



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:33 PM UTC

PDB ID : 3IS9 / pdb_00003is9
Title : Crystal structure of the HIV-1 reverse transcriptase (RT) in complex with the alkenyldiarylmethane (ADAM) Non-nucleoside RT Inhibitor dimethyl 3,3'-(6-methoxy-6-oxohex-1-ene-1,1-diyl)bis(5-cyano-6-methoxybenzoate).
Authors : Ho, W.C.; Bauman, J.D.; Das, K.; Arnold, E.
Deposited on : 2009-08-25
Resolution : 2.55 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

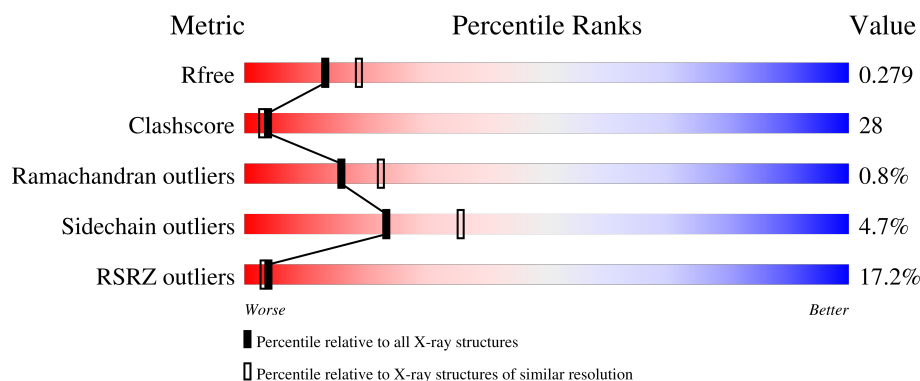
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	558	20% 52% 42% 5%
2	B	428	13% 54% 39% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8103 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4501	2913	748	833	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P03366
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

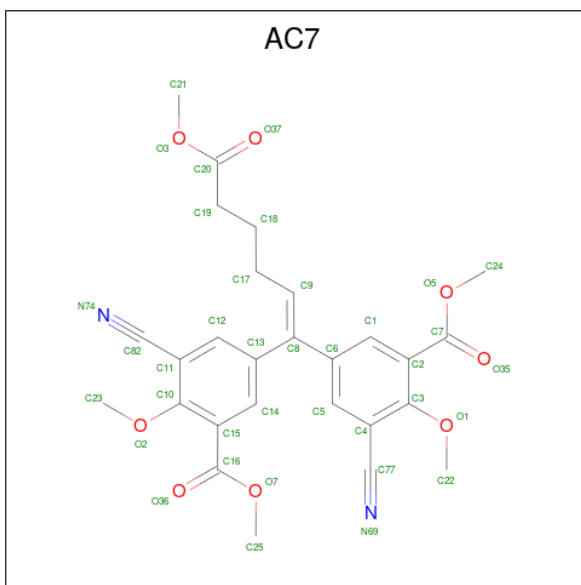
- Molecule 2 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total	C	N	O	S	0	0	0
			3441	2244	568	622	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is dimethyl 3,3'-(6-methoxy-6-oxohex-1-ene-1,1-diyl)bis(5-cyano-6-methoxybenzoate) (CCD ID: AC7) (formula: C₂₇H₂₆N₂O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			37	27	2	8		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	65	Total O 65 65	0	0
4	B	59	Total O 59 59	0	0

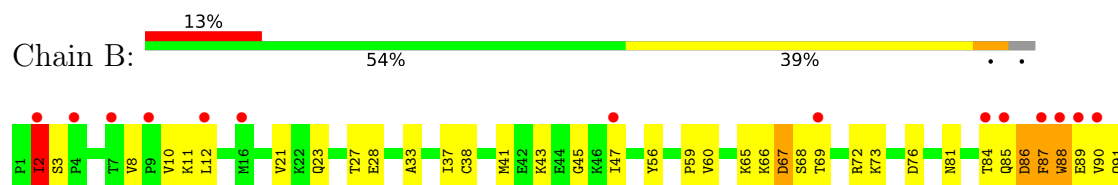
3 Residue-property plots

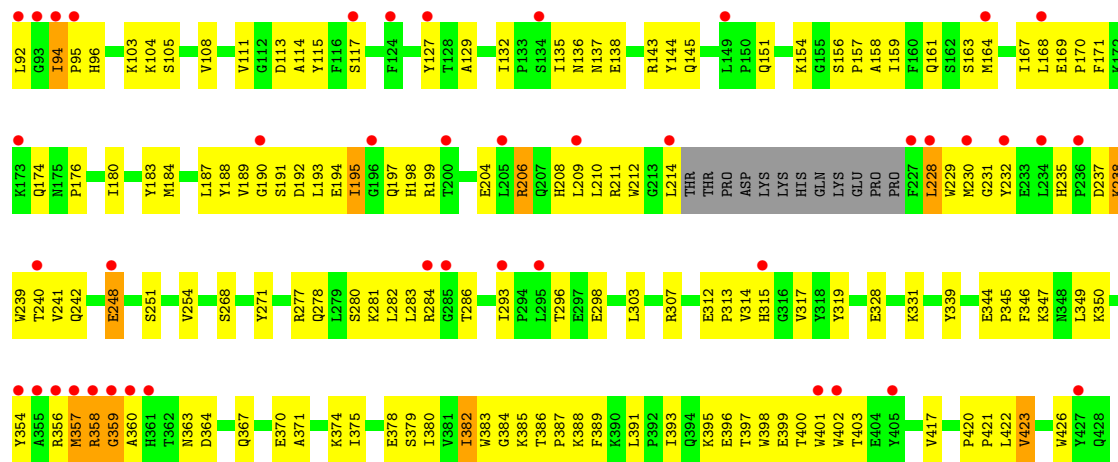
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: Reverse transcriptase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.82Å 73.73Å 108.69Å 90.00° 99.55° 90.00°	Depositor
Resolution (Å)	40.00 – 2.55 40.00 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.6 (40.00-2.55) 85.9 (40.00-2.74)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.72Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.250 , 0.282 0.266 , 0.279	Depositor DCC
R_{free} test set	1414 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.7	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	0.91	EDS
Total number of atoms	8103	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: AC7

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	0.49	1/4619 (0.0%)	0.96	19/6278 (0.3%)
2	B	0.50	0/3541	0.94	10/4810 (0.2%)
All	All	0.49	1/8160 (0.0%)	0.95	29/11088 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ASP	CG-OD1	5.36	1.35	1.25

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	LEU	N-CA-C	-8.92	101.64	111.36
2	B	2	ILE	N-CA-C	8.29	119.82	107.80
1	A	309	ILE	N-CA-C	-8.15	104.81	112.96
1	A	391	LEU	N-CA-C	7.45	120.07	110.39
1	A	223	LYS	N-CA-C	7.37	119.94	108.96
1	A	382	ILE	N-CA-C	7.28	118.08	110.72
1	A	66	LYS	N-CA-C	7.20	121.10	110.30
1	A	545	ASN	N-CA-C	-6.83	105.48	113.88
1	A	259	LYS	N-CA-C	-6.58	105.12	113.02
2	B	382	ILE	N-CA-C	6.44	117.22	110.72
2	B	356	ARG	N-CA-C	6.33	119.66	110.42
1	A	184	MET	N-CA-C	6.32	117.92	108.31
1	A	184	MET	CB-CA-C	-6.19	109.42	116.54
1	A	508	ALA	N-CA-C	-6.10	105.80	113.18
1	A	305	GLU	N-CA-C	-5.97	105.85	113.02
1	A	112	GLY	N-CA-C	-5.91	106.43	113.99
1	A	147	ASN	N-CA-C	-5.75	104.98	113.61
2	B	358	ARG	N-CA-C	5.73	119.08	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	THR	N-CA-C	5.67	118.91	110.52
1	A	308	GLU	N-CA-C	-5.42	106.53	114.39
1	A	222	GLN	N-CA-C	-5.39	104.32	112.99
1	A	493	VAL	N-CA-C	5.28	115.16	107.88
2	B	69	THR	N-CA-C	-5.26	106.86	113.28
1	A	138	GLU	N-CA-C	-5.20	106.17	112.88
2	B	349	LEU	N-CA-C	-5.17	107.00	113.72
2	B	389	PHE	N-CA-C	5.08	118.23	110.20
2	B	198	HIS	N-CA-C	-5.08	107.22	113.41
2	B	189	VAL	N-CA-C	5.06	115.33	107.28
2	B	391	LEU	N-CA-C	5.06	116.03	109.65

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	4501	0	4554	262	0
2	B	3441	0	3476	212	0
3	A	37	0	26	3	0
4	A	65	0	0	3	0
4	B	59	0	0	2	0
All	All	8103	0	8056	453	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 28.

