Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 08:30 am BST

PDB ID	:	3H0A
Title	:	Crystal Structure of Peroxisome Proliferator-Activated Receptor Gamma (PPARg) and Retinoic Acid Receptor Alpha (RXRa) 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)

The following versions of software and data (see references ⓘ) were used in the production of this report:

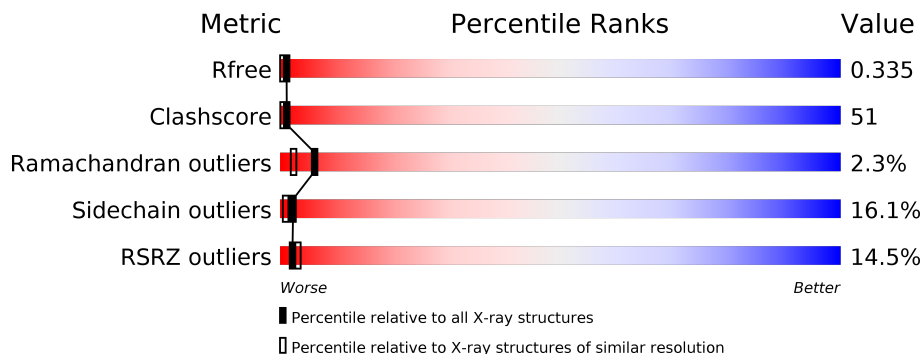|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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	Percentile Ranks	Value
Rfree		0.335
Clashscore		51
Ramachandran outliers		2.3%
Sidechain outliers		16.1%
RSRZ outliers		14.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 on 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 <=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	24% (upper bar) — 21% / 54% / 17% / 8%
2	D	272	3% (upper bar) — 59% / 32% / 6% / ·
3	B	12	75% (upper bar) — 25% / 50% / 17% / 8%
3	E	12	33% / 58% / 8%

2 Entry composition (i)

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.

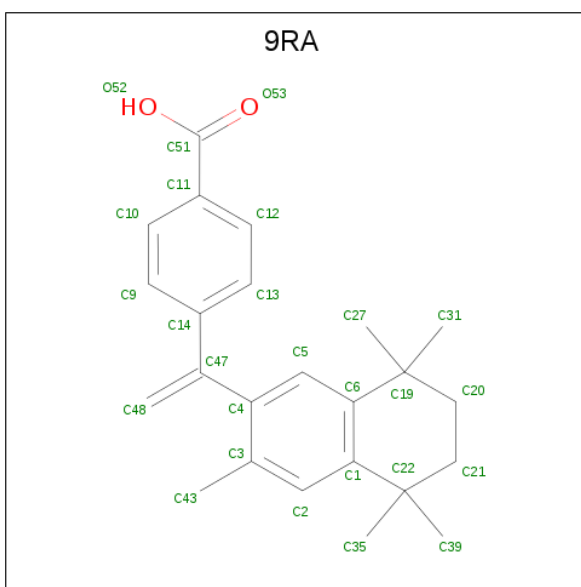| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1661	1066	285	300	10			

- 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 (three-letter code: 9RA) (formula: $C_{24}H_{28}O_2$).

9RA

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 (three-letter code: D30) (formula: $C_{31}H_{29}F_3O_5S$).

D30
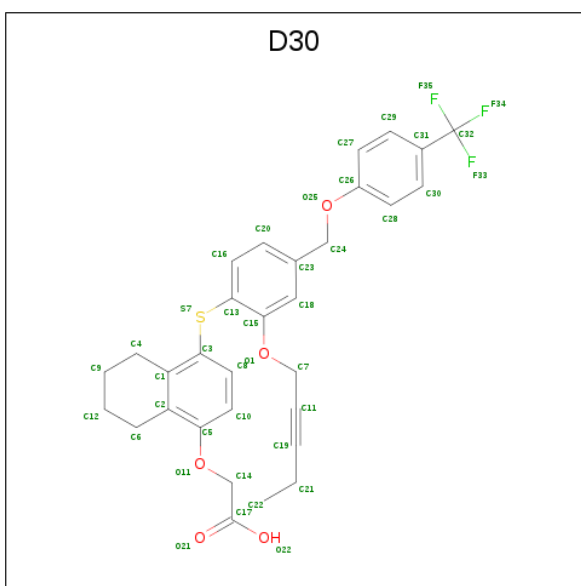
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	F	O	S	0	0
			40	31	3	5	1		

