



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:30 AM UTC

PDB ID : 3QO9 / pdb_00003qo9
Title : Crystal structure of HIV-1 Reverse Transcriptase (RT) in complex with TSAO-T, a non-nucleoside RT inhibitor (NNRTI)
Authors : Das, K.; Arnold, E.
Deposited on : 2011-02-09
Resolution : 2.60 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

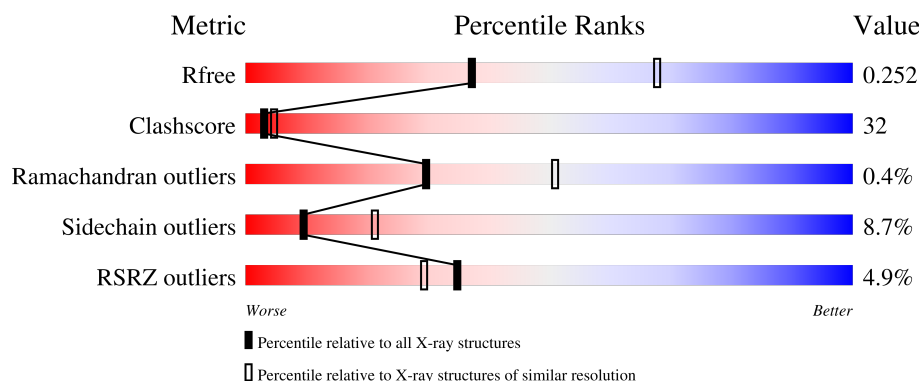
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	557	 4% 48% 41% 9% ..
2	B	428	 6% 45% 41% 10% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7987 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	553	Total	C	N	O	S	0	0	0
			4500	2912	749	832	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	160	SER	PHE	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

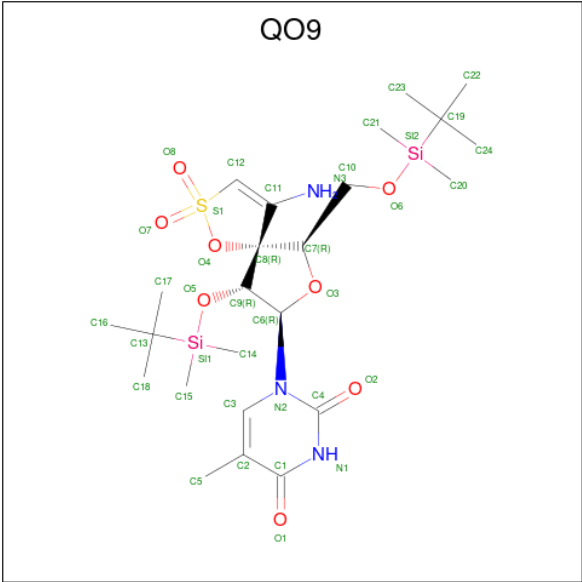
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3413	2225	564	617	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 1-[(5R,6R,8R,9R)-4-amino-9-{[tert-butyl(dimethyl)silyl]oxy}-6-({[tert-butyl(dimethyl)silyl]oxy}methyl)-2,2-dioxido-1,7-dioxa-2-thiaspiro[4.4]non-3-en-8-yl]-5-methylpyrimidine-2,4(1H,3H)-dione (CCD ID: QO9) (formula: C₂₄H₄₃N₃O₈SSi₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	Si	0	0
			38	24	3	8	1	2		

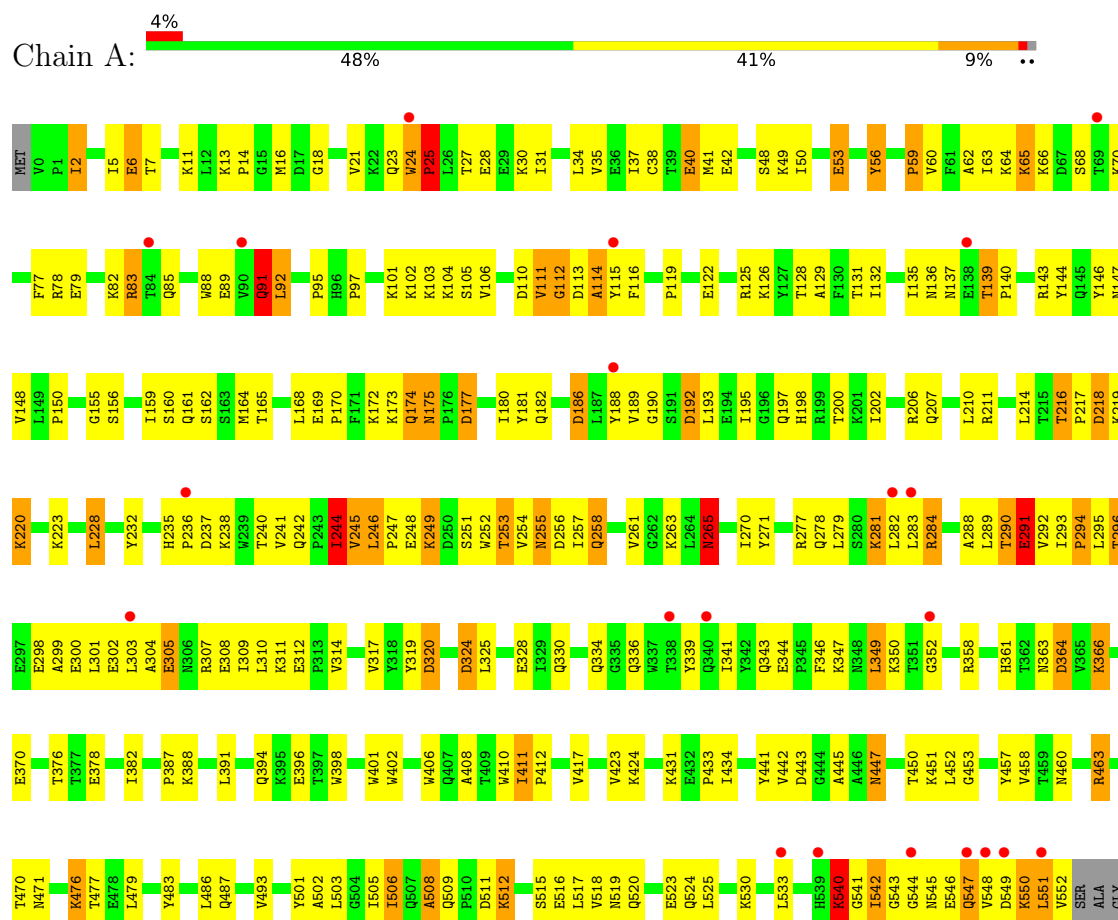
- Molecule 4 is water.

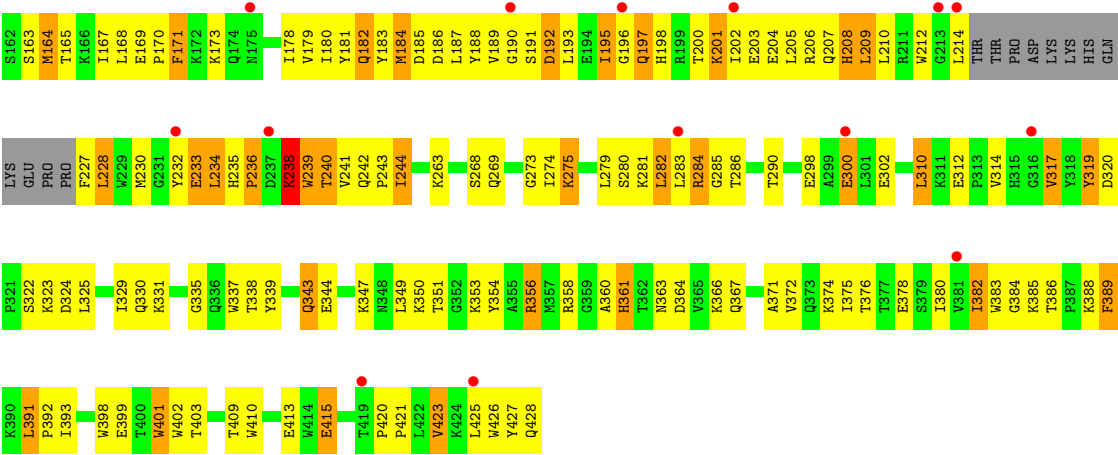
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		
4	B	11	Total	O	0	0
			11	11		

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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.76Å 72.59Å 108.97Å 90.00° 98.75° 90.00°	Depositor
Resolution (Å)	48.27 – 2.60 48.27 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.27-2.60) 96.5 (48.27-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.286 0.247 , 0.252	Depositor DCC
R_{free} test set	1465 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7987	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: QO9

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	0.52	0/4617	1.17	48/6274 (0.8%)
2	B	0.52	0/3511	1.16	38/4768 (0.8%)
All	All	0.52	0/8128	1.16	86/11042 (0.8%)

There are no bond length outliers.