All (453) 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:220:LYS:O	1:A:221:HIS:CG	2.04	1.11
1:A:430:GLU:HG3	1:A:434:ILE:HD11	1.33	1.10
1:A:542:ILE:HD12	2:B:283:LEU:HD12	1.35	1.09
1:A:223:LYS:HD3	3:A:556:AC7:H25	1.37	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:LYS:HD3	2:B:239:TRP:CD1	1.92	1.04
2:B:400:THR:CG2	2:B:401:TRP:NE1	2.22	1.02
1:A:542:ILE:HD12	2:B:283:LEU:CD1	1.91	1.00
1:A:541:GLY:HA2	1:A:546:GLU:HG3	1.47	0.95
1:A:542:ILE:CD1	2:B:283:LEU:HD12	1.96	0.94
2:B:357:MET:HG3	2:B:358:ARG:N	1.80	0.93
2:B:357:MET:SD	2:B:370:GLU:OE1	2.30	0.90
2:B:11:LYS:H	2:B:85:GLN:HE21	1.18	0.90
1:A:441:TYR:HB3	1:A:544:GLY:O	1.72	0.89
1:A:544:GLY:CA	2:B:286:THR:HG22	2.03	0.88
1:A:544:GLY:HA2	2:B:286:THR:CG2	2.05	0.87
2:B:400:THR:HG21	2:B:401:TRP:NE1	1.90	0.86
1:A:544:GLY:HA3	2:B:286:THR:HG22	1.54	0.86
2:B:41:MET:HE1	2:B:73:LYS:HE2	1.56	0.86
2:B:238:LYS:HG2	2:B:239:TRP:N	1.91	0.85
1:A:223:LYS:HD3	3:A:556:AC7:C25	2.06	0.85
2:B:2:ILE:O	2:B:117:SER:HB2	1.77	0.85
1:A:220:LYS:O	1:A:221:HIS:CD2	2.29	0.84
2:B:37:ILE:HG22	2:B:41:MET:HE2	1.57	0.83
2:B:400:THR:HG22	2:B:401:TRP:NE1	1.94	0.83
1:A:254:VAL:HB	1:A:290:THR:HA	1.61	0.83
1:A:503:LEU:HD11	1:A:535:TRP:HB2	1.60	0.82
2:B:354:TYR:OH	2:B:357:MET:SD	2.36	0.82
1:A:70:LYS:HG2	1:A:71:TRP:H	1.44	0.82
1:A:220:LYS:C	1:A:221:HIS:ND1	2.38	0.82
1:A:458:VAL:HG12	1:A:464:GLN:HG2	1.60	0.81
1:A:543:GLY:C	1:A:545:ASN:H	1.86	0.81
2:B:238:LYS:CD	2:B:239:TRP:CD1	2.64	0.81
2:B:400:THR:HB	2:B:401:TRP:CD1	2.15	0.81
1:A:2:ILE:HD13	1:A:2:ILE:H	1.46	0.81
1:A:23:GLN:HE21	1:A:23:GLN:HA	1.45	0.80
1:A:253:THR:H	1:A:256:ASP:HB2	1.44	0.79
1:A:94:ILE:HD13	1:A:94:ILE:H	1.45	0.79
1:A:220:LYS:O	1:A:221:HIS:ND1	2.16	0.79
1:A:426:TRP:HB3	1:A:526:ILE:CD1	2.13	0.78
1:A:541:GLY:CA	1:A:546:GLU:HG3	2.14	0.78
2:B:206:ARG:HH11	2:B:206:ARG:HB2	1.48	0.78
1:A:543:GLY:HA2	1:A:546:GLU:HB2	1.64	0.77
1:A:544:GLY:CA	2:B:286:THR:CG2	2.63	0.77
2:B:8:VAL:HB	2:B:159:ILE:HD12	1.67	0.77
2:B:96:HIS:CE1	2:B:384:GLY:N	2.52	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:HG3	1:A:197:GLN:HE21	1.50	0.76
1:A:220:LYS:C	1:A:221:HIS:CG	2.62	0.76
2:B:170:PRO:HB2	2:B:208:HIS:CE1	2.20	0.76
2:B:354:TYR:OH	2:B:357:MET:HG2	1.86	0.76
2:B:41:MET:HE1	2:B:73:LYS:CE	2.15	0.75
1:A:206:ARG:NH2	1:A:218:ASP:HA	2.01	0.75
1:A:439:THR:H	1:A:460:ASN:ND2	1.85	0.75
2:B:163:SER:O	2:B:167:ILE:HG13	1.87	0.75
2:B:359:GLY:HA3	2:B:367:GLN:HG3	1.66	0.75
2:B:402:TRP:CE2	2:B:403:THR:HG23	2.20	0.75
2:B:400:THR:HG22	2:B:401:TRP:CE2	2.20	0.75
1:A:376:THR:HG21	2:B:401:TRP:CZ2	2.22	0.74
1:A:543:GLY:H	1:A:546:GLU:HG2	1.50	0.74
2:B:238:LYS:HD3	2:B:239:TRP:NE1	2.02	0.74
2:B:354:TYR:OH	2:B:357:MET:CG	2.36	0.74
1:A:503:LEU:CD1	1:A:535:TRP:HB2	2.18	0.73
1:A:317:VAL:HG11	1:A:347:LYS:HG3	1.68	0.73
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.03	0.73
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.70	0.73
1:A:266:TRP:O	1:A:269:GLN:HG2	1.89	0.73
1:A:543:GLY:H	1:A:546:GLU:CG	2.02	0.73
2:B:33:ALA:O	2:B:37:ILE:HG12	1.87	0.72
1:A:66:LYS:O	1:A:67:ASP:HB2	1.89	0.72
2:B:400:THR:CG2	2:B:401:TRP:CD1	2.72	0.72
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.72	0.72
2:B:11:LYS:H	2:B:85:GLN:NE2	1.87	0.71
2:B:400:THR:HG22	2:B:401:TRP:CD1	2.25	0.71
1:A:458:VAL:HG23	2:B:286:THR:HG21	1.70	0.71
1:A:277:ARG:NH1	1:A:334:GLN:HB3	2.05	0.70
2:B:277:ARG:NH1	2:B:281:LYS:HZ2	1.89	0.70
2:B:89:GLU:HB2	2:B:91:GLN:HE21	1.55	0.70
1:A:220:LYS:O	1:A:221:HIS:CE1	2.45	0.69
1:A:26:LEU:HB2	1:A:31:ILE:HD11	1.75	0.69
1:A:285:GLY:O	1:A:286:THR:HG23	1.93	0.69
1:A:424:LYS:HB2	4:A:580:HOH:O	1.92	0.69
2:B:240:THR:O	2:B:350:LYS:HD2	1.92	0.69
2:B:254:VAL:HG22	2:B:293:ILE:HD11	1.75	0.69
1:A:69:THR:CG2	1:A:70:LYS:N	2.56	0.69
1:A:219:LYS:H	1:A:219:LYS:HD2	1.57	0.69
2:B:400:THR:HG21	2:B:401:TRP:HE1	1.58	0.68
1:A:444:GLY:HA2	1:A:552:VAL:HG11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:MET:HG3	2:B:358:ARG:H	1.56	0.68
1:A:441:TYR:CB	1:A:544:GLY:O	2.42	0.68
1:A:69:THR:HG22	1:A:70:LYS:N	2.09	0.67
1:A:426:TRP:HB3	1:A:526:ILE:HD11	1.77	0.67
2:B:359:GLY:HA3	2:B:367:GLN:CG	2.24	0.67
2:B:358:ARG:O	2:B:360:ALA:N	2.27	0.67
1:A:285:GLY:O	1:A:286:THR:CG2	2.42	0.67
2:B:65:LYS:HD3	2:B:230:MET:SD	2.35	0.67
2:B:67:ASP:OD1	2:B:67:ASP:C	2.37	0.67
2:B:423:VAL:HG12	2:B:426:TRP:CZ3	2.29	0.67
1:A:31:ILE:O	1:A:35:VAL:HG23	1.95	0.67
2:B:400:THR:CB	2:B:401:TRP:CD1	2.77	0.67
1:A:257:ILE:O	1:A:261:VAL:HG23	1.95	0.67
2:B:371:ALA:O	2:B:375:ILE:HG12	1.96	0.66
1:A:307:ARG:O	1:A:311:LYS:HB2	1.96	0.66
1:A:444:GLY:CA	1:A:552:VAL:HG11	2.25	0.66
1:A:373:GLN:HE22	2:B:397:THR:HG23	1.61	0.66
2:B:357:MET:SD	2:B:370:GLU:CD	2.79	0.65
2:B:94:ILE:HG12	2:B:94:ILE:O	1.96	0.65
1:A:277:ARG:HH11	1:A:334:GLN:HB3	1.61	0.65
2:B:206:ARG:HB2	2:B:206:ARG:NH1	2.11	0.65
2:B:358:ARG:C	2:B:360:ALA:H	2.02	0.65
1:A:426:TRP:HB3	1:A:526:ILE:HD12	1.77	0.65
1:A:219:LYS:HD2	1:A:219:LYS:N	2.13	0.64
2:B:402:TRP:CE2	2:B:403:THR:CG2	2.81	0.64
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.79	0.64
1:A:356:ARG:HD3	1:A:367:GLN:NE2	2.12	0.64
1:A:129:ALA:HA	1:A:144:TYR:O	1.98	0.64
1:A:543:GLY:C	1:A:545:ASN:N	2.54	0.63
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.28	0.63
2:B:400:THR:CG2	2:B:401:TRP:CE2	2.80	0.63
2:B:358:ARG:C	2:B:360:ALA:N	2.50	0.63
1:A:285:GLY:C	1:A:286:THR:HG23	2.24	0.63
1:A:65:LYS:HE3	1:A:68:SER:HB3	1.80	0.63
1:A:73:LYS:HE3	1:A:75:VAL:HG23	1.81	0.63
2:B:210:LEU:O	2:B:210:LEU:HD23	1.99	0.62
1:A:23:GLN:HA	1:A:23:GLN:NE2	2.13	0.62
2:B:87:PHE:CD2	2:B:158:ALA:CB	2.82	0.62
1:A:42:GLU:OE1	1:A:49:LYS:HG3	2.00	0.62
2:B:193:LEU:HB3	2:B:197:GLN:HG3	1.82	0.62
1:A:454:LYS:O	1:A:552:VAL:HG13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ARG:NH2	2:B:151:GLN:NE2	2.48	0.61
1:A:369:THR:O	1:A:373:GLN:HG2	2.00	0.61
1:A:199:ARG:O	1:A:203:GLU:HG2	2.00	0.61
1:A:211:ARG:HG2	1:A:211:ARG:HH11	1.64	0.61
1:A:474:ASN:O	1:A:478:GLU:HG3	2.01	0.61
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.81	0.61
2:B:380:ILE:HD11	2:B:386:THR:HG22	1.83	0.60
1:A:373:GLN:NE2	2:B:397:THR:HA	2.15	0.60
2:B:238:LYS:CG	2:B:239:TRP:N	2.60	0.60
1:A:272:PRO:HG3	1:A:351:THR:HG21	1.84	0.60
2:B:229:TRP:O	2:B:229:TRP:CE3	2.54	0.60
1:A:2:ILE:H	1:A:2:ILE:CD1	2.13	0.60
1:A:260:LEU:O	1:A:264:LEU:HB2	2.01	0.60
1:A:107:THR:HG22	1:A:108:VAL:N	2.17	0.60
2:B:281:LYS:HD2	2:B:284:ARG:NH1	2.17	0.60
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.84	0.59
1:A:253:THR:H	1:A:256:ASP:CB	2.14	0.59
1:A:230:MET:HE2	1:A:230:MET:H	1.68	0.59
2:B:194:GLU:HG2	2:B:197:GLN:HG2	1.84	0.59
2:B:229:TRP:O	2:B:229:TRP:CD2	2.56	0.59
1:A:287:LYS:NZ	1:A:287:LYS:HB3	2.17	0.58
2:B:209:LEU:O	2:B:214:LEU:HB2	2.03	0.58
1:A:182:GLN:HB3	1:A:187:LEU:CD2	2.33	0.58
1:A:160:PHE:CZ	1:A:164:MET:HE3	2.39	0.58
1:A:107:THR:OG1	1:A:202:ILE:HD11	2.04	0.58
2:B:238:LYS:CG	2:B:239:TRP:CD1	2.86	0.58
