



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:28 AM EDT

PDB ID : 2I4P / pdb_00002i4p
Title : Crystal structure of the complex between PPARgamma and the partial agonist LT127 (ureidofibrate derivative). Structure obtained from crystals of the apo-form soaked for 30 days.
Authors : Pochetti, G.; Mazza, F.
Deposited on : 2006-08-22
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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

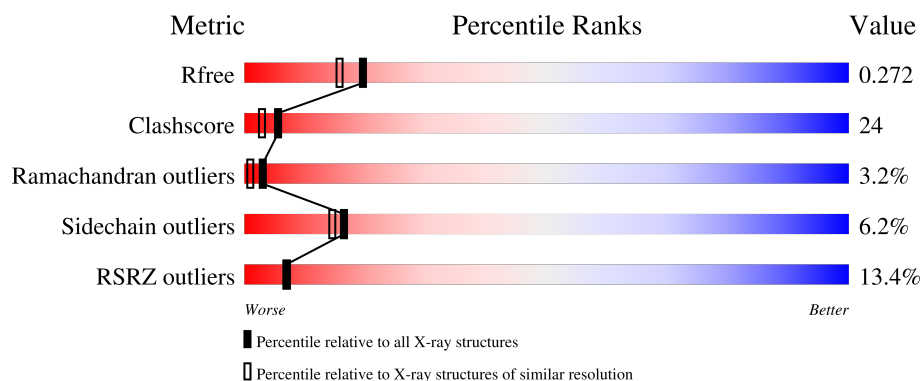
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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	286	9% 56% 34% 6%
1	B	286	15% 58% 30% 6% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DRH	A	999	X	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4478 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.

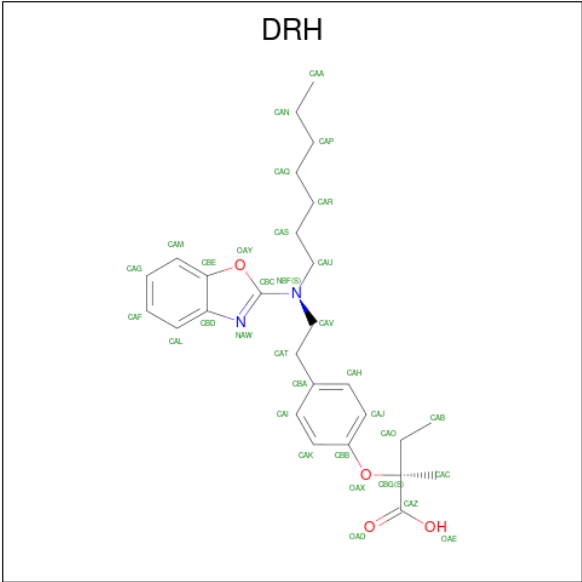
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	78	0	0
			2166	1397	354	405	10			
1	B	270	Total	C	N	O	S	107	0	0
			2166	1397	354	405	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	GLY	-	cloning artifact	UNP P37231
A	192	SER	-	cloning artifact	UNP P37231
A	193	HIS	-	cloning artifact	UNP P37231
A	194	MET	-	cloning artifact	UNP P37231
B	191	GLY	-	cloning artifact	UNP P37231
B	192	SER	-	cloning artifact	UNP P37231
B	193	HIS	-	cloning artifact	UNP P37231
B	194	MET	-	cloning artifact	UNP P37231

- Molecule 2 is (2S)-2-(4-{2-[1,3-BENZOXAZOL-2-YL(HEPTYL)AMINO]ETHYL}PHENOXY)-2-METHYLBUTANOIC ACID (CCD ID: DRH) (formula: C₂₇H₃₆N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	27	2	4		

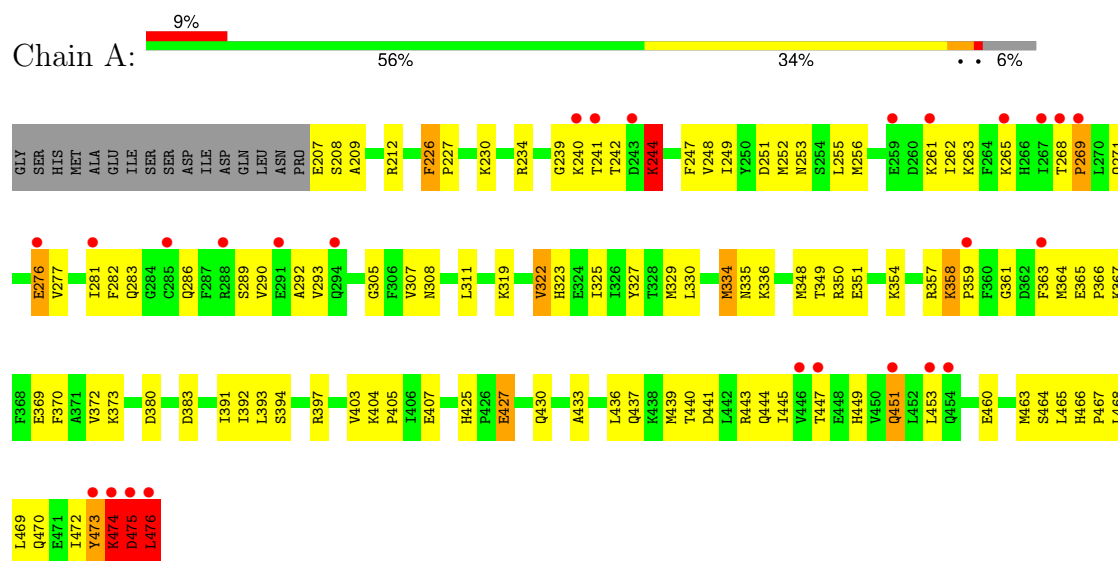
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total	O	0	0
			67	67		
3	B	46	Total	O	0	0
			46	46		

