



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 03:25 AM EDT

PDB ID : 3H0A / pdb_00003h0a
Title : Crystal Structure of Peroxisome Proliferator-Activated Receptor Gamma (PPAR γ) and Retinoic Acid Receptor Alpha (RXR α) in Complex with 9-cis Retinoic Acid, Co-activator Peptide, and a Partial Agonist
Authors : Wang, Z.; Sudom, A.; Walker, N.P.
Deposited on : 2009-04-08
Resolution : 2.10 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

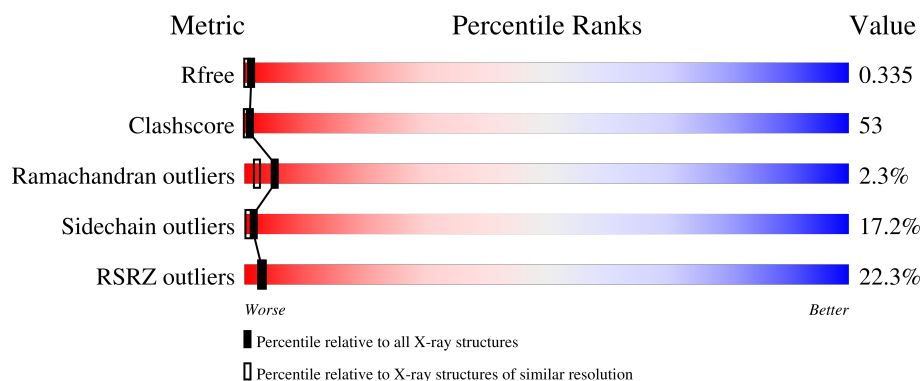
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	228	
2	D	272	
3	B	12	
3	E	12	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4147 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 Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1661	1066	285	300	10			

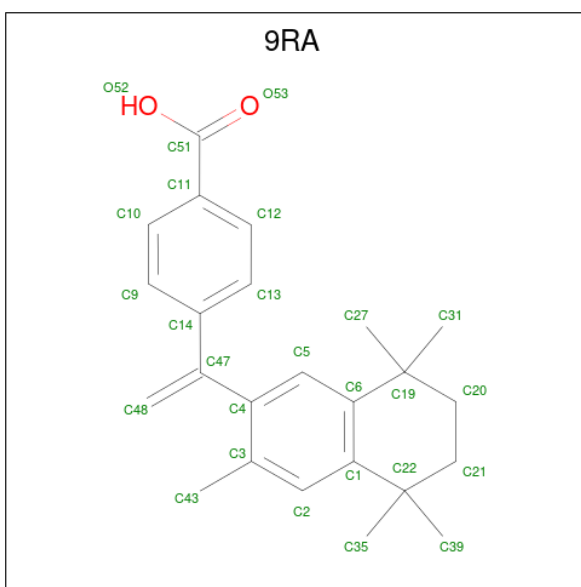
- Molecule 2 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	265	Total	C	N	O	S	0	2	0
			2135	1375	351	399	10			

- Molecule 3 is a protein called Nuclear receptor coactivator 1, Co-activator Peptide.

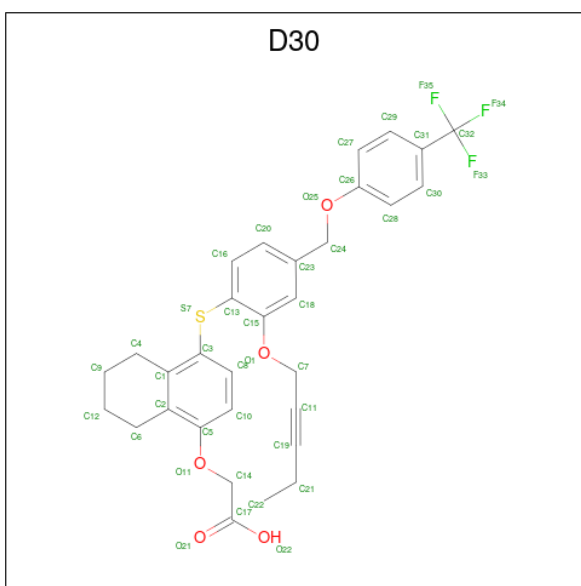
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	11	Total	C	N	O	0	0	0
			86	55	15	16			
3	E	12	Total	C	N	O	0	0	0
			94	59	16	19			

- Molecule 4 is 4-[1-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-yl)ethenyl]benzoic acid (CCD ID: 9RA) (formula: C₂₄H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			26	24	2		

- Molecule 5 is [(4-{[2-(pent-2-yn-1-yloxy)-4-{[4-(trifluoromethyl)phenoxy]methyl}phenyl]sulfanyl}-5,6,7,8-tetrahydronaphthalen-1-yl)oxy]acetic acid (CCD ID: D30) (formula: $C_{31}H_{29}F_3O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	F	O	S	0	0
			40	31	3	5	1		

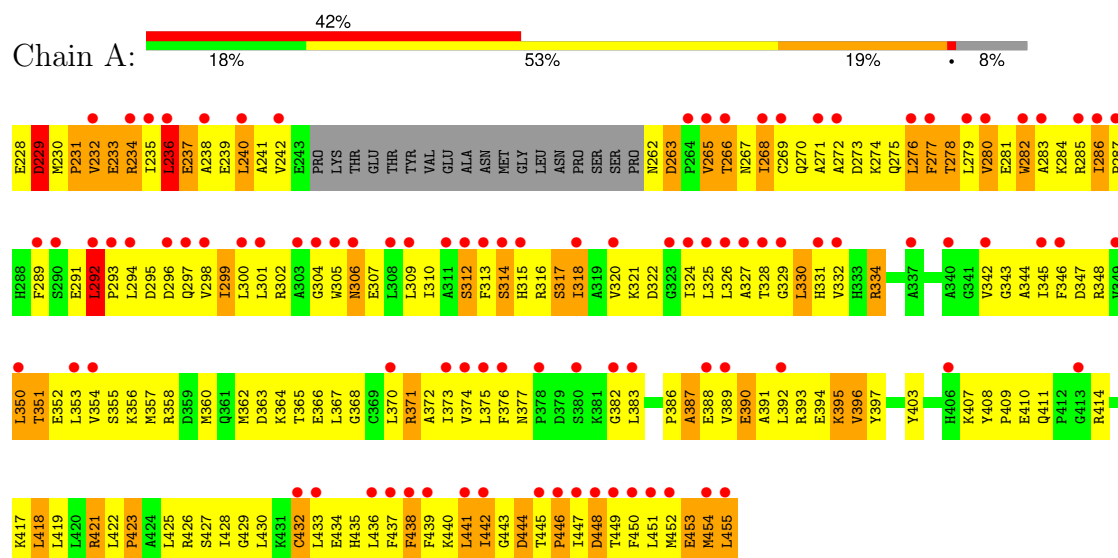
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total 9	O 9	0	0
6	D	93	Total 93	O 93	0	0
6	E	3	Total 3	O 3	0	0

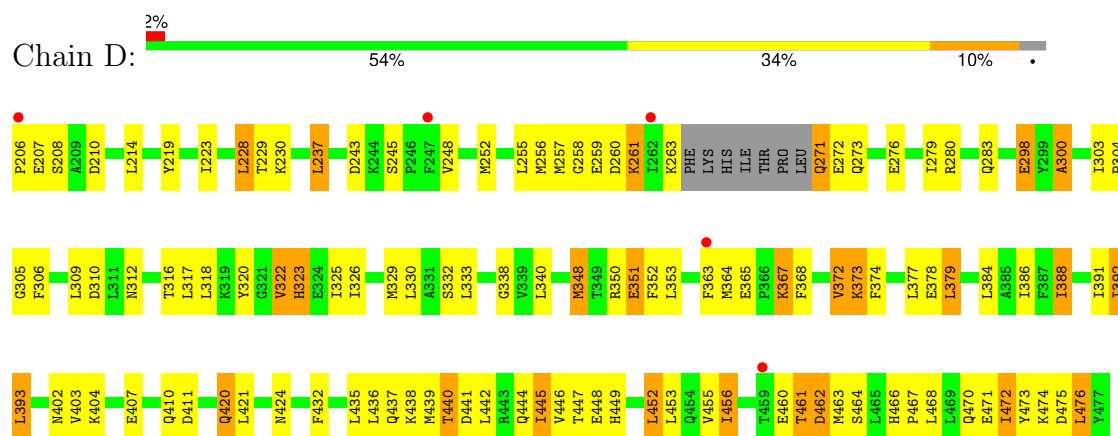
3 Residue-property plots

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.