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540	LYS	N-CA-C	-11.12	96.92	113.61
1	A	91	GLN	N-CA-C	11.10	123.12	111.14
2	B	132	ILE	N-CA-C	-10.02	97.63	107.55
2	B	391	LEU	N-CA-C	9.75	121.94	109.65
2	B	361	HIS	N-CA-C	-9.34	102.08	112.72
1	A	64	LYS	N-CA-C	-9.18	94.22	109.46
1	A	56	TYR	N-CA-C	8.44	121.42	110.53
2	B	96	HIS	N-CA-C	-8.37	98.74	110.29
2	B	92	LEU	N-CA-C	8.32	121.40	111.33
2	B	312	GLU	CA-C-N	7.99	128.61	120.14
2	B	312	GLU	C-N-CA	7.99	128.61	120.14
1	A	551	LEU	N-CA-C	-7.82	103.88	113.19
1	A	65	LYS	N-CA-C	7.71	122.00	109.59
1	A	218	ASP	N-CA-C	-7.64	94.52	110.80
1	A	320	ASP	CA-C-N	7.62	128.31	119.47
1	A	320	ASP	C-N-CA	7.62	128.31	119.47
1	A	296	THR	N-CA-C	-7.46	98.76	109.96
1	A	114	ALA	N-CA-C	-7.45	103.10	111.07
2	B	235	HIS	CA-C-N	7.31	128.29	120.47
2	B	235	HIS	C-N-CA	7.31	128.29	120.47
1	A	542	ILE	N-CA-C	7.21	119.45	108.71
1	A	349	LEU	N-CA-C	-7.13	102.54	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	234	LEU	N-CA-C	7.11	120.77	108.76
2	B	118	VAL	CA-C-N	7.06	127.05	119.78
2	B	118	VAL	C-N-CA	7.06	127.05	119.78
1	A	25	PRO	N-CA-C	-7.03	97.99	112.47
1	A	493	VAL	N-CA-C	7.02	117.61	108.35
2	B	238	LYS	N-CA-C	-6.94	98.43	107.73
1	A	547	GLN	N-CA-C	-6.93	103.81	111.36
2	B	239	TRP	N-CA-C	-6.89	99.37	110.32
2	B	401	TRP	N-CA-C	6.84	123.13	114.31
1	A	382	ILE	N-CA-C	6.82	118.43	111.00
1	A	290	THR	N-CA-C	6.81	120.95	111.56
1	A	255	ASN	N-CA-C	-6.78	103.81	111.14
1	A	40	GLU	N-CA-C	-6.75	103.85	111.07
2	B	343	GLN	N-CA-C	-6.74	105.69	114.04
1	A	281	LYS	N-CA-C	6.71	122.44	111.37
2	B	349	LEU	N-CA-C	-6.47	105.54	113.50
2	B	192	ASP	N-CA-C	-6.44	106.14	112.97
2	B	6	GLU	N-CA-C	6.38	122.53	113.02
2	B	184	MET	CB-CA-C	-6.38	109.23	116.63
1	A	66	LYS	N-CA-C	6.32	120.08	111.17
1	A	200	THR	N-CA-C	-6.30	104.11	110.97
1	A	258	GLN	N-CA-C	-6.30	103.71	111.33
2	B	155	GLY	N-CA-C	-6.29	104.86	115.62
1	A	516	GLU	N-CA-C	-6.12	105.91	113.19
2	B	319	TYR	N-CA-C	-6.12	101.47	110.52
1	A	244	ILE	CB-CA-C	-6.10	101.60	110.63
1	A	310	LEU	N-CA-C	6.07	120.29	113.01
1	A	508	ALA	N-CA-C	-6.03	105.88	113.72
2	B	68	SER	N-CA-C	6.00	118.81	109.52
2	B	38	CYS	N-CA-C	5.96	118.57	111.71
2	B	161	GLN	N-CA-C	5.91	117.39	111.07
1	A	92	LEU	N-CA-C	5.90	119.37	110.64
1	A	192	ASP	N-CA-C	-5.88	103.25	110.65
2	B	389	PHE	N-CA-C	5.88	119.17	110.48
2	B	240	THR	N-CA-C	-5.84	104.82	111.07
2	B	413	GLU	N-CA-C	-5.83	101.11	110.14
2	B	273	GLY	N-CA-C	5.75	120.79	114.40
2	B	300	GLU	N-CA-C	-5.74	104.40	111.40
1	A	410	TRP	N-CA-C	5.67	117.62	108.32
1	A	220	LYS	N-CA-C	-5.62	101.87	110.30
1	A	112	GLY	N-CA-C	-5.58	105.89	113.37
1	A	59	PRO	N-CA-C	5.57	119.60	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	88	TRP	N-CA-C	5.55	117.85	109.41
1	A	319	TYR	N-CA-C	5.51	118.91	110.20
1	A	245	VAL	N-CA-C	-5.41	100.33	108.12
1	A	341	ILE	N-CA-C	-5.40	100.70	108.53
1	A	175	ASN	CA-C-N	5.37	125.04	119.56
1	A	175	ASN	C-N-CA	5.37	125.04	119.56
2	B	236	PRO	N-CA-C	5.31	123.78	114.75
1	A	53	GLU	N-CA-C	-5.25	105.98	112.38
1	A	291	GLU	N-CA-C	5.22	117.32	109.23
2	B	386	THR	CA-C-N	5.19	125.40	120.31
2	B	386	THR	C-N-CA	5.19	125.40	120.31
1	A	388	LYS	N-CA-C	-5.18	101.26	109.96
2	B	269	GLN	N-CA-C	-5.17	105.83	111.82
1	A	364	ASP	N-CA-C	5.14	117.55	111.33
2	B	21	VAL	N-CA-C	5.12	115.34	108.17
2	B	164	MET	N-CA-C	-5.12	105.78	111.36
1	A	165	THR	N-CA-C	-5.09	105.62	111.07
1	A	131	THR	N-CA-C	5.08	117.19	108.90
1	A	411	ILE	CB-CA-C	-5.07	105.21	110.13
2	B	7	THR	N-CA-C	5.06	117.98	110.14
1	A	265	ASN	N-CA-C	-5.05	105.68	111.14
1	A	147	ASN	N-CA-C	-5.00	106.59	113.30

