THR:HG22	1:A:255:ASN:H	1.58	0.69
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.73	0.69
1:A:92:LEU:HD12	1:A:92:LEU:O	1.94	0.68
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.74	0.68
1:A:105:SER:HB2	1:A:198:HIS:CD2	2.27	0.68
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.28	0.68
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.28	0.68
2:B:63:ILE:HD11	2:B:72:ARG:HD3	1.76	0.67
2:B:203:GLU:HG3	2:B:207:GLN:NE2	2.09	0.67
1:A:111:VAL:HG12	1:A:114:ALA:HB2	1.76	0.67
1:A:518:VAL:O	1:A:522:ILE:HG13	1.94	0.67
1:A:500:GLN:HE21	2:B:422:LEU:CD1	2.08	0.66
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.77	0.66
2:B:244:ILE:HD13	2:B:266:TRP:HZ3	1.60	0.66
2:B:420:PRO:O	2:B:423:VAL:HG12	1.95	0.66
1:A:347:LYS:O	1:A:347:LYS:HG2	1.94	0.66
2:B:205:LEU:O	2:B:209:LEU:HG	1.95	0.66
1:A:500:GLN:HE21	2:B:422:LEU:HD12	1.59	0.65
2:B:193:LEU:CD2	2:B:201:LYS:HD2	2.26	0.65
1:A:411:ILE:O	1:A:412:PRO:O	2.15	0.65
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.79	0.65
1:A:134:SER:HB3	1:A:140:PRO:O	1.96	0.64
1:A:191:SER:OG	1:A:193:LEU:HG	1.97	0.64
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.32	0.64
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.78	0.64
2:B:193:LEU:HD12	2:B:193:LEU:H	1.63	0.64
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.62	0.64
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.31	0.64
2:B:169:GLU:O	2:B:173:LYS:HG3	1.96	0.64
1:A:28:GLU:OE1	1:A:135:ILE:HG22	1.97	0.64
1:A:296:THR:HG22	1:A:297:GLU:H	1.61	0.64
1:A:62:ALA:C	1:A:63:ILE:HD12	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.32	0.64
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.33	0.63
1:A:40:GLU:OE2	1:A:40:GLU:HA	1.99	0.63
1:A:319:TYR:OH	1:A:385:LYS:HE2	1.98	0.63
2:B:195:ILE:HG13	2:B:199:ARG:HE	1.63	0.62
1:A:91:GLN:HE21	2:B:137:ASN:HB3	1.64	0.62
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.34	0.62
1:A:53:GLU:O	1:A:55:PRO:HD3	2.00	0.62
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.82	0.62
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.35	0.62
2:B:13:LYS:HB2	2:B:16:MET:SD	2.40	0.61
1:A:296:THR:HG22	1:A:297:GLU:N	2.15	0.61
1:A:61:PHE:CE2	1:A:74:LEU:HG	2.35	0.61
1:A:207:GLN:HA	1:A:207:GLN:HE21	1.63	0.61
2:B:66:LYS:HE3	2:B:230:MET:CG	2.27	0.61
1:A:27:THR:HG23	1:A:30:LYS:CB	2.30	0.61
1:A:110:ASP:O	1:A:112:GLY:N	2.34	0.61
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.36	0.61
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.65	0.61
1:A:89:GLU:HG2	1:A:90:VAL:H	1.64	0.60
1:A:249:LYS:NZ	1:A:256:ASP:HB3	2.16	0.60
2:B:372:VAL:HG13	2:B:389:PHE:CZ	2.37	0.60
2:B:66:LYS:HZ2	2:B:67:ASP:HB2	1.66	0.60
1:A:376:THR:HG23	1:A:386:THR:HG22	1.82	0.60
1:A:111:VAL:CG1	1:A:114:ALA:HB2	2.32	0.60
2:B:166:LYS:O	2:B:169:GLU:HG3	2.02	0.59
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.84	0.59
2:B:191:SER:HB2	2:B:193:LEU:CD1	2.32	0.59
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.85	0.59
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.85	0.59