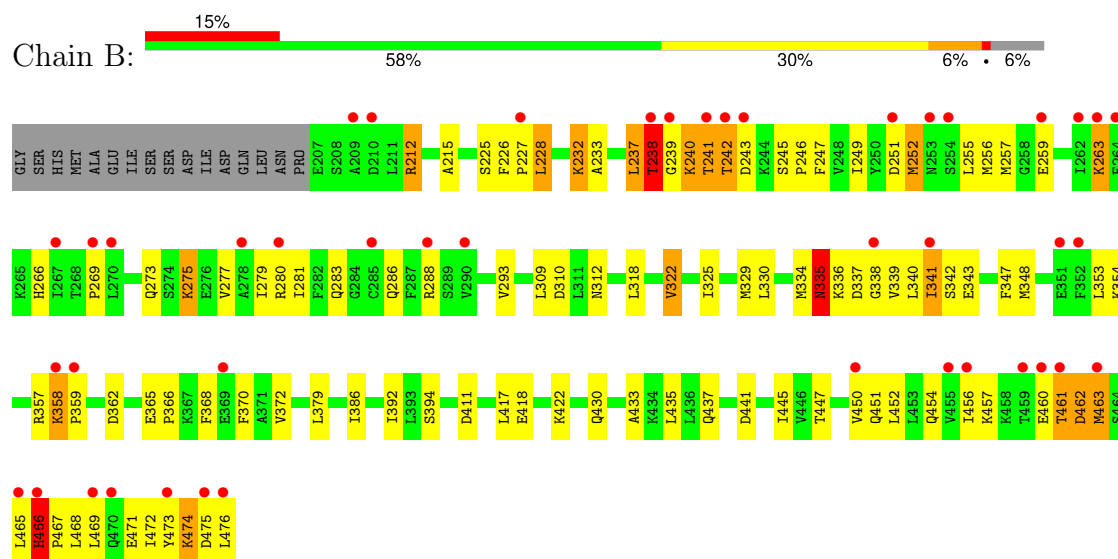
3 Residue-property plots [i](#)

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: Peroxisome proliferator-activated receptor gamma



- Molecule 1: Peroxisome proliferator-activated receptor gamma



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.54Å 60.91Å 118.35Å 90.00° 103.08° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10 8.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (8.00-2.10) 83.7 (8.00-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.272 , 0.295 0.277 , 0.272	Depositor DCC
R_{free} test set	1609 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.52 , 74.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4478	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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: DRH

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	0.51	2/2203 (0.1%)	1.08	19/2967 (0.6%)
1	B	0.42	0/2203	0.88	3/2967 (0.1%)
All	All	0.47	2/4406 (0.0%)	0.99	22/5934 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	473	TYR	CA-C	7.05	1.62	1.52
1	A	476	LEU	C-OXT	6.17	1.35	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	ASP	N-CA-C	12.65	131.76	107.98
1	A	474	LYS	CA-C-N	12.31	142.04	122.34
1	A	474	LYS	C-N-CA	12.31	142.04	122.34
1	A	242	THR	N-CA-C	-7.94	104.48	114.56
1	A	475	ASP	CA-C-N	-7.50	108.20	121.70
1	A	475	ASP	C-N-CA	-7.50	108.20	121.70
1	A	226	PHE	CA-C-N	7.18	127.02	119.05
1	A	226	PHE	C-N-CA	7.18	127.02	119.05
1	A	475	ASP	CA-C-O	-7.09	113.64	121.58
1	B	241	THR	N-CA-C	-6.95	102.36	111.74
1	A	475	ASP	N-CA-CB	-6.94	100.22	110.49
1	A	475	ASP	CB-CA-C	-6.91	100.08	111.68
1	A	474	LYS	N-CA-C	-6.68	96.57	110.80
1	A	240	LYS	N-CA-C	-6.62	104.78	112.86
1	B	225	SER	N-CA-C	6.23	120.08	112.23
1	A	476	LEU	CA-C-O	5.88	138.63	121.00
1	A	244	LYS	N-CA-C	5.84	117.45	110.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	ASN	N-CA-C	-5.62	100.94	108.86
1	A	248	VAL	N-CA-C	5.59	116.36	108.36
1	A	322	VAL	N-CA-C	5.49	116.13	110.36
1	A	334	MET	N-CA-C	5.42	118.41	109.85
1	B	335	ASN	N-CA-C	-5.07	101.71	108.86

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	2166	0	2232	105	0
1	B	2166	0	2232	88	0
2	A	33	0	35	22	0
3	A	67	0	0	11	0
3	B	46	0	0	8	0
All	All	4478	0	4499	201	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 24.

