



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:40 AM GMT

PDB ID : 2I4Z  
Title : Crystal structure of the complex between PPARgamma and the partial agonist LT127 (ureidofibrate derivative). This structure has been obtained from crystals soaked for 6 hours.  
Authors : Pochetti, G.; Mazza, F.  
Deposited on : 2006-08-23  
Resolution : 2.25 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

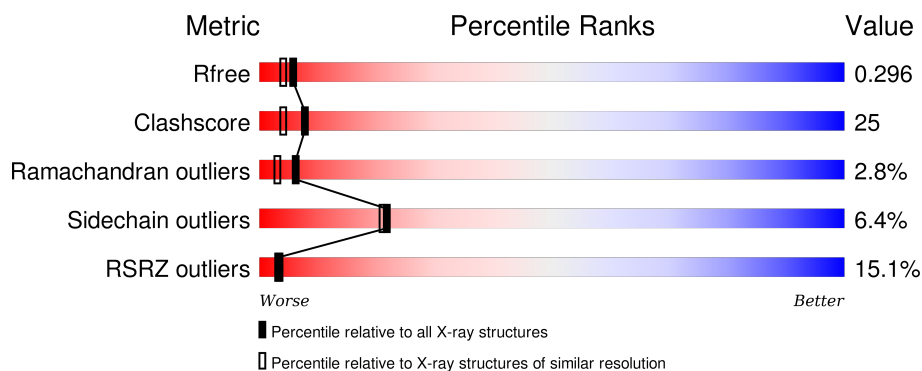
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>8%</div> <div>59%</div> <div>32%</div> <div>• 6%</div> </div>
1	B	286	<div> <div>19%</div> <div>59%</div> <div>30%</div> <div>5% 6%</div> </div>

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	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4634 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.

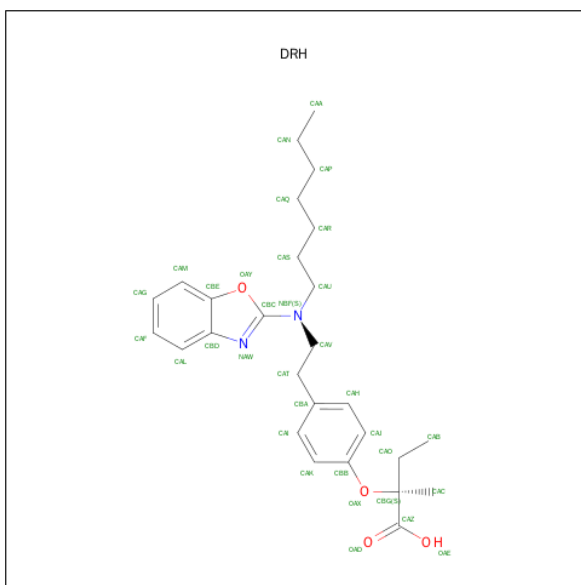
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	77	6	0
			2222	1432	367	413	10			
1	B	270	Total	C	N	O	S	107	2	0
			2184	1408	358	408	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 (three-letter code: DRH) (formula: C<sub>27</sub>H<sub>36</sub>N<sub>2</sub>O<sub>4</sub>).