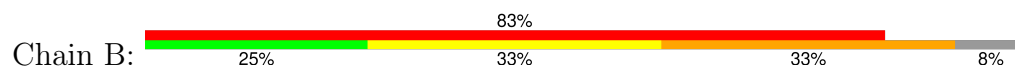
• Molecule 1: Retinoic acid receptor RXR-alpha

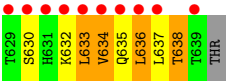


• Molecule 2: Peroxisome proliferator-activated receptor gamma

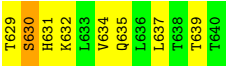


• Molecule 3: Nuclear receptor coactivator 1, Co-activator Peptide





● Molecule 3: Nuclear receptor coactivator 1, Co-activator Peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.26Å 53.83Å 67.11Å 90.00° 107.74° 90.00°	Depositor
Resolution (Å)	28.46 – 2.10 28.46 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (28.46-2.10) 97.7 (28.46-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.246 , 0.342 0.245 , 0.335	Depositor DCC
R_{free} test set	1758 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4147	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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: 9RA, D30

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	0.77	0/1693	1.18	12/2288 (0.5%)
2	D	1.32	6/2181 (0.3%)	1.38	11/2936 (0.4%)
3	B	0.78	0/86	1.20	1/116 (0.9%)
3	E	1.25	0/94	1.32	0/126
All	All	1.11	6/4054 (0.1%)	1.29	24/5466 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	309	LEU	N-CA	6.16	1.53	1.45
2	D	379	LEU	C-O	-5.98	1.16	1.23
2	D	410	GLN	C-O	5.54	1.30	1.24
2	D	392	ILE	CG1-CD1	5.36	1.72	1.51
2	D	420	GLN	N-CA	5.09	1.52	1.46
2	D	411	ASP	N-CA	5.03	1.52	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	372	VAL	N-CA-C	-9.32	98.95	111.44
1	A	229	ASP	N-CA-C	-8.75	101.57	113.30
3	B	636	LEU	N-CA-C	-8.57	101.92	112.38
1	A	280	VAL	N-CA-C	-8.23	102.79	110.53
2	D	461	THR	CB-CA-C	-7.99	105.35	115.89
2	D	392	ILE	N-CA-C	7.89	118.67	110.62
1	A	292	LEU	CA-C-N	7.76	129.54	119.84
1	A	292	LEU	C-N-CA	7.76	129.54	119.84
2	D	391	ILE	N-CA-C	7.46	117.58	110.42
1	A	432	CYS	N-CA-C	-7.34	103.22	111.07
1	A	234	ARG	N-CA-C	-6.86	104.64	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	GLY	N-CA-C	-6.67	104.23	112.77
1	A	411	GLN	CA-C-N	-6.62	112.89	120.04
1	A	411	GLN	C-N-CA	-6.62	112.89	120.04
2	D	393	LEU	N-CA-C	-5.60	103.75	111.81
1	A	236	LEU	N-CA-C	-5.53	105.41	111.82
2	D	300	ALA	N-CA-C	-5.51	104.50	111.11
2	D	322	VAL	N-CA-C	5.39	117.79	111.05
2	D	298	GLU	N-CA-C	-5.36	105.60	111.82
1	A	397	TYR	N-CA-C	-5.21	105.30	110.97
2	D	248	VAL	N-CA-C	5.20	115.84	107.73
2	D	462	ASP	N-CA-C	-5.20	106.18	112.88
2	D	316	THR	N-CA-C	5.08	117.21	111.11
1	A	282	TRP	N-CA-C	5.07	117.54	111.71

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	1661	0	1696	309	0
2	D	2135	0	2195	109	0
3	B	86	0	95	7	0
3	E	94	0	102	16	0
4	A	26	0	27	7	0
5	D	40	0	28	0	0
6	A	9	0	0	2	0
6	D	93	0	0	4	0
6	E	3	0	0	1	0
All	All	4147	0	4143	438	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 53.