All (201) 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:475:ASP:O	1:A:476:LEU:CB	1.66	1.36
1:A:330:LEU:HD22	2:A:999:DRH:HAT1	1.36	1.06
1:A:473:TYR:O	1:A:474:LYS:HG3	1.59	1.01
2:A:999:DRH:OAD	2:A:999:DRH:HAK	1.59	1.00
1:B:430:GLN:HG3	1:B:433:ALA:HB3	1.53	0.91
1:B:293:VAL:HG21	1:B:476:LEU:HD11	1.51	0.89
1:A:247:PHE:HB2	1:A:261:LYS:HD3	1.54	0.89
1:B:293:VAL:HG22	1:B:322:VAL:HG21	1.57	0.86
1:B:325:ILE:HG22	1:B:329:MET:HE2	1.59	0.84
1:A:244:LYS:HE2	3:A:8:HOH:O	1.76	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:HIS:NE2	2:A:999:DRH:HAC1	1.93	0.83
1:A:329:MET:SD	2:A:999:DRH:HAA3	2.20	0.82
1:B:335:ASN:HD22	1:B:335:ASN:C	1.86	0.81
1:B:212:ARG:HH11	1:B:212:ARG:HB3	1.47	0.80
1:A:253:ASN:HA	1:A:256:MET:HE3	1.62	0.80
1:A:330:LEU:HD13	2:A:999:DRH:HAV2	1.63	0.80
1:B:335:ASN:ND2	1:B:337:ASP:H	1.79	0.79
1:A:357:ARG:HG2	1:A:359:PRO:HD2	1.65	0.79
1:B:341:ILE:HD13	1:B:342:SER:H	1.47	0.78
1:B:358:LYS:N	1:B:358:LYS:HE3	2.00	0.76
1:A:261:LYS:HE2	1:A:262:ILE:HG13	1.66	0.76
1:A:475:ASP:O	1:A:476:LEU:CG	2.34	0.75
1:A:241:THR:HB	3:A:15:HOH:O	1.85	0.74
2:A:999:DRH:HAK	2:A:999:DRH:CAZ	2.19	0.72
1:A:473:TYR:O	1:A:474:LYS:CG	2.37	0.71
1:B:341:ILE:HD13	3:B:6:HOH:O	1.88	0.71
1:A:330:LEU:HD13	2:A:999:DRH:CAV	2.20	0.71
1:A:475:ASP:O	1:A:476:LEU:HB2	0.93	0.71
1:B:451:GLN:O	1:B:454:GLN:HG2	1.91	0.70
1:A:249:ILE:HD12	1:A:255:LEU:HA	1.72	0.69
2:A:999:DRH:OAD	2:A:999:DRH:CAK	2.39	0.69
1:B:358:LYS:HE3	1:B:358:LYS:H	1.58	0.68
1:B:336:LYS:HG2	1:B:372:VAL:HG22	1.74	0.68
1:A:440:THR:O	1:A:444:GLN:HG2	1.94	0.68
1:A:349:THR:HG22	1:A:351:GLU:H	1.60	0.66
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.78	0.66
1:B:240:LYS:HG3	1:B:241:THR:H	1.63	0.64
1:A:440:THR:HB	3:B:39:HOH:O	1.97	0.63
1:A:311:LEU:C	1:A:311:LEU:HD23	2.24	0.63
1:B:341:ILE:CD1	1:B:342:SER:H	2.12	0.63
1:B:335:ASN:C	1:B:335:ASN:ND2	2.56	0.62
1:B:466:HIS:N	1:B:467:PRO:CD	2.62	0.62
1:A:474:LYS:H	1:A:475:ASP:HB2	1.64	0.62
1:B:467:PRO:C	1:B:469:LEU:H	2.07	0.62
2:A:999:DRH:OAY	2:A:999:DRH:HAT2	2.00	0.61
1:A:329:MET:SD	2:A:999:DRH:CAA	2.88	0.60
1:B:441:ASP:O	1:B:445:ILE:HG12	2.01	0.60
1:B:411:ASP:HB2	3:B:22:HOH:O	2.02	0.60
1:A:430:GLN:HG3	1:A:433:ALA:HB3	1.82	0.59
1:A:268:THR:N	1:A:269:PRO:HD2	2.17	0.59
1:A:268:THR:H	1:A:269:PRO:HD2	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:HD23	1:B:232:LYS:HB3	1.85	0.58
1:B:228:LEU:CD2	1:B:232:LYS:HB3	2.34	0.58
1:A:391:ILE:HD13	1:A:439:MET:HE3	1.85	0.57
1:A:466:HIS:ND1	1:A:467:PRO:HD2	2.20	0.57
1:B:447:THR:O	1:B:450:VAL:HG22	2.04	0.56
1:A:441:ASP:O	1:A:445:ILE:HG12	2.06	0.56
1:B:335:ASN:ND2	1:B:338:GLY:H	2.04	0.56
1:A:226:PHE:CG	1:A:329:MET:HE1	2.40	0.55
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.36	0.55
1:A:292:ALA:CB	2:A:999:DRH:HAQ1	2.36	0.55
1:B:251:ASP:HB2	3:B:23:HOH:O	2.05	0.55
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.87	0.55
1:B:335:ASN:HD21	1:B:338:GLY:N	2.05	0.55
1:B:325:ILE:CG2	1:B:329:MET:HE2	2.35	0.54
1:A:336:LYS:HE2	1:A:372:VAL:HG11	1.89	0.54
1:A:208:SER:O	1:A:212:ARG:HG2	2.07	0.54