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

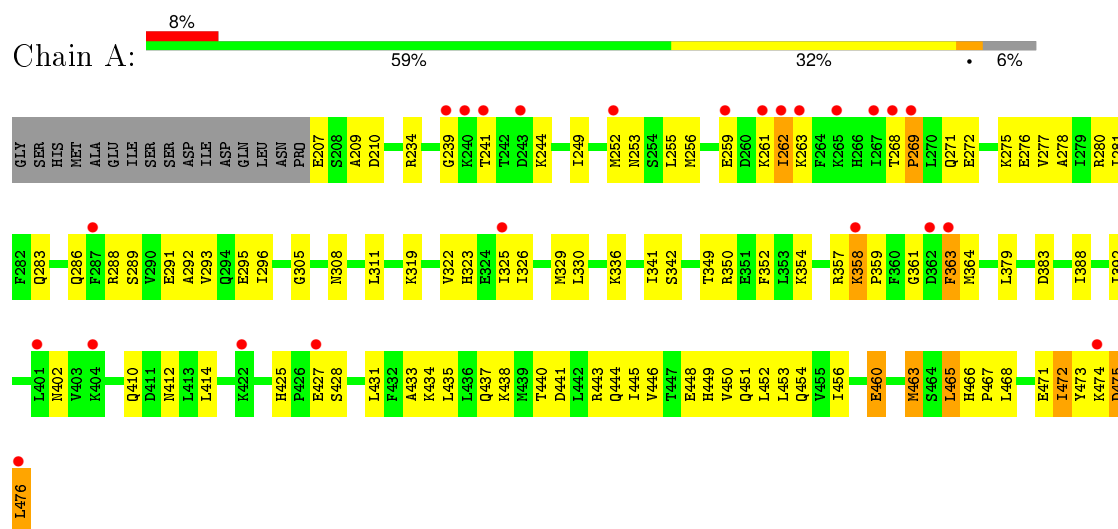
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	119	Total O 119 119	10	0
3	B	76	Total O 76 76	8	0

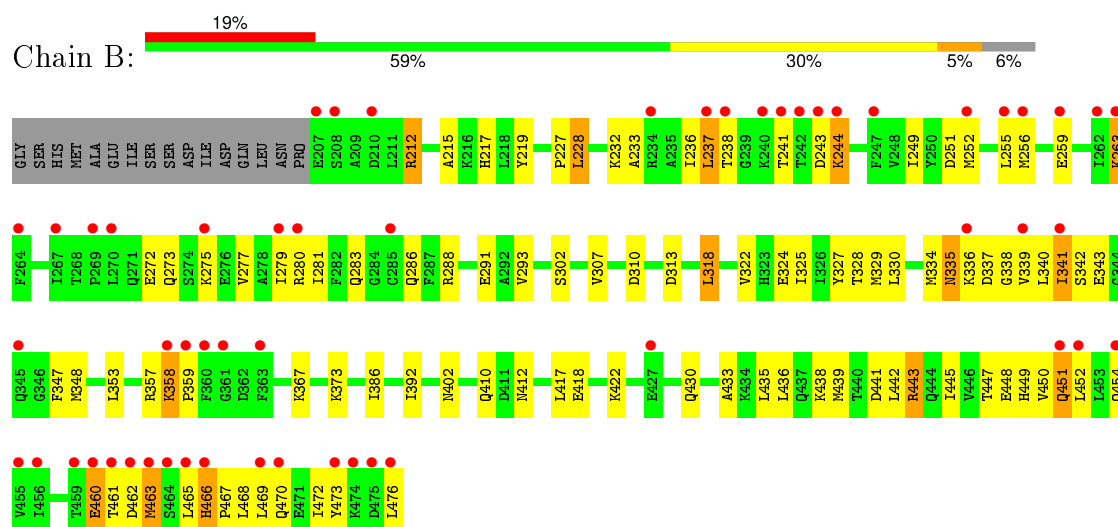
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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, $\alpha$ , $\beta$ , $\gamma$	93.00 Å   60.14 Å   118.08 Å 90.00°   103.70°   90.00°	Depositor
Resolution (Å)	8.00 – 2.25 27.32 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.8 (8.00-2.25) 97.7 (27.32-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.24 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.238   ,   0.290 0.243   ,   0.296	Depositor DCC
$R_{free}$ test set	1424 reflections (4.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 70.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 29624 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4634	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.38	0/2258	0.57	0/3034
1	B	0.34	0/2221	0.55	0/2990
All	All	0.36	0/4479	0.56	0/6024

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2222	0	2298	130	0
1	B	2184	0	2251	88	0
2	A	33	0	35	28	0
3	A	119	0	0	15	0
3	B	76	0	0	8	0
All	All	4634	0	4584	218	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 25.