All (438) 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:292:LEU:HB3	1:A:293:PRO:CD	1.44	1.47
1:A:292:LEU:CB	1:A:293:PRO:HD3	1.64	1.27
1:A:302:ARG:NH2	1:A:454:MET:HB2	1.54	1.19
1:A:292:LEU:HB3	1:A:293:PRO:HD2	1.20	1.18
1:A:326:LEU:HB2	1:A:330:LEU:HD23	1.23	1.15
1:A:292:LEU:CB	1:A:293:PRO:CD	2.19	1.14
1:A:440:LYS:NZ	1:A:441:LEU:HG	1.63	1.14
1:A:292:LEU:CD1	1:A:293:PRO:HD3	1.77	1.14
2:D:437:GLN:O	2:D:440:THR:HB	1.47	1.13
1:A:292:LEU:CG	1:A:293:PRO:HD3	1.78	1.13
1:A:272:ALA:O	1:A:276:LEU:HD22	1.52	1.09
1:A:292:LEU:HD12	1:A:293:PRO:HD3	1.33	1.09
1:A:330:LEU:HD22	1:A:330:LEU:N	1.66	1.07
1:A:452:MET:O	1:A:454:MET:N	1.86	1.07
1:A:241:ALA:HB1	1:A:285:ARG:NH1	1.70	1.06
2:D:228:LEU:HD12	2:D:333:LEU:HD21	1.33	1.06
1:A:373:ILE:HG23	1:A:393:ARG:HD2	1.35	1.05
1:A:266:THR:HB	1:A:446:PRO:HD2	1.33	1.05
1:A:330:LEU:H	1:A:330:LEU:CD2	1.65	1.04
1:A:435:HIS:HE1	6:A:118:HOH:O	1.43	1.01
1:A:231:PRO:HG2	1:A:234:ARG:HB2	1.41	1.00
1:A:266:THR:OG1	1:A:446:PRO:HG2	1.61	1.00
1:A:242:VAL:HG21	1:A:282:TRP:HB2	1.41	0.99
1:A:302:ARG:HH21	1:A:454:MET:HB2	1.21	0.99
2:D:363:PHE:HE2	2:D:456:ILE:CD1	1.73	0.99
1:A:268:ILE:HD11	1:A:332:VAL:HG21	1.00	0.98
1:A:268:ILE:HD11	1:A:332:VAL:CG2	1.92	0.98
1:A:292:LEU:HD12	1:A:293:PRO:CD	1.94	0.97
2:D:461:THR:HG23	2:D:463:MET:H	1.29	0.97
1:A:231:PRO:HD2	1:A:287:PRO:HG2	1.46	0.97
1:A:268:ILE:CD1	1:A:332:VAL:HG21	1.93	0.97
2:D:228:LEU:CD1	2:D:333:LEU:HD21	1.94	0.96
1:A:330:LEU:HD22	1:A:330:LEU:H	0.81	0.95
1:A:237:GLU:OE2	1:A:237:GLU:HA	1.66	0.95
1:A:306:ASN:O	1:A:310:ILE:HG13	1.66	0.95
3:E:629:THR:OG1	3:E:630:SER:N	1.95	0.94
1:A:279:LEU:HD22	1:A:309:LEU:HD13	1.50	0.94
1:A:328:THR:HB	1:A:330:LEU:HD21	1.45	0.94
1:A:307:GLU:OE2	1:A:426:ARG:HA	1.66	0.94
1:A:440:LYS:HZ2	1:A:441:LEU:HG	1.29	0.93
1:A:445:THR:HG23	1:A:446:PRO:HD2	1.52	0.92
1:A:390:GLU:HG3	1:A:391:ALA:N	1.82	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASP:HA	1:A:276:LEU:HD23	1.52	0.91
2:D:466:HIS:HD2	2:D:468:LEU:H	1.16	0.91
1:A:407:LYS:HG2	1:A:408:TYR:CE2	2.05	0.91
1:A:276:LEU:HD21	1:A:451:LEU:HD23	1.52	0.91
1:A:286:ILE:O	1:A:289:PHE:HB3	1.71	0.89
1:A:376:PHE:C	1:A:389:VAL:CG1	2.46	0.88
1:A:302:ARG:NH2	1:A:454:MET:CB	2.36	0.88
2:D:363:PHE:HE2	2:D:456:ILE:HD11	1.39	0.87
2:D:322:VAL:O	2:D:326:ILE:HG13	1.74	0.87
1:A:281:GLU:O	1:A:284:LYS:HG2	1.74	0.86
1:A:241:ALA:HB1	1:A:285:ARG:HH12	1.35	0.86
1:A:241:ALA:CB	1:A:285:ARG:NH1	2.39	0.86
2:D:363:PHE:CE2	2:D:456:ILE:CD1	2.58	0.85
1:A:440:LYS:HD3	1:A:441:LEU:N	1.92	0.85
1:A:262:ASN:C	1:A:267:ASN:HD21	1.84	0.85
1:A:269:CYS:O	1:A:451:LEU:HD11	1.77	0.85
2:D:466:HIS:CD2	2:D:467:PRO:HD2	2.12	0.84
1:A:366:GLU:CD	1:A:414:ARG:HH21	1.85	0.84
1:A:326:LEU:CB	1:A:330:LEU:HD23	2.06	0.84
1:A:376:PHE:HA	1:A:389:VAL:HG13	1.60	0.83
2:D:237:LEU:HD11	2:D:340:LEU:HG	1.61	0.83
1:A:440:LYS:HZ3	1:A:441:LEU:HG	1.38	0.83
1:A:347:ASP:HA	1:A:350:LEU:HD12	1.60	0.82
1:A:374:VAL:HG23	1:A:422:LEU:HD21	1.63	0.81
1:A:362:MET:HA	1:A:414:ARG:HH22	1.46	0.81
2:D:206:PRO:HD2	2:D:208:SER:HB2	1.62	0.81
1:A:326:LEU:HB2	1:A:330:LEU:CD2	2.09	0.80
1:A:318:ILE:HD11	1:A:357:MET:HB2	1.61	0.80
2:D:363:PHE:CE2	2:D:456:ILE:HD13	2.15	0.80
2:D:258:GLY:HA2	2:D:261:LYS:HE2	1.63	0.79
2:D:461:THR:CG2	2:D:463:MET:HG3	2.11	0.79
1:A:282:TRP:HH2	1:A:371:ARG:O	1.66	0.79
2:D:466:HIS:O	2:D:470:GLN:HG3	1.81	0.79
2:D:461:THR:OG1	2:D:462:ASP:N	2.16	0.79
1:A:367:LEU:O	1:A:371:ARG:HG3	1.83	0.78
1:A:376:PHE:CA	1:A:389:VAL:HG13	2.14	0.78
1:A:445:THR:CG2	1:A:446:PRO:HD2	2.13	0.78
3:E:635:GLN:O	3:E:639:THR:HG23	1.84	0.78
1:A:231:PRO:CD	1:A:287:PRO:HG2	2.14	0.77
1:A:376:PHE:HB3	1:A:393:ARG:HB2	1.66	0.77
1:A:302:ARG:HH21	1:A:454:MET:CB	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:VAL:HG11	1:A:403:TYR:HB2	1.66	0.76
1:A:273:ASP:OD1	1:A:448:ASP:HB2	1.85	0.76
2:D:300:ALA:HA	2:D:303:ILE:HD12	1.68	0.76
1:A:454:MET:O	1:A:455:LEU:HB3	1.85	0.76
1:A:241:ALA:CB	1:A:285:ARG:HH11	1.99	0.75
1:A:238:ALA:HB1	1:A:282:TRP:CD1	2.21	0.75
1:A:438:PHE:CZ	1:A:439:PHE:CE1	2.74	0.75
2:D:445:ILE:HD11	6:D:19:HOH:O	1.87	0.75
1:A:452:MET:C	1:A:454:MET:H	1.92	0.74
1:A:266:THR:CB	1:A:446:PRO:HG2	2.16	0.74
1:A:266:THR:OG1	1:A:446:PRO:CG	2.35	0.74
3:B:634:VAL:O	3:B:638:THR:HG23	1.88	0.73
1:A:348:ARG:NH2	1:A:428:ILE:HG13	2.02	0.73
2:D:364:MET:O	2:D:367:LYS:HB2	1.89	0.73
2:D:384:LEU:O	2:D:388:ILE:HG13	1.89	0.73
1:A:302:ARG:NH2	1:A:453:GLU:O	2.20	0.73
1:A:407:LYS:CG	1:A:408:TYR:CE2	2.72	0.72
1:A:286:ILE:O	1:A:289:PHE:CB	2.37	0.72
1:A:423:PRO:O	1:A:426:ARG:N	2.22	0.72
1:A:275:GLN:HB3	1:A:309:LEU:HD11	1.72	0.72
2:D:260:ASP:OD2	2:D:261:LYS:HD3	1.90	0.71
2:D:441:ASP:O	2:D:444:GLN:N	2.21	0.71
1:A:292:LEU:HG	1:A:388:GLU:OE2	1.91	0.71
3:E:629:THR:O	3:E:631:HIS:N	2.23	0.71
2:D:461:THR:HG23	2:D:463:MET:N	2.03	0.70
1:A:302:ARG:HH22	1:A:454:MET:HB2	1.49	0.70
1:A:355:SER:HA	1:A:358:ARG:NH1	2.06	0.70
1:A:353:LEU:HD13	1:A:425:LEU:HD13	1.74	0.70
1:A:374:VAL:CG2	1:A:422:LEU:HD21	2.22	0.69
1:A:266:THR:O	1:A:270:GLN:HG3	1.92	0.69
1:A:263:ASP:C	1:A:267:ASN:HD22	2.00	0.69
1:A:266:THR:HB	1:A:446:PRO:CD	2.16	0.69
1:A:273:ASP:HA	1:A:276:LEU:CD2	2.21	0.69
1:A:275:GLN:O	1:A:278:THR:HG23	1.92	0.68
1:A:436:LEU:HD21	4:A:500:9RA:H2	1.75	0.68
1:A:320:VAL:HG11	1:A:331:HIS:HE1	1.58	0.68
2:D:466:HIS:CD2	2:D:468:LEU:H	2.05	0.68
2:D:471:GLU:OE1	3:E:632:LYS:HG3	1.94	0.68
1:A:366:GLU:OE1	1:A:414:ARG:NH2	2.26	0.68
1:A:328:THR:HB	1:A:330:LEU:CD2	2.24	0.67
2:D:441:ASP:O	2:D:444:GLN:HB3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLY:C	1:A:306:ASN:N	2.49	0.67
1:A:292:LEU:CD1	1:A:293:PRO:CD	2.60	0.67
2:D:260:ASP:OD2	2:D:261:LYS:CD	2.43	0.67
1:A:312:SER:OG	1:A:371:ARG:NH1	2.27	0.67
1:A:231:PRO:CG	1:A:234:ARG:HB2	2.21	0.66
1:A:315:HIS:CG	1:A:367:LEU:HD22	2.29	0.66
1:A:389:VAL:HG12	1:A:389:VAL:O	1.95	0.66
2:D:403:VAL:O	2:D:407:GLU:HG3	1.95	0.66
1:A:266:THR:HB	1:A:445:THR:HG23	1.77	0.66
2:D:276:GLU:O	2:D:280:ARG:HG3	1.94	0.66
1:A:443:GLY:O	1:A:444:ASP:HB2	1.96	0.66
1:A:455:LEU:C	1:A:455:LEU:HD12	2.22	0.65
1:A:343:GLY:O	1:A:346:PHE:HB3	1.95	0.65
2:D:303:ILE:O	6:D:92:HOH:O	2.15	0.65
1:A:437:PHE:CE1	1:A:455:LEU:HB2	2.31	0.65
1:A:382:GLY:O	1:A:383:LEU:HD12	1.96	0.65
1:A:387:ALA:HA	1:A:390:GLU:HB3	1.78	0.65
1:A:373:ILE:HG23	1:A:393:ARG:CD	2.21	0.65
1:A:280:VAL:O	1:A:284:LYS:HD3	1.97	0.64
1:A:315:HIS:ND1	1:A:367:LEU:HD22	2.12	0.64
1:A:266:THR:CB	1:A:446:PRO:HD2	2.19	0.64
2:D:229:THR:HG22	6:D:66:HOH:O	1.98	0.64
