Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:28 am BST

PDB ID	:	1NYX
Title	:	Ligand binding domain of the human peroxisome proliferator activated receptor gamma in complex with an agonist
Authors	:	Ebdrup, S.; Pettersson, I.; Rasmussen, H.B.; Deussen, H.-J.; Frost Jensen, A.; Mortensen, S.B.; Fleckner, J.; Pridal, L.; Nygaard, L.; Sauerberg, P.
Deposited on	:	2003-02-14
Resolution	:	2.65 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 following versions of software and data (see references ①) were used in the production of this report:

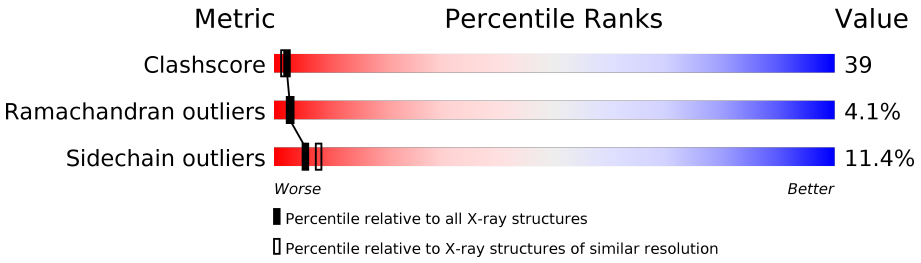
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.65 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))
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	276	37% 48% 8% • 6%
1	B	276	33% 51% 8% • 7%

2 Entry composition

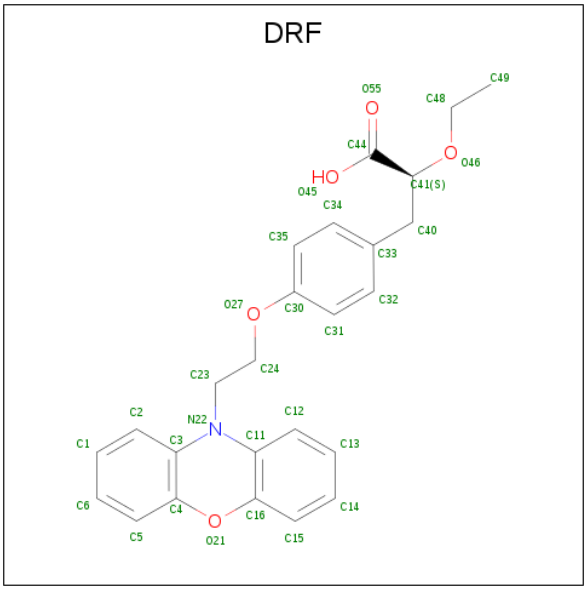
There are 3 unique types of molecules in this entry. The entry contains 4272 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 peroxisome proliferator activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	3	0
			2087	1342	341	393	11			
1	B	258	Total	C	N	O	S	0	0	0
			2069	1339	339	382	9			

- Molecule 2 is (2S)-2-ETHOXY-3-{4-[2-(10H-PHENOXAZIN-10-YL)ETHOXY]PHENYL}PROPANOIC ACID (three-letter code: DRF) (formula: $C_{25}H_{25}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	25	1	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	39	Total O 39 39	0	0

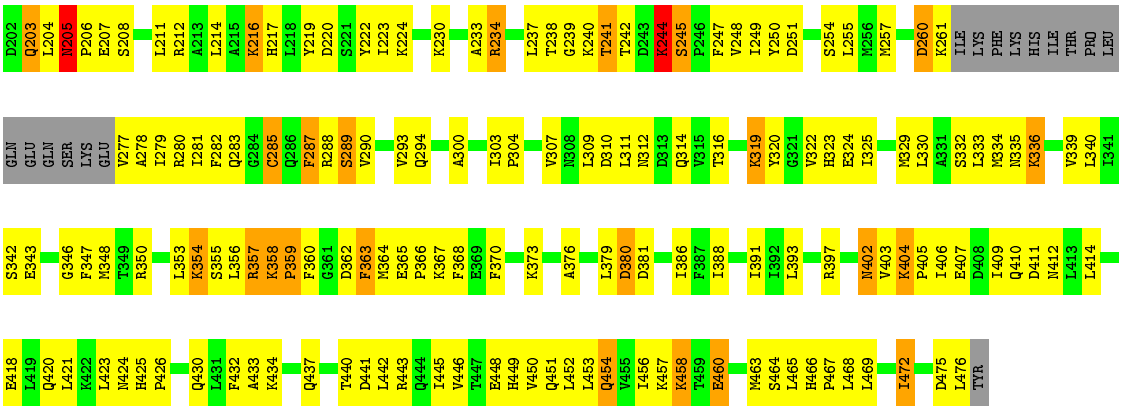
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