2:B:254:VAL:HG23	2:B:291:GLU:O	2.03	0.59
2:B:79:GLU:O	2:B:83:ARG:HG3	2.03	0.59
1:A:56:TYR:O	1:A:143:ARG:NH2	2.31	0.59
1:A:108:VAL:C	1:A:109:LEU:HD23	2.28	0.58
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.37	0.58
1:A:27:THR:HG23	1:A:30:LYS:CG	2.33	0.58
1:A:265:ASN:N	1:A:265:ASN:HD22	2.01	0.58
1:A:498:ASP:O	1:A:535:TRP:NE1	2.34	0.58
2:B:6:GLU:HG2	2:B:6:GLU:O	2.02	0.58
2:B:33:ALA:O	2:B:37:ILE:HG13	2.02	0.58
1:A:136:ASN:OD1	1:A:139:THR:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ASP:O	1:A:178:ILE:HD13	2.03	0.58
2:B:168:LEU:C	2:B:170:PRO:HD2	2.28	0.58
1:A:54:ASN:ND2	1:A:126:LYS:HB2	2.19	0.58
1:A:522:ILE:O	1:A:526:ILE:HG13	2.04	0.57
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.49	0.57
2:B:113:ASP:OD1	2:B:214:LEU:HD11	2.05	0.57
1:A:129:ALA:HA	1:A:144:TYR:O	2.04	0.57
1:A:178:ILE:HG22	1:A:179:VAL:N	2.19	0.57
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.34	0.57
2:B:276:VAL:O	2:B:277:ARG:C	2.48	0.57
1:A:132:ILE:HB	1:A:142:ILE:HG13	1.87	0.57
1:A:194:GLU:O	1:A:197:GLN:N	2.38	0.57
1:A:37:ILE:O	1:A:41:MET:HG3	2.05	0.57
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.40	0.57
1:A:195:ILE:HD13	1:A:195:ILE:N	2.12	0.57
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.86	0.57
2:B:239:TRP:HB3	2:B:350:LYS:NZ	2.19	0.57
1:A:89:GLU:CG	1:A:90:VAL:N	2.67	0.56
2:B:66:LYS:CG	2:B:230:MET:HA	2.34	0.56
2:B:197:GLN:O	2:B:201:LYS:HG3	2.05	0.56
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.41	0.56
2:B:175:ASN:N	2:B:176:PRO:HD3	2.20	0.56
2:B:175:ASN:HB3	2:B:178:ILE:HD12	1.86	0.56
1:A:170:PRO:HA	1:A:173:LYS:HE3	1.88	0.56
2:B:203:GLU:CG	2:B:207:GLN:HE22	2.18	0.56
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.88	0.56
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.06	0.55
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.53	0.55
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.88	0.55
2:B:193:LEU:HD12	2:B:193:LEU:N	2.20	0.55
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.32	0.55
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.42	0.55
2:B:208:HIS:NE2	2:B:212:TRP:HZ3	2.05	0.55
1:A:363:ASN:ND2	1:A:401:TRP:CZ3	2.75	0.54
1:A:226:PRO:HA	1:A:234:LEU:O	2.07	0.54
1:A:116:PHE:CD2	1:A:116:PHE:N	2.73	0.54
1:A:406:TRP:O	2:B:331:LYS:HB3	2.08	0.54
2:B:66:LYS:CE	2:B:230:MET:HG3	2.30	0.54
2:B:379:SER:CB	2:B:387:PRO:HD3	2.38	0.54
1:A:89:GLU:HG2	1:A:90:VAL:N	2.22	0.54
1:A:292:VAL:C	1:A:293:ILE:HD12	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:GLN:NE2	2:B:421:PRO:HB3	2.23	0.54
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.38	0.54
1:A:396:GLU:HG3	1:A:397:THR:N	2.20	0.54
2:B:60:VAL:HG11	2:B:130:PHE:CD1	2.43	0.54
1:A:28:GLU:OE1	1:A:135:ILE:CG2	2.56	0.54
1:A:61:PHE:N	1:A:61:PHE:CD2	2.75	0.54
1:A:257:ILE:HD13	1:A:282:LEU:HD13	1.90	0.54
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.42	0.54
1:A:393:ILE:HD12	1:A:423:VAL:HG21	1.90	0.54
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.43	0.53
1:A:340:GLN:CB	1:A:351:THR:HG22	2.39	0.53