3:B:633:LEU:HG	3:B:636:LEU:HD23	1.80	0.64
1:A:304:GLY:C	1:A:306:ASN:H	2.05	0.64
1:A:301:LEU:O	1:A:305:TRP:HB3	1.97	0.63
2:D:320:TYR:CE2	2:D:476:LEU:HD12	2.34	0.63
1:A:376:PHE:O	1:A:389:VAL:HG12	1.98	0.63
1:A:270:GLN:HA	1:A:448:ASP:OD1	1.97	0.63
1:A:277:PHE:N	1:A:277:PHE:CD1	2.67	0.62
1:A:275:GLN:C	1:A:278:THR:HG23	2.24	0.62
1:A:436:LEU:HD11	4:A:500:9RA:H43A	1.80	0.62
2:D:438:LYS:C	2:D:440:THR:H	2.07	0.62
2:D:318:LEU:HD11	3:E:637:LEU:HD21	1.80	0.62
2:D:255:LEU:HD12	2:D:256:MET:HE2	1.81	0.62
2:D:261:LYS:HG2	2:D:261:LYS:O	2.00	0.62
2:D:363:PHE:HZ	2:D:453:LEU:HD23	1.64	0.62
1:A:231:PRO:HD2	1:A:287:PRO:CG	2.27	0.62
1:A:233:GLU:C	1:A:235:ILE:H	2.07	0.62
1:A:376:PHE:CA	1:A:389:VAL:CG1	2.75	0.61
2:D:310:ASP:OD1	2:D:312:ASN:HB2	1.99	0.61
1:A:289:PHE:CE1	1:A:297:GLN:HG2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LEU:HG	1:A:437:PHE:CE2	2.36	0.61
1:A:276:LEU:CD2	1:A:451:LEU:HD23	2.28	0.61
2:D:333:LEU:HD23	2:D:340:LEU:HD12	1.83	0.61
2:D:466:HIS:HD2	2:D:468:LEU:N	1.94	0.61
2:D:473:TYR:O	2:D:474:LYS:C	2.44	0.61
1:A:263:ASP:O	1:A:267:ASN:ND2	2.32	0.61
1:A:438:PHE:CE2	1:A:439:PHE:CZ	2.89	0.60
1:A:292:LEU:HD12	1:A:293:PRO:CG	2.31	0.60
1:A:242:VAL:HG23	1:A:242:VAL:O	2.01	0.60
1:A:376:PHE:C	1:A:389:VAL:HG12	2.24	0.59
1:A:437:PHE:HE1	1:A:455:LEU:HB2	1.67	0.59
1:A:313:PHE:O	1:A:317:SER:OG	2.21	0.59
1:A:454:MET:O	1:A:455:LEU:CB	2.50	0.59
2:D:441:ASP:O	2:D:444:GLN:CB	2.51	0.59
1:A:237:GLU:OE2	1:A:237:GLU:CA	2.46	0.58
1:A:289:PHE:CZ	1:A:297:GLN:OE1	2.57	0.58
1:A:316:ARG:O	1:A:316:ARG:HG2	2.02	0.58
1:A:275:GLN:HA	1:A:278:THR:CG2	2.33	0.58
1:A:348:ARG:O	1:A:352:GLU:HB2	2.04	0.58
1:A:277:PHE:H	1:A:277:PHE:HD1	1.49	0.57
1:A:233:GLU:C	1:A:235:ILE:N	2.56	0.57
1:A:392:LEU:HA	1:A:395:LYS:HG3	1.86	0.57
2:D:279:ILE:O	2:D:283:GLN:HG3	2.04	0.57
1:A:326:LEU:HD12	1:A:330:LEU:HB2	1.86	0.57
2:D:421:LEU:CD1	2:D:432:PHE:HA	2.35	0.57
1:A:273:ASP:N	1:A:451:LEU:HD21	2.19	0.57
1:A:275:GLN:HA	1:A:278:THR:HG21	1.86	0.57
1:A:374:VAL:CG2	1:A:422:LEU:CD2	2.82	0.56
1:A:295:ASP:O	1:A:298:VAL:HB	2.06	0.56
2:D:325:ILE:HD11	2:D:392:ILE:HG12	1.87	0.56
2:D:329:MET:CG	2:D:388:ILE:HD11	2.35	0.56
2:D:363:PHE:CZ	2:D:453:LEU:HD23	2.40	0.56
1:A:292:LEU:CG	1:A:388:GLU:OE2	2.54	0.56
1:A:277:PHE:O	1:A:280:VAL:HB	2.06	0.56
1:A:266:THR:CB	1:A:446:PRO:CG	2.82	0.56
2:D:436:LEU:O	2:D:439:MET:HB2	2.06	0.56
3:E:629:THR:O	3:E:630:SER:C	2.49	0.56
3:E:631:HIS:HA	3:E:634:VAL:HG22	1.87	0.56
1:A:296:ASP:OD1	1:A:299:ILE:HD13	2.06	0.56
1:A:421:ARG:NH1	1:A:421:ARG:HA	2.21	0.56
1:A:348:ARG:NH2	1:A:428:ILE:CG1	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:630:SER:O	3:E:630:SER:OG	2.23	0.55
1:A:289:PHE:CE1	1:A:297:GLN:OE1	2.59	0.55
1:A:445:THR:O	1:A:447:ILE:HG13	2.06	0.55
1:A:292:LEU:CB	1:A:388:GLU:OE2	2.55	0.55
1:A:315:HIS:ND1	1:A:367:LEU:CD2	2.70	0.55
2:D:402:ASN:HB2	6:D:86:HOH:O	2.06	0.55
1:A:307:GLU:HA	1:A:310:ILE:HD12	1.89	0.55
1:A:448:ASP:OD1	1:A:451:LEU:CD1	2.56	0.54
1:A:296:ASP:OD2	1:A:382:GLY:O	2.26	0.54
1:A:351:THR:HA	1:A:355:SER:HB3	1.89	0.54
2:D:466:HIS:CD2	2:D:467:PRO:CD	2.88	0.54
1:A:322:ASP:HB3	1:A:334:ARG:HG2	1.88	0.54
1:A:417:LYS:O	1:A:418:LEU:C	2.49	0.54
3:E:631:HIS:HA	3:E:634:VAL:CG2	2.37	0.54
1:A:302:ARG:NH2	1:A:454:MET:CG	2.71	0.54
1:A:407:LYS:HG2	1:A:408:TYR:HE2	1.68	0.54
2:D:329:MET:HG2	2:D:388:ILE:HD11	1.89	0.54
2:D:461:THR:HG21	2:D:463:MET:HG3	1.90	0.54
1:A:296:ASP:OD1	1:A:299:ILE:CD1	2.56	0.54
1:A:442:ILE:CG2	1:A:443:GLY:N	2.70	0.54
1:A:265:VAL:CG1	1:A:266:THR:HG22	2.38	0.54
2:D:318:LEU:CD1	3:E:637:LEU:HD21	2.38	0.54
1:A:348:ARG:HH21	1:A:428:ILE:HG13	1.72	0.54
1:A:447:ILE:HG22	1:A:452:MET:HG2	1.89	0.54
1:A:242:VAL:CG2	1:A:282:TRP:HB2	2.25	0.53
2:D:237:LEU:CD1	2:D:340:LEU:HG	2.36	0.53
2:D:363:PHE:CZ	2:D:456:ILE:HD13	2.43	0.53
1:A:354:VAL:HG12	1:A:358:ARG:HH22	1.72	0.53
1:A:455:LEU:C	1:A:455:LEU:CD1	2.81	0.53
1:A:232:VAL:HG11	1:A:403:TYR:CB	2.35	0.53
1:A:353:LEU:CD1	1:A:425:LEU:HD13	2.37	0.53
1:A:374:VAL:HG12	1:A:374:VAL:O	2.09	0.53
2:D:252:MET:O	2:D:256:MET:HG2	2.09	0.53
1:A:407:LYS:CG	1:A:408:TYR:CD2	2.92	0.53
1:A:267:ASN:O	1:A:270:GLN:HB2	2.09	0.52
1:A:421:ARG:HA	1:A:421:ARG:HH11	1.73	0.52
1:A:433:LEU:HG	1:A:437:PHE:CZ	2.44	0.52
1:A:388:GLU:C	1:A:390:GLU:H	2.16	0.52
1:A:239:GLU:OE2	1:A:282:TRP:NE1	2.42	0.52
1:A:426:ARG:O	1:A:430:LEU:HD23	2.09	0.52
2:D:442:LEU:C	2:D:444:GLN:N	2.65	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLU:C	1:A:284:LYS:HG2	2.35	0.52
1:A:273:ASP:OD1	1:A:448:ASP:CB	2.55	0.52
1:A:282:TRP:CH2	1:A:371:ARG:O	2.55	0.52
1:A:283:ALA:O	1:A:289:PHE:CE2	2.62	0.52
1:A:426:ARG:O	1:A:430:LEU:CD2	2.58	0.52
1:A:436:LEU:HD11	4:A:500:9RA:C43	2.39	0.52
1:A:440:LYS:HD3	1:A:441:LEU:CA	2.39	0.52
1:A:236:LEU:HD22	1:A:240:LEU:HD22	1.92	0.52
1:A:304:GLY:O	1:A:305:TRP:C	2.53	0.52
2:D:323[B]:HIS:HE1	2:D:472:ILE:CG2	2.23	0.52
1:A:440:LYS:CD	1:A:441:LEU:N	2.69	0.51
2:D:442:LEU:C	2:D:444:GLN:H	2.18	0.51
1:A:354:VAL:CG1	1:A:358:ARG:HH22	2.23	0.51
1:A:374:VAL:O	1:A:374:VAL:CG1	2.59	0.51
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.45	0.51
1:A:389:VAL:CG1	1:A:389:VAL:O	2.56	0.51
1:A:445:THR:CG2	1:A:446:PRO:CD	2.86	0.51
1:A:354:VAL:HG12	1:A:358:ARG:NH2	2.25	0.51
1:A:382:GLY:O	1:A:383:LEU:CD1	2.59	0.51
2:D:440:THR:HG22	2:D:441:ASP:N	2.25	0.51
1:A:435:HIS:CE1	6:A:118:HOH:O	2.32	0.51
2:D:323[B]:HIS:HE1	2:D:472:ILE:HG21	1.75	0.51
1:A:327:ALA:N	4:A:500:9RA:O52	2.44	0.51
1:A:266:THR:CB	1:A:446:PRO:CD	2.85	0.50
1:A:376:PHE:CE1	1:A:392:LEU:HB2	2.46	0.50
1:A:306:ASN:OD1	1:A:310:ILE:HD11	2.11	0.50
1:A:419:LEU:O	1:A:422:LEU:HB2	2.11	0.50
1:A:310:ILE:HB	1:A:425:LEU:HD11	1.93	0.50
1:A:376:PHE:C	1:A:389:VAL:HG11	2.32	0.50
1:A:322:ASP:O	1:A:334:ARG:HG2	2.12	0.50
1:A:344:ALA:C	1:A:346:PHE:N	2.70	0.50
3:B:635:GLN:C	3:B:637:LEU:N	2.67	0.50
1:A:228:GLU:OE1	1:A:229:ASP:HB2	2.12	0.49
1:A:292:LEU:HD12	1:A:293:PRO:HG3	1.92	0.49
1:A:330:LEU:N	1:A:330:LEU:CD2	2.44	0.49
1:A:263:ASP:C	1:A:267:ASN:ND2	2.68	0.49
1:A:442:ILE:HG22	1:A:443:GLY:N	2.25	0.49
1:A:329:GLY:N	1:A:330:LEU:HD22	2.26	0.49
1:A:448:ASP:OD1	1:A:451:LEU:HD11	2.12	0.49
3:E:639:THR:HG22	6:E:42:HOH:O	2.12	0.49
1:A:315:HIS:O	1:A:318:ILE:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:PHE:O	1:A:451:LEU:C	2.54	0.49
1:A:268:ILE:HD12	1:A:326:LEU:HD11	1.94	0.49
1:A:229:ASP:HB3	1:A:395:LYS:HD2	1.94	0.49
2:D:261:LYS:HD3	2:D:261:LYS:H	1.79	0.48
2:D:474:LYS:HD3	2:D:475:ASP:OD2	2.12	0.48