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.90	0.54
1:B:433:ALA:O	1:B:437:GLN:HG2	2.07	0.54
1:A:370:PHE:HA	1:A:373:LYS:HE2	1.89	0.53
2:A:999:DRH:HAL	3:A:116:HOH:O	2.07	0.53
1:B:237:LEU:O	1:B:239:GLY:N	2.41	0.53
1:B:255:LEU:CD2	1:B:281:ILE:HD11	2.39	0.53
1:B:252:MET:O	1:B:256:MET:HG2	2.09	0.53
1:B:365:GLU:N	1:B:366:PRO:HD2	2.24	0.53
1:B:256:MET:HE1	1:B:280:ARG:HH12	1.74	0.52
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.40	0.52
1:B:466:HIS:N	1:B:467:PRO:HD2	2.23	0.52
1:A:252:MET:HE1	1:A:277:VAL:HB	1.92	0.52
1:A:475:ASP:O	1:A:476:LEU:HG	2.08	0.51
1:A:349:THR:HG21	3:A:91:HOH:O	2.09	0.51
1:B:335:ASN:ND2	1:B:338:GLY:N	2.58	0.51
1:A:286:GLN:N	2:A:999:DRH:HAB1	2.26	0.51
1:A:230:LYS:O	1:A:234:ARG:HG2	2.10	0.51
1:A:282:PHE:CE2	1:A:463:MET:HE1	2.45	0.51
1:B:473:TYR:O	1:B:474:LYS:HB2	2.11	0.51
1:B:343:GLU:O	1:B:343:GLU:HG3	2.11	0.51
1:A:289:SER:O	1:A:293:VAL:HG23	2.12	0.50
1:A:277:VAL:O	1:A:281:ILE:HG13	2.12	0.50
2:A:999:DRH:CBC	3:A:18:HOH:O	2.59	0.50
1:B:247:PHE:HE1	1:B:257:MET:HE2	1.77	0.50
1:A:262:ILE:HG22	1:A:263:LYS:N	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ILE:HG21	1:A:348:MET:HE2	1.94	0.49
1:B:358:LYS:H	1:B:358:LYS:CE	2.22	0.49
1:A:207:GLU:HG3	1:A:209:ALA:HB3	1.93	0.49
1:A:404:LYS:N	1:A:405:PRO:HD2	2.28	0.49
1:A:255:LEU:HD21	1:A:277:VAL:HG23	1.95	0.49
1:B:228:LEU:HD22	1:B:233:ALA:HB2	1.95	0.49
1:A:391:ILE:CD1	1:A:439:MET:HE3	2.42	0.49
1:A:453:LEU:HD21	3:A:1:HOH:O	2.12	0.48
1:A:256:MET:O	1:A:268:THR:HG23	2.13	0.48
1:B:242:THR:HA	3:B:61:HOH:O	2.13	0.48
1:B:336:LYS:HE3	1:B:372:VAL:HG11	1.96	0.48
1:A:263:LYS:HB3	3:A:86:HOH:O	2.14	0.48
1:A:286:GLN:CA	2:A:999:DRH:HAB1	2.44	0.48
1:A:380:ASP:HB2	3:A:32:HOH:O	2.13	0.48
1:A:433:ALA:O	1:A:437:GLN:HG3	2.13	0.48
1:B:358:LYS:HB2	1:B:359:PRO:HD3	1.96	0.48
1:A:292:ALA:HB1	2:A:999:DRH:HAQ1	1.96	0.47
1:A:330:LEU:HD22	2:A:999:DRH:CAT	2.26	0.47
1:B:335:ASN:ND2	1:B:337:ASP:N	2.56	0.47
1:A:437:GLN:O	1:A:440:THR:HG22	2.15	0.47
1:B:310:ASP:OD2	1:B:312:ASN:HB2	2.14	0.47
1:A:349:THR:HG22	1:A:351:GLU:N	2.28	0.47
1:B:288:ARG:HB3	3:B:13:HOH:O	2.13	0.47
1:B:457:LYS:O	1:B:461:THR:HG23	2.15	0.47
1:A:330:LEU:HD13	2:A:999:DRH:CAT	2.44	0.47
1:B:334:MET:HG2	1:B:339:VAL:HB	1.95	0.47
1:A:403:VAL:O	1:A:407:GLU:HG3	2.15	0.46
1:A:256:MET:HG2	1:A:268:THR:O	2.15	0.46
1:B:467:PRO:C	1:B:469:LEU:N	2.73	0.46
1:B:418:GLU:O	1:B:422:LYS:HG3	2.14	0.46
1:B:255:LEU:CD2	1:B:277:VAL:HG13	2.45	0.46
1:B:452:LEU:O	1:B:456:ILE:HG13	2.16	0.46
1:B:463:MET:HG3	1:B:465:LEU:H	1.80	0.46
1:A:436:LEU:O	1:A:439:MET:HB2	2.16	0.46
1:A:286:GLN:NE2	1:A:465:LEU:HA	2.31	0.46
1:A:307:VAL:HG22	3:A:10:HOH:O	2.15	0.46
1:B:275:LYS:HA	1:B:275:LYS:HE3	1.99	0.45
1:B:465:LEU:O	1:B:466:HIS:HB2	2.16	0.45
1:A:292:ALA:HB2	2:A:999:DRH:HAQ1	1.99	0.45
1:B:465:LEU:O	1:B:466:HIS:CB	2.64	0.45
1:A:262:ILE:HG22	1:A:263:LYS:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:999:DRH:HAC2	3:A:1:HOH:O	2.17	0.45
1:B:215:ALA:HA	1:B:386:ILE:CD1	2.47	0.45
1:B:342:SER:O	1:B:343:GLU:HB3	2.16	0.45