1:A:350:LYS:HG2	1:A:351:THR:N	2.23	0.53
1:A:480:GLN:HG2	1:A:517:LEU:HD11	1.88	0.53
2:B:169:GLU:N	2:B:170:PRO:HD2	2.23	0.53
2:B:186:ASP:OD1	2:B:228:LEU:HD12	2.09	0.53
1:A:5:ILE:HG13	1:A:6:GLU:N	2.22	0.53
1:A:366:LYS:HE3	1:A:405:TYR:OH	2.09	0.53
2:B:278:GLN:NE2	2:B:298:GLU:HB2	2.22	0.53
2:B:167:ILE:HG23	2:B:212:TRP:CE3	2.43	0.53
1:A:183:TYR:CD1	1:A:184:MET:HG2	2.43	0.53
1:A:61:PHE:N	1:A:61:PHE:HD2	2.06	0.53
1:A:194:GLU:O	1:A:195:ILE:C	2.51	0.53
2:B:118:VAL:HB	2:B:149:LEU:HG	1.91	0.53
2:B:295:LEU:H	2:B:295:LEU:CD1	2.21	0.53
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.43	0.52
1:A:278:GLN:NE2	1:A:278:GLN:HA	2.22	0.52
2:B:257:ILE:HG21	2:B:283:LEU:HD13	1.90	0.52
1:A:178:ILE:HD12	1:A:191:SER:HB2	1.89	0.52
1:A:239:TRP:HZ2	1:A:349:LEU:O	1.92	0.52
2:B:308:GLU:HA	2:B:311:LYS:HG3	1.91	0.52
1:A:174:GLN:O	1:A:176:PRO:HD2	2.09	0.52
2:B:66:LYS:HG2	2:B:230:MET:CA	2.39	0.52
2:B:183:TYR:OH	2:B:386:THR:HG23	2.10	0.52
2:B:327:ALA:O	2:B:389:PHE:HA	2.09	0.52
2:B:17:ASP:CG	2:B:18:GLY:H	2.18	0.52
1:A:95:PRO:HB3	2:B:136:ASN:O	2.09	0.52
1:A:254:VAL:O	1:A:258:GLN:HG3	2.09	0.52
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.92	0.52
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.90	0.52
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.92	0.52
2:B:170:PRO:HG2	2:B:171:PHE:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:TRP:HA	2:B:229:TRP:CE3	2.46	0.52
1:A:94:ILE:HD13	1:A:230:MET:HE1	1.92	0.51
2:B:270:ILE:O	2:B:272:PRO:HD3	2.10	0.51
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.45	0.51
2:B:376:THR:O	2:B:377:THR:C	2.54	0.51
1:A:18:GLY:HA3	1:A:56:TYR:CE1	2.45	0.51
1:A:417:VAL:O	1:A:417:VAL:HG13	2.10	0.51
2:B:335:GLY:O	2:B:355:ALA:HA	2.11	0.51
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.92	0.51
2:B:195:ILE:HG23	2:B:196:GLY:N	2.26	0.51
2:B:205:LEU:HD22	2:B:209:LEU:HG	1.93	0.51
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.46	0.51
1:A:170:PRO:O	1:A:173:LYS:HG2	2.10	0.51
1:A:440:PHE:HZ	1:A:463:ARG:HH21	1.59	0.51
2:B:173:LYS:O	2:B:176:PRO:HD3	2.10	0.51
1:A:116:PHE:HE1	3:A:1302:PO4:O1	1.94	0.51
1:A:261:VAL:O	1:A:265:ASN:ND2	2.44	0.51
1:A:109:LEU:HD23	1:A:109:LEU:N	2.26	0.51
1:A:328:GLU:O	1:A:339:TYR:HA	2.11	0.50
1:A:433:PRO:HB3	2:B:289:LEU:HD23	1.93	0.50
2:B:110:ASP:HB3	2:B:226:PRO:HG2	1.93	0.50
2:B:202:ILE:HG21	2:B:227:PHE:HE1	1.75	0.50
2:B:206:ARG:NH2	2:B:226:PRO:HA	2.25	0.50
2:B:193:LEU:HD21	2:B:201:LYS:HZ2	1.75	0.50
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.46	0.50
1:A:254:VAL:HG22	1:A:293:ILE:CD1	2.40	0.50
1:A:332:GLN:HB3	1:A:336:GLN:HB3	1.92	0.50
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.76	0.50
1:A:440:PHE:CD2	1:A:459:THR:HG22	2.47	0.50
1:A:253:THR:O	1:A:254:VAL:C	2.53	0.50
1:A:41:MET:HE1	3:A:1302:PO4:O2	2.12	0.50
1:A:108:VAL:HA	1:A:187:LEU:O	2.11	0.50
1:A:118:VAL:HB	1:A:149:LEU:HG	1.92	0.50
1:A:197:GLN:HA	1:A:197:GLN:OE1	2.10	0.50
2:B:195:ILE:CG2	2:B:196:GLY:N	2.75	0.50
1:A:72:ARG:HG2	1:A:73:LYS:N	2.27	0.50
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.94	0.49