1:A:53:GLU:H	1:A:53:GLU:CD	2.11	0.58
1:A:258:GLN:HB2	1:A:283:LEU:HD22	1.85	0.58
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.85	0.58
1:A:65:LYS:HE3	1:A:68:SER:CB	2.34	0.57
2:B:396:GLU:CD	2:B:396:GLU:H	2.13	0.57
1:A:17:ASP:O	1:A:83:ARG:HD3	2.05	0.57
1:A:92:LEU:HD12	1:A:92:LEU:O	2.03	0.57
2:B:87:PHE:CD2	2:B:158:ALA:HB1	2.40	0.57
1:A:31:ILE:CD1	1:A:133:PRO:HG2	2.33	0.57
1:A:73:LYS:NZ	1:A:130:PHE:CZ	2.72	0.57
1:A:224:GLU:HA	1:A:227:PHE:HE2	1.69	0.57
1:A:417:VAL:HG22	1:A:419:THR:HG22	1.86	0.57
2:B:238:LYS:HG2	2:B:239:TRP:CD1	2.40	0.57
1:A:303:LEU:O	1:A:306:ASN:HB2	2.04	0.56
2:B:357:MET:CG	2:B:358:ARG:H	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HH11	1:A:277:ARG:HG2	1.71	0.56
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.41	0.56
2:B:10:VAL:HA	2:B:85:GLN:NE2	2.21	0.56
2:B:208:HIS:O	2:B:211:ARG:HG2	2.06	0.56
2:B:88:TRP:O	2:B:89:GLU:C	2.48	0.56
1:A:175:ASN:O	1:A:178:ILE:HG13	2.06	0.55
1:A:278:GLN:HB2	1:A:302:GLU:OE2	2.05	0.55
1:A:458:VAL:CG2	2:B:286:THR:HG21	2.35	0.55
2:B:167:ILE:HG22	2:B:167:ILE:O	2.06	0.55
2:B:402:TRP:CZ2	2:B:403:THR:CG2	2.89	0.55
1:A:293:ILE:CG2	1:A:294:PRO:HD2	2.36	0.55
2:B:135:ILE:O	2:B:138:GLU:HG3	2.07	0.55
2:B:68:SER:H	2:B:230:MET:CE	2.20	0.55
1:A:31:ILE:HD11	1:A:133:PRO:HG2	1.88	0.54
1:A:361:HIS:NE2	1:A:505:ILE:HD12	2.22	0.54
2:B:240:THR:O	2:B:350:LYS:HA	2.06	0.54
2:B:402:TRP:CZ2	2:B:403:THR:HG22	2.43	0.54
1:A:107:THR:HG22	1:A:108:VAL:H	1.72	0.54
2:B:239:TRP:O	2:B:240:THR:C	2.51	0.54
1:A:366:LYS:HE2	1:A:405:TYR:OH	2.08	0.54
2:B:89:GLU:C	2:B:91:GLN:H	2.15	0.54
1:A:94:ILE:HD13	1:A:94:ILE:N	2.20	0.54
2:B:84:THR:O	2:B:85:GLN:C	2.51	0.54
2:B:206:ARG:HH21	2:B:229:TRP:HA	1.73	0.54
1:A:429:LEU:HD11	1:A:506:ILE:CG2	2.37	0.53
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.89	0.53
2:B:96:HIS:CD2	2:B:383:TRP:HA	2.43	0.53
1:A:178:ILE:C	1:A:178:ILE:HD12	2.33	0.53
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.24	0.53
1:A:97:PRO:HA	1:A:100:LEU:HG	1.91	0.53
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.90	0.53
1:A:74:LEU:HD13	1:A:74:LEU:O	2.09	0.53
2:B:67:ASP:O	2:B:68:SER:C	2.52	0.53
1:A:46:LYS:HD3	1:A:116:PHE:CD1	2.44	0.53
1:A:246:LEU:HB3	1:A:307:ARG:HH12	1.74	0.53
2:B:72:ARG:HG2	2:B:72:ARG:HH11	1.73	0.53
1:A:2:ILE:HD13	1:A:2:ILE:N	2.20	0.53
1:A:483:TYR:O	1:A:487:GLN:HG3	2.09	0.53
2:B:239:TRP:O	2:B:242:GLN:NE2	2.42	0.53
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.08	0.52
2:B:113:ASP:HB2	2:B:228:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ALA:CB	1:A:214:LEU:HD22	2.40	0.52
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.10	0.52
1:A:73:LYS:HE3	1:A:75:VAL:CG2	2.39	0.52
1:A:217:PRO:O	1:A:219:LYS:NZ	2.42	0.52
2:B:96:HIS:CE1	2:B:384:GLY:CA	2.93	0.52
2:B:11:LYS:N	2:B:85:GLN:HE21	1.99	0.52
1:A:225:PRO:HB3	1:A:235:HIS:ND1	2.25	0.52
1:A:10:VAL:HG12	1:A:11:LYS:N	2.24	0.52
1:A:70:LYS:CG	1:A:71:TRP:H	2.19	0.52
2:B:3:SER:HA	2:B:117:SER:O	2.10	0.51
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.45	0.51
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.45	0.51
1:A:211:ARG:HG2	1:A:211:ARG:NH1	2.24	0.51
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.50	0.51
2:B:56:TYR:O	2:B:129:ALA:HB3	2.09	0.51
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.40	0.51
2:B:174:GLN:O	2:B:176:PRO:HD3	2.10	0.51
1:A:16:MET:HE2	1:A:83:ARG:NH1	2.26	0.51
1:A:391:LEU:C	1:A:417:VAL:HG12	2.35	0.51
1:A:257:ILE:HA	1:A:260:LEU:HB3	1.93	0.51
2:B:169:GLU:OE2	2:B:169:GLU:HA	2.10	0.51
1:A:378:GLU:O	1:A:382:ILE:HG12	2.10	0.50
1:A:91:GLN:NE2	1:A:183:TYR:HE1	2.09	0.50
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.47	0.50
1:A:245:VAL:HG13	1:A:245:VAL:O	2.12	0.50
1:A:542:ILE:O	1:A:542:ILE:HG22	2.10	0.50
1:A:207:GLN:O	1:A:210:LEU:HB3	2.11	0.50
1:A:206:ARG:HH22	1:A:218:ASP:HA	1.74	0.50
1:A:457:TYR:CD1	1:A:457:TYR:C	2.90	0.50
2:B:156:SER:N	2:B:157:PRO:HD2	2.26	0.50
2:B:423:VAL:HG12	2:B:426:TRP:HZ3	1.73	0.50
1:A:328:GLU:O	1:A:339:TYR:HA	2.12	0.49
2:B:169:GLU:C	2:B:171:PHE:H	2.19	0.49
1:A:117:SER:HB2	1:A:214:LEU:CD2	2.42	0.49
2:B:254:VAL:HG22	2:B:293:ILE:CD1	2.41	0.49
1:A:225:PRO:HG3	1:A:236:PRO:HD3	1.94	0.49
2:B:167:ILE:HG12	2:B:212:TRP:CE3	2.47	0.49
1:A:356:ARG:HH11	1:A:362:THR:HG21	1.78	0.49
1:A:544:GLY:HA2	2:B:286:THR:HG23	1.89	0.49
1:A:295:LEU:HD12	1:A:295:LEU:N	2.27	0.49
2:B:317:VAL:HG22	2:B:347:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG22	1:A:90:VAL:O	2.13	0.49
2:B:91:GLN:CD	2:B:161:GLN:HE22	2.19	0.49
2:B:400:THR:HB	2:B:401:TRP:HD1	1.74	0.49
2:B:395:LYS:HE2	2:B:399:GLU:OE1	2.13	0.49
1:A:307:ARG:HH11	1:A:307:ARG:HG2	1.77	0.48
2:B:251:SER:HB3	4:B:456:HOH:O	2.13	0.48
2:B:113:ASP:O	2:B:114:ALA:C	2.56	0.48
2:B:357:MET:CG	2:B:358:ARG:N	2.57	0.48
1:A:255:ASN:HB3	1:A:259:LYS:HD3	1.95	0.48
2:B:76:ASP:OD1	2:B:76:ASP:C	2.55	0.48
1:A:78:ARG:O	1:A:82:LYS:HG3	2.13	0.48
1:A:135:ILE:H	1:A:135:ILE:HD12	1.78	0.48
1:A:249:LYS:HD3	1:A:256:ASP:OD1	2.13	0.48
1:A:447:ASN:OD1	1:A:450:THR:HG23	2.13	0.48
2:B:87:PHE:CD2	2:B:158:ALA:HB3	2.47	0.48
1:A:450:THR:O	1:A:451:LYS:HB2	2.13	0.48
2:B:72:ARG:NH2	2:B:151:GLN:HE22	2.11	0.48
2:B:81:ASN:OD1	2:B:154:LYS:N	2.38	0.48
1:A:284:ARG:HG2	1:A:284:ARG:HH11	1.79	0.48
2:B:164:MET:O	2:B:168:LEU:HG	2.14	0.48
1:A:29:GLU:HG3	1:A:30:LYS:N	2.28	0.48
1:A:76:ASP:OD1	1:A:78:ARG:HD3	2.13	0.48
1:A:360:ALA:O	1:A:514:GLU:HG2	2.14	0.48
2:B:328:GLU:O	2:B:339:TYR:HA	2.14	0.48
1:A:224:GLU:HB2	1:A:225:PRO:HD2	1.95	0.48
1:A:285:GLY:C	1:A:286:THR:CG2	2.87	0.48
2:B:248:GLU:O	2:B:248:GLU:HG2	2.13	0.47
2:B:280:SER:O	2:B:283:LEU:HB2	2.14	0.47
1:A:503:LEU:HD13	2:B:422:LEU:CD1	2.44	0.47
1:A:541:GLY:C	1:A:546:GLU:HG3	2.39	0.47
2:B:379:SER:OG	2:B:387:PRO:HD3	2.15	0.47
2:B:206:ARG:HH11	2:B:206:ARG:CB	2.25	0.47
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.97	0.47
2:B:170:PRO:HB2	2:B:208:HIS:HE1	1.74	0.47
1:A:77:PHE:O	1:A:78:ARG:C	2.58	0.47
1:A:311:LYS:O	1:A:313:PRO:HD3	2.14	0.47
1:A:417:VAL:O	1:A:417:VAL:HG13	2.14	0.47
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.77	0.47
1:A:116:PHE:O	1:A:148:VAL:HG11	2.15	0.47
1:A:198:HIS:C	1:A:200:THR:N	2.72	0.47
2:B:238:LYS:HG2	2:B:239:TRP:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:LYS:O	2:B:85:GLN:HG2	2.15	0.47
1:A:287:LYS:O	1:A:288:ALA:HB3	2.15	0.47
2:B:312:GLU:HB3	2:B:313:PRO:HD2	1.96	0.47
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.97	0.47
2:B:277:ARG:O	2:B:281:LYS:HG2	2.15	0.46
2:B:68:SER:H	2:B:230:MET:HE3	1.80	0.46
2:B:278:GLN:NE2	2:B:298:GLU:HB3	2.30	0.46
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.97	0.46
1:A:210:LEU:C	1:A:212:TRP:H	2.23	0.46
1:A:454:LYS:HB2	1:A:552:VAL:O	2.15	0.46
2:B:96:HIS:NE2	2:B:383:TRP:CA	2.79	0.46
1:A:66:LYS:O	1:A:67:ASP:CB	2.61	0.46
2:B:67:ASP:OD1	2:B:68:SER:N	2.49	0.46
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.97	0.46