1:B:468:LEU:O	1:B:472:ILE:HG13	2.17	0.45
1:A:330:LEU:O	1:A:334:MET:HG3	2.18	0.44
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.46	0.44
1:A:239:GLY:C	1:A:241:THR:N	2.72	0.44
1:B:430:GLN:NE2	1:B:433:ALA:HB2	2.31	0.44
1:A:383:ASP:OD2	1:A:425:HIS:HE1	2.00	0.44
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.81	0.44
1:B:255:LEU:HD23	1:B:277:VAL:HG13	2.00	0.44
2:A:999:DRH:OAY	2:A:999:DRH:CAT	2.65	0.44
1:B:259:GLU:OE1	1:B:280:ARG:NH2	2.47	0.44
1:A:336:LYS:HD3	1:A:350:ARG:NH1	2.33	0.44
1:A:323:HIS:CE1	1:A:473:TYR:CE2	3.06	0.44
1:A:207:GLU:HG3	1:A:209:ALA:H	1.82	0.43
1:B:463:MET:C	1:B:465:LEU:H	2.27	0.43
1:B:469:LEU:HD13	1:B:469:LEU:O	2.17	0.43
1:A:325:ILE:HD11	1:A:392:ILE:HG13	2.00	0.43
1:A:469:LEU:O	1:A:473:TYR:CD1	2.71	0.43
1:B:226:PHE:HA	1:B:227:PRO:HD3	1.87	0.43
1:A:394:SER:O	1:A:397:ARG:HG2	2.19	0.43
1:A:427:GLU:H	1:A:427:GLU:CD	2.26	0.43
1:B:379:LEU:HD21	1:B:435:LEU:HD22	1.99	0.43
1:B:215:ALA:HA	1:B:386:ILE:HD11	2.01	0.43
1:B:237:LEU:HD21	1:B:340:LEU:HG	2.01	0.43
1:B:379:LEU:HD12	3:B:84:HOH:O	2.17	0.43
1:A:251:ASP:OD1	1:A:251:ASP:C	2.61	0.43
1:B:237:LEU:HB3	1:B:238:THR:H	1.64	0.42
1:A:263:LYS:HZ1	1:A:265:LYS:HE2	1.84	0.42
1:A:290:VAL:HG13	1:A:468:LEU:HD23	2.01	0.42
1:B:269:PRO:HA	1:B:280:ARG:NH2	2.34	0.42
1:B:370:PHE:HE1	1:B:441:ASP:HB2	1.84	0.42
1:A:336:LYS:HD3	1:A:350:ARG:HH12	1.84	0.42
1:A:447:THR:O	1:A:451:GLN:HG3	2.19	0.42
1:B:354:LYS:HD3	1:B:365:GLU:CG	2.49	0.42
1:B:368:PHE:O	1:B:372:VAL:HG23	2.20	0.42
1:A:252:MET:O	1:A:256:MET:HG3	2.20	0.42
1:A:464:SER:C	1:A:465:LEU:HD23	2.45	0.42
1:B:245:SER:HA	1:B:246:PRO:HD3	1.91	0.42
1:A:226:PHE:CD2	1:A:329:MET:HE1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLU:O	1:A:373:LYS:HG3	2.20	0.42
1:B:475:ASP:O	1:B:476:LEU:HB3	2.20	0.42
1:A:276:GLU:OE2	1:A:357:ARG:CZ	2.68	0.41
1:A:364:MET:O	1:A:365:GLU:C	2.62	0.41
1:B:249:ILE:HD12	1:B:255:LEU:HA	2.01	0.41
1:A:319:LYS:O	1:A:472:ILE:HG23	2.19	0.41
1:A:393:LEU:CD2	1:A:393:LEU:N	2.82	0.41
1:B:286:GLN:HB3	1:B:473:TYR:CE2	2.55	0.41
1:B:348:MET:SD	1:B:353:LEU:HD21	2.60	0.41
1:A:370:PHE:HA	1:A:373:LYS:CE	2.50	0.41
1:B:279:ILE:O	1:B:283:GLN:HG3	2.20	0.41
1:A:330:LEU:CD2	2:A:999:DRH:HAT1	2.26	0.41
1:A:207:GLU:HA	3:A:90:HOH:O	2.19	0.41
1:A:475:ASP:C	1:A:476:LEU:CG	2.87	0.41
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.55	0.41
1:A:439:MET:HE1	3:B:74:HOH:O	2.20	0.41
1:B:457:LYS:NZ	1:B:461:THR:HG21	2.36	0.41
1:A:357:ARG:O	1:A:358:LYS:C	2.63	0.41
1:A:365:GLU:N	1:A:366:PRO:HD2	2.36	0.41
1:B:309:LEU:O	1:B:310:ASP:C	2.64	0.41
1:B:467:PRO:O	1:B:468:LEU:HB3	2.20	0.41
1:A:354:LYS:HA	1:A:361:GLY:O	2.21	0.40
1:B:255:LEU:HD22	1:B:281:ILE:HD11	2.02	0.40
1:B:386:ILE:HB	1:B:417:LEU:HD13	2.03	0.40
1:A:226:PHE:HA	1:A:227:PRO:HD3	1.87	0.40
1:A:327:TYR:CD1	1:A:367:LYS:HD2	2.57	0.40
1:A:397:ARG:HH11	1:A:443:ARG:NH2	2.19	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	268/286 (94%)	254 (95%)	10 (4%)	4 (2%)	8	4
1	B	268/286 (94%)	235 (88%)	20 (8%)	13 (5%)	1	0
All	All	536/572 (94%)	489 (91%)	30 (6%)	17 (3%)	3	1