2:D:330:LEU:HD21	2:D:364:MET:HE1	1.96	0.48
1:A:320:VAL:HG11	1:A:331:HIS:CE1	2.45	0.48
1:A:366:GLU:OE2	1:A:414:ARG:NH2	2.44	0.48
1:A:238:ALA:CB	1:A:282:TRP:CD1	2.94	0.48
1:A:344:ALA:C	1:A:346:PHE:H	2.20	0.48
1:A:356:LYS:O	1:A:360:MET:HG2	2.14	0.48
1:A:392:LEU:HD23	1:A:395:LYS:HE2	1.95	0.48
1:A:273:ASP:O	1:A:277:PHE:CE1	2.67	0.47
1:A:441:LEU:HD23	1:A:441:LEU:HA	1.75	0.47
3:E:631:HIS:C	3:E:634:VAL:HG22	2.39	0.47
1:A:265:VAL:CG1	1:A:266:THR:N	2.78	0.47
2:D:317:LEU:HD13	2:D:392:ILE:O	2.14	0.47
1:A:440:LYS:HZ2	1:A:441:LEU:CG	2.13	0.47
2:D:260:ASP:OD2	2:D:261:LYS:HD2	2.12	0.47
1:A:386:PRO:C	1:A:388:GLU:H	2.22	0.47
1:A:231:PRO:HG2	1:A:234:ARG:CB	2.29	0.47
1:A:348:ARG:HH21	1:A:428:ILE:CG1	2.27	0.47
3:B:632:LYS:O	3:B:632:LYS:HG2	2.13	0.47
1:A:315:HIS:CE1	1:A:364:LYS:HE3	2.50	0.47
2:D:260:ASP:OD2	2:D:261:LYS:N	2.45	0.47
2:D:420:GLN:O	2:D:424:ASN:CB	2.63	0.47
1:A:432:CYS:O	1:A:435:HIS:HB2	2.15	0.47
1:A:376:PHE:HA	1:A:389:VAL:CG1	2.37	0.46
1:A:390:GLU:CG	1:A:391:ALA:N	2.62	0.46
2:D:462:ASP:O	2:D:463:MET:C	2.58	0.46
1:A:262:ASN:C	1:A:262:ASN:OD1	2.58	0.46
1:A:275:GLN:NE2	1:A:327:ALA:HB1	2.30	0.46
2:D:460:GLU:C	2:D:461:THR:HG22	2.41	0.46
1:A:268:ILE:HG23	4:A:500:9RA:H9	1.97	0.46
1:A:274:LYS:HZ2	1:A:274:LYS:HG2	1.61	0.46
1:A:366:GLU:OE1	1:A:414:ARG:NE	2.48	0.46
1:A:362:MET:HE2	1:A:418:LEU:HD12	1.98	0.46
2:D:320:TYR:CD2	2:D:476:LEU:CD1	2.98	0.46
1:A:296:ASP:OD1	1:A:299:ILE:HB	2.15	0.46
3:E:632:LYS:O	3:E:635:GLN:HB3	2.16	0.46
1:A:302:ARG:HH22	1:A:454:MET:CB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:348:MET:CE	2:D:353:LEU:CD2	2.94	0.46
1:A:321:LYS:N	1:A:321:LYS:HD3	2.31	0.46
2:D:363:PHE:CE2	2:D:456:ILE:HD11	2.31	0.46
1:A:287:PRO:C	1:A:289:PHE:H	2.22	0.46
1:A:238:ALA:HB2	1:A:285:ARG:HG3	1.98	0.45
1:A:273:ASP:O	1:A:277:PHE:HE1	1.99	0.45
1:A:274:LYS:HZ2	1:A:327:ALA:HB1	1.81	0.45
1:A:353:LEU:O	1:A:357:MET:HG3	2.16	0.45
2:D:338:GLY:C	2:D:368:PHE:HE1	2.25	0.45
1:A:238:ALA:O	1:A:242:VAL:HG22	2.17	0.45
3:E:631:HIS:CA	3:E:634:VAL:HG22	2.46	0.45
1:A:268:ILE:CD1	1:A:268:ILE:N	2.80	0.45
2:D:435:LEU:HD12	2:D:435:LEU:O	2.17	0.45
2:D:348:MET:CE	2:D:353:LEU:HD21	2.47	0.45
2:D:350:ARG:HE	2:D:365:GLU:CD	2.25	0.45
2:D:367:LYS:HD3	2:D:367:LYS:N	2.31	0.45
1:A:242:VAL:HG11	1:A:282:TRP:N	2.32	0.45
2:D:206:PRO:HG2	2:D:208:SER:H	1.82	0.45
2:D:444:GLN:O	2:D:447:THR:N	2.50	0.45
3:B:638:THR:O	3:B:638:THR:OG1	2.32	0.45
1:A:262:ASN:C	1:A:267:ASN:ND2	2.65	0.44
2:D:351:GLU:O	2:D:352:PHE:C	2.59	0.44
2:D:446:VAL:O	2:D:449:HIS:HB3	2.17	0.44
1:A:237:GLU:O	1:A:238:ALA:C	2.59	0.44
1:A:375:LEU:C	1:A:377:ASN:H	2.26	0.44
1:A:353:LEU:CD1	1:A:425:LEU:CD1	2.96	0.44
2:D:219:TYR:CD1	2:D:219:TYR:C	2.94	0.44
2:D:230:LYS:HE2	2:D:379:LEU:O	2.18	0.44
1:A:277:PHE:CZ	1:A:450:PHE:HD1	2.34	0.44
1:A:266:THR:CG2	1:A:446:PRO:HG2	2.47	0.44
1:A:376:PHE:CE1	1:A:392:LEU:CB	3.00	0.44
2:D:305:GLY:O	2:D:306:PHE:C	2.59	0.44
2:D:320:TYR:CE2	2:D:476:LEU:CD1	3.00	0.44
2:D:444:GLN:O	2:D:447:THR:OG1	2.25	0.44
1:A:232:VAL:O	1:A:365:THR:HG23	2.18	0.44
2:D:455:VAL:O	2:D:455:VAL:HG12	2.18	0.44
1:A:289:PHE:CE2	1:A:297:GLN:OE1	2.71	0.43
1:A:407:LYS:HG3	1:A:408:TYR:CD2	2.53	0.43
2:D:438:LYS:C	2:D:440:THR:N	2.73	0.43
1:A:448:ASP:OD1	1:A:451:LEU:HD12	2.18	0.43
1:A:438:PHE:CE2	1:A:439:PHE:CE1	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:VAL:C	1:A:300:LEU:N	2.76	0.43
2:D:207:GLU:O	2:D:210:ASP:HB2	2.19	0.43
2:D:393:LEU:N	2:D:393:LEU:HD22	2.33	0.43
2:D:214:LEU:HD13	2:D:304:PRO:HG2	2.01	0.43
2:D:223:ILE:HD13	2:D:223:ILE:HA	1.85	0.43
2:D:325:ILE:HD11	2:D:392:ILE:CG1	2.48	0.43
1:A:322:ASP:O	1:A:334:ARG:CG	2.66	0.43
2:D:452:LEU:HA	2:D:452:LEU:HD12	1.64	0.43
4:A:500:9RA:H39B	4:A:500:9RA:H20A	1.75	0.43
1:A:433:LEU:O	1:A:434:GLU:C	2.61	0.42
1:A:317:SER:HB3	1:A:324:ILE:HA	2.01	0.42
2:D:377:LEU:O	2:D:378:GLU:C	2.61	0.42
1:A:310:ILE:O	1:A:314:SER:HB2	2.19	0.42
1:A:366:GLU:OE1	1:A:414:ARG:CZ	2.67	0.42
1:A:436:LEU:O	1:A:440:LYS:HB2	2.20	0.42
3:E:631:HIS:O	3:E:634:VAL:CG2	2.67	0.42
1:A:362:MET:HG2	1:A:363:ASP:N	2.33	0.42
1:A:354:VAL:CG1	1:A:358:ARG:NH2	2.82	0.42
1:A:231:PRO:CD	1:A:287:PRO:CG	2.93	0.42
1:A:266:THR:OG1	1:A:446:PRO:CB	2.67	0.42
1:A:417:LYS:O	1:A:421:ARG:HG2	2.19	0.42
1:A:437:PHE:HE1	1:A:455:LEU:HA	1.85	0.42
1:A:284:LYS:HA	1:A:284:LYS:HD2	1.91	0.42
1:A:370:LEU:C	1:A:372:ALA:H	2.28	0.42
1:A:445:THR:O	1:A:447:ILE:CG1	2.68	0.42
1:A:266:THR:OG1	1:A:446:PRO:HB2	2.20	0.42
1:A:287:PRO:C	1:A:289:PHE:N	2.77	0.42
2:D:329:MET:HB3	2:D:329:MET:HE2	1.86	0.41
1:A:268:ILE:HG22	1:A:269:CYS:N	2.35	0.41
1:A:374:VAL:HG22	1:A:422:LEU:CD2	2.49	0.41
1:A:407:LYS:C	1:A:409:PRO:HD3	2.45	0.41
4:A:500:9RA:H13	4:A:500:9RA:H48	1.81	0.41
1:A:231:PRO:C	1:A:233:GLU:N	2.79	0.41
1:A:265:VAL:HG12	1:A:266:THR:HG22	2.00	0.41
1:A:265:VAL:HG13	1:A:266:THR:N	2.36	0.41
1:A:296:ASP:O	1:A:300:LEU:HB2	2.21	0.41
1:A:300:LEU:HG	1:A:375:LEU:O	2.19	0.41
1:A:231:PRO:C	1:A:233:GLU:H	2.27	0.41
1:A:388:GLU:C	1:A:390:GLU:N	2.79	0.41
2:D:348:MET:HE2	2:D:348:MET:HB3	1.58	0.41
1:A:305:TRP:O	1:A:309:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LEU:O	1:A:396:VAL:HG23	2.19	0.41
1:A:278:THR:OG1	1:A:279:LEU:N	2.54	0.41
1:A:304:GLY:O	1:A:306:ASN:N	2.53	0.41
2:D:228:LEU:HD11	2:D:333:LEU:HD21	1.93	0.41
2:D:261:LYS:CD	2:D:261:LYS:H	2.33	0.41
1:A:280:VAL:O	1:A:284:LYS:CD	2.67	0.41
1:A:353:LEU:O	1:A:354:VAL:C	2.64	0.41
1:A:228:GLU:HB3	1:A:229:ASP:H	1.58	0.41
2:D:219:TYR:CE1	2:D:223:ILE:CG1	3.04	0.41
3:B:633:LEU:CG	3:B:636:LEU:HD23	2.47	0.41
3:B:634:VAL:O	3:B:634:VAL:CG1	2.69	0.41
1:A:440:LYS:HD3	1:A:440:LYS:C	2.45	0.40
2:D:271:GLN:HB2	2:D:272:GLU:H	1.65	0.40
3:E:631:HIS:O	3:E:634:VAL:HG22	2.21	0.40
1:A:266:THR:HG21	1:A:446:PRO:HG2	2.02	0.40
1:A:275:GLN:O	1:A:278:THR:CG2	2.67	0.40
1:A:294:LEU:O	1:A:295:ASP:C	2.63	0.40
1:A:426:ARG:NH1	2:D:440:THR:HG23	2.36	0.40
1:A:430:LEU:HD11	2:D:444:GLN:HE21	1.86	0.40
1:A:437:PHE:HD1	1:A:455:LEU:O	2.04	0.40
2:D:441:ASP:O	2:D:444:GLN:CA	2.69	0.40
1:A:269:CYS:HB2	1:A:451:LEU:HD13	2.04	0.40
1:A:271:ALA:HB1	1:A:327:ALA:HB3	2.04	0.40
1:A:368:GLY:O	1:A:372:ALA:HB2	2.21	0.40
2:D:455:VAL:O	2:D:455:VAL:CG1	2.69	0.40
2:D:373:LYS:O	2:D:374:PHE:C	2.62	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	206/228 (90%)	152 (74%)	45 (22%)	9 (4%)	2	0
2	D	263/272 (97%)	247 (94%)	15 (6%)	1 (0%)	30	29
3	B	9/12 (75%)	4 (44%)	5 (56%)	0	100	100
3	E	10/12 (83%)	9 (90%)	0	1 (10%)	0	0
All	All	488/524 (93%)	412 (84%)	65 (13%)	11 (2%)	5	2