2:B:65:LYS:HB2	2:B:230:MET:SD	2.56	0.46
1:A:7:THR:HG23	4:A:610:HOH:O	2.14	0.46
1:A:77:PHE:O	1:A:80:LEU:N	2.48	0.46
1:A:278:GLN:O	1:A:282:LEU:HG	2.15	0.46
2:B:194:GLU:N	2:B:194:GLU:OE1	2.49	0.46
2:B:283:LEU:O	2:B:284:ARG:C	2.57	0.46
1:A:255:ASN:O	1:A:259:LYS:HB2	2.16	0.46
1:A:269:GLN:HA	1:A:351:THR:O	2.15	0.46
2:B:10:VAL:HA	2:B:85:GLN:HE22	1.80	0.46
2:B:85:GLN:O	2:B:85:GLN:HG3	2.16	0.46
1:A:40:GLU:HG3	1:A:41:MET:N	2.31	0.46
2:B:12:LEU:HG	2:B:127:TYR:CE1	2.52	0.45
1:A:181:TYR:HD2	1:A:188:TYR:CD1	2.34	0.45
1:A:257:ILE:O	1:A:260:LEU:HB3	2.16	0.45
1:A:282:LEU:HD13	1:A:295:LEU:HA	1.98	0.45
1:A:199:ARG:HA	1:A:202:ILE:HD12	1.98	0.45
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.98	0.45
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.52	0.45
1:A:278:GLN:O	1:A:299:ALA:HB2	2.17	0.45
1:A:546:GLU:OE1	1:A:546:GLU:HA	2.16	0.45
2:B:91:GLN:O	2:B:92:LEU:HB2	2.16	0.45
2:B:65:LYS:CB	2:B:230:MET:SD	3.04	0.45
2:B:357:MET:HE2	2:B:357:MET:HB2	1.83	0.45
1:A:252:TRP:HB3	1:A:257:ILE:HG13	1.97	0.45
1:A:306:ASN:O	1:A:310:LEU:N	2.44	0.45
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.51	0.45
1:A:270:ILE:O	1:A:272:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:NH1	1:A:334:GLN:O	2.50	0.45
1:A:293:ILE:HG23	1:A:294:PRO:HD2	1.97	0.45
2:B:96:HIS:NE2	2:B:382:ILE:C	2.75	0.45
1:A:73:LYS:HE2	1:A:146:TYR:OH	2.16	0.45
2:B:89:GLU:C	2:B:91:GLN:N	2.72	0.45
2:B:303:LEU:O	2:B:307:ARG:HB2	2.17	0.45
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.98	0.45
1:A:542:ILE:HD13	2:B:283:LEU:HD12	1.92	0.45
2:B:90:VAL:HG12	2:B:90:VAL:O	2.16	0.45
1:A:543:GLY:O	1:A:545:ASN:N	2.44	0.45
1:A:23:GLN:HE22	1:A:60:VAL:H	1.66	0.44
1:A:8:VAL:HG21	1:A:159:ILE:HG23	1.99	0.44
1:A:223:LYS:HB2	3:A:556:AC7:H25	1.98	0.44
2:B:8:VAL:O	2:B:10:VAL:HG23	2.17	0.44
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.32	0.44
2:B:315:HIS:ND1	2:B:315:HIS:C	2.74	0.44
2:B:331:LYS:NZ	2:B:364:ASP:OD1	2.50	0.44
1:A:438:GLU:CD	1:A:461:LYS:HD3	2.42	0.44
1:A:543:GLY:CA	1:A:546:GLU:HB2	2.43	0.44
1:A:281:LYS:O	1:A:284:ARG:HD2	2.17	0.44
2:B:350:LYS:NZ	2:B:378:GLU:OE1	2.50	0.44
2:B:229:TRP:O	2:B:229:TRP:CG	2.71	0.44
1:A:74:LEU:HD13	1:A:74:LEU:C	2.42	0.44
2:B:423:VAL:HG12	2:B:426:TRP:CE3	2.52	0.44
1:A:94:ILE:HB	1:A:95:PRO:CD	2.46	0.44
1:A:115:TYR:HA	1:A:160:PHE:CD2	2.53	0.44
1:A:94:ILE:HB	1:A:95:PRO:HD2	2.00	0.44
2:B:96:HIS:CE1	2:B:383:TRP:C	2.96	0.44
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.18	0.43
2:B:95:PRO:O	2:B:96:HIS:C	2.59	0.43
2:B:108:VAL:O	2:B:231:GLY:HA2	2.18	0.43
1:A:231:GLY:C	1:A:242:GLN:HG3	2.43	0.43
1:A:246:LEU:CB	1:A:307:ARG:HH12	2.30	0.43
1:A:406:TRP:CE2	1:A:407:GLN:HG3	2.52	0.43
1:A:542:ILE:HD12	2:B:283:LEU:HD13	1.89	0.43
2:B:345:PRO:O	2:B:346:PHE:HB2	2.17	0.43
1:A:231:GLY:O	1:A:242:GLN:HG3	2.18	0.43
2:B:43:LYS:C	2:B:45:GLY:H	2.26	0.43
2:B:103:LYS:HD2	2:B:191:SER:C	2.43	0.43
1:A:198:HIS:C	1:A:200:THR:H	2.25	0.43
1:A:287:LYS:H	1:A:287:LYS:HG2	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLN:NE2	2:B:397:THR:OG1	2.52	0.43
2:B:115:TYR:OH	2:B:157:PRO:HA	2.18	0.43
1:A:7:THR:HG21	4:A:612:HOH:O	2.17	0.43
1:A:207:GLN:OE1	1:A:207:GLN:C	2.61	0.43
1:A:222:GLN:C	1:A:223:LYS:HG3	2.42	0.43
1:A:175:ASN:N	1:A:176:PRO:HD3	2.34	0.43
2:B:194:GLU:O	2:B:195:ILE:C	2.62	0.43
1:A:50:ILE:HG13	1:A:143:ARG:HB3	2.01	0.43
1:A:148:VAL:O	1:A:150:PRO:HD3	2.19	0.43
1:A:253:THR:HA	1:A:291:GLU:O	2.19	0.43
1:A:283:LEU:C	1:A:283:LEU:HD12	2.44	0.43
1:A:390:LYS:HB3	1:A:390:LYS:HE3	1.71	0.43
2:B:66:LYS:HG3	2:B:67:ASP:H	1.82	0.43
2:B:89:GLU:HB3	2:B:91:GLN:HG3	2.01	0.43
1:A:26:LEU:HB2	1:A:31:ILE:CD1	2.45	0.43
1:A:442:VAL:HG12	1:A:457:TYR:HB3	2.00	0.43
1:A:69:THR:CG2	1:A:70:LYS:H	2.30	0.43
1:A:156:SER:N	1:A:157:PRO:CD	2.82	0.43
1:A:320:ASP:C	1:A:320:ASP:OD1	2.62	0.43
1:A:254:VAL:H	1:A:291:GLU:H	1.67	0.42
2:B:251:SER:HA	4:B:484:HOH:O	2.19	0.42
2:B:363:ASN:OD1	2:B:363:ASN:C	2.62	0.42
1:A:439:THR:H	1:A:460:ASN:HD21	1.63	0.42
2:B:96:HIS:NE2	2:B:383:TRP:C	2.77	0.42
1:A:444:GLY:HA2	1:A:552:VAL:CG1	2.47	0.42
1:A:540:LYS:O	2:B:280:SER:HB3	2.19	0.42
2:B:171:PHE:HE1	2:B:204:GLU:HG2	1.83	0.42
1:A:246:LEU:HD21	1:A:310:LEU:CD1	2.50	0.42
1:A:460:ASN:H	1:A:460:ASN:HD22	1.66	0.42
1:A:518:VAL:O	1:A:522:ILE:HG12	2.20	0.42
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.50	0.42
2:B:379:SER:CB	2:B:387:PRO:HD3	2.49	0.42
1:A:253:THR:N	1:A:256:ASP:HB2	2.22	0.42
2:B:339:TYR:CD1	2:B:375:ILE:HD12	2.55	0.42
2:B:277:ARG:NH1	2:B:281:LYS:NZ	2.64	0.42
1:A:103:LYS:HA	1:A:192:ASP:OD1	2.19	0.42
2:B:268:SER:HA	2:B:271:TYR:O	2.20	0.42
2:B:401:TRP:CD1	2:B:401:TRP:N	2.87	0.42
1:A:50:ILE:CG1	1:A:143:ARG:HB3	2.49	0.42
1:A:111:VAL:C	1:A:113:ASP:N	2.75	0.42
1:A:336:GLN:C	1:A:337:TRP:CD1	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASN:OD1	1:A:363:ASN:C	2.62	0.42
2:B:28:GLU:HB2	2:B:135:ILE:HD11	2.02	0.42
2:B:136:ASN:O	2:B:137:ASN:C	2.62	0.42
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.55	0.42
1:A:223:LYS:O	1:A:224:GLU:HB3	2.20	0.41
1:A:301:LEU:O	1:A:305:GLU:HG3	2.20	0.41
1:A:221:HIS:C	1:A:222:GLN:HG3	2.45	0.41
2:B:111:VAL:HG11	2:B:187:LEU:HD22	2.02	0.41
1:A:5:ILE:HD12	1:A:5:ILE:N	2.35	0.41
1:A:241:VAL:CG2	1:A:271:TYR:HE1	2.32	0.41
2:B:357:MET:CG	2:B:370:GLU:OE1	2.68	0.41
1:A:380:ILE:HD12	2:B:27:THR:HG22	2.03	0.41
2:B:358:ARG:O	2:B:359:GLY:C	2.62	0.41
1:A:538:ALA:O	1:A:540:LYS:HG2	2.21	0.41
2:B:23:GLN:OE1	2:B:60:VAL:HG12	2.20	0.41
2:B:72:ARG:HH22	2:B:151:GLN:NE2	2.18	0.41
1:A:182:GLN:H	1:A:182:GLN:HG3	1.72	0.41
1:A:449:GLU:H	1:A:449:GLU:CD	2.28	0.41
2:B:315:HIS:ND1	2:B:315:HIS:O	2.53	0.41
1:A:363:ASN:HA	1:A:511:ASP:CG	2.45	0.41
2:B:43:LYS:C	2:B:45:GLY:N	2.79	0.41
2:B:67:ASP:H	2:B:230:MET:HE2	1.86	0.41
2:B:237:ASP:HB2	2:B:238:LYS:H	1.65	0.41
2:B:239:TRP:C	2:B:241:VAL:N	2.78	0.41
2:B:232:TYR:OH	2:B:374:LYS:HE2	2.20	0.41
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.87	0.40
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.56	0.40
2:B:104:LYS:NZ	2:B:192:ASP:HB3	2.36	0.40
2:B:105:SER:O	2:B:190:GLY:HA2	2.22	0.40
1:A:23:GLN:NE2	1:A:23:GLN:CA	2.74	0.40
1:A:304:ALA:C	1:A:306:ASN:H	2.28	0.40
1:A:438:GLU:HG3	1:A:461:LYS:HD3	2.03	0.40
1:A:491:LEU:HB3	1:A:529:GLU:HG3	2.03	0.40
1:A:503:LEU:HD12	1:A:535:TRP:CD1	2.56	0.40
2:B:211:ARG:CB	2:B:211:ARG:HH11	2.35	0.40
1:A:224:GLU:O	1:A:225:PRO:C	2.64	0.40
1:A:281:LYS:O	1:A:281:LYS:HD3	2.21	0.40
1:A:449:GLU:CD	1:A:449:GLU:N	2.80	0.40
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.93	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	552/558 (99%)	487 (88%)	62 (11%)	3 (0%)	24	34
2	B	412/428 (96%)	354 (86%)	53 (13%)	5 (1%)	10	13
All	All	964/986 (98%)	841 (87%)	115 (12%)	8 (1%)	16	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	359	GLY
1	A	92	LEU
2	B	86	ASP
2	B	87	PHE
1	A	85	GLN
1	A	225	PRO
2	B	195	ILE
2	B	423	VAL