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	PRO
1	A	474	LYS
1	B	237	LEU
1	B	357	ARG
1	B	394	SER
1	B	462	ASP
1	B	466	HIS
1	A	358	LYS
1	B	238	THR
1	B	240	LYS
1	B	242	THR
1	B	263	LYS
1	A	276	GLU
1	B	266	HIS
1	B	474	LYS
1	B	463	MET
1	B	243	ASP

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	243/257 (95%)	233 (96%)	10 (4%)	27	29
1	B	243/257 (95%)	223 (92%)	20 (8%)	10	8
All	All	486/514 (95%)	456 (94%)	30 (6%)	16	14

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	LYS
1	A	271	GLN
1	A	283	GLN
1	A	363	PHE
1	A	427	GLU
1	A	451	GLN
1	A	460	GLU
1	A	470	GLN
1	A	475	ASP
1	A	476	LEU
1	B	212	ARG
1	B	228	LEU
1	B	232	LYS
1	B	238	THR
1	B	252	MET
1	B	263	LYS
1	B	273	GLN
1	B	275	LYS
1	B	318	LEU
1	B	322	VAL
1	B	330	LEU
1	B	335	ASN
1	B	341	ILE
1	B	358	LYS
1	B	362	ASP
1	B	460	GLU
1	B	461	THR
1	B	462	ASP
1	B	466	HIS
1	B	471	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	286	GLN
1	A	308	ASN
1	A	314	GLN
1	A	402	ASN
1	A	410	GLN
1	A	412	ASN
1	A	425	HIS
1	A	430	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	451	GLN
1	A	454	GLN
1	A	470	GLN
1	B	217	HIS
1	B	253	ASN
1	B	308	ASN
1	B	323	HIS
1	B	335	ASN
1	B	410	GLN
1	B	412	ASN
1	B	430	GLN
1	B	444	GLN
1	B	470	GLN

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 oligosaccharides 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	DRH	A	999	-	34,35,35	0.93	1 (2%)	41,47,47	1.92	7 (17%)

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	DRH	A	999	-	1/1/3/3	13/30/30/30	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	DRH	CBD-NAW	-3.20	1.33	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	DRH	OAY-CBC-NAW	-6.57	110.41	116.47
2	A	999	DRH	CBD-NAW-CBC	6.51	108.56	103.42
2	A	999	DRH	CAM-CBE-CBD	-3.11	119.84	123.62
2	A	999	DRH	CBG-OAX-CBB	3.09	125.68	121.00
2	A	999	DRH	OAY-CBE-CAM	3.02	132.84	126.49
2	A	999	DRH	CAU-NBF-CBC	-2.68	115.12	120.65
2	A	999	DRH	OAX-CBG-CAZ	2.51	113.25	109.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	999	DRH	NBF

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	999	DRH	OAD-CAZ-CBG-OAX
2	A	999	DRH	CAT-CAV-NBF-CBC
2	A	999	DRH	CAS-CAU-NBF-CAV
2	A	999	DRH	CAT-CAV-NBF-CAU
2	A	999	DRH	CAS-CAU-NBF-CBC
2	A	999	DRH	OAE-CAZ-CBG-CAC
2	A	999	DRH	OAE-CAZ-CBG-OAX
2	A	999	DRH	CAJ-CBB-OAX-CBG
2	A	999	DRH	CAK-CBB-OAX-CBG
2	A	999	DRH	CAV-CAT-CBA-CAH
2	A	999	DRH	CAV-CAT-CBA-CAI
2	A	999	DRH	CBA-CAT-CAV-NBF

Continued on next page...