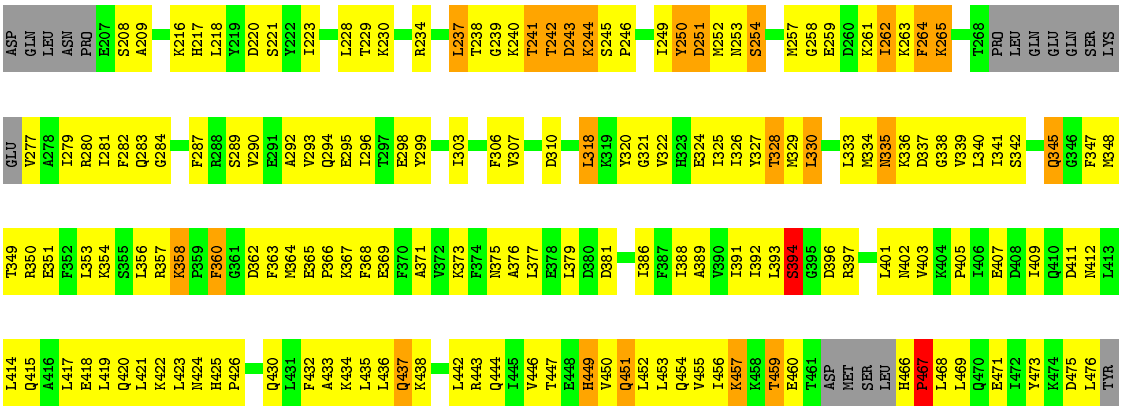
- Molecule 1: peroxisome proliferator activated receptor gamma

Chain A:



- Molecule 1: peroxisome proliferator activated receptor gamma

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	91.55Å 62.09Å 117.74Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	29.97 – 2.65	Depositor
% Data completeness (in resolution range)	80.0 (29.97-2.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX 2000	Depositor
R, R_{free}	0.237 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4272	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DRF

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	0.43	0/2141	0.66	0/2886
1	B	0.42	0/2103	0.64	0/2831
All	All	0.42	0/4244	0.65	0/5717

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	TYR	Sidechain

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	2087	0	2144	162	0
1	B	2069	0	2137	172	0
2	A	31	0	23	6	0
3	A	46	0	0	5	0
3	B	39	0	0	12	0
All	All	4272	0	4304	329	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 39.