1:A:409:THR:O	2:B:364:ASP:HB2	2.12	0.49
1:A:424:LYS:HE3	1:A:426:TRP:CE2	2.46	0.49
2:B:170:PRO:HA	2:B:173:LYS:NZ	2.27	0.49
1:A:57:ASN:HA	1:A:129:ALA:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:HA	1:A:149:LEU:HD12	1.93	0.49
1:A:178:ILE:HD11	1:A:193:LEU:HD11	1.94	0.49
1:A:91:GLN:O	1:A:93:GLY:N	2.44	0.49
1:A:201:LYS:O	1:A:204:GLU:HB3	2.12	0.49
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.47	0.49
1:A:90:VAL:O	1:A:91:GLN:HB2	2.12	0.49
2:B:195:ILE:HD11	2:B:233:GLU:HG3	1.94	0.49
1:A:178:ILE:CD1	1:A:191:SER:HB2	2.43	0.49
1:A:457:TYR:CD1	1:A:457:TYR:C	2.91	0.49
1:A:249:LYS:HZ1	1:A:256:ASP:HB3	1.77	0.49
1:A:507:GLN:HE22	2:B:421:PRO:HB3	1.76	0.49
2:B:295:LEU:N	2:B:295:LEU:CD1	2.73	0.49
1:A:253:THR:O	1:A:256:ASP:N	2.46	0.49
1:A:368:LEU:O	1:A:372:VAL:HG23	2.13	0.49
1:A:293:ILE:HD12	1:A:293:ILE:N	2.28	0.48
2:B:425:LEU:HD23	2:B:425:LEU:O	2.12	0.48
1:A:99:GLY:HA3	2:B:136:ASN:ND2	2.28	0.48
1:A:115:TYR:CD1	1:A:156:SER:HB3	2.48	0.48
1:A:363:ASN:HB2	1:A:511:ASP:OD2	2.13	0.48
2:B:64:LYS:HE2	2:B:68:SER:O	2.13	0.48
1:A:100:LEU:C	1:A:101:LYS:HD2	2.38	0.48
1:A:465:LYS:HD2	1:A:484:LEU:CD2	2.44	0.48
1:A:478:GLU:CD	1:A:499:SER:HB2	2.38	0.48
1:A:102:LYS:HG2	1:A:103:LYS:N	2.28	0.48
1:A:188:TYR:CD2	4:A:999:H16:HF1	2.49	0.48
2:B:40:GLU:OE2	2:B:40:GLU:HA	2.13	0.48
1:A:91:GLN:O	1:A:92:LEU:C	2.56	0.48
1:A:115:TYR:HB3	1:A:149:LEU:HB2	1.96	0.48
1:A:218:ASP:O	1:A:222:GLN:HG3	2.14	0.48
1:A:460:ASN:OD1	1:A:461:ARG:HG3	2.13	0.48
2:B:105:SER:O	2:B:190:GLY:HA2	2.13	0.48
2:B:174:GLN:C	2:B:176:PRO:HD3	2.38	0.48
2:B:239:TRP:HB3	2:B:350:LYS:HZ1	1.76	0.48
1:A:245:VAL:HG23	1:A:245:VAL:O	2.14	0.48
2:B:24:TRP:CD1	2:B:25:PRO:HD2	2.49	0.48
2:B:27:THR:OG1	2:B:30:LYS:HG2	2.13	0.48
2:B:66:LYS:HD2	2:B:67:ASP:N	2.29	0.48
2:B:193:LEU:HD21	2:B:201:LYS:NZ	2.29	0.48
2:B:254:VAL:O	2:B:258:GLN:HG3	2.13	0.48
2:B:380:ILE:O	2:B:384:GLY:N	2.46	0.48
1:A:24:TRP:HZ3	1:A:61:PHE:CG	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.29	0.47
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.35	0.47
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.49	0.47
2:B:328:GLU:CG	2:B:390:LYS:HD2	2.45	0.47
1:A:27:THR:HG23	1:A:30:LYS:HG3	1.94	0.47
1:A:106:VAL:HA	1:A:189:VAL:O	2.13	0.47
1:A:113:ASP:HB2	1:A:116:PHE:CD2	2.49	0.47
2:B:249:LYS:HD3	2:B:251:SER:O	2.15	0.47
2:B:379:SER:HB2	2:B:387:PRO:HD3	1.96	0.47
1:A:164:MET:O	1:A:168:LEU:HG	2.14	0.47
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.49	0.47
2:B:12:LEU:O	2:B:13:LYS:C	2.56	0.47
2:B:98:ALA:O	2:B:101:LYS:HG2	2.13	0.47
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.44	0.47
2:B:172:ARG:O	2:B:176:PRO:HG3	2.14	0.47
1:A:60:VAL:HG22	1:A:75:VAL:HG22	1.97	0.47
1:A:156:SER:HB2	1:A:157:PRO:CD	2.35	0.47
1:A:393:ILE:HD12	1:A:423:VAL:CG2	2.44	0.47
1:A:399:GLU:HG3	1:A:402:TRP:CZ3	2.49	0.47
1:A:49:LYS:HA	1:A:143:ARG:O	2.15	0.47
1:A:505:ILE:O	1:A:510:PRO:HD3	2.15	0.47
1:A:45:GLY:O	1:A:147:ASN:ND2	2.40	0.47
1:A:73:LYS:HZ3	1:A:75:VAL:HG23	1.80	0.47
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.47	0.47