- 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 and DNA 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.
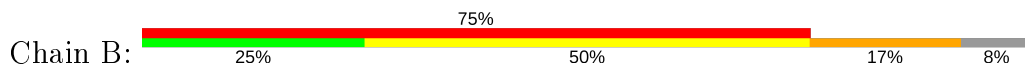
- Molecule 1: Retinoic acid receptor RXR-alpha
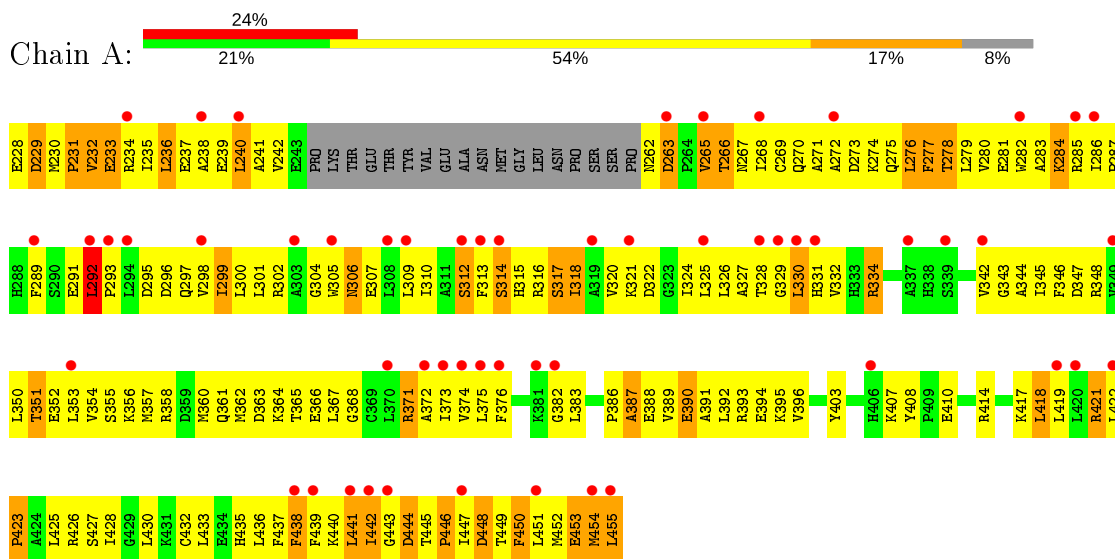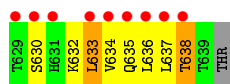

- Molecule 2: Peroxisome proliferator-activated receptor gamma
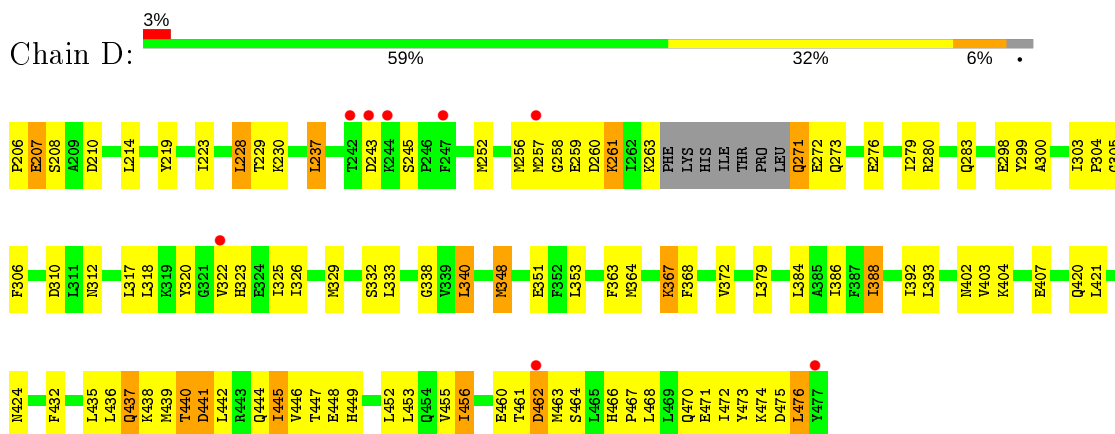
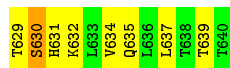- Molecule 3: Nuclear receptor coactivator 1, Co-activator Peptide

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

Chain E:

33% 58% 8%

4 Data and refinement statistics (i)

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) 97.8 (28.46-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [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 , 61.0	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.27$	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.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.61	0/1693	0.81	0/2288
2	D	1.00	1/2181 (0.0%)	1.01	1/2936 (0.0%)
3	B	0.51	0/86	0.72	0/116
3	E	0.94	0/94	1.01	0/126
All	All	0.84	1/4054 (0.0%)	0.93	1/5466 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	299	TYR	CD2-CE2	-5.68	1.30	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	340	LEU	CA-CB-CG	5.66	128.31	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1661	0	1696	298	0
2	D	2135	0	2195	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	420	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 51.

All (420) 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:N	1:A:330:LEU:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:330:LEU:HD22	0.81	0.95
1:A:237:GLU:HA	1:A:237:GLU:OE2	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
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: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: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:376:PHE:C	1:A:389:VAL:CG1	2.46	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:262:ASN:C	1:A:267:ASN:HD21	1.84	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:366:GLU:CD	1:A:414:ARG:HH21	1.85	0.79
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
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: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:355:SER:HA	1:A:358:ARG:NH1	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ARG:HH22	1:A:454:MET:HB2	1.49	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:452:MET:C	1:A:454:MET:H	1.92	0.69
1:A:266:THR:O	1:A:270:GLN:HG3	1.92	0.69
1:A:273:ASP:HA	1:A:276:LEU:CD2	2.21	0.69
1:A:266:THR:HB	1:A:446:PRO:CD	2.16	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
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: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
1:A:263:ASP:C	1:A:267:ASN:HD22	2.00	0.64
1:A:376:PHE:CA	1:A:389:VAL:CG1	2.75	0.64
1:A:436:LEU:HD11	4:A:500:9RA:H43	1.79	0.64
3:B:633:LEU:HG	3:B:636:LEU:HD23	1.80	0.64
2:D:229:THR:HG22	6:D:66:HOH:O	1.98	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