All (329) 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:293:VAL:HG22	1:A:322:VAL:HG21	1.27	1.16
1:B:327:TYR:OH	1:B:449:HIS:CE1	2.10	1.04
1:B:327:TYR:HH	1:B:449:HIS:CE1	1.77	1.01
1:A:249:ILE:HD12	1:A:255:LEU:HA	1.51	0.91
1:A:289:SER:HB3	2:A:101:DRF:H32	1.52	0.91
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.58	0.85
1:B:457:LYS:HE2	1:B:457:LYS:HA	1.57	0.85
1:B:303:ILE:HD11	1:B:392:ILE:HD12	1.59	0.84
1:B:335:ASN:HD22	1:B:337:ASP:H	1.24	0.84
1:B:244:LYS:HA	1:B:244:LYS:NZ	1.92	0.83
1:B:293:VAL:HG21	1:B:476:LEU:HD13	1.58	0.83
1:B:340:LEU:O	1:B:341:ILE:HD12	1.79	0.83
1:A:334:MET:HG2	1:A:339:VAL:HG23	1.62	0.82
1:B:451:GLN:O	1:B:454:GLN:HG2	1.81	0.80
1:A:277:VAL:HG13	1:A:278:ALA:H	1.46	0.80
1:B:335:ASN:ND2	1:B:337:ASP:H	1.80	0.79
1:A:208:SER:HA	1:A:211:LEU:HD12	1.63	0.79
1:A:293:VAL:HG22	1:A:322:VAL:CG2	2.11	0.79
1:A:440:THR:HG21	1:B:443:ARG:HG2	1.64	0.78
1:A:411:ASP:OD1	1:B:434:LYS:HE2	1.83	0.78
1:B:325:ILE:HD11	1:B:391:ILE:HB	1.65	0.78
1:B:457:LYS:CE	1:B:457:LYS:HA	2.14	0.78
1:A:212:ARG:HH21	1:A:216:LYS:HE3	1.49	0.77
1:B:299:TYR:HE2	3:B:32:HOH:O	1.67	0.77
1:B:394:SER:HA	3:B:57:HOH:O	1.85	0.77
1:A:446:VAL:O	1:A:450:VAL:HG23	1.87	0.75
1:A:203:GLN:HG3	1:A:204:LEU:H	1.48	0.75
1:A:402:ASN:HD22	1:A:402:ASN:N	1.86	0.74
1:B:327:TYR:OH	1:B:449:HIS:ND1	2.14	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LYS:HB3	1:A:404:LYS:NZ	2.02	0.74
1:A:279:ILE:HG22	1:A:283[B]:GLN:OE1	1.88	0.73
1:B:250:TYR:HB3	1:B:349:THR:HG21	1.69	0.73
1:B:244:LYS:HA	1:B:244:LYS:HZ2	1.53	0.72
1:A:212:ARG:HH11	1:A:423:LEU:HD12	1.55	0.72
1:B:449:HIS:C	1:B:449:HIS:CD2	2.63	0.72
1:B:466:HIS:N	1:B:467:PRO:HD2	2.05	0.71
1:A:219:TYR:CZ	1:A:223:ILE:HD11	2.25	0.71
1:B:402:ASN:HA	3:B:31:HOH:O	1.89	0.71
1:B:262:ILE:O	1:B:262:ILE:HD13	1.91	0.71
1:B:402:ASN:O	1:B:405:PRO:HD2	1.92	0.69
1:B:257:MET:HB3	1:B:261:LYS:HE2	1.74	0.69
1:B:335:ASN:HD22	1:B:335:ASN:C	1.96	0.69
1:B:405:PRO:O	1:B:409:ILE:HG13	1.93	0.68
1:A:244:LYS:HA	1:A:244:LYS:NZ	2.08	0.68
1:B:241:THR:O	1:B:243:ASP:N	2.20	0.68
1:B:320:TYR:HB3	1:B:397:ARG:HD2	1.75	0.68
1:A:442:LEU:O	1:A:446:VAL:HG23	1.94	0.67
1:A:443:ARG:HG2	3:A:70:HOH:O	1.94	0.67
1:A:285[A]:CYS:SG	2:A:101:DRF:H241	2.35	0.67
1:A:309:LEU:HD13	1:A:406:ILE:HG12	1.76	0.67
1:A:219:TYR:CE1	1:A:223:ILE:HD11	2.30	0.67
1:A:244:LYS:HZ3	1:A:244:LYS:HA	1.61	0.66
1:A:464:SER:HA	3:A:10:HOH:O	1.94	0.66
1:A:279:ILE:O	1:A:282:PHE:HB3	1.95	0.66
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.78	0.66
1:A:290:VAL:O	1:A:294:GLN:HG3	1.96	0.66
1:A:402:ASN:N	1:A:402:ASN:ND2	2.42	0.65
1:B:327:TYR:OH	1:B:449:HIS:HE1	1.78	0.65
1:A:335:ASN:HD21	1:A:347:PHE:HE1	1.45	0.65
1:A:441:ASP:O	1:A:445:ILE:HG13	1.97	0.65
1:A:359:PRO:HG2	1:A:360:PHE:CD1	2.33	0.64
1:A:472:ILE:O	1:A:472:ILE:HD13	1.97	0.63
1:B:457:LYS:HE2	1:B:457:LYS:CA	2.28	0.63
1:B:310:ASP:OD1	1:B:401:LEU:HD12	1.98	0.63
1:B:262:ILE:O	1:B:263:LYS:HB3	1.97	0.63
1:B:335:ASN:HD22	1:B:337:ASP:N	1.94	0.63
1:B:358:LYS:HE3	1:B:358:LYS:HA	1.80	0.63
1:B:334:MET:HE2	1:B:368:PHE:HA	1.80	0.62
1:A:364:MET:CE	1:A:367:LYS:HG3	2.29	0.62
1:B:430:GLN:HG3	1:B:433:ALA:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ILE:O	1:B:349:THR:HG23	2.00	0.62
1:B:377:LEU:HB2	1:B:379:LEU:HD13	1.82	0.62
1:A:307:VAL:HA	1:A:314:GLN:OE1	2.00	0.61
1:B:253:ASN:O	1:B:257:MET:HG3	2.01	0.61
1:B:363:PHE:O	1:B:367:LYS:HE2	2.00	0.61
1:A:311:LEU:HD23	1:A:311:LEU:C	2.20	0.61
1:A:285[A]:CYS:SG	2:A:101:DRF:C35	2.89	0.61
1:A:212:ARG:NH1	1:A:423:LEU:HD12	2.15	0.60
1:A:454:GLN:O	1:A:457:LYS:HB3	2.01	0.60
1:A:458:LYS:HB3	1:A:458:LYS:NZ	2.17	0.60
1:B:299:TYR:CE2	3:B:32:HOH:O	2.47	0.60