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	4500	0	4565	288	0
2	B	3413	0	3443	230	0
3	A	38	0	31	3	0
4	A	25	0	0	2	0
4	B	11	0	0	0	0
All	All	7987	0	8039	505	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 (505) 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)
2:B:46:LYS:HE3	2:B:116:PHE:HB3	1.20	1.16
1:A:253:THR:HG23	1:A:256:ASP:HB2	1.35	1.05
2:B:164:MET:HE2	2:B:187:LEU:HD11	1.39	1.04
1:A:447:ASN:HB3	1:A:450:THR:HG22	1.40	1.03
1:A:68:SER:HB3	1:A:70:LYS:HE3	1.41	1.02
2:B:232:TYR:HE2	2:B:374:LYS:HZ1	1.04	0.98
2:B:178:ILE:HD11	2:B:201:LYS:HD3	1.44	0.97
2:B:111:VAL:HG11	2:B:187:LEU:HD12	1.43	0.96
2:B:44:GLU:HG3	2:B:46:LYS:HG2	1.49	0.94
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.50	0.94
2:B:193:LEU:HB3	2:B:197:GLN:HG3	1.50	0.93
1:A:541:GLY:HA2	1:A:546:GLU:OE1	1.72	0.90
2:B:170:PRO:HG3	2:B:212:TRP:HE1	1.36	0.90
1:A:40:GLU:HG3	1:A:41:MET:N	1.88	0.89
2:B:170:PRO:HG2	2:B:208:HIS:NE2	1.87	0.89
1:A:217:PRO:HG2	1:A:219:LYS:HB2	1.55	0.89
1:A:128:THR:HG21	1:A:146:TYR:HB2	1.54	0.88
2:B:282:LEU:HD12	2:B:282:LEU:H	1.39	0.87
1:A:550:LYS:NZ	1:A:550:LYS:HB3	1.90	0.86
2:B:154:LYS:HG3	2:B:184:MET:HE3	1.54	0.86
1:A:542:ILE:HG23	2:B:283:LEU:HB3	1.58	0.86
2:B:371:ALA:O	2:B:375:ILE:HG13	1.74	0.86
2:B:197:GLN:NE2	2:B:201:LYS:HB2	1.92	0.85
1:A:317:VAL:HG23	1:A:349:LEU:HD23	1.56	0.85
2:B:63:ILE:HD13	2:B:74:LEU:HD23	1.56	0.84
1:A:544:GLY:O	1:A:548:VAL:N	2.08	0.84
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.60	0.84
1:A:502:ALA:O	1:A:506:ILE:HG22	1.78	0.84
1:A:253:THR:H	1:A:256:ASP:CB	1.91	0.83
1:A:544:GLY:O	1:A:548:VAL:HG23	1.79	0.83
2:B:197:GLN:HE22	2:B:201:LYS:HB2	1.41	0.82
1:A:111:VAL:HG21	1:A:164:MET:HE3	1.62	0.81
1:A:441:TYR:CB	1:A:544:GLY:HA3	2.10	0.81
1:A:543:GLY:HA2	2:B:285:GLY:O	1.79	0.81
2:B:363:ASN:O	2:B:367:GLN:HG3	1.79	0.81
1:A:447:ASN:HB3	1:A:450:THR:CG2	2.12	0.80
1:A:254:VAL:HG21	1:A:288:ALA:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:LYS:HE3	2:B:116:PHE:CB	2.09	0.79
1:A:441:TYR:HB2	1:A:544:GLY:HA3	1.62	0.79
1:A:255:ASN:HB2	1:A:289:LEU:HD23	1.65	0.78
1:A:255:ASN:HB2	1:A:289:LEU:CD2	2.13	0.77
2:B:198:HIS:O	2:B:201:LYS:HB3	1.85	0.77
2:B:353:LYS:HZ2	2:B:428:GLN:HE21	1.30	0.77
2:B:87:PHE:N	2:B:87:PHE:CD2	2.51	0.77
2:B:87:PHE:N	2:B:87:PHE:HD2	1.83	0.77
2:B:104:LYS:O	2:B:236:PRO:HD2	1.84	0.77
1:A:283:LEU:HB2	1:A:284:ARG:HH12	1.50	0.77
1:A:284:ARG:NE	1:A:358:ARG:HH22	1.83	0.76
2:B:241:VAL:HG13	2:B:351:THR:HG23	1.67	0.76
1:A:458:VAL:HG13	1:A:548:VAL:HG22	1.67	0.76
2:B:181:TYR:HB3	2:B:188:TYR:HB2	1.69	0.75
2:B:87:PHE:HD2	2:B:87:PHE:H	1.36	0.74
1:A:328:GLU:HG2	1:A:330:GLN:NE2	2.04	0.73
1:A:293:ILE:HG23	1:A:294:PRO:HD2	1.70	0.72
1:A:541:GLY:HA2	1:A:546:GLU:CD	2.14	0.72
1:A:541:GLY:C	1:A:546:GLU:HB2	2.14	0.72
1:A:443:ASP:HB3	1:A:548:VAL:CG1	2.19	0.72
2:B:279:LEU:HA	2:B:282:LEU:HD11	1.72	0.72
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.25	0.72
2:B:185:ASP:CG	2:B:409:THR:HG21	2.15	0.71
1:A:13:LYS:HB2	1:A:16:MET:SD	2.31	0.71
1:A:111:VAL:O	1:A:111:VAL:HG13	1.90	0.71
1:A:450:THR:HG23	1:A:452:LEU:H	1.56	0.71
1:A:517:LEU:HA	4:A:580:HOH:O	1.89	0.70
1:A:254:VAL:HB	1:A:289:LEU:HA	1.72	0.70
2:B:353:LYS:NZ	2:B:428:GLN:HE21	1.88	0.70
2:B:244:ILE:HB	2:B:310:LEU:HD13	1.73	0.70
1:A:253:THR:H	1:A:256:ASP:HB3	1.57	0.69
1:A:447:ASN:CB	1:A:450:THR:HG22	2.20	0.69
1:A:511:ASP:O	1:A:512:LYS:HE3	1.92	0.68
2:B:154:LYS:C	2:B:157:PRO:HD2	2.19	0.68
2:B:13:LYS:HB3	2:B:16:MET:SD	2.33	0.68
1:A:136:ASN:O	1:A:137:ASN:HB2	1.94	0.68
1:A:328:GLU:HG2	1:A:330:GLN:HE21	1.58	0.67
1:A:23:GLN:HE21	1:A:24:TRP:HB2	1.59	0.67
1:A:442:VAL:O	1:A:545:ASN:ND2	2.27	0.67
2:B:268:SER:HB3	2:B:274:ILE:HB	1.76	0.66
1:A:344:GLU:OE2	1:A:347:LYS:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:LYS:HG3	2:B:14:PRO:N	2.09	0.66
2:B:275:LYS:HD2	2:B:302:GLU:HG3	1.76	0.66
1:A:544:GLY:C	1:A:548:VAL:HG23	2.20	0.66
2:B:195:ILE:HG13	2:B:196:GLY:H	1.60	0.66
2:B:238:LYS:NZ	2:B:351:THR:O	2.28	0.66
2:B:169:GLU:N	2:B:170:PRO:HD2	2.10	0.66
1:A:232:TYR:O	1:A:242:GLN:NE2	2.21	0.65
1:A:235:HIS:HB2	1:A:238:LYS:O	1.96	0.65
2:B:67:ASP:HB2	2:B:230:MET:CG	2.26	0.65
1:A:546:GLU:HA	1:A:549:ASP:HB2	1.77	0.65
2:B:281:LYS:O	2:B:284:ARG:HD2	1.97	0.65
1:A:366:LYS:NZ	1:A:370:GLU:OE2	2.29	0.65
1:A:110:ASP:CB	1:A:219:LYS:HB3	2.26	0.65
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.79	0.64
2:B:5:ILE:HG23	2:B:5:ILE:O	1.96	0.64
1:A:23:GLN:NE2	1:A:24:TRP:HB2	2.12	0.64
2:B:44:GLU:HG3	2:B:46:LYS:CG	2.26	0.64
1:A:253:THR:HA	1:A:291:GLU:O	1.98	0.64
1:A:283:LEU:HB2	1:A:284:ARG:NH1	2.12	0.64
1:A:550:LYS:HB3	1:A:550:LYS:HZ3	1.63	0.64
1:A:443:ASP:HB3	1:A:548:VAL:HG11	1.80	0.63
2:B:160:PHE:HD2	2:B:160:PHE:O	1.81	0.63
2:B:275:LYS:HE3	2:B:302:GLU:HA	1.79	0.63
1:A:114:ALA:HA	1:A:214:LEU:HD22	1.80	0.63
1:A:295:LEU:HD22	1:A:300:GLU:OE1	1.98	0.63
1:A:320:ASP:H	1:A:343:GLN:HE22	1.45	0.63
1:A:540:LYS:HA	1:A:540:LYS:CE	2.29	0.63
1:A:251:SER:HA	1:A:292:VAL:HG13	1.80	0.63
1:A:547:GLN:HA	1:A:550:LYS:NZ	2.13	0.63
2:B:363:ASN:ND2	2:B:366:LYS:HB2	2.14	0.63
1:A:49:LYS:HG2	1:A:144:TYR:CE2	2.33	0.63
2:B:183:TYR:HE1	2:B:384:GLY:O	1.82	0.63
1:A:24:TRP:CZ3	1:A:59:PRO:HB2	2.34	0.62
1:A:28:GLU:HG3	1:A:135:ILE:HG23	1.80	0.62
1:A:252:TRP:O	1:A:293:ILE:N	2.32	0.62
2:B:378:GLU:O	2:B:382:ILE:HD12	1.99	0.62
1:A:317:VAL:CG2	1:A:349:LEU:HD23	2.29	0.62
1:A:545:ASN:O	1:A:549:ASP:CB	2.48	0.62
2:B:13:LYS:HG3	2:B:14:PRO:CD	2.30	0.62
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.34	0.62
2:B:167:ILE:HG23	2:B:212:TRP:CG	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:HB2	1:A:252:TRP:CH2	2.34	0.62
2:B:164:MET:CE	2:B:187:LEU:HD11	2.22	0.61
1:A:198:HIS:O	1:A:202:ILE:HG12	1.99	0.61
1:A:282:LEU:HD23	1:A:282:LEU:O	2.00	0.61