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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	0.63
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
2:D:318:LEU:HD11	3:E:637:LEU:HD21	1.80	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
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
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
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:455:LEU:HD12	1:A:455:LEU:C	2.22	0.60
1:A:242:VAL:O	1:A:242:VAL:HG23	2.01	0.60
1:A:304:GLY:C	1:A:306:ASN:H	2.05	0.59
1:A:437:PHE:HE1	1:A:455:LEU:HB2	1.67	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:233:GLU:C	1:A:235:ILE:N	2.56	0.58
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:HG2	1:A:316:ARG:O	2.02	0.58
1:A:275:GLN:HA	1:A:278:THR:CG2	2.33	0.58
1:A:275:GLN:C	1:A:278:THR:HG23	2.24	0.58
1:A:348:ARG:O	1:A:352:GLU:HB2	2.04	0.58
1:A:277:PHE:HD1	1:A:277:PHE:H	1.49	0.57
1:A:392:LEU:HA	1:A:395:LYS:HG3	1.86	0.57
1:A:233:GLU:C	1:A:235:ILE:H	2.07	0.57
2:D:279:ILE:O	2:D:283:GLN:HG3	2.04	0.57
2:D:438:LYS:C	2:D:440:THR:H	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:ILE:HD11	2:D:392:ILE:HG12	1.87	0.56
2:D:473:TYR:O	2:D:474:LYS:C	2.44	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:313:PHE:O	1:A:317:SER:OG	2.21	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: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:HA	1:A:421:ARG:NH1	2.21	0.56
1:A:348:ARG:NH2	1:A:428:ILE:CG1	2.68	0.55
3:E:630:SER:OG	3:E:630:SER:O	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
2:D:348:MET:HE2	2:D:353:LEU:CD2	2.37	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
3:E:631:HIS:HA	3:E:634:VAL:CG2	2.37	0.54
1:A:407:LYS:HG2	1:A:408:TYR:HE2	1.68	0.54
1:A:302:ARG:NH2	1:A:454:MET:CG	2.71	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:348:MET:HE2	2:D:353:LEU:HD21	1.90	0.53
2:D:363:PHE:CZ	2:D:456:ILE:HD13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:HG12	1:A:358:ARG:HH22	1.72	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
1:A:232:VAL:HG11	1:A:403:TYR:CB	2.35	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:376:PHE:C	1:A:389:VAL:HG12	2.24	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: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
1:A:273:ASP:OD1	1:A:448:ASP:CB	2.55	0.52
1:A:283:ALA:O	1:A:289:PHE:CE2	2.62	0.52
1:A:282:TRP:CH2	1:A:371:ARG:O	2.55	0.52
1:A:426:ARG:O	1:A:430:LEU:CD2	2.58	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
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
1:A:354:VAL:CG1	1:A:358:ARG:HH22	2.23	0.51
1:A:374:VAL:CG1	1:A:374:VAL:O	2.59	0.51
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.45	0.51
1:A:389:VAL:O	1:A:389:VAL:CG1	2.56	0.51
1:A:436:LEU:HD11	4:A:500:9RA:C43	2.39	0.51
1:A:445:THR:CG2	1:A:446:PRO:CD	2.86	0.51
3:E:629:THR:O	3:E:630:SER:C	2.49	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:442:ILE:HG22	1:A:443:GLY:N	2.25	0.50
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:322:ASP:O	1:A:334:ARG:HG2	2.12	0.50
1:A:228:GLU:OE1	1:A:229:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:417:LYS:O	1:A:418:LEU:C	2.49	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
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:H	2:D:261:LYS:HD3	1.79	0.48
2:D:474:LYS:HD3	2:D:475:ASP:OD2	2.12	0.48
1:A:455:LEU:CD1	1:A:455:LEU:C	2.81	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:356:LYS:O	1:A:360:MET:HG2	2.14	0.48
1:A:388:GLU:C	1:A:390:GLU:H	2.16	0.48
1:A:392:LEU:HD23	1:A:395:LYS:HE2	1.95	0.48
3:B:632:LYS:HG2	3:B:632:LYS:O	2.13	0.48
1:A:273:ASP:O	1:A:277:PHE:CE1	2.67	0.47
1:A:441:LEU:HA	1:A:441:LEU:HD23	1.75	0.47
1:A:265:VAL:CG1	1:A:266:THR:N	2.78	0.47
1:A:360:MET:HE3	1:A:417:LYS:HD2	1.95	0.47
2:D:317:LEU:HD13	2:D:392:ILE:O	2.14	0.47
2:D:442:LEU:C	2:D:444:GLN:N	2.65	0.47
1:A:281:GLU:C	1:A:284:LYS:HG2	2.35	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:304:GLY:O	1:A:305:TRP:C	2.53	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