2:B:98:ALA:O	2:B:101:LYS:HE3	2.15	0.47
1:A:93:GLY:O	2:B:137:ASN:HB3	2.14	0.46
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.50	0.46
1:A:470:THR:O	1:A:471:ASP:HB2	2.15	0.46
2:B:331:LYS:O	2:B:424:LYS:HE3	2.15	0.46
1:A:61:PHE:CZ	1:A:74:LEU:HD23	2.50	0.46
1:A:202:ILE:O	1:A:205:LEU:HB3	2.16	0.46
2:B:160:PHE:O	2:B:160:PHE:CD1	2.68	0.46
1:A:91:GLN:C	1:A:93:GLY:N	2.72	0.46
1:A:102:LYS:HZ3	1:A:237:ASP:HB2	1.80	0.46
1:A:116:PHE:H	1:A:116:PHE:HD2	1.58	0.46
2:B:163:SER:O	2:B:167:ILE:HG13	2.16	0.46
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.50	0.46
1:A:33:ALA:HB2	1:A:71:TRP:CD1	2.51	0.46
1:A:160:PHE:C	1:A:160:PHE:CD2	2.94	0.46
2:B:96:HIS:CE1	2:B:381:VAL:O	2.69	0.46
2:B:393:ILE:HG12	2:B:394:GLN:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LYS:NZ	2:B:67:ASP:HB2	2.30	0.46
2:B:167:ILE:O	2:B:208:HIS:HE1	1.98	0.46
2:B:298:GLU:CD	2:B:298:GLU:H	2.24	0.46
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.97	0.46
2:B:344:GLU:HG2	2:B:345:PRO:HD2	1.98	0.46
1:A:239:TRP:CZ2	1:A:349:LEU:O	2.69	0.46
2:B:57:ASN:ND2	2:B:143:ARG:NH1	2.53	0.46
2:B:227:PHE:CB	2:B:231:GLY:HA2	2.34	0.46
1:A:63:ILE:HD12	1:A:63:ILE:N	2.31	0.46
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.97	0.46
1:A:108:VAL:HG13	1:A:223:LYS:HB2	1.98	0.46
2:B:40:GLU:OE2	2:B:43:LYS:HD2	2.16	0.45
2:B:208:HIS:CE1	2:B:212:TRP:HZ3	2.34	0.45
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.80	0.45
1:A:31:ILE:HD13	1:A:133:PRO:O	2.17	0.45
1:A:73:LYS:HZ3	1:A:75:VAL:CG2	2.30	0.45
1:A:340:GLN:HA	1:A:351:THR:HA	1.98	0.45
1:A:479:LEU:HD12	1:A:479:LEU:N	2.32	0.45
2:B:423:VAL:HG13	2:B:424:LYS:N	2.31	0.45
1:A:30:LYS:CD	1:A:62:ALA:HB3	2.43	0.45
1:A:194:GLU:O	1:A:196:GLY:N	2.49	0.45
2:B:206:ARG:NH1	2:B:227:PHE:CE2	2.85	0.45
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.51	0.45
1:A:264:LEU:HD13	1:A:276:VAL:HG12	1.99	0.45
1:A:420:PRO:HA	1:A:421:PRO:C	2.40	0.45
1:A:434:ILE:HB	1:A:437:ALA:HB3	1.99	0.45
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.52	0.45
2:B:257:ILE:O	2:B:260:LEU:HB3	2.17	0.45
2:B:297:GLU:HA	2:B:300:GLU:HB2	1.99	0.45
1:A:472:THR:CB	1:A:476:LYS:HE3	2.46	0.45
2:B:197:GLN:O	2:B:198:HIS:C	2.59	0.45
1:A:241:VAL:O	1:A:242:GLN:C	2.60	0.45
1:A:406:TRP:HH2	2:B:418:ASN:OD1	2.00	0.45
1:A:193:LEU:HD13	1:A:197:GLN:HG3	1.99	0.44
2:B:228:LEU:HD23	2:B:228:LEU:HA	1.73	0.44
1:A:469:LEU:CD2	1:A:480:GLN:HG3	2.42	0.44
1:A:479:LEU:HD11	1:A:501:TYR:CE2	2.52	0.44
1:A:115:TYR:N	1:A:115:TYR:CD2	2.86	0.44
1:A:170:PRO:O	1:A:171:PHE:C	2.60	0.44
2:B:253:THR:HA	2:B:292:VAL:HA	1.98	0.44
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:HG3	1:A:237:ASP:HA	1.98	0.44
1:A:344:GLU:HB3	1:A:347:LYS:HD3	1.99	0.44
2:B:113:ASP:HB2	2:B:214:LEU:HD12	1.99	0.44
1:A:228:LEU:HD12	1:A:228:LEU:N	2.32	0.44
1:A:237:ASP:OD2	1:A:237:ASP:N	2.48	0.44
1:A:361:HIS:O	1:A:362:THR:HG23	2.16	0.44
2:B:303:LEU:HD22	2:B:307:ARG:HG3	2.00	0.44
1:A:164:MET:HE1	1:A:187:LEU:HD22	2.00	0.44
1:A:498:ASP:HA	1:A:536:VAL:O	2.18	0.44
2:B:120:LEU:O	2:B:121:ASP:C	2.59	0.44