1:A:357:ARG:HH12	1:A:460:GLU:CD	2.05	0.59
1:A:204:LEU:O	1:A:205:ASN:HB2	2.01	0.59
1:A:281:ILE:HG23	2:A:101:DRF:H6	1.83	0.59
1:A:404:LYS:N	1:A:405:PRO:HD2	2.18	0.59
1:A:220:ASP:OD1	1:A:224:LYS:HE3	2.02	0.59
1:B:433:ALA:O	1:B:437:GLN:HG2	2.01	0.59
1:A:230:LYS:HE2	1:A:379:LEU:O	2.02	0.59
1:B:434:LYS:HA	1:B:437:GLN:NE2	2.17	0.59
1:A:325:ILE:HD13	1:A:388:ILE:HG23	1.83	0.59
1:B:446:VAL:O	1:B:450:VAL:HG13	2.02	0.59
1:A:249:ILE:HD12	1:A:255:LEU:CA	2.30	0.58
1:A:277:VAL:HG13	1:A:278:ALA:N	2.16	0.58
1:B:303:ILE:CD1	1:B:392:ILE:HD12	2.31	0.58
1:B:324:GLU:OE2	1:B:443:ARG:HD2	2.03	0.58
1:A:336:LYS:HD3	1:A:350:ARG:HH12	1.69	0.58
1:A:237:LEU:HD13	1:A:335:ASN:HD22	1.68	0.57
1:A:300:ALA:O	1:A:303:ILE:HG13	2.03	0.57
1:A:336:LYS:HD3	1:A:350:ARG:NH1	2.19	0.57
1:A:307:VAL:HG22	3:A:18:HOH:O	2.04	0.57
1:B:277:VAL:O	1:B:281:ILE:HG13	2.04	0.57
1:B:321:GLY:O	1:B:325:ILE:HG12	2.04	0.57
1:B:449:HIS:C	1:B:449:HIS:HD2	2.06	0.57
1:B:336:LYS:O	1:B:350:ARG:HD3	2.05	0.57
1:B:348:MET:SD	1:B:353:LEU:HD21	2.44	0.57
1:B:425:HIS:N	1:B:426:PRO:HD3	2.20	0.57
1:B:379:LEU:HG	3:B:74:HOH:O	2.04	0.57
1:A:310:ASP:OD2	1:A:312:ASN:HB2	2.05	0.56
1:B:252:MET:SD	1:B:277:VAL:HG11	2.44	0.56
1:A:244:LYS:HZ2	1:A:245:SER:H	1.53	0.56
1:A:403:VAL:C	1:A:405:PRO:HD2	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LEU:HD11	1:B:435:LEU:HD23	1.88	0.56
1:A:234:ARG:N	1:A:234:ARG:HD2	2.20	0.56
1:A:325:ILE:HG13	1:A:391:ILE:HG21	1.86	0.56
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.35	0.56
1:A:277:VAL:HA	1:A:280:ARG:NH2	2.20	0.56
1:A:433:ALA:HA	1:B:436:LEU:HD13	1.88	0.56
1:A:430:GLN:O	1:A:434:LYS:HG2	2.06	0.55
1:B:339:VAL:HG22	1:B:340:LEU:O	2.06	0.55
1:B:389:ALA:N	3:B:32:HOH:O	2.39	0.55
1:A:425:HIS:N	1:A:426:PRO:HD3	2.22	0.55
1:B:240:LYS:O	1:B:242:THR:HG22	2.07	0.55
1:B:279:ILE:O	1:B:283:GLN:HG3	2.06	0.55
1:A:364:MET:HE3	1:A:367:LYS:HG3	1.88	0.55
1:A:342:SER:O	1:A:343:GLU:HB2	2.07	0.55
1:B:298:GLU:O	1:B:298:GLU:HG2	2.05	0.55
1:B:303:ILE:HG21	1:B:393:LEU:HD21	1.88	0.54
1:A:433:ALA:CB	1:B:414:LEU:HD13	2.37	0.54
1:B:434:LYS:O	1:B:437:GLN:HG3	2.07	0.54
1:A:311:LEU:O	1:A:311:LEU:HD23	2.08	0.54
1:B:442:LEU:O	1:B:446:VAL:HG23	2.07	0.54
1:A:334:MET:CG	1:A:339:VAL:HG23	2.37	0.54
1:A:316:THR:O	1:A:319:LYS:HB3	2.08	0.54
1:B:403:VAL:O	1:B:403:VAL:HG12	2.08	0.54
1:B:371:ALA:O	1:B:375:ASN:ND2	2.40	0.54
1:A:433:ALA:O	1:A:437:GLN:HG3	2.09	0.53
1:B:345:GLN:CA	1:B:345:GLN:HE21	2.22	0.53
1:B:454:GLN:CG	1:B:455:VAL:N	2.71	0.53
1:B:292:ALA:O	1:B:295:GLU:N	2.41	0.53
1:B:353:LEU:O	1:B:356:LEU:HG	2.09	0.53
1:A:443:ARG:HG3	3:B:79:HOH:O	2.09	0.53
1:B:335:ASN:C	1:B:335:ASN:ND2	2.62	0.53
1:A:217:HIS:HE1	3:A:73:HOH:O	1.92	0.53
1:B:328:THR:OG1	1:B:442:LEU:HD11	2.08	0.53
1:B:237:LEU:HD22	1:B:335:ASN:OD1	2.09	0.53
1:B:257:MET:CB	1:B:261:LYS:HE2	2.38	0.53
1:A:250:TYR:CE2	1:A:254:SER:OG	2.58	0.53
1:A:260:ASP:O	1:A:261:LYS:HB2	2.08	0.53
1:A:330:LEU:O	1:A:334:MET:HG3	2.09	0.53
1:B:341:ILE:HG23	1:B:342:SER:N	2.24	0.53
1:B:263:LYS:HG3	1:B:264:PHE:N	2.23	0.53
1:B:335:ASN:ND2	1:B:337:ASP:N	2.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LYS:O	1:B:376:ALA:HB3	2.09	0.53
1:B:452:LEU:O	1:B:456:ILE:HG23	2.08	0.52
1:B:341:ILE:HG12	1:B:348:MET:HE3	1.91	0.52
1:A:334:MET:HG2	1:A:339:VAL:CG2	2.35	0.52
1:A:359:PRO:HG2	1:A:360:PHE:HD1	1.72	0.52
1:B:417:LEU:HB3	1:B:432:PHE:HE1	1.73	0.52
1:B:434:LYS:HA	1:B:437:GLN:HE21	1.74	0.52
1:A:230:LYS:O	1:A:233:ALA:HB3	2.10	0.52
1:B:228:LEU:HD13	1:B:333:LEU:HD22	1.91	0.52
1:B:241:THR:HG22	1:B:242:THR:H	1.75	0.52
1:A:360:PHE:HD1	1:A:360:PHE:H	1.57	0.52
1:B:257:MET:O	1:B:261:LYS:HG3	2.10	0.52
1:B:360:PHE:CD2	1:B:360:PHE:N	2.77	0.52