2:D:442:LEU:C	2:D:444:GLN:H	2.18	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:376:PHE:C	1:A:389:VAL:HG11	2.32	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
1:A:275:GLN:NE2	1:A:327:ALA:HB1	2.30	0.46
1:A:274:LYS:HZ2	1:A:274:LYS:HG2	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLU:OE1	1:A:414:ARG:NE	2.48	0.46
1:A:268:ILE:HG23	4:A:500:9RA:H9	1.97	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
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:274:LYS:HZ2	1:A:327:ALA:HB1	1.81	0.45
1:A:273:ASP:O	1:A:277:PHE:HE1	1.99	0.45
1:A:238:ALA:HB2	1:A:285:ARG:HG3	1.98	0.45
1:A:353:LEU:O	1:A:357:MET:HG3	2.16	0.45
3:B:635:GLN:C	3:B:637:LEU:N	2.67	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:N	1:A:268:ILE:CD1	2.80	0.45
2:D:435:LEU:O	2:D:435:LEU:HD12	2.17	0.45
1:A:263:ASP:C	1:A:267:ASN:ND2	2.68	0.45
2:D:367:LYS:N	2:D:367:LYS:HD3	2.31	0.45
1:A:242:VAL:HG11	1:A:282:TRP:N	2.32	0.45
3:B:638:THR:OG1	3:B:638:THR:O	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
2:D:446:VAL:O	2:D:449:HIS:HB3	2.17	0.44
1:A:450:PHE:O	1:A:451:LEU:C	2.54	0.44
1:A:353:LEU:CD1	1:A:425:LEU:CD1	2.96	0.44
2:D:230:LYS:HE2	2:D:379:LEU:O	2.18	0.44
1:A:230:MET:HB2	1:A:230:MET:HE2	1.73	0.44
1:A:277:PHE:CZ	1:A:450:PHE:HD1	2.34	0.44
1:A:376:PHE:CE1	1:A:392:LEU:CB	3.00	0.44
1:A:266:THR:CG2	1:A:446:PRO:HG2	2.47	0.44
2:D:444:GLN:O	2:D:447:THR:OG1	2.25	0.44
2:D:320:TYR:CE2	2:D:476:LEU:CD1	3.00	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:348:MET:CE	2:D:353:LEU:HD21	2.47	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:344:ALA:C	1:A:346:PHE:N	2.70	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
1:A:344:ALA:C	1:A:346:PHE:H	2.20	0.43
2:D:223:ILE:HA	2:D:223:ILE:HD13	1.85	0.43
2:D:214:LEU:HD13	2:D:304:PRO:HG2	2.01	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:348:MET:HB3	2:D:348:MET:HE2	1.73	0.43
3:E:631:HIS:C	3:E:634:VAL:HG22	2.39	0.43
2:D:452:LEU:HD12	2:D:452:LEU:HA	1.64	0.43
4:A:500:9RA:H20A	4:A:500:9RA:H39B	1.75	0.43
1:A:317:SER:HB3	1:A:324:ILE:HA	2.01	0.42
1:A:386:PRO:C	1:A:388:GLU:H	2.22	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:445:THR:O	1:A:447:ILE:CG1	2.68	0.42
2:D:462:ASP:O	2:D:463:MET:C	2.58	0.42
1:A:262:ASN:OD1	1:A:262:ASN:C	2.58	0.42
1:A:266:THR:OG1	1:A:446:PRO:HB2	2.20	0.42
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
4:A:500:9RA:H13	4:A:500:9RA:H48	1.81	0.41
2:D:460:GLU:C	2:D:461:THR:HG22	2.41	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:305:TRP:O	1:A:309:LEU:HB2	2.20	0.41
1:A:287:PRO:C	1:A:289:PHE:H	2.22	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLY:O	1:A:306:ASN:N	2.53	0.41
2:D:261:LYS:H	2:D:261:LYS:CD	2.33	0.41
2:D:228:LEU:HD11	2:D:333:LEU:HD21	1.93	0.41
1:A:280:VAL:O	1:A:284:LYS:CD	2.67	0.41
2:D:219:TYR:CE1	2:D:223:ILE:CG1	3.04	0.41
2:D:305:GLY:O	2:D:306:PHE:C	2.59	0.41
1:A:228:GLU:HB3	1:A:229:ASP:H	1.58	0.41
3:B:634:VAL:CG1	3:B:634:VAL:O	2.69	0.41
3:B:633:LEU:CG	3:B:636:LEU:HD23	2.47	0.41
1:A:262:ASN:C	1:A:267:ASN:ND2	2.65	0.40
2:D:271:GLN:HB2	2:D:272:GLU:H	1.65	0.40
2:D:338:GLY:C	2:D:368:PHE:HE1	2.25	0.40
3:E:631:HIS:O	3:E:634:VAL:HG22	2.21	0.40
1:A:237:GLU:O	1:A:238:ALA:C	2.59	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: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:CG1	2:D:455:VAL:O	2.69	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	206/228 (90%)	152 (74%)	45 (22%)	9 (4%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	263/272 (97%)	247 (94%)	15 (6%)	1 (0%)	34	32
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%)	6	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 (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	181/197 (92%)	141 (78%)	40 (22%)	1	0
2	D	240/245 (98%)	212 (88%)	28 (12%)	5	3
3	B	11/12 (92%)	8 (73%)	3 (27%)	0	0
3	E	12/12 (100%)	12 (100%)	0	100	100
All	All	444/466 (95%)	373 (84%)	71 (16%)	2	1