1:A:277:ARG:HG3	1:A:277:ARG:HH11	1.82	0.44
2:B:17:ASP:CG	2:B:18:GLY:N	2.75	0.44
2:B:158:ALA:O	2:B:161:GLN:CB	2.65	0.44
1:A:28:GLU:OE1	1:A:135:ILE:HA	2.18	0.44
1:A:356:ARG:CZ	1:A:358:ARG:HG2	2.48	0.44
1:A:19:PRO:HD3	1:A:80:LEU:HD13	2.00	0.43
1:A:58:THR:CG2	1:A:76:ASP:O	2.66	0.43
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.53	0.43
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.18	0.43
1:A:121:ASP:O	1:A:122:GLU:C	2.61	0.43
1:A:178:ILE:CG2	1:A:179:VAL:N	2.80	0.43
1:A:270:ILE:HG23	1:A:271:TYR:N	2.34	0.43
1:A:116:PHE:CE1	3:A:1302:PO4:O3	2.72	0.43
1:A:219:LYS:HA	1:A:222:GLN:CD	2.43	0.43
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.99	0.43
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.48	0.43
1:A:156:SER:CB	1:A:157:PRO:HD3	2.35	0.43
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.54	0.43
2:B:320:ASP:OD2	2:B:323:LYS:HG2	2.19	0.43
1:A:118:VAL:HG13	1:A:119:PRO:HD2	2.01	0.43
2:B:57:ASN:ND2	2:B:143:ARG:HH11	2.13	0.43
1:A:503:LEU:HD22	1:A:535:TRP:CB	2.47	0.43
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.54	0.42
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.19	0.42
2:B:325:LEU:HB3	2:B:387:PRO:HA	2.01	0.42
1:A:320:ASP:OD2	1:A:322:SER:OG	2.36	0.42
2:B:27:THR:O	2:B:28:GLU:C	2.62	0.42
2:B:199:ARG:CZ	2:B:233:GLU:OE1	2.67	0.42
1:A:106:VAL:O	1:A:225:PRO:HD3	2.19	0.42
1:A:112:GLY:O	1:A:113:ASP:C	2.62	0.42
1:A:115:TYR:O	1:A:149:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:SER:HB2	1:A:493:VAL:HG22	2.01	0.42
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.54	0.42
2:B:378:GLU:O	2:B:379:SER:C	2.63	0.42
1:A:116:PHE:HE1	3:A:1302:PO4:P	2.42	0.42
1:A:176:PRO:C	1:A:178:ILE:H	2.28	0.42
1:A:207:GLN:HE21	1:A:207:GLN:CA	2.29	0.42
1:A:439:THR:O	1:A:459:THR:HA	2.20	0.42
2:B:17:ASP:OD1	2:B:56:TYR:OH	2.32	0.42
1:A:88:TRP:HB2	2:B:54:ASN:O	2.20	0.42
1:A:465:LYS:HD2	1:A:484:LEU:HD21	2.01	0.42
2:B:229:TRP:HA	2:B:229:TRP:HE3	1.81	0.42
1:A:89:GLU:O	1:A:90:VAL:C	2.63	0.42
2:B:21:VAL:HG12	2:B:22:LYS:O	2.19	0.42
2:B:389:PHE:CD1	2:B:389:PHE:N	2.88	0.42
1:A:155:GLY:O	1:A:156:SER:C	2.63	0.42
1:A:483:TYR:CZ	1:A:520:GLN:HB3	2.54	0.42
2:B:148:VAL:HG23	2:B:149:LEU:N	2.34	0.42
2:B:161:GLN:O	2:B:164:MET:HB3	2.20	0.42
2:B:193:LEU:H	2:B:193:LEU:CD1	2.29	0.42
2:B:241:VAL:HG11	2:B:313:PRO:HG3	2.02	0.42
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.42	0.42
2:B:233:GLU:H	2:B:233:GLU:HG2	1.66	0.42
2:B:265:ASN:O	2:B:268:SER:OG	2.34	0.42
2:B:278:GLN:HB3	2:B:299:ALA:HB2	2.02	0.42
2:B:162:SER:C	2:B:164:MET:N	2.75	0.42
1:A:229:TRP:O	1:A:230:MET:C	2.63	0.41
2:B:58:THR:HG21	2:B:77:PHE:CD2	2.55	0.41
2:B:348:ASN:HD22	2:B:351:THR:HG22	1.82	0.41
1:A:136:ASN:OD1	1:A:139:THR:CG2	2.68	0.41
1:A:171:PHE:CE2	1:A:175:ASN:ND2	2.89	0.41
2:B:332:GLN:HB2	2:B:336:GLN:O	2.19	0.41
1:A:61:PHE:HE2	1:A:74:LEU:HG	1.84	0.41
1:A:93:GLY:O	2:B:137:ASN:CB	2.68	0.41
1:A:134:SER:OG	1:A:139:THR:O	2.37	0.41
1:A:247:PRO:O	1:A:307:ARG:NH2	2.48	0.41
1:A:253:THR:HG22	1:A:255:ASN:N	2.31	0.41
1:A:516:GLU:O	1:A:517:LEU:C	2.62	0.41