1:A:265:ASN:N	1:A:265:ASN:HD22	1.98	0.61
2:B:193:LEU:HB3	2:B:197:GLN:CG	2.25	0.61
2:B:204:GLU:O	2:B:208:HIS:HB3	2.00	0.61
1:A:129:ALA:HA	1:A:144:TYR:O	2.00	0.60
2:B:279:LEU:N	2:B:302:GLU:OE1	2.30	0.60
1:A:102:LYS:HG2	1:A:103:LYS:N	2.14	0.60
2:B:170:PRO:CG	2:B:208:HIS:NE2	2.62	0.60
1:A:37:ILE:O	1:A:40:GLU:HG2	2.01	0.60
1:A:540:LYS:HA	1:A:540:LYS:HE2	1.84	0.60
2:B:391:LEU:HB3	2:B:393:ILE:HG22	1.83	0.60
1:A:548:VAL:HA	1:A:551:LEU:HD12	1.84	0.60
2:B:178:ILE:HD11	2:B:201:LYS:CD	2.27	0.60
1:A:277:ARG:NH1	1:A:334:GLN:HB3	2.16	0.60
2:B:167:ILE:HA	2:B:212:TRP:CE2	2.37	0.60
2:B:356:ARG:HH11	2:B:356:ARG:HG2	1.65	0.60
2:B:232:TYR:HE2	2:B:374:LYS:NZ	1.90	0.60
1:A:545:ASN:O	1:A:549:ASP:CG	2.45	0.60
1:A:174:GLN:O	1:A:174:GLN:HG3	2.00	0.60
1:A:441:TYR:HB3	1:A:544:GLY:HA3	1.83	0.60
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.83	0.59
1:A:290:THR:O	1:A:290:THR:HG22	2.01	0.59
1:A:110:ASP:HB2	1:A:219:LYS:HB3	1.82	0.59
1:A:95:PRO:HG2	3:A:556:QO9:H22A	1.84	0.59
1:A:13:LYS:HB3	1:A:14:PRO:CD	2.30	0.59
1:A:180:ILE:HD13	1:A:189:VAL:HG13	1.84	0.59
1:A:253:THR:H	1:A:256:ASP:HB2	1.67	0.59
1:A:294:PRO:O	1:A:295:LEU:HG	2.03	0.59
2:B:329:ILE:O	2:B:392:PRO:HG3	2.03	0.59
2:B:385:LYS:O	2:B:385:LYS:HG3	2.03	0.59
1:A:104:LYS:HD2	1:A:192:ASP:OD1	2.03	0.59
1:A:148:VAL:O	1:A:150:PRO:HD3	2.03	0.59
1:A:246:LEU:N	1:A:246:LEU:HD23	2.18	0.59
1:A:24:TRP:CE3	1:A:59:PRO:HB2	2.37	0.59
1:A:303:LEU:O	1:A:307:ARG:HG3	2.03	0.59
1:A:325:LEU:HG	1:A:387:PRO:HB3	1.85	0.58
2:B:111:VAL:HG11	2:B:187:LEU:CD1	2.26	0.58
1:A:289:LEU:HD23	1:A:289:LEU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:ND2	1:A:450:THR:H	2.00	0.58
2:B:350:LYS:HG3	2:B:351:THR:N	2.18	0.58
1:A:40:GLU:CG	1:A:41:MET:N	2.66	0.58
2:B:205:LEU:O	2:B:209:LEU:HB2	2.04	0.58
2:B:171:PHE:HZ	2:B:204:GLU:HB3	1.68	0.58
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.85	0.58
2:B:164:MET:HE2	2:B:187:LEU:CD1	2.24	0.58
2:B:324:ASP:HA	2:B:385:LYS:HZ3	1.69	0.58
2:B:89:GLU:OE1	2:B:94:ILE:HG12	2.04	0.57
2:B:323:LYS:O	2:B:385:LYS:NZ	2.37	0.57
2:B:360:ALA:HB3	2:B:363:ASN:HB3	1.86	0.57
1:A:550:LYS:O	1:A:552:VAL:HG23	2.03	0.57
2:B:356:ARG:HH11	2:B:356:ARG:CG	2.17	0.57
2:B:205:LEU:O	2:B:205:LEU:HD23	2.02	0.57
2:B:79:GLU:O	2:B:83:ARG:HG3	2.04	0.57
2:B:196:GLY:O	2:B:200:THR:HG23	2.04	0.57
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.85	0.57
2:B:67:ASP:HB2	2:B:230:MET:HG2	1.86	0.57
1:A:277:ARG:HB2	1:A:336:GLN:HE21	1.68	0.57
2:B:330:GLN:NE2	2:B:338:THR:OG1	2.37	0.57
1:A:102:LYS:NZ	1:A:236:PRO:O	2.37	0.57
2:B:205:LEU:HD23	2:B:205:LEU:C	2.30	0.57
2:B:360:ALA:O	2:B:367:GLN:NE2	2.37	0.57
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.87	0.57
1:A:398:TRP:CH2	1:A:411:ILE:HG13	2.39	0.56
2:B:233:GLU:O	2:B:234:LEU:HD23	2.05	0.56
2:B:344:GLU:HB2	2:B:347:LYS:HB2	1.87	0.56
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.40	0.56
2:B:182:GLN:HG3	2:B:187:LEU:CD2	2.35	0.56
2:B:353:LYS:HE3	2:B:428:GLN:HG2	1.87	0.56
2:B:195:ILE:HG13	2:B:196:GLY:N	2.21	0.56
1:A:544:GLY:O	1:A:548:VAL:CG2	2.52	0.56
1:A:550:LYS:HB3	1:A:550:LYS:HZ2	1.67	0.56
1:A:78:ARG:O	1:A:82:LYS:HG3	2.06	0.56
1:A:506:ILE:HG21	1:A:533:LEU:HD21	1.86	0.56
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.46	0.56
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.35	0.56
1:A:278:GLN:HE21	1:A:298:GLU:HB2	1.70	0.56
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.41	0.55
1:A:253:THR:CG2	1:A:256:ASP:HB2	2.23	0.55
2:B:111:VAL:CG1	2:B:187:LEU:HD12	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLY:O	1:A:115:TYR:HB2	2.06	0.55
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.72	0.55
1:A:177:ASP:OD1	1:A:177:ASP:C	2.50	0.55
1:A:284:ARG:CD	1:A:358:ARG:HH22	2.19	0.55
2:B:104:LYS:CG	2:B:192:ASP:HA	2.37	0.55
2:B:154:LYS:CG	2:B:184:MET:HE3	2.31	0.55
2:B:99:GLY:O	2:B:103:LYS:HG2	2.07	0.55
2:B:156:SER:N	2:B:157:PRO:HD2	2.21	0.55
2:B:193:LEU:CB	2:B:197:GLN:HG3	2.31	0.55
2:B:353:LYS:CE	2:B:428:GLN:HE21	2.19	0.55
1:A:128:THR:CG2	1:A:146:TYR:H	2.20	0.55
2:B:361:HIS:O	2:B:361:HIS:ND1	2.39	0.55
2:B:183:TYR:CE1	2:B:384:GLY:O	2.60	0.55
1:A:128:THR:CG2	1:A:146:TYR:HD2	2.20	0.55
1:A:433:PRO:HB2	2:B:290:THR:HG22	1.88	0.55
1:A:13:LYS:CB	1:A:14:PRO:HD2	2.31	0.54
1:A:451:LYS:HE2	1:A:471:ASN:HA	1.89	0.54
1:A:445:ALA:O	1:A:453:GLY:HA3	2.07	0.54
2:B:13:LYS:HE3	2:B:14:PRO:HG2	1.89	0.54
2:B:279:LEU:O	2:B:282:LEU:CD1	2.55	0.54
1:A:162:SER:OG	2:B:52:PRO:HD3	2.07	0.54
1:A:253:THR:N	1:A:256:ASP:HB3	2.23	0.54
2:B:314:VAL:HB	2:B:317:VAL:HG21	1.90	0.54
1:A:186:ASP:OD2	1:A:220:LYS:HD2	2.06	0.54
1:A:542:ILE:N	1:A:546:GLU:HB2	2.22	0.54
2:B:240:THR:HG23	2:B:241:VAL:N	2.23	0.54
2:B:324:ASP:HA	2:B:385:LYS:NZ	2.22	0.54
1:A:92:LEU:HD12	1:A:92:LEU:H	1.73	0.54
1:A:284:ARG:HE	1:A:358:ARG:HH22	1.54	0.54
1:A:550:LYS:C	1:A:552:VAL:H	2.16	0.54
1:A:207:GLN:HB3	1:A:211:ARG:NH2	2.23	0.53
2:B:228:LEU:N	2:B:228:LEU:HD23	2.23	0.53
1:A:156:SER:O	1:A:160:SER:HB2	2.06	0.53
2:B:169:GLU:HB3	2:B:173:LYS:NZ	2.23	0.53
1:A:105:SER:O	1:A:190:GLY:HA2	2.08	0.53
2:B:126:LYS:HA	2:B:145:GLN:OE1	2.09	0.53
1:A:296:THR:O	1:A:299:ALA:HB3	2.09	0.53
2:B:154:LYS:O	2:B:157:PRO:HD2	2.08	0.53
2:B:160:PHE:O	2:B:160:PHE:CD2	2.61	0.53
2:B:181:TYR:CG	2:B:182:GLN:N	2.77	0.53
1:A:217:PRO:O	1:A:219:LYS:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:HG23	1:A:271:TYR:CD1	2.43	0.53
1:A:31:ILE:O	1:A:35:VAL:HG23	2.09	0.53
1:A:83:ARG:NH1	1:A:83:ARG:HG2	2.24	0.52
1:A:283:LEU:CB	1:A:284:ARG:HH12	2.20	0.52
1:A:445:ALA:O	1:A:477:THR:HG21	2.08	0.52
1:A:42:GLU:OE1	1:A:49:LYS:HE2	2.09	0.52
1:A:458:VAL:CG2	2:B:286:THR:HG21	2.39	0.52
2:B:154:LYS:HG3	2:B:184:MET:CE	2.35	0.52
1:A:49:LYS:HG2	1:A:144:TYR:HE2	1.73	0.52
1:A:228:LEU:N	1:A:228:LEU:HD23	2.23	0.52