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	ASP
1	A	233	GLU
1	A	236	LEU
1	A	240	LEU
1	A	263	ASP
1	A	265	VAL
1	A	266	THR
1	A	276	LEU
1	A	277	PHE
1	A	278	THR
1	A	284	LYS
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	351	THR
1	A	361	GLN
1	A	390	GLU
1	A	394	GLU
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
1	A	450	PHE
1	A	455	LEU
2	D	207	GLU
2	D	228	LEU
2	D	237	LEU

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Mol	Chain	Res	Type
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	332	SER
2	D	348	MET
2	D	351	GLU
2	D	367	LYS
2	D	372	VAL
2	D	386	ILE
2	D	388	ILE
2	D	404	LYS
2	D	437	GLN
2	D	440	THR
2	D	441	ASP
2	D	448	GLU
2	D	456	ILE
2	D	462	ASP
2	D	464	SER
2	D	476	LEU
3	B	630	SER
3	B	633	LEU
3	B	638	THR

Some 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
2	D	253	ASN
2	D	345	GLN
2	D	375	ASN
2	D	415	GLN
2	D	437	GLN
2	D	444	GLN

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Mol	Chain	Res	Type
2	D	466	HIS

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

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	-	26,28,28	1.71	4 (15%)	41,44,44	1.30	7 (17%)
5	D30	D	500	-	40,43,43	1.14	2 (5%)	54,59,59	1.29	6 (11%)

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	-	-	7/8/31/31	0/3/3/3
5	D30	D	500	-	-	2/23/33/33	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	5.19	1.49	1.40
5	D	500	D30	C3-S7	-5.03	1.70	1.78
4	A	500	9RA	C4-C3	4.67	1.48	1.40
5	D	500	D30	C13-S7	-4.14	1.72	1.78
4	A	500	9RA	C11-C51	3.63	1.50	1.47
4	A	500	9RA	C4-C47	2.13	1.51	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	500	D30	C24-O25-C26	3.91	127.31	117.65
4	A	500	9RA	C14-C47-C48	-3.34	117.88	121.35
5	D	500	D30	O1-C15-C13	3.19	119.87	116.07
5	D	500	D30	C7-O1-C15	2.87	123.08	117.24
5	D	500	D30	O11-C5-C2	2.53	119.36	115.71
4	A	500	9RA	C22-C1-C6	-2.31	120.22	122.70
4	A	500	9RA	C13-C14-C47	-2.30	119.36	121.20
5	D	500	D30	C14-O11-C5	2.28	122.24	117.76
4	A	500	9RA	C4-C47-C14	2.25	121.16	118.33
4	A	500	9RA	C2-C3-C4	2.21	119.71	118.03
4	A	500	9RA	C43-C3-C4	-2.21	119.37	122.79
5	D	500	D30	O1-C15-C18	-2.09	118.77	123.58
4	A	500	9RA	C20-C21-C22	-2.02	106.29	113.97

There are no chirality outliers.
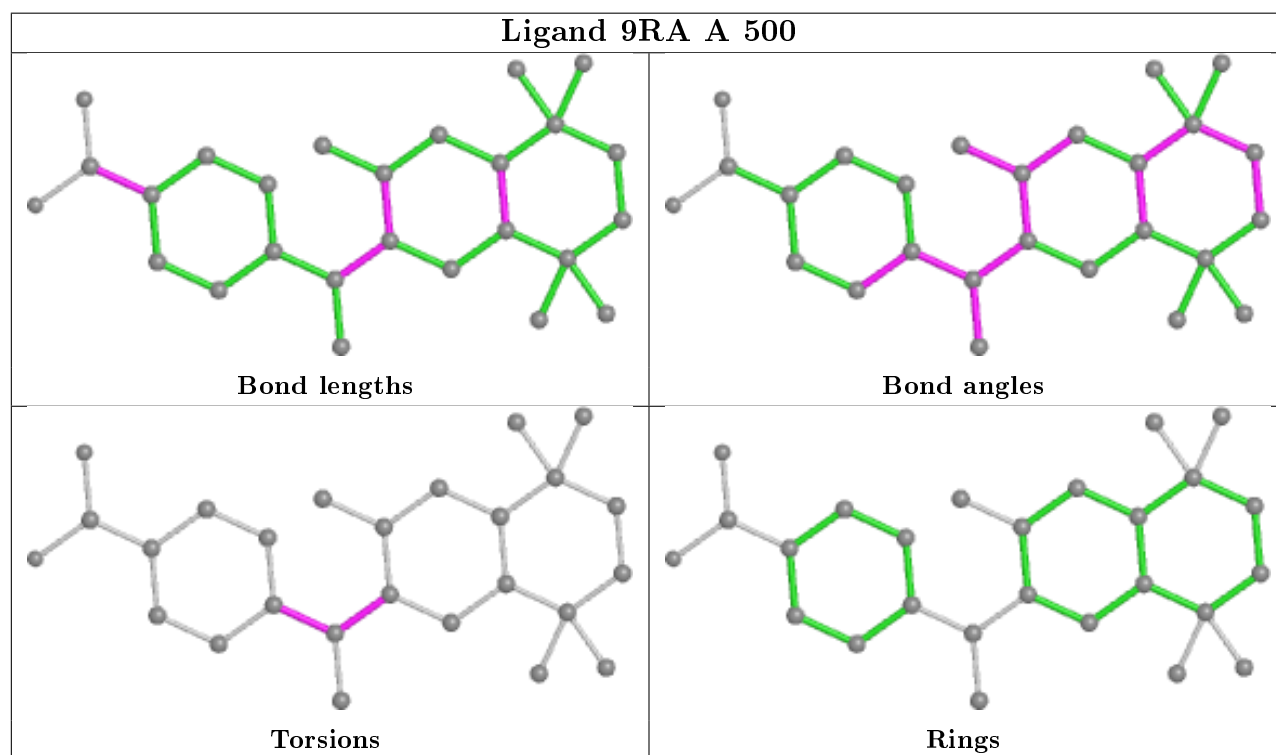
All (9) torsion outliers are listed below:

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
4	A	500	9RA	C9-C14-C47-C48
4	A	500	9RA	C9-C14-C47-C4
4	A	500	9RA	C3-C4-C47-C48
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 then 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.

Ligand 9RA A 500

Bond lengths

Bond angles

Torsions

Rings

Ligand D30 D 500

Bond lengths

Bond angles

Torsions

Rings
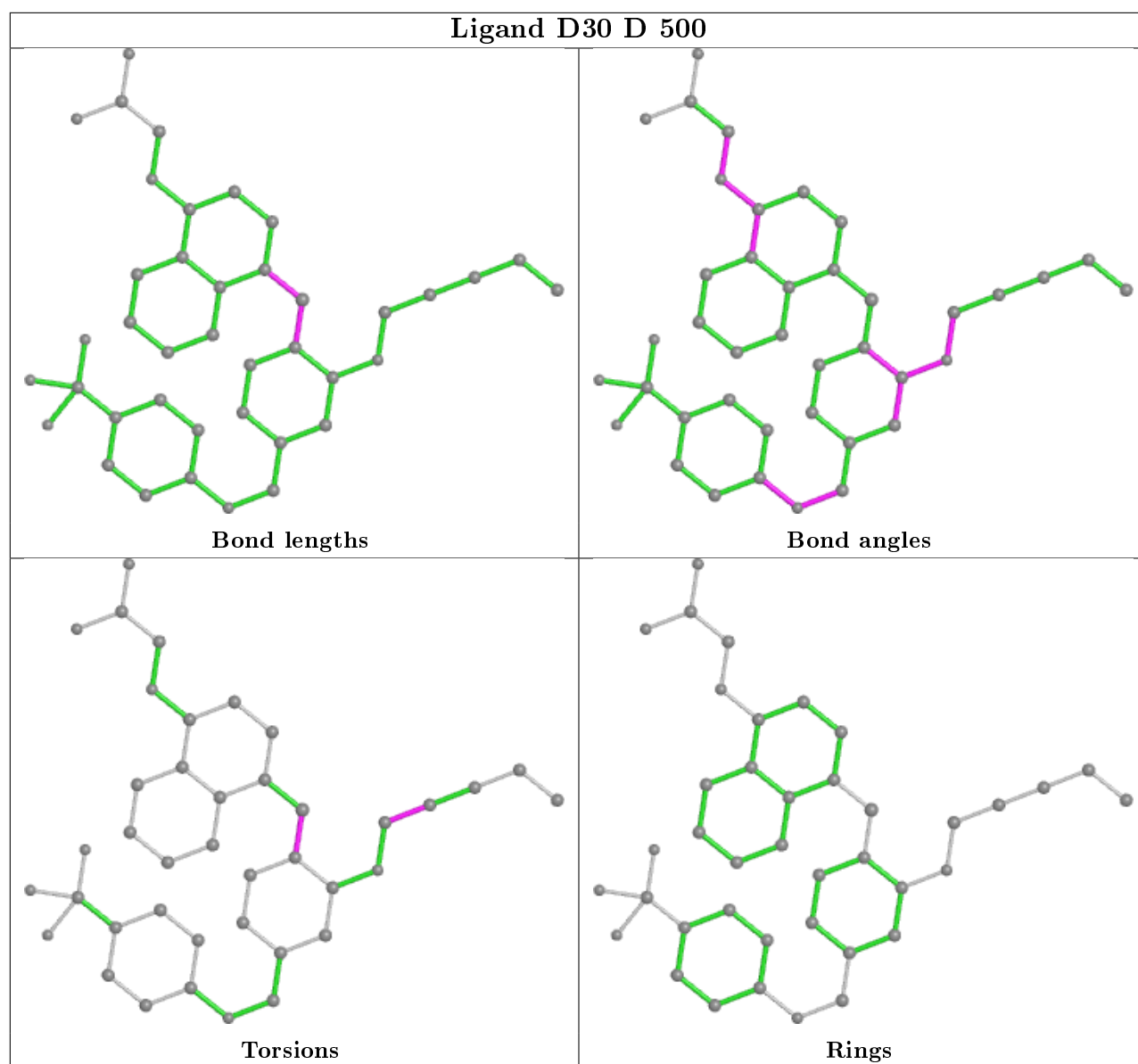
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	210/228 (92%)	1.47	55 (26%)	0	0	34, 64, 81, 84	0
2	D	265/272 (97%)	-0.00	8 (3%)	50	56	11, 27, 57, 70	0
3	B	11/12 (91%)	3.55	9 (81%)	0	0	113, 115, 119, 119	0
3	E	12/12 (100%)	-0.07	0	100	100	18, 30, 41, 45	0
All	All	498/524 (95%)	0.69	72 (14%)	2	3	11, 44, 81, 119	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	438	PHE	6.4
3	B	635	GLN	6.3
1	A	240	LEU	6.0
1	A	331	HIS	5.8
1	A	447	ILE	5.5
3	B	630	SER	5.5
1	A	451	LEU	5.2
3	B	637	LEU	5.1
1	A	265	VAL	4.8
1	A	441	LEU	4.8
1	A	342	VAL	4.7
1	A	309	LEU	4.5
1	A	298	VAL	4.4
1	A	319	ALA	4.2
1	A	330	LEU	4.1
1	A	337	ALA	4.1
1	A	285	ARG	4.1
1	A	442	ILE	4.0
1	A	325	LEU	3.9
3	B	634	VAL	3.8
3	B	631	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	477	TYR	3.6
1	A	422	LEU	3.5
1	A	308	LEU	3.5
1	A	439	PHE	3.5
1	A	328	THR	3.4
2	D	242	THR	3.4
1	A	339	SER	3.4
1	A	294	LEU	3.3
1	A	374	VAL	3.3
1	A	406	HIS	3.2
1	A	353	LEU	3.2
1	A	373	ILE	3.1
1	A	370	LEU	3.1
3	B	633	LEU	3.1
1	A	263	ASP	3.0
2	D	244	LYS	3.0
1	A	272	ALA	3.0
3	B	629	THR	2.9
1	A	314	SER	2.9
3	B	638	THR	2.9
3	B	636	LEU	2.9
1	A	382	GLY	2.8
1	A	292	LEU	2.8
1	A	420	LEU	2.8
1	A	234	ARG	2.7
2	D	462	ASP	2.7
1	A	455	LEU	2.7
1	A	321	LYS	2.6
1	A	443	GLY	2.6
1	A	329	GLY	2.6
1	A	313	PHE	2.6
1	A	419	LEU	2.6
1	A	303	ALA	2.5
2	D	247	PHE	2.5
1	A	305	TRP	2.4
1	A	268	ILE	2.4
1	A	375	LEU	2.4
1	A	286	ILE	2.4
1	A	381	LYS	2.3
1	A	293	PRO	2.3
2	D	322	VAL	2.3
1	A	376	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	243	ASP	2.3
1	A	312	SER	2.2
1	A	238	ALA	2.2
1	A	349	VAL	2.1
2	D	257	MET	2.1
1	A	289	PHE	2.1
1	A	454	MET	2.0
1	A	282	TRP	2.0
1	A	372	ALA	2.0