Continued from previous page...

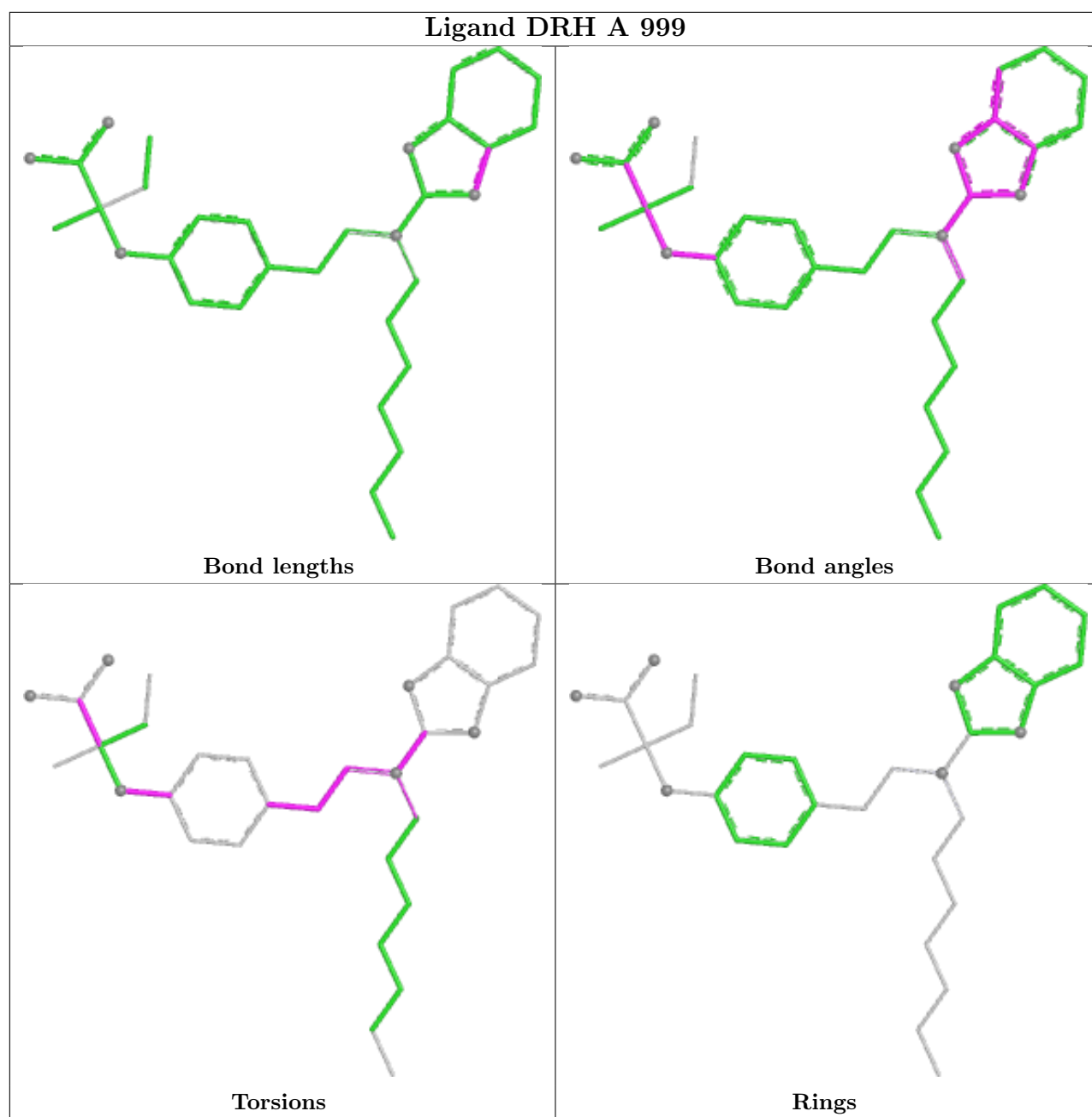
Mol	Chain	Res	Type	Atoms
2	A	999	DRH	OAY-CBC-NBF-CAU