1:A:160:PHE:CE2	1:A:164:MET:HG2	2.55	0.41
2:B:259:LYS:HE2	2:B:259:LYS:HB3	1.95	0.41
1:A:203:GLU:O	1:A:207:GLN:HG2	2.20	0.41
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:O	1:A:213:GLY:N	2.54	0.41
1:A:340:GLN:HB3	1:A:340:GLN:HE21	1.65	0.41
1:A:402:TRP:CG	1:A:403:THR:N	2.87	0.41
2:B:7:THR:HG22	2:B:119:PRO:HG2	2.02	0.41
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.56	0.41
1:A:212:TRP:C	1:A:214:LEU:N	2.77	0.41
1:A:236:PRO:HA	4:A:999:H16:H9	2.02	0.41
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.20	0.41
1:A:480:GLN:O	1:A:481:ALA:C	2.63	0.41
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.50	0.41
2:B:125:ARG:HG2	2:B:146:TYR:O	2.21	0.41
2:B:259:LYS:O	2:B:260:LEU:C	2.64	0.41
2:B:345:PRO:O	2:B:346:PHE:HB2	2.20	0.41
2:B:366:LYS:O	2:B:367:GLN:C	2.64	0.41
1:A:362:THR:O	1:A:512:GLN:HG2	2.21	0.41
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.54	0.41
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.56	0.40
1:A:212:TRP:O	1:A:214:LEU:N	2.53	0.40
1:A:270:ILE:O	1:A:272:PRO:HD3	2.20	0.40
1:A:391:LEU:C	1:A:417:VAL:HG12	2.46	0.40
1:A:476:LYS:HD3	1:A:517:LEU:HD12	2.04	0.40
2:B:276:VAL:O	2:B:279:LEU:N	2.54	0.40
1:A:208:HIS:O	1:A:211:ARG:HB2	2.21	0.40
1:A:249:LYS:HZ3	1:A:256:ASP:HB3	1.86	0.40
1:A:270:ILE:HG23	1:A:271:TYR:CD2	2.57	0.40
1:A:278:GLN:HG3	1:A:298:GLU:HB3	2.03	0.40
2:B:278:GLN:NE2	2:B:298:GLU:CB	2.84	0.40
1:A:7:THR:HG21	1:A:121:ASP:HA	2.04	0.40
1:A:13:LYS:HE3	1:A:84:THR:O	2.22	0.40
2:B:365:VAL:O	2:B:366:LYS:C	2.65	0.40
1:A:109:LEU:N	1:A:109:LEU:CD2	2.83	0.40
2:B:97:PRO:C	2:B:99:GLY:N	2.79	0.40
2:B:208:HIS:CE1	2:B:212:TRP:CZ3	3.10	0.40
2:B:368:LEU:O	2:B:371:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	510/560 (91%)	453 (89%)	42 (8%)	15 (3%)	3	12
2	B	393/440 (89%)	338 (86%)	49 (12%)	6 (2%)	8	26
All	All	903/1000 (90%)	791 (88%)	91 (10%)	21 (2%)	5	16

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	91	GLN
1	A	92	LEU
1	A	137	ASN
1	A	156	SER
1	A	412	PRO
1	A	472	THR
1	A	111	VAL
1	A	195	ILE
1	A	402	TRP
1	A	268	SER
1	A	345	PRO
2	B	250	ASP
2	B	286	THR
1	A	121	ASP
1	A	170	PRO
1	A	356	ARG
2	B	166	LYS
2	B	158	ALA
2	B	277	ARG
2	B	167	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	466/499 (93%)	426 (91%)	40 (9%)	10	29
2	B	366/400 (92%)	350 (96%)	16 (4%)	25	58
All	All	832/899 (92%)	776 (93%)	56 (7%)	15	40

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	20	LYS
1	A	27	THR
1	A	36	GLU
1	A	39	THR
1	A	61	PHE
1	A	92	LEU
1	A	105	SER
1	A	107	THR
1	A	109	LEU
1	A	115	TYR
1	A	116	PHE
1	A	135	ILE
1	A	138	GLU
1	A	162	SER
1	A	164	MET
1	A	195	ILE
1	A	205	LEU
1	A	215	THR
1	A	265	ASN
1	A	275	LYS
1	A	287	LYS
1	A	289	LEU
1	A	301	LEU
1	A	317	VAL
1	A	336	GLN
1	A	340	GLN

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Mol	Chain	Res	Type
1	A	345	PRO
1	A	348	ASN
1	A	356	ARG
1	A	361	HIS
1	A	362	THR
1	A	391	LEU
1	A	396	GLU
1	A	400	THR
1	A	443	ASP
1	A	484	LEU
1	A	487	GLN
1	A	493	VAL
1	A	517	LEU
2	B	6	GLU
2	B	10	VAL
2	B	55	PRO
2	B	70	LYS
2	B	122	GLU