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

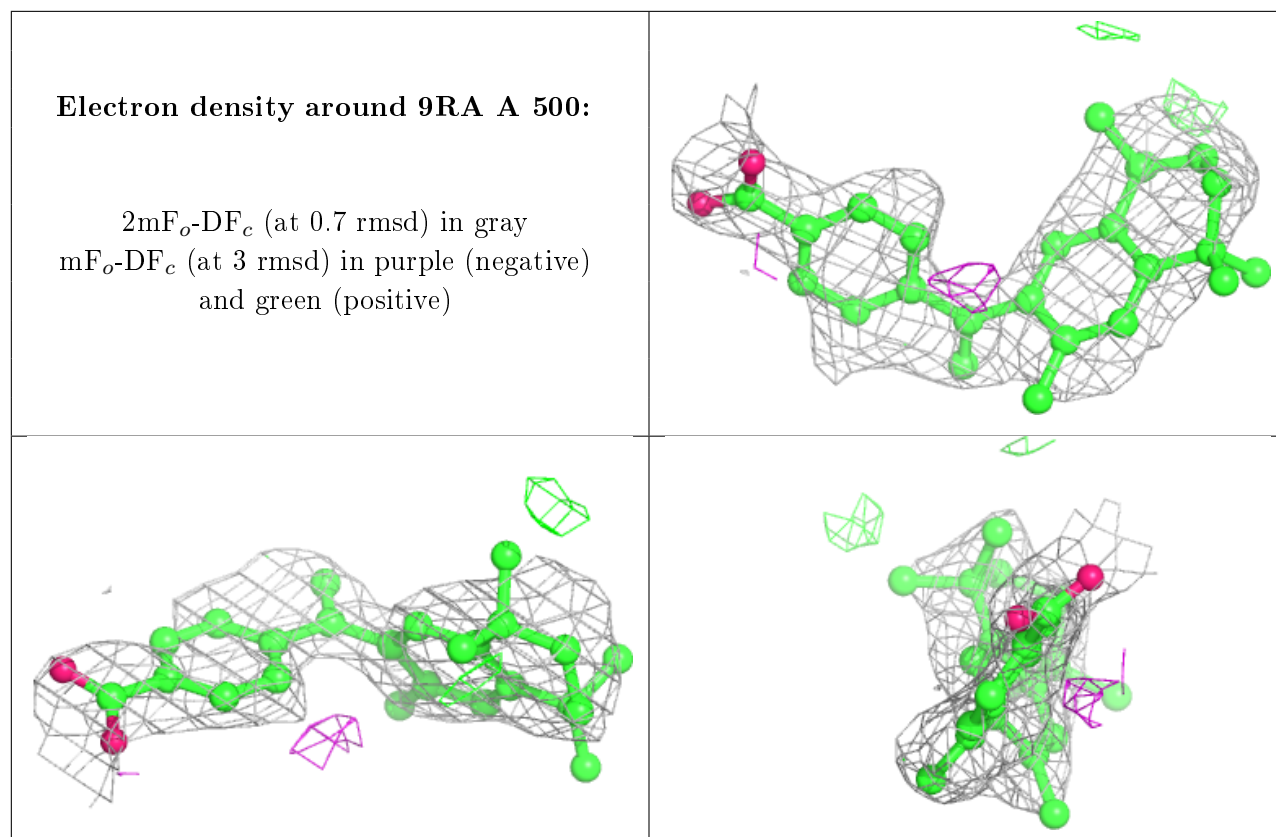There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