There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	DRH	22	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	262/286 (91%)	0.62	26 (9%) 13 13	8, 45, 66, 75	2 (0%)
1	B	261/286 (91%)	0.89	44 (16%) 4 4	7, 45, 79, 90	7 (2%)
All	All	523/572 (91%)	0.76	70 (13%) 7 7	7, 45, 74, 90	9 (1%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	ILE	12.1
1	A	267	ILE	8.2
1	A	268	THR	6.8
1	B	264	PHE	5.8
1	A	476	LEU	5.5
1	B	285	CYS	4.9
1	A	473	TYR	4.8
1	A	243	ASP	4.8
1	B	241	THR	4.6
1	B	288	ARG	3.9
1	B	270	LEU	3.8
1	B	461	THR	3.7
1	B	242	THR	3.6
1	B	459	THR	3.6
1	B	238	THR	3.5
1	A	269	PRO	3.5
1	A	359	PRO	3.5
1	A	240	LYS	3.3
1	B	465	LEU	3.3
1	B	473	TYR	3.2
1	A	451	GLN	3.1
1	B	460	GLU	3.1
1	B	476	LEU	3.0
1	B	466	HIS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	263	LYS	2.9
1	B	475	ASP	2.9
1	B	338	GLY	2.9
1	B	455	VAL	2.8
1	B	280	ARG	2.7
1	B	456	ILE	2.7
1	A	474	LYS	2.7
1	A	453	LEU	2.6
1	A	446	VAL	2.6
1	B	210	ASP	2.6
1	B	259	GLU	2.5
1	A	241	THR	2.5
1	A	265	LYS	2.4
1	B	254	SER	2.3
1	B	262	ILE	2.3
1	B	341	ILE	2.3
1	A	475	ASP	2.3
1	A	288	ARG	2.3
1	B	239	GLY	2.3
1	A	276	GLU	2.3
1	A	363	PHE	2.3
1	B	351	GLU	2.3
1	A	281	ILE	2.3
1	B	227	PRO	2.3
1	A	285	CYS	2.3
1	B	253	ASN	2.2
1	B	209	ALA	2.2
1	B	352	PHE	2.2
1	B	269	PRO	2.2
1	B	359	PRO	2.2
1	A	447	THR	2.2
1	A	259	GLU	2.1
1	A	291	GLU	2.1
1	B	470	GLN	2.1
1	B	469	LEU	2.1
1	B	358	LYS	2.1
1	B	369	GLU	2.1
1	B	450	VAL	2.1
1	B	278	ALA	2.1
1	B	463	MET	2.1
1	A	454	GLN	2.1
1	B	243	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	290	VAL	2.0
1	A	294	GLN	2.0
1	B	251	ASP	2.0
1	A	261	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

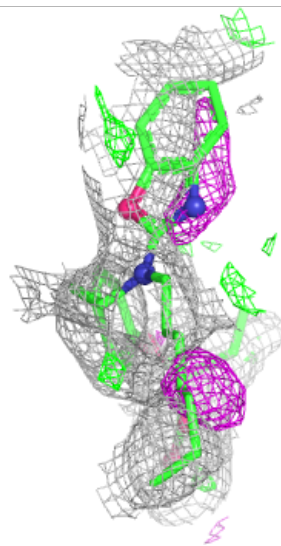
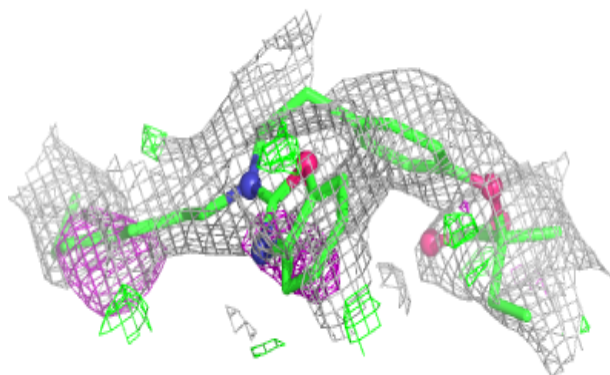
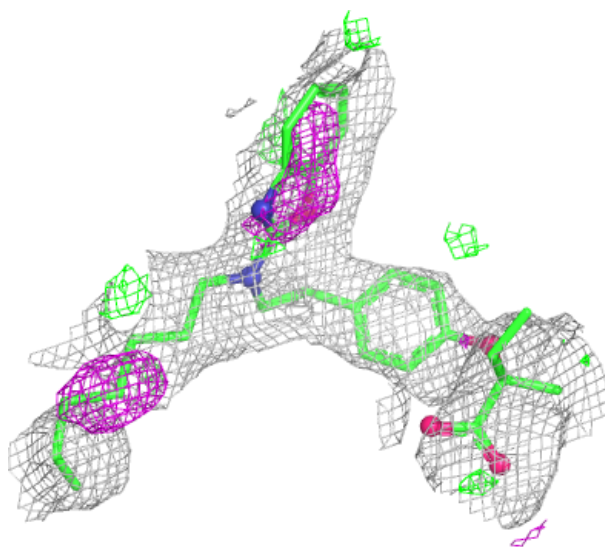
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DRH	A	999	33/33	0.59	0.15	63,71,72,72	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 DRH A 999:

$2mF_o-DF_c$ (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.