1:A:450:THR:HG23	1:A:452:LEU:N	2.25	0.52
2:B:5:ILE:O	2:B:5:ILE:CG2	2.57	0.52
2:B:90:VAL:HG22	2:B:90:VAL:O	2.08	0.52
1:A:541:GLY:CA	1:A:546:GLU:HG2	2.39	0.52
2:B:279:LEU:O	2:B:282:LEU:HD13	2.10	0.52
1:A:78:ARG:HG2	1:A:82:LYS:HE3	1.92	0.52
1:A:441:TYR:HB3	1:A:544:GLY:CA	2.40	0.52
2:B:240:THR:HG23	2:B:241:VAL:H	1.75	0.52
2:B:104:LYS:HG3	2:B:192:ASP:HA	1.91	0.51
1:A:112:GLY:O	1:A:116:PHE:CD2	2.63	0.51
1:A:406:TRP:CD2	2:B:420:PRO:HB3	2.45	0.51
2:B:67:ASP:HB2	2:B:230:MET:HG3	1.91	0.51
2:B:70:LYS:HG2	2:B:71:TRP:O	2.10	0.51
2:B:165:THR:O	2:B:169:GLU:HG3	2.10	0.51
2:B:399:GLU:HA	2:B:402:TRP:CD1	2.45	0.51
2:B:239:TRP:N	2:B:239:TRP:CE3	2.78	0.51
1:A:219:LYS:O	1:A:220:LYS:C	2.50	0.51
1:A:251:SER:OG	1:A:292:VAL:HG22	2.10	0.51
2:B:325:LEU:HD23	2:B:343:GLN:CG	2.41	0.51
1:A:23:GLN:NE2	1:A:24:TRP:H	2.09	0.51
1:A:77:PHE:O	1:A:78:ARG:C	2.53	0.51
2:B:33:ALA:O	2:B:37:ILE:HG13	2.11	0.51
2:B:195:ILE:CG1	2:B:196:GLY:N	2.73	0.51
2:B:29:GLU:CD	2:B:71:TRP:HZ2	2.19	0.51
1:A:299:ALA:O	1:A:302:GLU:HG2	2.11	0.51
1:A:542:ILE:CG2	2:B:283:LEU:HB3	2.36	0.50
1:A:424:LYS:HB2	4:A:581:HOH:O	2.10	0.50
1:A:91:GLN:NE2	1:A:92:LEU:N	2.58	0.50
3:A:556:QO9:HN3	3:A:556:QO9:H10A	1.76	0.50
2:B:167:ILE:HG23	2:B:212:TRP:CD1	2.47	0.50
2:B:60:VAL:HG23	2:B:75:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:LEU:HD23	2:B:214:LEU:HD22	1.93	0.50
1:A:366:LYS:O	1:A:370:GLU:HG3	2.11	0.50
1:A:106:VAL:HA	1:A:189:VAL:O	2.12	0.50
1:A:523:GLU:OE1	1:A:523:GLU:HA	2.07	0.50
2:B:169:GLU:N	2:B:170:PRO:CD	2.75	0.50
2:B:201:LYS:HA	2:B:201:LYS:NZ	2.27	0.50
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.47	0.50
1:A:125:ARG:O	1:A:128:THR:HB	2.12	0.49
1:A:486:LEU:HB3	1:A:524:GLN:HB3	1.94	0.49
2:B:197:GLN:C	2:B:197:GLN:CD	2.79	0.49
1:A:545:ASN:O	1:A:549:ASP:HB2	2.11	0.49
2:B:398:TRP:NE1	2:B:402:TRP:CD1	2.80	0.49
1:A:411:ILE:HG22	1:A:412:PRO:O	2.12	0.49
2:B:142:ILE:HG22	2:B:144:TYR:CE1	2.47	0.49
2:B:107:THR:HG23	2:B:198:HIS:HE2	1.77	0.49
1:A:541:GLY:HA2	1:A:546:GLU:CG	2.41	0.49
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.95	0.49
2:B:353:LYS:CE	2:B:428:GLN:HG2	2.42	0.49
2:B:388:LYS:CE	2:B:415:GLU:HG2	2.42	0.49
1:A:257:ILE:O	1:A:261:VAL:HG23	2.13	0.49
1:A:441:TYR:CB	1:A:544:GLY:CA	2.86	0.49
1:A:2:ILE:HD11	1:A:210:LEU:O	2.13	0.49
2:B:239:TRP:N	2:B:239:TRP:HE3	2.10	0.49
1:A:48:SER:O	1:A:144:TYR:HA	2.12	0.49
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.95	0.49
1:A:104:LYS:N	1:A:192:ASP:OD1	2.43	0.49
1:A:483:TYR:O	1:A:487:GLN:HG3	2.13	0.49
1:A:476:LYS:HG3	1:A:517:LEU:HD23	1.95	0.49
1:A:542:ILE:HG21	2:B:283:LEU:HD13	1.93	0.49
2:B:195:ILE:O	2:B:196:GLY:C	2.56	0.49
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.95	0.48
1:A:11:LYS:O	1:A:85:GLN:HB3	2.13	0.48
1:A:83:ARG:HG2	1:A:83:ARG:HH11	1.77	0.48
1:A:89:GLU:HG3	1:A:91:GLN:H	1.78	0.48
2:B:65:LYS:HG3	2:B:66:LYS:N	2.28	0.48
1:A:172:LYS:HE2	1:A:180:ILE:HB	1.94	0.48
1:A:27:THR:OG1	1:A:30:LYS:HG3	2.13	0.48
1:A:128:THR:HG21	1:A:146:TYR:CB	2.35	0.48
1:A:181:TYR:HB2	1:A:188:TYR:HB2	1.95	0.48
1:A:460:ASN:HA	2:B:286:THR:O	2.14	0.48
1:A:541:GLY:CA	1:A:546:GLU:CG	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LYS:HG2	2:B:71:TRP:N	2.28	0.48
1:A:508:ALA:C	1:A:509:GLN:HG3	2.38	0.48
2:B:284:ARG:HH11	2:B:284:ARG:HB3	1.76	0.48
1:A:102:LYS:HE3	1:A:236:PRO:O	2.12	0.48
1:A:206:ARG:NE	1:A:216:THR:O	2.31	0.48
2:B:201:LYS:HA	2:B:201:LYS:HZ3	1.77	0.48
2:B:12:LEU:HD12	2:B:16:MET:O	2.12	0.48
2:B:275:LYS:CD	2:B:302:GLU:HG3	2.41	0.48
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.48	0.48
1:A:210:LEU:O	1:A:210:LEU:HG	2.13	0.48
1:A:279:LEU:HG	1:A:302:GLU:OE1	2.12	0.48
1:A:312:GLU:O	1:A:314:VAL:HG23	2.14	0.48
1:A:458:VAL:HG23	2:B:286:THR:HG21	1.95	0.48
1:A:111:VAL:O	1:A:111:VAL:CG1	2.62	0.47
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.48	0.47
1:A:547:GLN:HA	1:A:550:LYS:HZ1	1.78	0.47
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.50	0.47
1:A:245:VAL:C	1:A:246:LEU:HD23	2.38	0.47
1:A:102:LYS:CG	1:A:103:LYS:N	2.77	0.47
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.45	0.47
2:B:380:ILE:O	2:B:384:GLY:N	2.46	0.47
2:B:203:GLU:O	2:B:207:GLN:HB2	2.15	0.47
1:A:102:LYS:CE	1:A:236:PRO:O	2.63	0.47
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.80	0.47
1:A:284:ARG:HD3	1:A:358:ARG:HH22	1.79	0.47
2:B:65:LYS:HG3	2:B:66:LYS:H	1.80	0.47
1:A:277:ARG:HH11	1:A:334:GLN:HB3	1.80	0.47
2:B:115:TYR:OH	2:B:157:PRO:HA	2.15	0.47
1:A:417:VAL:O	1:A:417:VAL:HG13	2.15	0.47
2:B:168:LEU:C	2:B:170:PRO:HD2	2.39	0.47
2:B:209:LEU:HD23	2:B:214:LEU:CD2	2.45	0.47
2:B:263:LYS:HG3	2:B:426:TRP:CD1	2.50	0.47
1:A:541:GLY:C	1:A:546:GLU:CB	2.87	0.46
2:B:227:PHE:HB3	2:B:228:LEU:HD23	1.97	0.46
2:B:96:HIS:ND1	2:B:97:PRO:HD2	2.30	0.46
1:A:68:SER:CB	1:A:70:LYS:HE3	2.30	0.46
1:A:515:SER:C	1:A:517:LEU:H	2.21	0.46
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.97	0.46
1:A:450:THR:O	1:A:451:LYS:HB2	2.16	0.46
2:B:105:SER:O	2:B:190:GLY:HA2	2.16	0.46
2:B:335:GLY:HA2	2:B:367:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:CD1	1:A:189:VAL:HG13	2.45	0.46
2:B:34:LEU:CD2	2:B:73:LYS:HG3	2.45	0.46
2:B:122:GLU:OE2	2:B:125:ARG:CZ	2.63	0.46
1:A:42:GLU:OE2	1:A:49:LYS:HG3	2.15	0.46
1:A:113:ASP:HA	1:A:116:PHE:CD2	2.51	0.46
2:B:182:GLN:HG3	2:B:187:LEU:HD21	1.98	0.46
1:A:515:SER:C	1:A:517:LEU:N	2.70	0.46
1:A:550:LYS:C	1:A:552:VAL:N	2.71	0.46
2:B:182:GLN:HG3	2:B:187:LEU:HD23	1.98	0.46
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.81	0.46
1:A:240:THR:HG23	1:A:241:VAL:O	2.16	0.46
2:B:13:LYS:CG	2:B:14:PRO:HD2	2.45	0.46
2:B:76:ASP:OD1	2:B:78:ARG:HG3	2.16	0.46
1:A:193:LEU:HD13	1:A:197:GLN:HG2	1.98	0.45
2:B:77:PHE:O	2:B:78:ARG:C	2.57	0.45
1:A:79:GLU:OE2	1:A:83:ARG:NE	2.50	0.45
1:A:293:ILE:CG2	1:A:294:PRO:HD2	2.45	0.45