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	LEU
1	A	453	GLU
1	A	454	MET
3	E	630	SER
2	D	445	ILE
1	A	371	ARG
1	A	387	ALA
1	A	446	PRO
1	A	231	PRO
1	A	232	VAL
1	A	423	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	181/197 (92%)	137 (76%)	44 (24%)	0	0
2	D	240/245 (98%)	211 (88%)	29 (12%)	4	2
3	B	11/12 (92%)	7 (64%)	4 (36%)	0	0
3	E	12/12 (100%)	12 (100%)	0	100	100
All	All	444/466 (95%)	367 (83%)	77 (17%)	1	1

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	ASP
1	A	230	MET
1	A	233	GLU
1	A	236	LEU
1	A	237	GLU
1	A	240	LEU
1	A	263	ASP
1	A	265	VAL
1	A	266	THR
1	A	268	ILE
1	A	276	LEU
1	A	277	PHE
1	A	278	THR
1	A	286	ILE
1	A	291	GLU
1	A	292	LEU
1	A	299	ILE
1	A	306	ASN
1	A	312	SER
1	A	314	SER
1	A	317	SER
1	A	318	ILE
1	A	325	LEU
1	A	330	LEU
1	A	334	ARG
1	A	342	VAL
1	A	345	ILE
1	A	350	LEU
1	A	351	THR
1	A	390	GLU
1	A	394	GLU
1	A	395	LYS
1	A	396	VAL
1	A	410	GLU
1	A	418	LEU
1	A	421	ARG
1	A	427	SER
1	A	438	PHE
1	A	441	LEU
1	A	442	ILE
1	A	444	ASP
1	A	448	ASP
1	A	449	THR