2	B	148	VAL
2	B	178	ILE
2	B	194	GLU
2	B	205	LEU
2	B	210	LEU
2	B	233	GLU
2	B	240	THR
2	B	242	GLN
2	B	250	ASP
2	B	295	LEU
2	B	303	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	182	GLN
1	A	207	GLN
1	A	208	HIS
1	A	222	GLN
1	A	242	GLN
1	A	265	ASN
1	A	336	GLN
1	A	407	GLN

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Mol	Chain	Res	Type
1	A	475	GLN
1	A	480	GLN
1	A	500	GLN
1	A	507	GLN
1	A	512	GLN
1	A	520	GLN
2	B	57	ASN
2	B	147	ASN
2	B	151	GLN
2	B	175	ASN
2	B	207	GLN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	336	GLN
2	B	348	ASN
2	B	394	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	CSD	A	280	1	4,7,8	2.09	1 (25%)	1,8,10	6.22	1 (100%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	280	1	-	2/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	3.87	1.51	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	6.22	117.06	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	PO4	A	1302	-	4,4,4	1.74	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	1300	-	4,4,4	1.61	0	6,6,6	0.47	0
4	H16	A	999	-	24,24,24	1.95	8 (33%)	28,33,33	1.22	4 (14%)
3	PO4	A	1301	-	4,4,4	1.69	0	6,6,6	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	H16	A	999	-	-	3/7/15/15	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	H16	C4-S4	4.44	1.83	1.76
4	A	999	H16	C6-N1	3.61	1.40	1.35
4	A	999	H16	C6-C5	3.22	1.49	1.44
4	A	999	H16	C3-C4	-3.13	1.39	1.45
4	A	999	H16	C10-C9	2.61	1.43	1.38
4	A	999	H16	CF-CA	2.41	1.60	1.51
4	A	999	H16	CE-CF	2.14	1.58	1.53
4	A	999	H16	C3-C2	2.09	1.44	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	H16	C2-N1-C6	-2.78	120.93	124.82
4	A	999	H16	C11-C5-C6	2.66	120.21	116.64
4	A	999	H16	C5-C6-N1	2.32	118.00	115.92
4	A	999	H16	O2-C6-C5	-2.27	121.76	124.56

There are no chirality outliers.

All (3) torsion outliers are listed below:

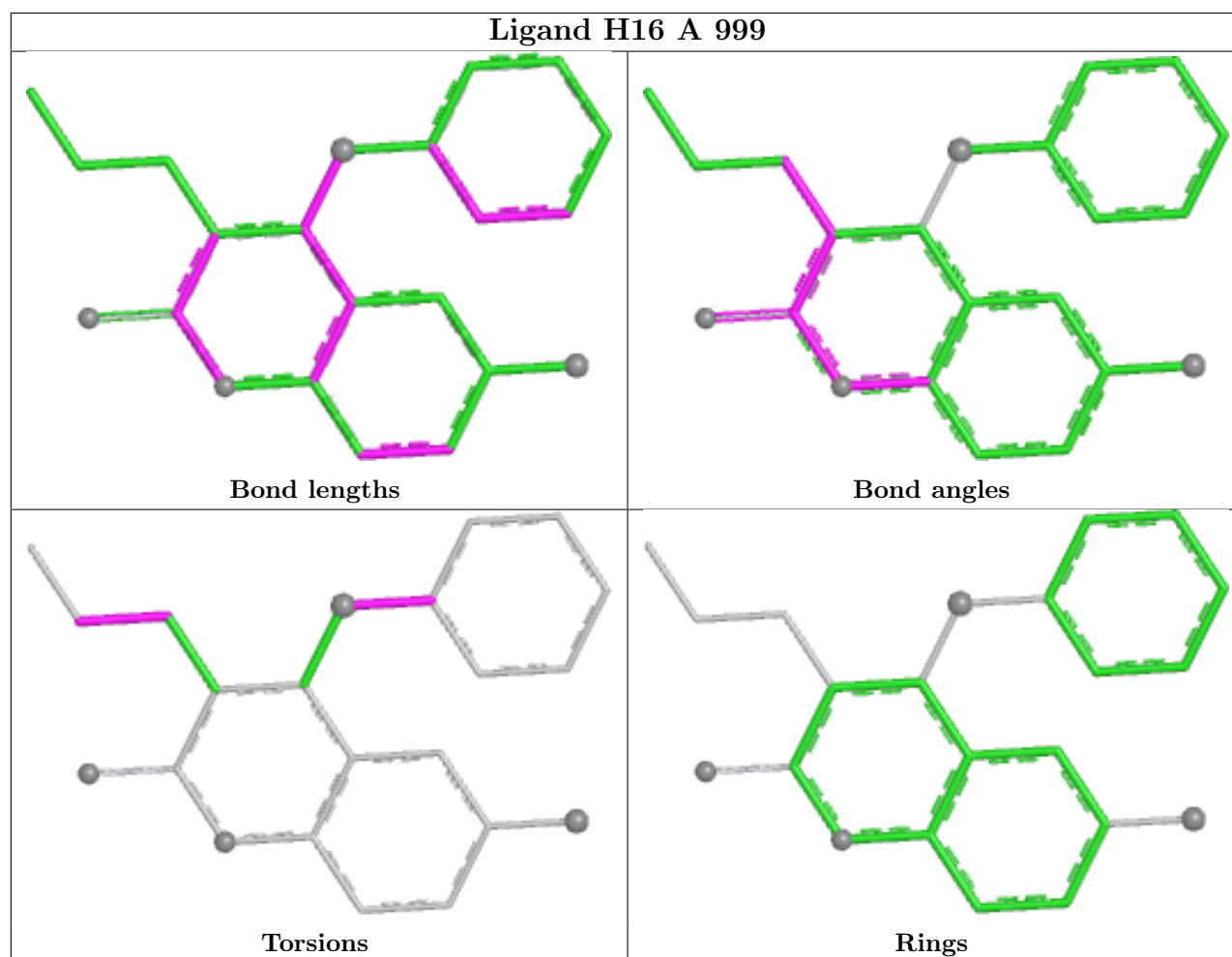
Mol	Chain	Res	Type	Atoms
4	A	999	H16	CB-CA-S4-C4
4	A	999	H16	CF-CA-S4-C4
4	A	999	H16	C5-C11-C12-C13

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1302	PO4	4	0
4	A	999	H16	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	516/560 (92%)	-0.43	1 (0%) 91 89	25, 63, 107, 131	0
2	B	401/440 (91%)	-0.45	0 100 100	25, 62, 110, 135	0
All	All	917/1000 (91%)	-0.44	1 (0%) 92 90	25, 62, 108, 135	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	TRP	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSD	A	280	8/9	0.97	0.05	48,54,61,78	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

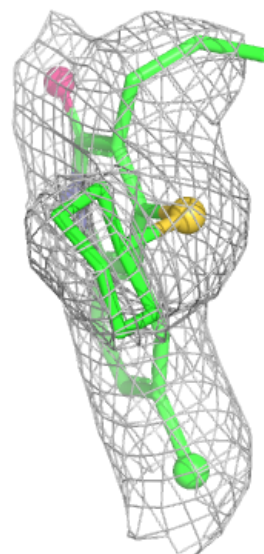
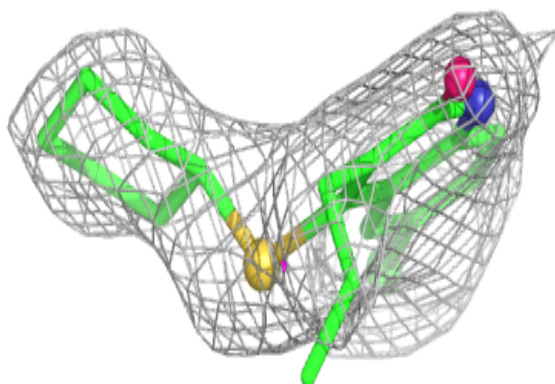
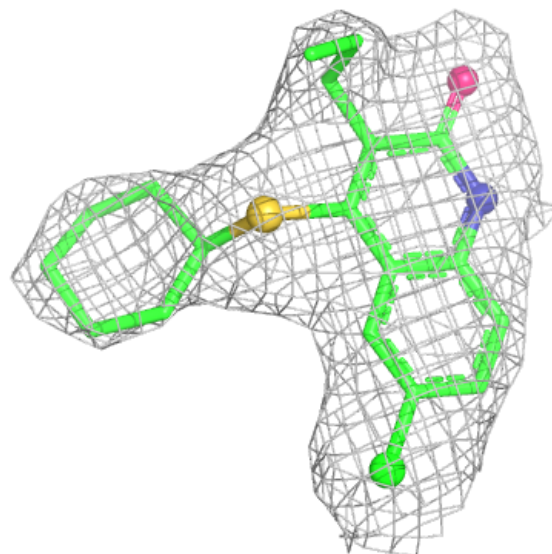
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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
3	PO4	A	1300	5/5	0.71	0.09	123,128,130,133	0
3	PO4	A	1301	5/5	0.82	0.15	121,133,134,136	0
3	PO4	A	1302	5/5	0.84	0.11	145,147,149,149	0
4	H16	A	999	22/22	0.97	0.07	26,48,56,59	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 H16 A 999:

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.