1:A:320:TYR:HB2	1:A:397:ARG:HD2	1.91	0.52
1:A:279:ILE:HG23	1:A:283[B]:GLN:HE22	1.75	0.51
1:B:258:GLY:O	1:B:262:ILE:HG22	2.09	0.51
1:B:341:ILE:CG2	1:B:342:SER:N	2.72	0.51
1:A:329:MET:HE1	1:A:388:ILE:HG13	1.92	0.51
1:A:353:LEU:C	1:A:355:SER:H	2.13	0.51
1:A:404:LYS:HZ3	1:A:404:LYS:HB3	1.74	0.51
1:A:363:PHE:CE2	1:A:456:ILE:HD11	2.46	0.51
2:A:101:DRF:H13	3:A:8:HOH:O	2.10	0.51
1:A:449:HIS:O	1:A:453:LEU:HB2	2.10	0.51
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.92	0.51
1:A:238:THR:C	1:A:240:LYS:H	2.14	0.50
1:A:247:PHE:CD2	1:A:248:VAL:N	2.80	0.50
1:B:290:VAL:HG21	1:B:473:TYR:HD1	1.75	0.50
1:B:277:VAL:N	3:B:21:HOH:O	2.45	0.50
1:B:330:LEU:HD13	1:B:334:MET:SD	2.52	0.50
1:A:320:TYR:O	1:A:397:ARG:CZ	2.60	0.50
1:A:323:HIS:CE1	1:A:472:ILE:HD12	2.46	0.50
1:B:217:HIS:HD2	1:B:218:LEU:HD23	1.77	0.50
1:B:403:VAL:N	3:B:31:HOH:O	2.45	0.50
1:B:358:LYS:CA	1:B:358:LYS:HE3	2.42	0.49
1:A:350:ARG:HG3	1:A:368:PHE:CD2	2.47	0.49
1:B:244:LYS:HA	1:B:244:LYS:HZ3	1.77	0.49
1:B:237:LEU:HD21	1:B:347:PHE:HE1	1.77	0.49
1:B:289:SER:O	1:B:292:ALA:N	2.46	0.49
1:A:380:ASP:OD2	1:A:424:ASN:ND2	2.42	0.48
1:B:223:ILE:HD12	1:B:229:THR:HG21	1.95	0.48
1:A:409:ILE:O	1:A:412:ASN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ALA:HA	1:A:303:ILE:CD1	2.43	0.48
1:A:393:LEU:O	1:A:410:GLN:OE1	2.32	0.48
1:B:245:SER:HB2	1:B:246:PRO:HD2	1.95	0.48
1:B:365:GLU:N	1:B:366:PRO:HD2	2.28	0.48
1:A:220:ASP:O	1:A:224:LYS:HG3	2.13	0.48
1:A:440:THR:HG21	1:B:443:ARG:CG	2.38	0.48
1:B:234:ARG:NH2	1:B:334:MET:O	2.37	0.48
1:B:216:LYS:HD3	1:B:220:ASP:OD2	2.14	0.48
1:B:237:LEU:O	1:B:239:GLY:N	2.47	0.48
1:B:326:ILE:HG22	1:B:327:TYR:N	2.29	0.47
1:A:323:HIS:HE1	1:A:472:ILE:HD12	1.78	0.47
1:A:230:LYS:HG3	1:A:332:SER:HB2	1.96	0.47
1:B:294:GLN:NE2	1:B:294:GLN:HA	2.29	0.47
1:A:360:PHE:CD1	1:A:360:PHE:N	2.81	0.47
1:B:217:HIS:CD2	1:B:218:LEU:HD23	2.50	0.47
1:B:453:LEU:O	1:B:456:ILE:HG12	2.14	0.47
1:B:334:MET:HG3	1:B:339:VAL:HB	1.96	0.47
1:B:345:GLN:HE21	1:B:345:GLN:HA	1.78	0.47
1:B:262:ILE:CD1	1:B:262:ILE:O	2.62	0.47
1:B:459:THR:HG22	1:B:460:GLU:N	2.30	0.47
1:A:222:TYR:CE2	1:A:381:ASP:OD1	2.68	0.47
1:B:364:MET:HA	1:B:367:LYS:HG2	1.95	0.47
1:A:244:LYS:HZ2	1:A:245:SER:N	2.12	0.47
1:A:211:LEU:O	1:A:214:LEU:HB3	2.16	0.46
1:A:348:MET:SD	1:A:353:LEU:HD21	2.55	0.46
1:B:430:GLN:HG3	1:B:433:ALA:CB	2.45	0.46
1:A:260:ASP:O	1:A:261:LYS:CB	2.63	0.46
1:A:242:THR:HG22	1:A:242:THR:O	2.16	0.46
1:B:447:THR:O	1:B:450:VAL:HG22	2.16	0.46
1:A:322:VAL:HG13	1:A:323:HIS:N	2.30	0.46
1:A:466:HIS:HA	1:A:467:PRO:HD3	1.89	0.46
1:A:466:HIS:HB3	1:A:469:LEU:HD23	1.98	0.46
1:B:354:LYS:HD3	1:B:365:GLU:HG3	1.98	0.45
1:B:403:VAL:O	1:B:407:GLU:HG3	2.16	0.45
1:A:205:ASN:ND2	1:A:206:PRO:HD2	2.31	0.45
1:A:373:LYS:O	1:A:376:ALA:HB3	2.16	0.45
1:A:357:ARG:NH1	1:A:460:GLU:OE1	2.50	0.45
1:B:456:ILE:HG13	1:B:457:LYS:N	2.30	0.45
1:A:222:TYR:HE2	1:A:381:ASP:OD1	1.98	0.45
1:B:263:LYS:CG	1:B:264:PHE:N	2.79	0.45
1:B:325:ILE:CD1	1:B:391:ILE:HB	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:GLN:HG3	1:B:455:VAL:N	2.31	0.45
1:B:354:LYS:HD3	1:B:365:GLU:CG	2.47	0.45
1:A:388:ILE:HD13	1:A:388:ILE:HA	1.87	0.45
1:B:208:SER:OG	1:B:209:ALA:N	2.48	0.45
1:A:280:ARG:HB2	1:A:280:ARG:HE	1.50	0.45
1:A:469:LEU:HA	1:A:472:ILE:HG22	1.99	0.45
1:B:290:VAL:HG21	1:B:473:TYR:CD1	2.51	0.45
1:A:287:PHE:CD1	1:A:288:ARG:N	2.85	0.45
1:A:354:LYS:HG2	1:A:354:LYS:O	2.16	0.45
1:A:393:LEU:O	1:A:410:GLN:HB2	2.16	0.45
1:B:242:THR:O	1:B:243:ASP:CB	2.65	0.45
1:B:345:GLN:NE2	1:B:345:GLN:HA	2.32	0.45
1:A:463:MET:HG2	1:A:464:SER:N	2.32	0.44
1:B:230:LYS:HB3	1:B:381:ASP:OD2	2.17	0.44
1:A:365:GLU:N	1:A:366:PRO:HD2	2.31	0.44