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	493/495 (100%)	469 (95%)	24 (5%)	22	34
2	B	378/390 (97%)	361 (96%)	17 (4%)	24	38
All	All	871/885 (98%)	830 (95%)	41 (5%)	23	36

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	46	LYS
1	A	72	ARG
1	A	73	LYS
1	A	74	LEU
1	A	78	ARG
1	A	91	GLN
1	A	94	ILE
1	A	101	LYS
1	A	139	THR
1	A	166	LYS
1	A	182	GLN
1	A	207	GLN
1	A	219	LYS
1	A	221	HIS
1	A	223	LYS
1	A	248	GLU
1	A	256	ASP
1	A	281	LYS
1	A	287	LYS
1	A	344	GLU
1	A	347	LYS
1	A	419	THR
1	A	512	LYS
2	B	2	ILE
2	B	67	ASP
2	B	86	ASP
2	B	88	TRP
2	B	94	ILE
2	B	145	GLN
2	B	180	ILE
2	B	206	ARG
2	B	228	LEU
2	B	235	HIS
2	B	238	LYS
2	B	248	GLU
2	B	314	VAL
2	B	344	GLU
2	B	357	MET
2	B	388	LYS
2	B	417	VAL

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	23	GLN
1	A	145	GLN
1	A	151	GLN
1	A	197	GLN
1	A	242	GLN
1	A	255	ASN
1	A	258	GLN
1	A	332	GLN
1	A	373	GLN
1	A	460	ASN
1	A	475	GLN
1	A	520	GLN
1	A	545	ASN
2	B	57	ASN
2	B	85	GLN
2	B	91	GLN
2	B	151	GLN
2	B	161	GLN
2	B	174	GLN
2	B	208	HIS
2	B	242	GLN
2	B	255	ASN
2	B	258	GLN
2	B	278	GLN
2	B	330	GLN
2	B	340	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AC7	A	556	-	38,38,38	3.22	13 (34%)	47,51,51	1.82	7 (14%)