2:B:98:ALA:HB1	2:B:101:LYS:NZ	2.32	0.45
1:A:25:PRO:HG2	1:A:25:PRO:O	2.17	0.45
2:B:320:ASP:CG	2:B:322:SER:HG	2.24	0.45
1:A:40:GLU:HG3	1:A:41:MET:H	1.73	0.45
1:A:139:THR:HG22	1:A:140:PRO:CD	2.46	0.45
1:A:324:ASP:OD1	1:A:324:ASP:N	2.49	0.45
2:B:376:THR:HG21	2:B:410:TRP:CE3	2.51	0.45
1:A:305:GLU:O	1:A:309:ILE:HG13	2.16	0.45
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.16	0.45
2:B:402:TRP:CH2	2:B:403:THR:HG22	2.52	0.45
1:A:111:VAL:HG22	1:A:114:ALA:HB3	1.99	0.45
2:B:242:GLN:HA	2:B:243:PRO:HD3	1.79	0.45
1:A:358:ARG:HG2	1:A:358:ARG:NH1	2.31	0.45
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.52	0.45
2:B:161:GLN:C	2:B:163:SER:H	2.24	0.45
2:B:356:ARG:CG	2:B:356:ARG:NH1	2.79	0.45
1:A:244:ILE:CG2	1:A:263:LYS:HB3	2.47	0.45
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.32	0.45
1:A:302:GLU:HG3	1:A:303:LEU:N	2.31	0.45
1:A:308:GLU:HA	1:A:311:LYS:HE3	1.98	0.45
1:A:350:LYS:HD3	1:A:378:GLU:OE2	2.16	0.45
1:A:128:THR:HG21	1:A:146:TYR:H	1.82	0.44
1:A:223:LYS:HD2	1:A:223:LYS:HA	1.85	0.44
2:B:372:VAL:HG13	2:B:389:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASN:OD1	1:A:363:ASN:C	2.60	0.44
2:B:11:LYS:O	2:B:12:LEU:HD23	2.18	0.44
2:B:75:VAL:HB	2:B:77:PHE:CE1	2.52	0.44
1:A:457:TYR:CD1	1:A:457:TYR:C	2.96	0.44
2:B:30:LYS:HG2	2:B:62:ALA:HB3	2.00	0.44
2:B:44:GLU:OE1	2:B:46:LYS:HG3	2.17	0.44
2:B:280:SER:O	2:B:283:LEU:HB2	2.18	0.44
2:B:354:TYR:CE1	2:B:356:ARG:HG3	2.53	0.44
2:B:421:PRO:HB2	2:B:423:VAL:HG22	1.98	0.44
1:A:447:ASN:HD22	1:A:450:THR:H	1.65	0.44
1:A:506:ILE:HD13	1:A:525:LEU:HD11	2.00	0.44
1:A:445:ALA:N	1:A:477:THR:OG1	2.50	0.44
1:A:249:LYS:HD3	1:A:256:ASP:OD1	2.17	0.44
2:B:164:MET:O	2:B:165:THR:C	2.61	0.44
2:B:195:ILE:HD12	2:B:196:GLY:N	2.33	0.44
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.98	0.43
1:A:544:GLY:O	1:A:548:VAL:CB	2.66	0.43
2:B:325:LEU:HD23	2:B:343:GLN:HG2	2.00	0.43
1:A:253:THR:OG1	1:A:254:VAL:N	2.50	0.43
2:B:191:SER:C	2:B:193:LEU:H	2.25	0.43
2:B:202:ILE:O	2:B:206:ARG:HB2	2.18	0.43
1:A:252:TRP:HA	1:A:256:ASP:OD1	2.18	0.43
2:B:181:TYR:HD2	2:B:188:TYR:CD1	2.36	0.43
1:A:257:ILE:O	1:A:258:GLN:C	2.62	0.43
2:B:13:LYS:HG3	2:B:14:PRO:HD2	2.00	0.43
1:A:155:GLY:O	1:A:159:ILE:HG13	2.19	0.43
2:B:34:LEU:HD22	2:B:73:LYS:HG3	2.01	0.43
2:B:282:LEU:HD12	2:B:282:LEU:N	2.20	0.43
1:A:278:GLN:HB2	1:A:302:GLU:OE1	2.18	0.43
2:B:160:PHE:O	2:B:163:SER:HB3	2.18	0.43
1:A:63:ILE:HG23	1:A:63:ILE:O	2.19	0.43
1:A:101:LYS:O	3:A:556:QO9:H12	2.18	0.43
1:A:282:LEU:O	1:A:282:LEU:CD2	2.66	0.43
1:A:301:LEU:O	1:A:304:ALA:HB3	2.19	0.43
2:B:170:PRO:HG3	2:B:212:TRP:NE1	2.18	0.43
2:B:376:THR:CG2	2:B:410:TRP:CZ3	3.01	0.43
1:A:2:ILE:HD12	1:A:211:ARG:C	2.44	0.42
2:B:191:SER:HB2	2:B:193:LEU:HG	2.00	0.42
1:A:344:GLU:HG3	1:A:347:LYS:HB2	2.01	0.42
2:B:72:ARG:HG3	2:B:73:LYS:N	2.34	0.42
2:B:108:VAL:CG1	2:B:186:ASP:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:ILE:HG12	2:B:189:VAL:HG13	2.02	0.42
2:B:279:LEU:C	2:B:282:LEU:CD1	2.92	0.42
1:A:161:GLN:HG2	1:A:182:GLN:NE2	2.34	0.42
1:A:391:LEU:C	1:A:417:VAL:HG12	2.44	0.42
2:B:353:LYS:HE3	2:B:428:GLN:NE2	2.35	0.42
2:B:388:LYS:HE2	2:B:415:GLU:HG2	2.01	0.42
1:A:50:ILE:CG1	1:A:143:ARG:HB3	2.49	0.42
1:A:168:LEU:HD13	1:A:180:ILE:HG21	2.00	0.42
1:A:546:GLU:OE1	1:A:546:GLU:HA	2.19	0.42
2:B:156:SER:N	2:B:157:PRO:CD	2.82	0.42
2:B:178:ILE:CG2	2:B:179:VAL:N	2.82	0.42
2:B:242:GLN:H	2:B:351:THR:HG1	1.61	0.42
1:A:49:LYS:HA	1:A:143:ARG:O	2.19	0.42
1:A:173:LYS:C	1:A:175:ASN:H	2.28	0.42
1:A:255:ASN:HB2	1:A:289:LEU:HD21	1.98	0.42
1:A:48:SER:O	1:A:144:TYR:HD2	2.03	0.42
1:A:128:THR:CG2	1:A:128:THR:O	2.66	0.42
1:A:503:LEU:HD12	1:A:503:LEU:HA	1.78	0.42
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.55	0.41
2:B:320:ASP:OD2	2:B:320:ASP:C	2.61	0.41
1:A:302:GLU:O	1:A:303:LEU:C	2.63	0.41
2:B:382:ILE:HB	2:B:383:TRP:CE3	2.56	0.41
2:B:399:GLU:HA	2:B:402:TRP:HD1	1.85	0.41
1:A:207:GLN:O	1:A:211:ARG:CZ	2.69	0.41
1:A:401:TRP:CD1	1:A:402:TRP:N	2.88	0.41
2:B:112:GLY:C	2:B:114:ALA:H	2.29	0.41
2:B:118:VAL:HA	2:B:119:PRO:HD3	1.90	0.41
2:B:391:LEU:HA	2:B:392:PRO:HD3	1.78	0.41
1:A:65:LYS:O	1:A:68:SER:HB2	2.20	0.41
1:A:128:THR:HG22	1:A:146:TYR:H	1.86	0.41
1:A:295:LEU:HD22	1:A:300:GLU:CD	2.45	0.41
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.55	0.41
1:A:89:GLU:HG2	1:A:92:LEU:HD12	2.03	0.41
2:B:339:TYR:CD1	2:B:339:TYR:C	2.99	0.41
2:B:427:TYR:O	2:B:428:GLN:OE1	2.37	0.41
1:A:128:THR:CG2	1:A:146:TYR:CD2	3.02	0.41
1:A:346:PHE:O	1:A:347:LYS:HG2	2.20	0.41
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.83	0.41
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.56	0.41
1:A:5:ILE:O	1:A:6:GLU:C	2.64	0.41
1:A:88:TRP:NE1	2:B:143:ARG:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:LYS:H	2:B:104:LYS:HG2	1.70	0.41
2:B:210:LEU:HA	2:B:214:LEU:HB3	2.02	0.41
1:A:2:ILE:HA	1:A:2:ILE:HD13	1.79	0.41
1:A:111:VAL:CG2	1:A:164:MET:HE3	2.41	0.41
1:A:278:GLN:OE1	1:A:278:GLN:HA	2.21	0.41
1:A:283:LEU:CB	1:A:284:ARG:NH1	2.80	0.41
1:A:452:LEU:HD23	1:A:470:THR:HA	2.03	0.41
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.56	0.40
1:A:114:ALA:O	1:A:115:TYR:C	2.63	0.40
2:B:13:LYS:HD2	2:B:14:PRO:HD2	2.03	0.40
2:B:233:GLU:H	2:B:233:GLU:HG2	1.51	0.40
2:B:283:LEU:HD23	2:B:283:LEU:HA	1.94	0.40
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.56	0.40
1:A:136:ASN:O	1:A:137:ASN:CB	2.67	0.40
1:A:301:LEU:O	1:A:304:ALA:N	2.54	0.40
1:A:479:LEU:HD13	1:A:518:VAL:HG22	2.03	0.40
1:A:506:ILE:CD1	1:A:525:LEU:HD11	2.51	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	551/557 (99%)	497 (90%)	51 (9%)	3 (0%)	24	46
2	B	408/428 (95%)	364 (89%)	43 (10%)	1 (0%)	43	66
All	All	959/985 (97%)	861 (90%)	94 (10%)	4 (0%)	30	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE