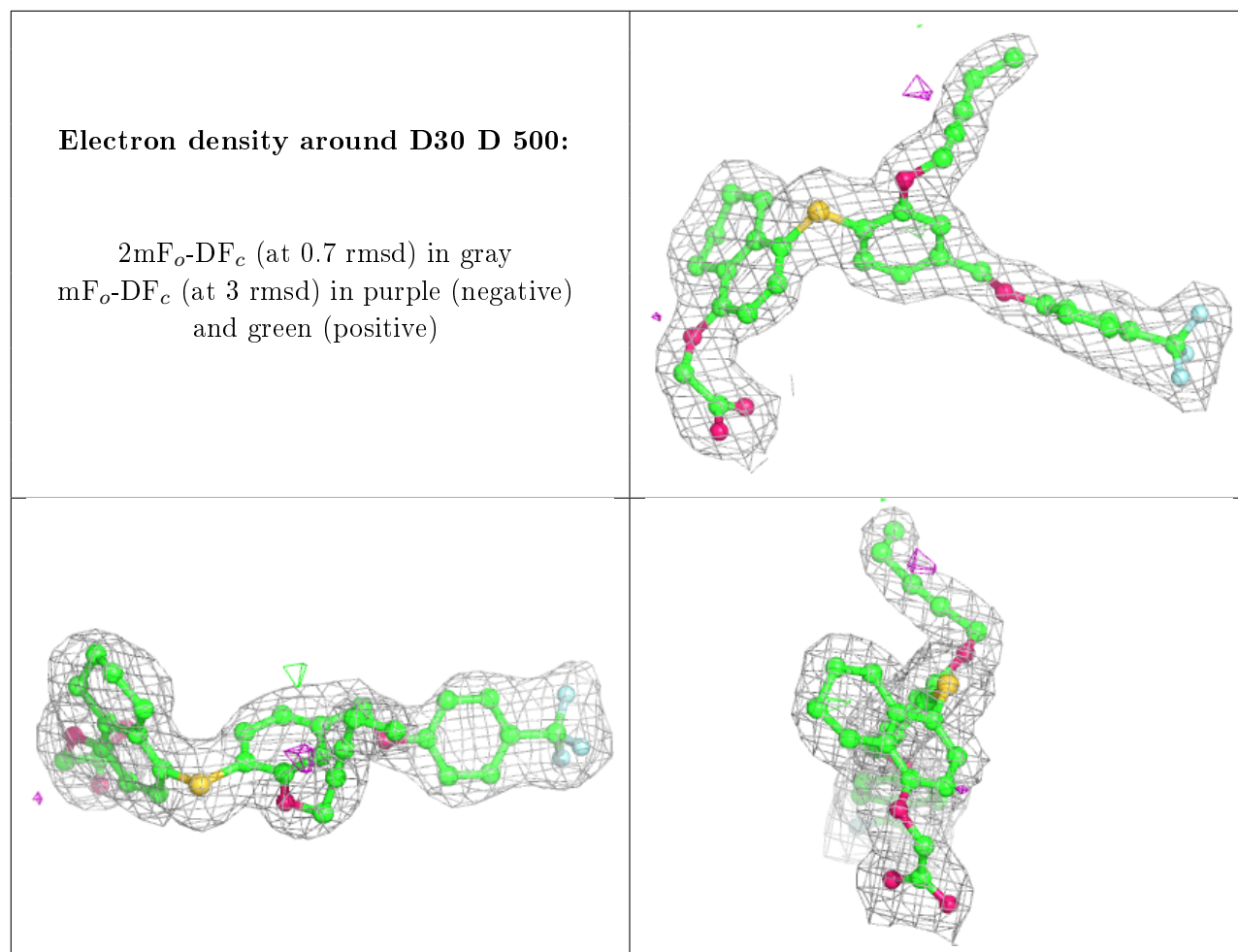## 6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	9RA	A	500	26/26	0.77	0.26	70,75,78,79	0
5	D30	D	500	40/40	0.92	0.12	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:

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

Electron density around D30 D 500:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.