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
3	AC7	A	556	-	-	5/37/37/37	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	556	AC7	C4-C77	-11.04	1.28	1.44
3	A	556	AC7	C11-C82	-9.14	1.31	1.44
3	A	556	AC7	O5-C7	5.79	1.46	1.33
3	A	556	AC7	C6-C8	5.13	1.56	1.49
3	A	556	AC7	O7-C16	5.09	1.44	1.33
3	A	556	AC7	O3-C20	4.19	1.46	1.33
3	A	556	AC7	C13-C8	3.85	1.54	1.49
3	A	556	AC7	C1-C6	3.27	1.44	1.39
3	A	556	AC7	C9-C8	3.24	1.37	1.34
3	A	556	AC7	C12-C13	2.59	1.43	1.39
3	A	556	AC7	C12-C11	2.50	1.43	1.39
3	A	556	AC7	C1-C2	2.38	1.43	1.39
3	A	556	AC7	C5-C6	2.09	1.42	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	556	AC7	O7-C16-C15	7.10	124.10	112.31
3	A	556	AC7	O5-C7-C2	4.53	119.83	112.31
3	A	556	AC7	O7-C16-O36	-3.59	116.48	123.46
3	A	556	AC7	C22-O1-C3	3.40	123.96	114.74
3	A	556	AC7	O5-C7-O35	-2.61	118.38	123.46
3	A	556	AC7	C24-O5-C7	2.42	120.46	115.81
3	A	556	AC7	C13-C8-C9	-2.34	118.81	121.76