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Mol	Chain	Res	Type
1	A	455	LEU
2	D	228	LEU
2	D	237	LEU
2	D	243	ASP
2	D	245	SER
2	D	257	MET
2	D	259	GLU
2	D	261	LYS
2	D	263	LYS
2	D	271	GLN
2	D	273	GLN
2	D	298	GLU
2	D	323[A]	HIS
2	D	323[B]	HIS
2	D	332	SER
2	D	348	MET
2	D	351	GLU
2	D	367	LYS
2	D	372	VAL
2	D	373	LYS
2	D	386	ILE
2	D	388	ILE
2	D	404	LYS
2	D	440	THR
2	D	448	GLU
2	D	452	LEU
2	D	456	ILE
2	D	464	SER
2	D	472	ILE
2	D	476	LEU
3	B	630	SER
3	B	633	LEU
3	B	634	VAL
3	B	638	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	275	GLN
1	A	331	HIS
1	A	335	ASN

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Mol	Chain	Res	Type
2	D	253	ASN
2	D	286	GLN
2	D	308	ASN
2	D	375	ASN
2	D	444	GLN
2	D	451	GLN
2	D	466	HIS

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 ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	9RA	A	500	-	28,28,28	1.62	4 (14%)	43,44,44	1.33	7 (16%)
5	D30	D	500	-	42,43,43	1.16	2 (4%)	56,59,59	1.29	7 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	9RA	A	500	-	-	6/12/31/31	0/3/3/3
5	D30	D	500	-	-	2/25/33/33	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	9RA	C1-C6	5.25	1.49	1.40
5	D	500	D30	C3-S7	-5.12	1.70	1.78
4	A	500	9RA	C4-C3	4.96	1.48	1.40
5	D	500	D30	C13-S7	-4.21	1.72	1.78
4	A	500	9RA	C4-C47	2.22	1.51	1.50
4	A	500	9RA	O52-C51	-2.08	1.24	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	500	D30	C24-O25-C26	4.07	127.31	117.62
4	A	500	9RA	C14-C47-C48	-3.30	117.88	121.46
5	D	500	D30	O1-C15-C13	3.19	119.87	116.07
5	D	500	D30	O11-C5-C2	2.59	119.36	115.75
5	D	500	D30	C7-O1-C15	2.52	123.08	117.45
4	A	500	9RA	C13-C14-C47	-2.34	119.36	121.20
4	A	500	9RA	C43-C3-C4	-2.32	119.37	122.81
4	A	500	9RA	C4-C47-C14	2.30	121.16	118.22
5	D	500	D30	O22-C17-C14	2.28	124.41	113.66
4	A	500	9RA	C22-C1-C6	-2.27	120.22	122.76
4	A	500	9RA	C2-C3-C4	2.27	119.71	117.97
5	D	500	D30	C14-O11-C5	2.22	122.24	117.60
5	D	500	D30	O1-C15-C18	-2.18	118.77	123.49
4	A	500	9RA	C20-C21-C22	-2.06	106.29	113.84

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	500	D30	C19-C11-C7-O1
5	D	500	D30	C15-C13-S7-C3
4	A	500	9RA	C5-C4-C47-C14
4	A	500	9RA	C5-C4-C47-C48
4	A	500	9RA	C13-C14-C47-C48

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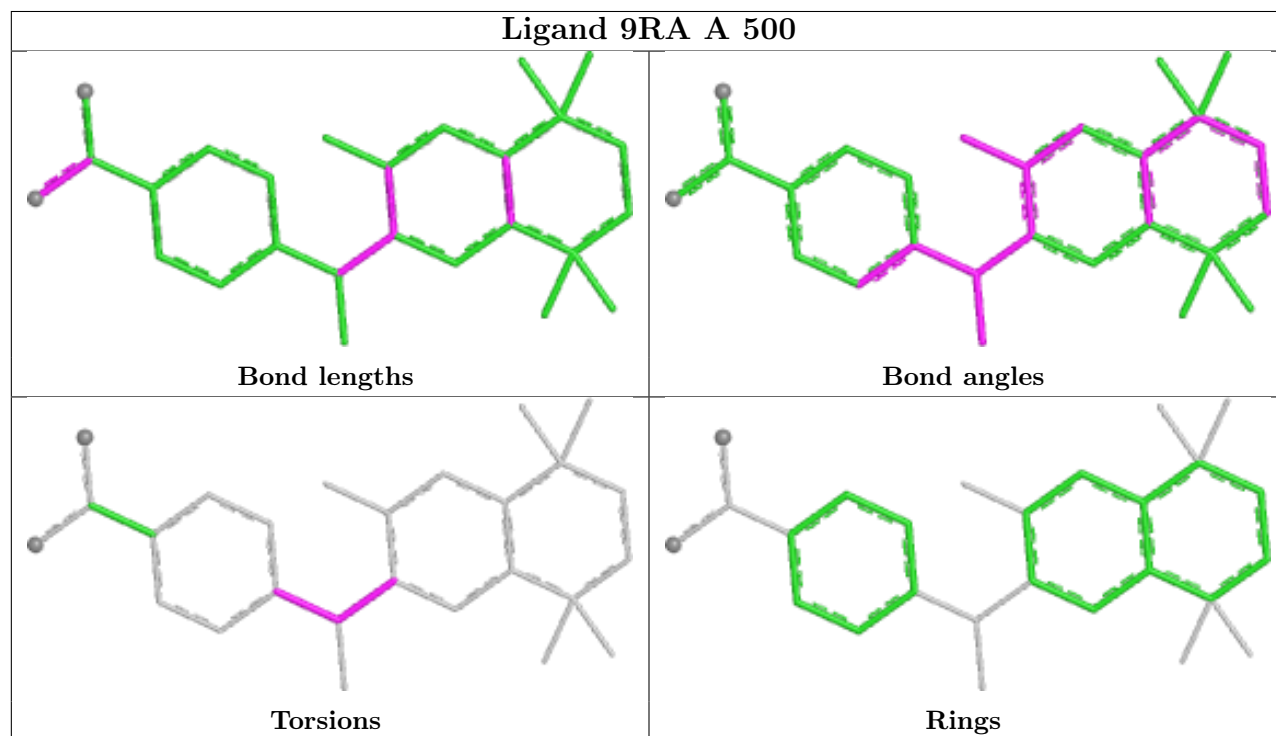
Mol	Chain	Res	Type	Atoms
4	A	500	9RA	C9-C14-C47-C48
4	A	500	9RA	C9-C14-C47-C4
4	A	500	9RA	C13-C14-C47-C4