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Mol	Chain	Res	Type
2	B	95	PRO
1	A	294	PRO
1	A	25	PRO

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	495/497 (100%)	452 (91%)	43 (9%)	9	21
2	B	374/390 (96%)	341 (91%)	33 (9%)	9	21
All	All	869/887 (98%)	793 (91%)	76 (9%)	9	21

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	6	GLU
1	A	24	TRP
1	A	53	GLU
1	A	60	VAL
1	A	83	ARG
1	A	91	GLN
1	A	111	VAL
1	A	122	GLU
1	A	126	LYS
1	A	139	THR
1	A	174	GLN
1	A	177	ASP
1	A	186	ASP
1	A	216	THR
1	A	218	ASP
1	A	228	LEU
1	A	237	ASP
1	A	244	ILE
1	A	246	LEU

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Mol	Chain	Res	Type
1	A	248	GLU
1	A	249	LYS
1	A	253	THR
1	A	265	ASN
1	A	281	LYS
1	A	284	ARG
1	A	291	GLU
1	A	305	GLU
1	A	324	ASP
1	A	361	HIS
1	A	366	LYS
1	A	394	GLN
1	A	396	GLU
1	A	431	LYS
1	A	447	ASN
1	A	463	ARG
1	A	476	LYS
1	A	506	ILE
1	A	512	LYS
1	A	519	ASN
1	A	520	GLN
1	A	540	LYS
1	A	550	LYS
2	B	7	THR
2	B	48	SER
2	B	67	ASP
2	B	74	LEU
2	B	84	THR
2	B	87	PHE
2	B	122	GLU
2	B	126	LYS
2	B	161	GLN
2	B	171	PHE
2	B	182	GLN
2	B	195	ILE
2	B	197	GLN
2	B	201	LYS
2	B	208	HIS
2	B	209	LEU
2	B	228	LEU
2	B	233	GLU
2	B	238	LYS

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Mol	Chain	Res	Type
2	B	244	ILE
2	B	275	LYS
2	B	282	LEU
2	B	284	ARG
2	B	298	GLU
2	B	300	GLU
2	B	310	LEU
2	B	317	VAL
2	B	356	ARG
2	B	358	ARG
2	B	382	ILE
2	B	415	GLU
2	B	423	VAL
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	91	GLN
1	A	137	ASN
1	A	161	GLN
1	A	182	GLN
1	A	207	GLN
1	A	265	ASN
1	A	278	GLN
1	A	306	ASN
1	A	315	HIS
1	A	336	GLN
1	A	343	GLN
1	A	394	GLN
1	A	428	GLN
1	A	447	ASN
1	A	475	GLN
1	A	487	GLN
1	A	545	ASN
1	A	547	GLN
2	B	161	GLN
2	B	197	GLN
2	B	207	GLN
2	B	330	GLN
2	B	336	GLN

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Mol	Chain	Res	Type
2	B	340	GLN
2	B	418	ASN
2	B	428	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	QO9	A	556	-	34,40,40	2.68	9 (26%)	47,68,68	1.99	13 (27%)

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	QO9	A	556	-	-	2/33/70/70	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	556	QO9	O2-C4	7.03	1.35	1.23
3	A	556	QO9	O1-C1	6.63	1.36	1.23
3	A	556	QO9	O8-S1	5.95	1.51	1.42
3	A	556	QO9	O7-S1	5.28	1.50	1.42
3	A	556	QO9	C3-C2	5.02	1.42	1.34
3	A	556	QO9	C5-C2	-4.96	1.38	1.50
3	A	556	QO9	C11-N3	3.37	1.41	1.34
3	A	556	QO9	C9-C6	2.70	1.56	1.53
3	A	556	QO9	C10-C7	2.55	1.56	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	556	QO9	C2-C1-N1	5.67	120.25	115.32
3	A	556	QO9	C8-C9-C6	-4.31	97.13	103.99
3	A	556	QO9	C1-N1-C4	-4.09	121.98	127.34
3	A	556	QO9	N1-C4-N2	4.00	120.09	114.89
3	A	556	QO9	O1-C1-C2	-3.63	120.76	124.92
3	A	556	QO9	O4-S1-O8	3.55	113.10	108.59
3	A	556	QO9	SI1-O5-C9	-3.50	115.64	127.82
3	A	556	QO9	O8-S1-O7	-3.21	108.57	115.55
3	A	556	QO9	C9-C6-N2	2.96	118.09	114.60
3	A	556	QO9	C3-N2-C4	-2.76	118.56	121.30
3	A	556	QO9	C5-C2-C1	2.42	121.37	118.78
3	A	556	QO9	SI2-O6-C10	-2.32	115.04	125.61
3	A	556	QO9	O4-S1-O7	2.29	111.50	108.59

There are no chirality outliers.