There are no chirality outliers.

All (5) torsion outliers are listed below:

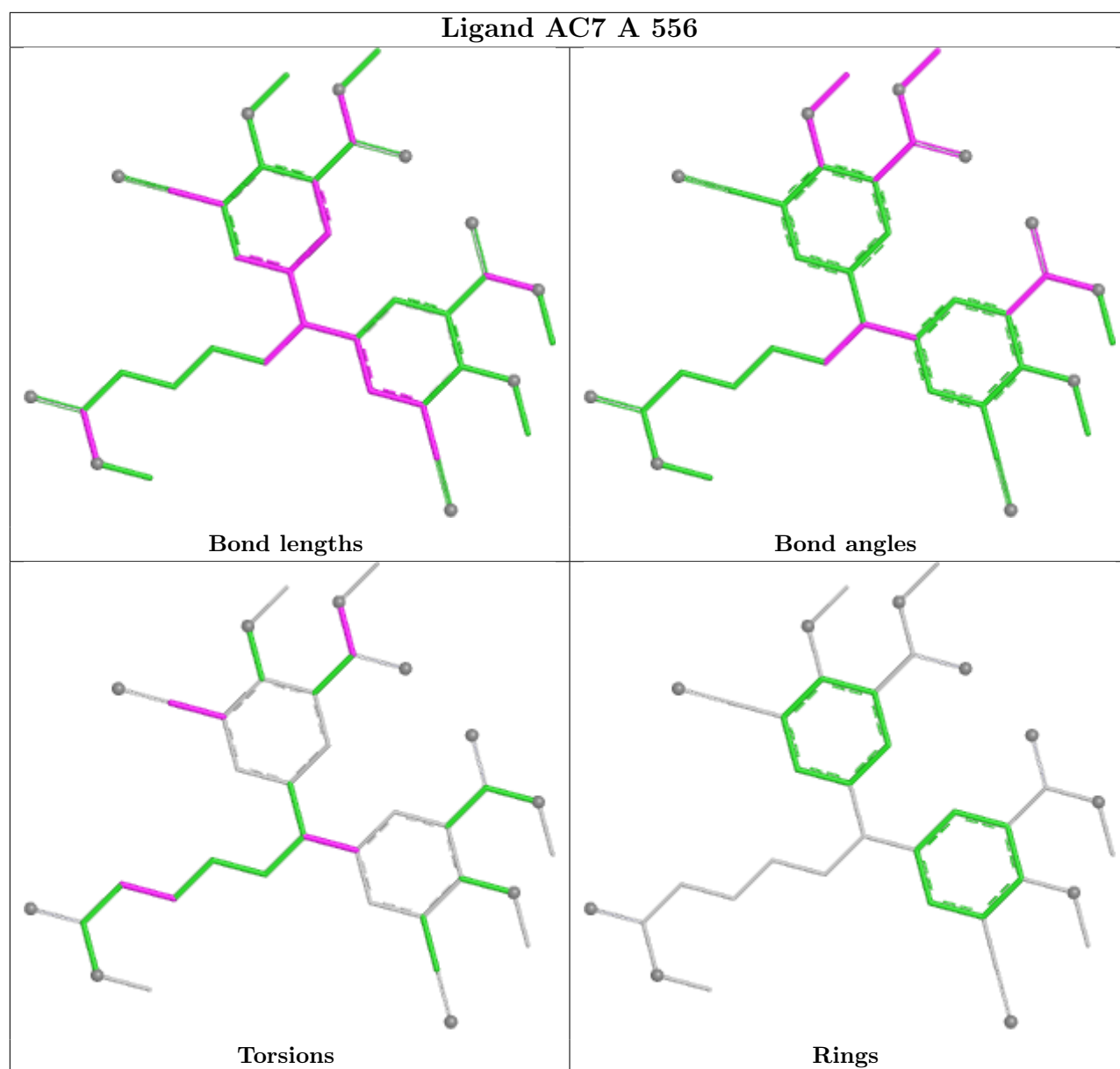
Mol	Chain	Res	Type	Atoms
3	A	556	AC7	C3-C4-C77-N69
3	A	556	AC7	C2-C7-O5-C24
3	A	556	AC7	O35-C7-O5-C24
3	A	556	AC7	C17-C18-C19-C20
3	A	556	AC7	C14-C13-C8-C9