1:B:257:MET:CA	1:B:261:LYS:HE2	2.48	0.44
1:B:241:THR:CG2	1:B:242:THR:H	2.29	0.44
1:A:404:LYS:N	1:A:405:PRO:CD	2.81	0.44
1:A:342:SER:H	2:A:101:DRF:C14	2.31	0.44
1:A:421:LEU:C	1:A:423:LEU:N	2.71	0.44
1:A:277:VAL:HA	1:A:280:ARG:HH21	1.83	0.44
1:B:241:THR:O	1:B:242:THR:HG22	2.18	0.44
1:B:228:LEU:HD13	1:B:333:LEU:CD2	2.48	0.44
1:B:375:ASN:HB3	3:B:20:HOH:O	2.18	0.44
1:B:345:GLN:HE21	1:B:345:GLN:N	2.16	0.43
1:A:418:GLU:HB2	1:A:432:PHE:CE2	2.53	0.43
1:B:296:ILE:O	1:B:299:TYR:HB3	2.18	0.43
1:A:451:GLN:O	1:A:454:GLN:HB2	2.19	0.43
1:A:211:LEU:O	1:A:214:LEU:N	2.49	0.43
1:A:363:PHE:CE2	1:A:456:ILE:CD1	3.02	0.43
1:B:469:LEU:C	1:B:471:GLU:N	2.71	0.43
1:A:257:MET:O	1:A:260:ASP:HB2	2.19	0.43
1:B:259:GLU:HG3	1:B:264:PHE:HD1	1.83	0.43
1:B:468:LEU:HD12	1:B:468:LEU:HA	1.83	0.43
1:B:241:THR:HG22	1:B:242:THR:N	2.32	0.43
1:A:356:LEU:O	1:A:357:ARG:C	2.57	0.43
1:B:307:VAL:HG13	3:B:56:HOH:O	2.19	0.43
1:A:205:ASN:ND2	1:A:206:PRO:CD	2.82	0.43
1:A:323:HIS:C	1:A:325:ILE:N	2.72	0.43
1:A:404:LYS:HZ2	1:A:404:LYS:HB3	1.80	0.43
1:B:466:HIS:N	1:B:467:PRO:CD	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:HA	1:A:283[B]:GLN:OE1	2.19	0.42
1:B:221:SER:HB2	1:B:299:TYR:HE1	1.84	0.42
1:B:393:LEU:HD22	1:B:393:LEU:N	2.34	0.42
1:B:457:LYS:HZ3	1:B:457:LYS:HA	1.84	0.42
1:A:465:LEU:HD12	1:A:466:HIS:H	1.84	0.42
1:B:263:LYS:HD3	1:B:264:PHE:H	1.83	0.42
1:B:367:LYS:HZ1	1:B:449:HIS:HB2	1.85	0.42
1:B:250:TYR:N	1:B:250:TYR:CD2	2.87	0.42
1:B:403:VAL:O	1:B:403:VAL:CG1	2.67	0.42
1:A:410:GLN:C	1:A:412:ASN:N	2.73	0.42
1:A:410:GLN:HE21	1:A:414:LEU:HD11	1.85	0.42
1:B:345:GLN:NE2	1:B:345:GLN:CA	2.82	0.42
1:A:320:TYR:O	1:A:397:ARG:NH1	2.53	0.42
1:A:309:LEU:CD1	1:A:406:ILE:HG12	2.48	0.42
1:A:449:HIS:CD2	1:A:453:LEU:HD22	2.55	0.42
1:A:458:LYS:HB3	1:A:458:LYS:HZ2	1.83	0.42
1:B:365:GLU:O	1:B:369:GLU:HG3	2.20	0.42
1:A:279:ILE:HD13	1:A:360:PHE:CZ	2.54	0.42
1:A:241:THR:O	1:A:241:THR:OG1	2.37	0.42
1:A:430:GLN:OE1	1:B:415:GLN:HG3	2.19	0.42
1:B:386:ILE:HD12	1:B:420:GLN:HG2	2.01	0.42
1:B:457:LYS:HA	1:B:457:LYS:NZ	2.33	0.42
1:B:282:PHE:CZ	1:B:456:ILE:HD13	2.54	0.42
1:A:279:ILE:CG2	1:A:283[B]:GLN:HE22	2.33	0.41
1:B:373:LYS:O	1:B:376:ALA:CB	2.68	0.41
1:A:424:ASN:ND2	1:A:425:HIS:HE1	2.19	0.41
1:B:335:ASN:ND2	1:B:338:GLY:H	2.18	0.41
1:A:300:ALA:HA	1:A:303:ILE:HG13	2.02	0.41
1:B:251:ASP:HB2	1:B:254:SER:OG	2.20	0.41
1:B:259:GLU:OE1	1:B:280:ARG:NH2	2.53	0.41
1:B:282:PHE:C	1:B:284:GLY:N	2.73	0.41
1:B:324:GLU:HG3	1:B:446:VAL:HG21	2.03	0.41
1:B:424:ASN:HD22	1:B:425:HIS:CE1	2.38	0.41
1:B:265:LYS:HB3	1:B:287:PHE:CZ	2.55	0.41
1:A:340:LEU:HD23	1:A:346:GLY:O	2.21	0.41
1:A:421:LEU:C	1:A:423:LEU:H	2.24	0.41
1:A:323:HIS:O	1:A:324:GLU:C	2.59	0.41
1:A:448:GLU:O	1:A:452:LEU:HG	2.20	0.41
1:B:306:PHE:HB3	3:B:56:HOH:O	2.20	0.41
1:A:277:VAL:HA	1:A:280:ARG:CZ	2.51	0.41
1:A:325:ILE:HD11	1:A:388:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ILE:O	1:B:329:MET:HG3	2.20	0.41
1:B:240:LYS:O	1:B:241:THR:C	2.59	0.41
1:B:325:ILE:O	1:B:325:ILE:HG22	2.21	0.40
1:A:370:PHE:HB2	1:A:445:ILE:HD11	2.03	0.40
1:A:469:LEU:HA	1:A:472:ILE:CG2	2.51	0.40
1:A:300:ALA:HA	1:A:303:ILE:HD11	2.04	0.40
1:A:410:GLN:C	1:A:412:ASN:H	2.25	0.40
1:B:318:LEU:C	1:B:320:TYR:N	2.74	0.40
1:B:419:LEU:O	1:B:423:LEU:HG	2.21	0.40
1:A:282:PHE:HD2	1:A:283[B]:GLN:HE21	1.70	0.40
1:A:386:ILE:HD12	1:A:420:GLN:CB	2.52	0.40
1:B:418:GLU:O	1:B:422:LYS:HG3	2.20	0.40
1:B:334:MET:CE	1:B:368:PHE:HA	2.47	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	260/276 (94%)	223 (86%)	25 (10%)	12 (5%)	2	2
1	B	252/276 (91%)	202 (80%)	41 (16%)	9 (4%)	3	4
All	All	512/552 (93%)	425 (83%)	66 (13%)	21 (4%)	3	3