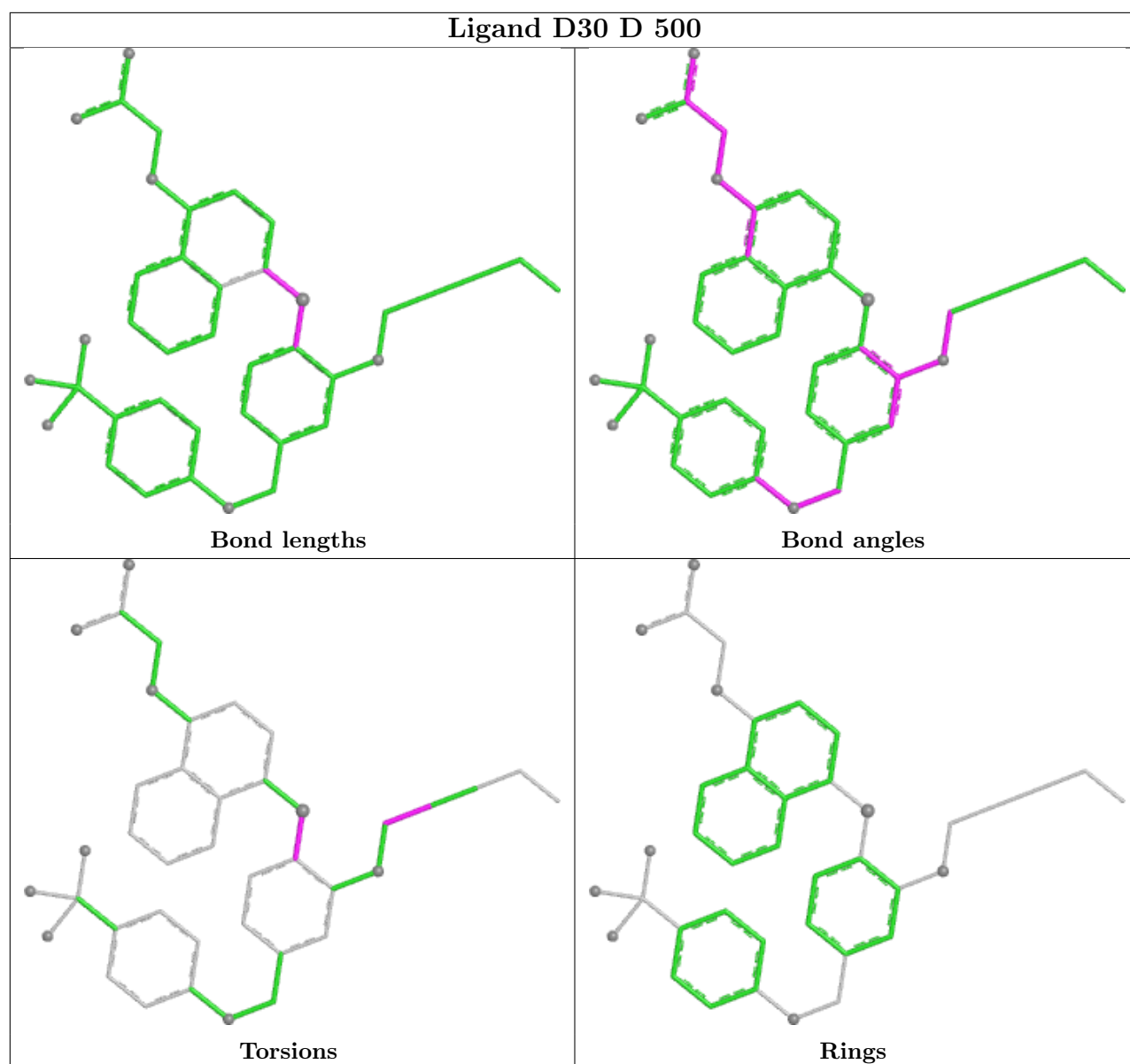
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	9RA	7	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	210/228 (92%)	2.03	96 (45%) 1 1	34, 64, 81, 84	0
2	D	265/272 (97%)	-0.07	5 (1%) 66 67	11, 27, 57, 70	2 (0%)
3	B	11/12 (91%)	3.94	10 (90%) 0 0	113, 115, 119, 119	0
3	E	12/12 (100%)	0.15	0 100 100	18, 30, 41, 45	0
All	All	498/524 (95%)	0.91	111 (22%) 3 3	11, 44, 81, 119	2 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	VAL	7.9
3	B	633	LEU	6.9
3	B	636	LEU	6.6
1	A	439	PHE	5.8
1	A	447	ILE	5.5
1	A	293	PRO	5.3
1	A	298	VAL	5.3
1	A	337	ALA	5.2
3	B	629	THR	5.2
1	A	451	LEU	5.1
1	A	438	PHE	4.9
1	A	342	VAL	4.9
3	B	637	LEU	4.8
1	A	332	VAL	4.6
1	A	313	PHE	4.6
1	A	272	ALA	4.4
1	A	282	TRP	4.1
1	A	455	LEU	4.1
1	A	309	LEU	4.1
1	A	328	THR	4.1
1	A	300	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	305	TRP	4.0
3	B	634	VAL	3.9
1	A	286	ILE	3.8
1	A	289	PHE	3.8
1	A	240	LEU	3.8
1	A	285	ARG	3.7
1	A	442	ILE	3.7
1	A	238	ALA	3.7
1	A	297	GLN	3.6
1	A	345	ILE	3.6
3	B	630	SER	3.6
1	A	268	ILE	3.5
1	A	441	LEU	3.5
1	A	292	LEU	3.5
1	A	383	LEU	3.5
1	A	340	ALA	3.4
1	A	353	LEU	3.4
1	A	308	LEU	3.3
1	A	376	PHE	3.3
1	A	279	LEU	3.3
1	A	314	SER	3.2
1	A	331	HIS	3.2
1	A	452	MET	3.2
1	A	450	PHE	3.1
1	A	294	LEU	3.1
3	B	632	LYS	3.1
1	A	446	PRO	3.0
1	A	234	ARG	3.0
1	A	454	MET	3.0
1	A	242	VAL	3.0
1	A	283	ALA	3.0
1	A	301	LEU	3.0
1	A	287	PRO	3.0
1	A	303	ALA	2.9
1	A	324	ILE	2.9
1	A	323	GLY	2.9
1	A	264	PRO	2.9
1	A	413	GLY	2.9
1	A	326	LEU	2.8
1	A	436	LEU	2.8
1	A	290	SER	2.8
1	A	449	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	280	VAL	2.8
1	A	327	ALA	2.8
1	A	266	THR	2.8
1	A	389	VAL	2.8
1	A	271	ALA	2.7
3	B	635	GLN	2.7
2	D	247	PHE	2.7
1	A	378	PRO	2.7
1	A	346	PHE	2.7
1	A	380	SER	2.7
1	A	232	VAL	2.7
1	A	320	VAL	2.7
2	D	459	THR	2.7
1	A	374	VAL	2.6
1	A	304	GLY	2.6
1	A	315	HIS	2.6
1	A	235	ILE	2.6
1	A	269	CYS	2.6
1	A	392	LEU	2.6
1	A	382	GLY	2.5
1	A	306	ASN	2.5
2	D	363	PHE	2.5
2	D	206	PRO	2.5
1	A	437	PHE	2.5
1	A	388	GLU	2.4
3	B	631	HIS	2.4
1	A	445	THR	2.4
1	A	236	LEU	2.3
1	A	276	LEU	2.3
1	A	432	CYS	2.3
1	A	312	SER	2.3
1	A	318	ILE	2.3
2	D	262	ILE	2.3
1	A	448	ASP	2.3
3	B	639	THR	2.3
1	A	406	HIS	2.2
1	A	325	LEU	2.2
1	A	350	LEU	2.2
1	A	311	ALA	2.2
1	A	375	LEU	2.2
1	A	433	LEU	2.1
1	A	349	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	354	VAL	2.1
1	A	277	PHE	2.1
1	A	329	GLY	2.1
1	A	370	LEU	2.1
1	A	296	ASP	2.0
1	A	373	ILE	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 monosaccharides in this entry.

6.4 Ligands [i](#)

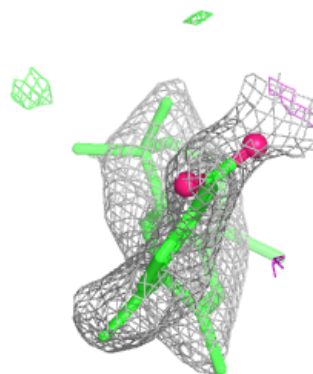
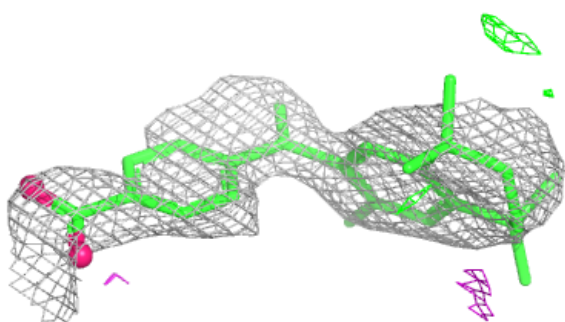
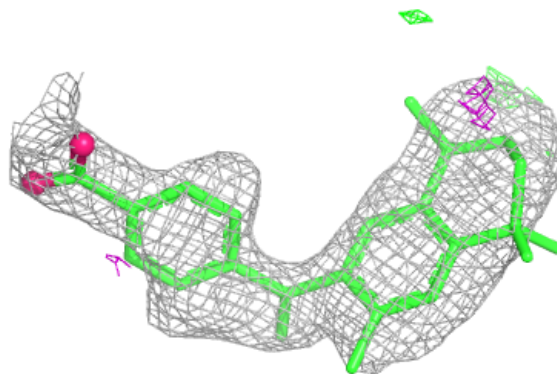
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	9RA	A	500	26/26	0.74	0.24	70,75,78,79	0
5	D30	D	500	40/40	0.93	0.09	16,31,42,47	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.

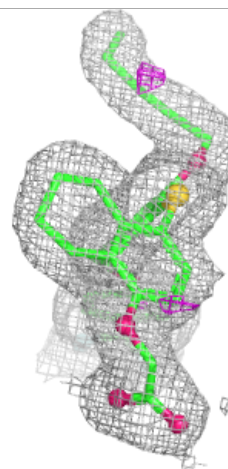
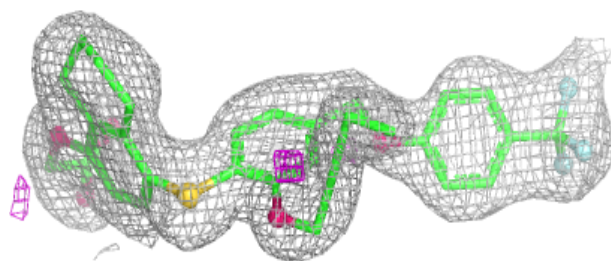
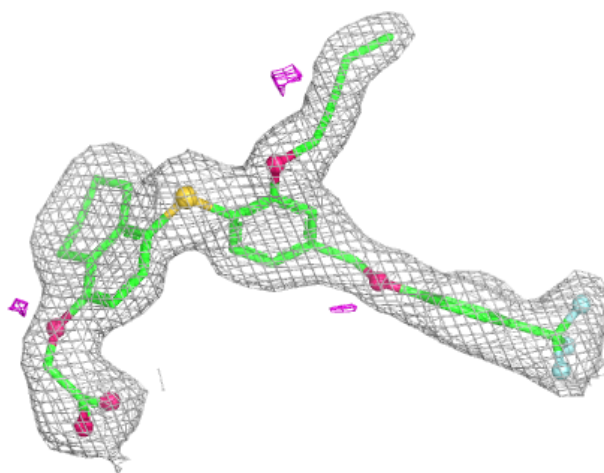
Electron density around 9RA A 500:

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



Electron density around D30 D 500:

$2mF_o-DF_c$ (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.