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	556	AC7	3	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	554/558 (99%)	1.22	110 (19%) 3 2	29, 78, 144, 186	0
2	B	416/428 (97%)	1.00	57 (13%) 6 5	36, 69, 145, 173	0
All	All	970/986 (98%)	1.13	167 (17%) 4 3	29, 73, 145, 186	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	548	VAL	6.8
1	A	552	VAL	6.5
1	A	547	GLN	6.4
1	A	551	LEU	5.5
1	A	553	SER	5.1
2	B	164	MET	5.1
1	A	549	ASP	5.0
1	A	283	LEU	4.7
1	A	247	PRO	4.7
1	A	545	ASN	4.6
2	B	214	LEU	4.6
2	B	94	ILE	4.5
2	B	2	ILE	4.4
1	A	109	LEU	4.4
2	B	401	TRP	4.4
1	A	317	VAL	4.3
2	B	228	LEU	4.3
2	B	90	VAL	4.3
1	A	270	ILE	4.2
1	A	100	LEU	4.2
2	B	93	GLY	4.1
1	A	257	ILE	4.1
2	B	357	MET	4.0
1	A	245	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	3.9
2	B	87	PHE	3.8
1	A	544	GLY	3.8
2	B	168	LEU	3.8
1	A	62	ALA	3.8
1	A	542	ILE	3.8
1	A	546	GLU	3.8
1	A	303	LEU	3.7
1	A	550	LYS	3.7
1	A	182	GLN	3.7
2	B	95	PRO	3.6
1	A	349	LEU	3.6
1	A	183	TYR	3.5
1	A	38	CYS	3.5
1	A	111	VAL	3.5
1	A	227	PHE	3.4
1	A	24	TRP	3.4
1	A	92	LEU	3.4
2	B	92	LEU	3.4
1	A	279	LEU	3.3
1	A	315	HIS	3.3
1	A	244	ILE	3.3
2	B	354	TYR	3.3
1	A	348	ASN	3.3
2	B	85	GLN	3.2
2	B	124	PHE	3.2
1	A	261	VAL	3.2
1	A	251	SER	3.2
1	A	75	VAL	3.2
1	A	292	VAL	3.2
1	A	252	TRP	3.2
1	A	225	PRO	3.0
2	B	359	GLY	3.0
1	A	280	SER	3.0
1	A	309	ILE	3.0
2	B	84	THR	3.0
2	B	427	TYR	3.0
2	B	4	PRO	2.9
1	A	223	LYS	2.9
1	A	90	VAL	2.9
2	B	232	TYR	2.9
1	A	236	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	554	ALA	2.9
1	A	1	PRO	2.8
1	A	239	TRP	2.8
1	A	282	LEU	2.8
2	B	209	LEU	2.8
1	A	364	ASP	2.8
1	A	241	VAL	2.8
2	B	200	THR	2.8
1	A	59	PRO	2.8
1	A	120	LEU	2.8
1	A	299	ALA	2.8
1	A	275	LYS	2.8
2	B	69	THR	2.7
2	B	173	LYS	2.7
1	A	108	VAL	2.7
1	A	214	LEU	2.7
1	A	232	TYR	2.7
1	A	274	ILE	2.7
1	A	188	TYR	2.7
1	A	71	TRP	2.7
1	A	26	LEU	2.6
2	B	88	TRP	2.6
2	B	360	ALA	2.6
1	A	318	TYR	2.6
2	B	358	ARG	2.6
2	B	248	GLU	2.6
1	A	216	THR	2.6
2	B	361	HIS	2.6
1	A	22	LYS	2.6
1	A	187	LEU	2.5
2	B	127	TYR	2.5
2	B	402	TRP	2.5
1	A	189	VAL	2.5
2	B	16	MET	2.5
1	A	218	ASP	2.5
1	A	88	TRP	2.5
2	B	230	MET	2.5
1	A	115	TYR	2.4
1	A	68	SER	2.4
2	B	405	TYR	2.4
2	B	227	PHE	2.4
1	A	106	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	332	GLN	2.4
2	B	295	LEU	2.4
2	B	315	HIS	2.4
1	A	496	VAL	2.4
2	B	134	SER	2.4
1	A	246	LEU	2.4
1	A	295	LEU	2.4
1	A	327	ALA	2.4
1	A	229	TRP	2.4
2	B	9	PRO	2.3
1	A	63	ILE	2.3
1	A	95	PRO	2.3
1	A	72	ARG	2.3
1	A	359	GLY	2.3
1	A	543	GLY	2.3
2	B	149	LEU	2.3
2	B	205	LEU	2.3
1	A	267	ALA	2.3
1	A	288	ALA	2.3
1	A	341	ILE	2.3
2	B	12	LEU	2.3
1	A	404	GLU	2.3
1	A	271	TYR	2.3
1	A	94	ILE	2.3
1	A	219	LYS	2.3
2	B	7	THR	2.2
2	B	285	GLY	2.2
1	A	260	LEU	2.2
1	A	132	ILE	2.2
2	B	47	ILE	2.2
2	B	284	ARG	2.2
1	A	334	GLN	2.2
2	B	190	GLY	2.2
2	B	196	GLY	2.2
1	A	77	PHE	2.2
1	A	238	LYS	2.2
1	A	310	LEU	2.1
2	B	117	SER	2.1
1	A	272	PRO	2.1
1	A	345	PRO	2.1
1	A	258	GLN	2.1
2	B	355	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	234	LEU	2.1
1	A	387	PRO	2.1
1	A	314	VAL	2.1
1	A	107	THR	2.1
2	B	240	THR	2.1
1	A	360	ALA	2.1
1	A	228	LEU	2.1
1	A	266	TRP	2.1
1	A	400	THR	2.1
2	B	293	ILE	2.1
1	A	329	ILE	2.0
2	B	236	PRO	2.0
2	B	356	ARG	2.0
1	A	234	LEU	2.0
1	A	264	LEU	2.0
2	B	89	GLU	2.0
1	A	541	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

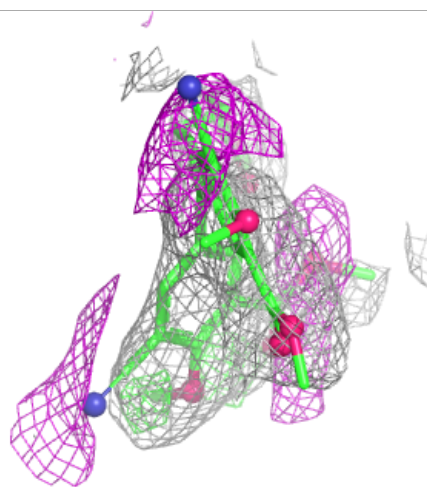
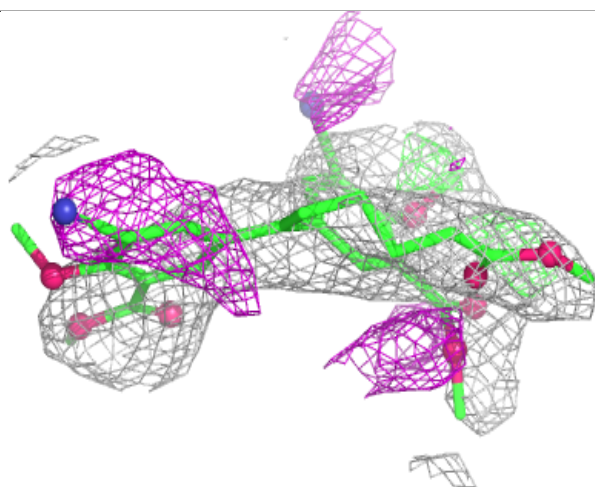
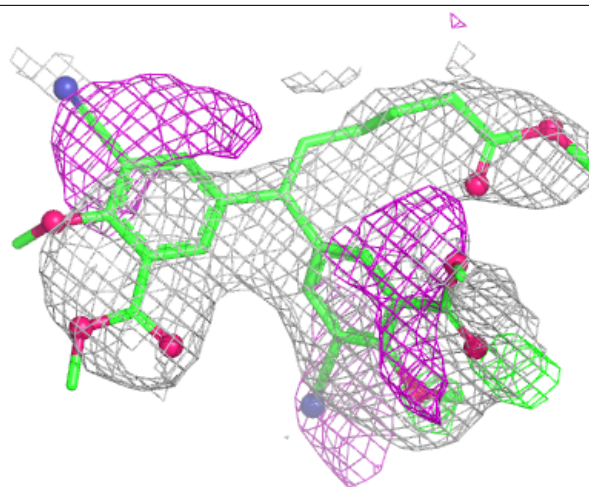
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	AC7	A	556	37/37	0.69	0.25	80,88,100,100	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 AC7 A 556:

$2mF_o-DF_c$ (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.