All (2) torsion outliers are listed below:

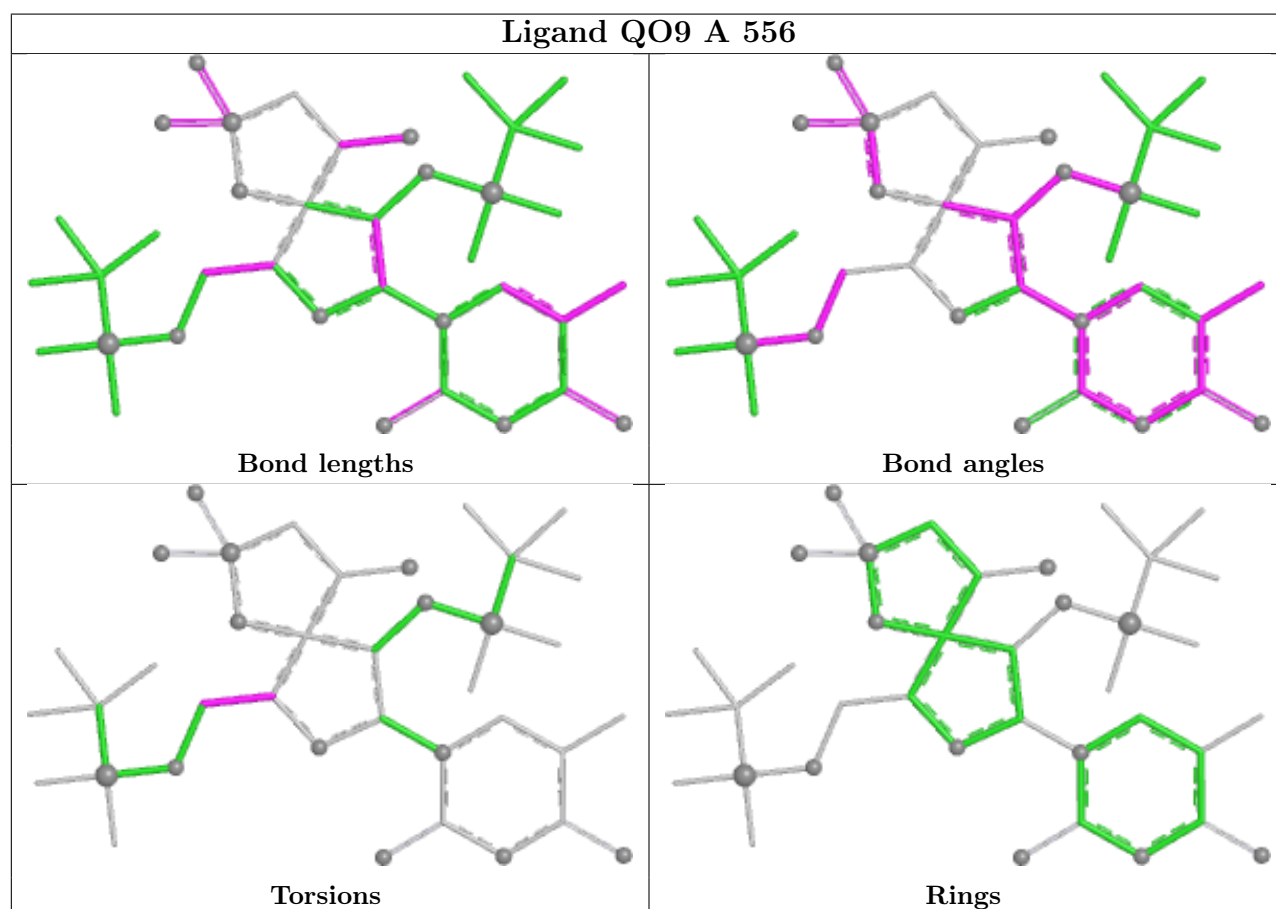
Mol	Chain	Res	Type	Atoms
3	A	556	QO9	O6-C10-C7-O3
3	A	556	QO9	O6-C10-C7-C8

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	556	QO9	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	553/557 (99%)	0.38	21 (3%) 44 38	47, 76, 133, 146	0
2	B	412/428 (96%)	0.58	26 (6%) 26 20	51, 81, 121, 144	0
All	All	965/985 (97%)	0.47	47 (4%) 35 29	47, 78, 126, 146	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	106	VAL	6.2
2	B	214	LEU	4.3
2	B	107	THR	4.0
1	A	551	LEU	3.8
2	B	196	GLY	3.6
2	B	91	GLN	3.6
1	A	236	PRO	3.5
1	A	547	GLN	3.1
1	A	549	ASP	3.1
2	B	141	GLY	3.0
2	B	94	ILE	2.9
2	B	283	LEU	2.9
2	B	190	GLY	2.8
2	B	108	VAL	2.8
2	B	111	VAL	2.8
1	A	283	LEU	2.7
2	B	300	GLU	2.7
1	A	352	GLY	2.7
2	B	381	VAL	2.7
2	B	109	LEU	2.7
2	B	153	TRP	2.7
2	B	175	ASN	2.6
1	A	282	LEU	2.5
2	B	150	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	340	GLN	2.4
2	B	316	GLY	2.4
2	B	419	THR	2.3
1	A	138	GLU	2.3
2	B	105	SER	2.3
1	A	24	TRP	2.3
1	A	548	VAL	2.3
1	A	533	LEU	2.3
1	A	338	THR	2.3
2	B	159	ILE	2.3
1	A	84	THR	2.2
2	B	425	LEU	2.2
2	B	213	GLY	2.2
1	A	90	VAL	2.2
2	B	202	ILE	2.2
2	B	237	ASP	2.1
1	A	69	THR	2.1
1	A	115	TYR	2.1
2	B	232	TYR	2.1
1	A	303	LEU	2.1
1	A	544	GLY	2.0
1	A	188	TYR	2.0
1	A	539	HIS	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](#)

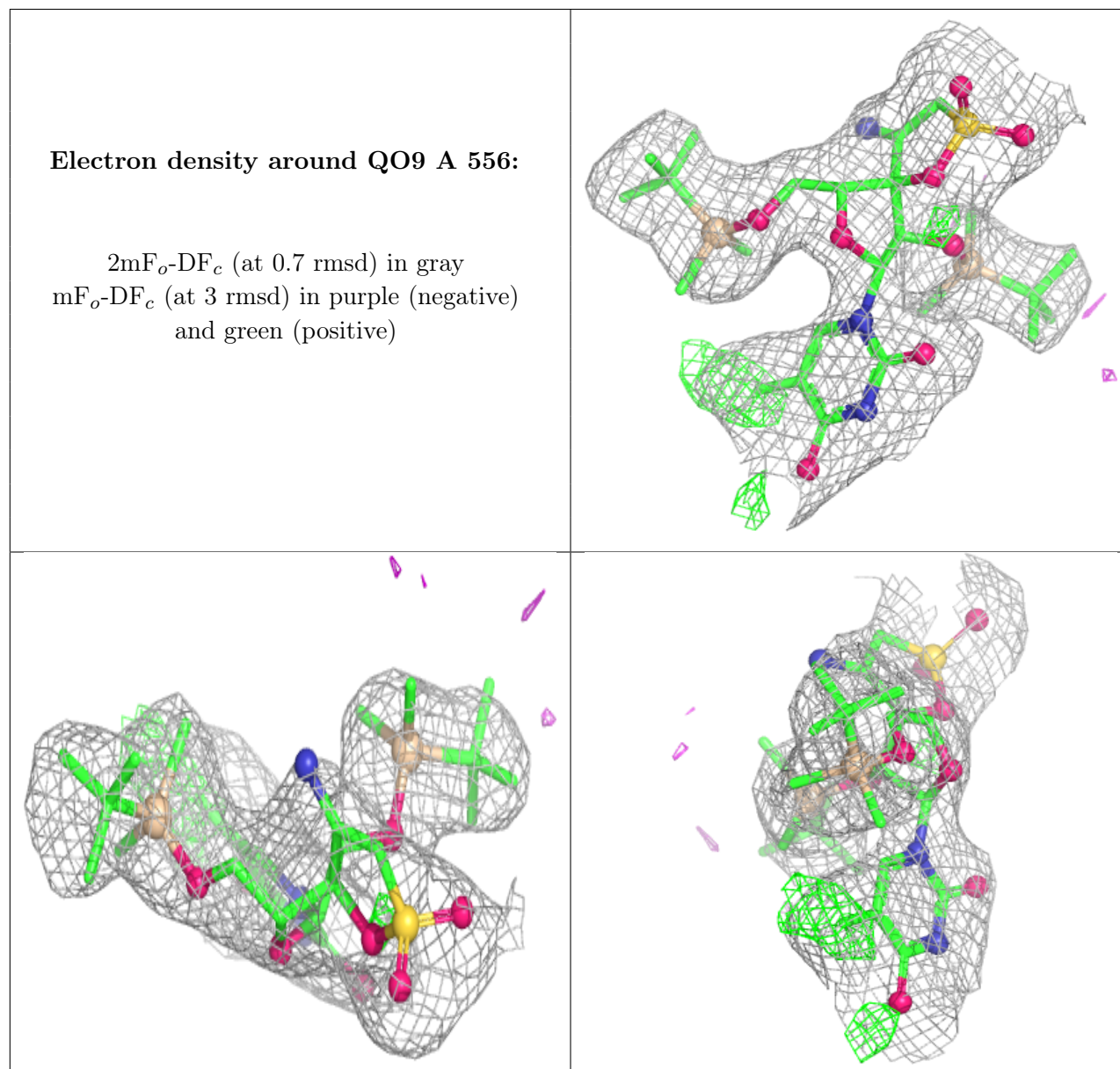
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	QO9	A	556	38/38	0.91	0.14	50,72,79,84	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.