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	LYS
1	B	241	THR
1	B	242	THR
1	B	394	SER
1	B	467	PRO

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Mol	Chain	Res	Type
1	A	354	LYS
1	B	238	THR
1	B	357	ARG
1	A	205	ASN
1	A	239	GLY
1	A	244	LYS
1	A	336	LYS
1	B	237	LEU
1	A	357	ARG
1	A	475	ASP
1	B	243	ASP
1	A	203	GLN
1	A	207	GLU
1	A	304	PRO
1	B	475	ASP
1	A	359	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	237/249 (95%)	211 (89%)	26 (11%)	6 9
1	B	231/249 (93%)	203 (88%)	28 (12%)	5 6
All	All	468/498 (94%)	414 (88%)	54 (12%)	5 7

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	216	LYS
1	A	234	ARG
1	A	241	THR
1	A	244	LYS
1	A	245	SER
1	A	251	ASP

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Mol	Chain	Res	Type
1	A	260	ASP
1	A	285[A]	CYS
1	A	285[B]	CYS
1	A	287	PHE
1	A	289	SER
1	A	319	LYS
1	A	333	LEU
1	A	362	ASP
1	A	363	PHE
1	A	380	ASP
1	A	402	ASN
1	A	404	LYS
1	A	407	GLU
1	A	454	GLN
1	A	458	LYS
1	A	460	GLU
1	A	468	LEU
1	A	472	ILE
1	A	476	LEU
1	B	244	LYS
1	B	251	ASP
1	B	254	SER
1	B	262	ILE
1	B	264	PHE
1	B	265	LYS
1	B	318	LEU
1	B	322	VAL
1	B	328	THR
1	B	330	LEU
1	B	335	ASN
1	B	345	GLN
1	B	351	GLU
1	B	358	LYS
1	B	360	PHE
1	B	362	ASP
1	B	394	SER
1	B	396	ASP
1	B	411	ASP
1	B	412	ASN
1	B	437	GLN
1	B	438	LYS
1	B	444	GLN

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Mol	Chain	Res	Type
1	B	449	HIS
1	B	451	GLN
1	B	457	LYS
1	B	459	THR
1	B	467	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	217	HIS
1	A	294	GLN
1	A	308	ASN
1	A	345	GLN
1	A	402	ASN
1	A	410	GLN
1	A	451	GLN
1	A	454	GLN
1	A	470	GLN
1	B	294	GLN
1	B	308	ASN
1	B	335	ASN
1	B	345	GLN
1	B	375	ASN
1	B	410	GLN
1	B	412	ASN
1	B	437	GLN
1	B	470	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	DRF	A	101	-	31,34,34	2.34	6 (19%)	40,46,46	1.46	8 (20%)

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
2	DRF	A	101	-	-	4/13/29/29	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	DRF	C40-C41	-6.96	1.42	1.53
2	A	101	DRF	O46-C41	6.67	1.56	1.43
2	A	101	DRF	C40-C33	-4.41	1.40	1.51
2	A	101	DRF	C11-C16	2.77	1.45	1.40
2	A	101	DRF	C3-C4	2.61	1.44	1.40
2	A	101	DRF	C12-C11	2.04	1.43	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	101	DRF	C24-O27-C30	-3.80	108.00	117.93
2	A	101	DRF	C40-C41-C44	3.53	119.26	111.66
2	A	101	DRF	O21-C16-C11	-3.06	118.75	121.39
2	A	101	DRF	C24-C23-N22	-2.87	109.54	113.02
2	A	101	DRF	O21-C4-C3	-2.73	119.04	121.39
2	A	101	DRF	C40-C33-C34	-2.54	115.86	120.91
2	A	101	DRF	O21-C4-C5	2.12	121.13	116.48
2	A	101	DRF	O21-C16-C15	2.06	121.00	116.48

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	DRF	C44-C41-O46-C48
2	A	101	DRF	C35-C30-O27-C24
2	A	101	DRF	C31-C30-O27-C24
2	A	101	DRF	C40-C41-O46-C48

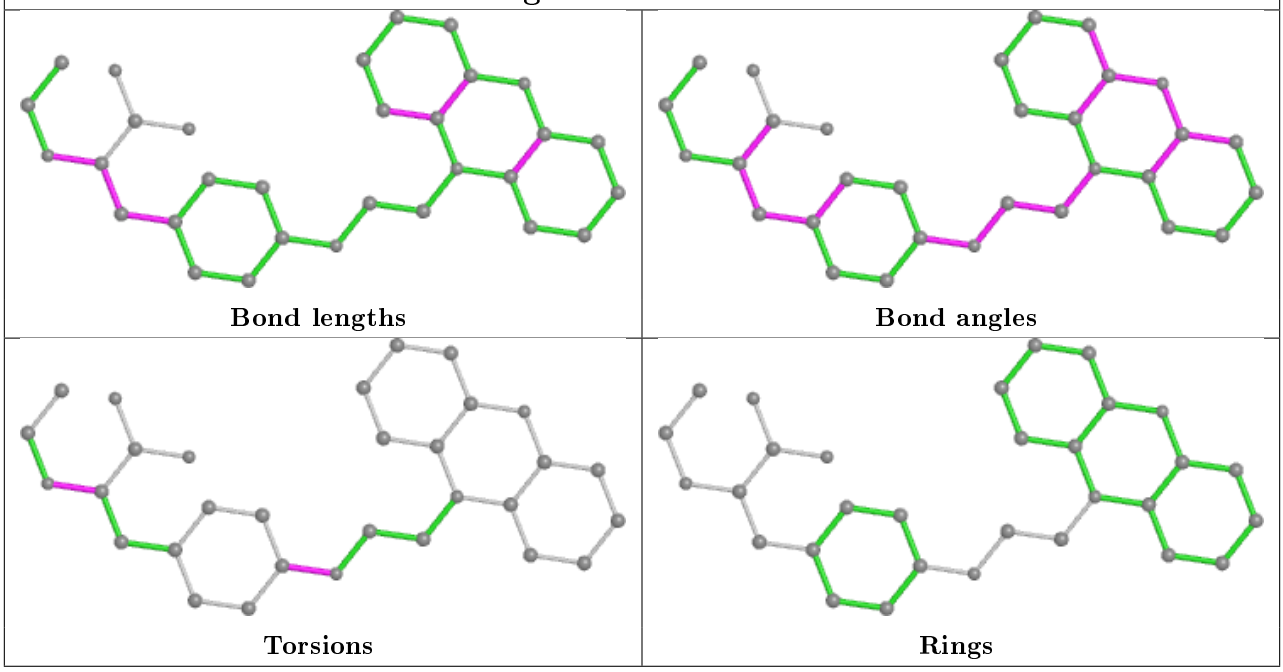
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	DRF	6	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 DRF A 101



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.