All (218) 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:B:212:ARG:HB3	1:B:212:ARG:HH11	1.27	0.99
1:B:293:VAL:HG22	1:B:322:VAL:HG21	1.51	0.92
1:B:293:VAL:HG21	1:B:476:LEU:HD11	1.48	0.92
1:B:402:ASN:HB3	3:B:484:HOH:O	1.72	0.88
1:A:286:GLN:NE2	1:A:465:LEU:HA	1.90	0.87
2:A:999:DRH:OAY	2:A:999:DRH:HAT2	1.78	0.82
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.61	0.82
1:B:430:GLN:HG3	1:B:433:ALA:HB3	1.61	0.81
1:A:286:GLN:HE22	1:A:465:LEU:HA	1.45	0.80
1:B:335:ASN:HD22	1:B:335:ASN:C	1.86	0.79
1:A:207:GLU:HB3	3:A:1086:HOH:O	1.82	0.79
1:B:335:ASN:ND2	1:B:337:ASP:H	1.82	0.77
1:B:466:HIS:NE2	1:B:469:LEU:HD12	1.99	0.77
1:A:475:ASP:O	1:A:476[A]:LEU:HB3	1.85	0.77
1:B:341:ILE:HD13	1:B:342:SER:H	1.50	0.75
1:A:349:THR:HG21	3:A:1114:HOH:O	1.87	0.74
1:A:471:GLU:OE2	1:A:474:LYS:HD3	1.86	0.74
1:A:474:LYS:O	1:A:475:ASP:HB2	1.86	0.73
1:A:349:THR:HG23	3:A:1008:HOH:O	1.88	0.73
1:B:467:PRO:HG3	3:B:551:HOH:O	1.88	0.73
1:A:329:MET:SD	2:A:999:DRH:HAA3	2.29	0.73
1:B:451:GLN:O	1:B:454:GLN:HG2	1.88	0.72
1:A:349:THR:HG22	1:A:352:PHE:H	1.54	0.72
1:A:473:TYR:HD2	1:A:476[B]:LEU:HD11	1.56	0.71
1:A:448:GLU:O	1:A:451:GLN:HG2	1.90	0.70
1:A:476[B]:LEU:HD22	3:A:1065:HOH:O	1.92	0.70
1:B:358:LYS:N	1:B:358:LYS:HE3	2.07	0.69
1:B:335:ASN:ND2	1:B:338:GLY:H	1.90	0.69
2:A:999:DRH:OAD	2:A:999:DRH:HAK	1.94	0.68
1:B:255:LEU:HD21	1:B:281:ILE:HD11	1.76	0.68
2:A:999:DRH:CAZ	2:A:999:DRH:HAK	2.24	0.68
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.77	0.67
1:B:279:ILE:O	1:B:283:GLN:HG3	1.94	0.67
1:B:463:MET:HG3	1:B:465:LEU:H	1.61	0.66
1:A:453:LEU:HD21	3:A:1000:HOH:O	1.95	0.65
1:B:441:ASP:O	1:B:445:ILE:HG12	1.97	0.65
1:B:367:LYS:HZ1	1:B:449:HIS:HB2	1.63	0.64
1:A:437:GLN:HG2	1:B:439:MET:HE1	1.80	0.63
1:A:450:VAL:HG21	1:A:476[B]:LEU:HD13	1.81	0.62
1:A:357:ARG:HG2	1:A:359:PRO:HD2	1.81	0.62
1:B:237:LEU:HD21	1:B:340:LEU:HG	1.82	0.61
1:A:326:ILE:HA	2:A:999:DRH:HAA2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ALA:HB1	2:A:999:DRH:HAN2	1.82	0.60
1:A:440:THR:O	1:A:444:GLN:HG2	2.01	0.60
1:A:325:ILE:HD13	1:A:388:ILE:HG23	1.83	0.60
1:A:262:ILE:HG22	1:A:263:LYS:H	1.65	0.60
1:A:473:TYR:HE1	3:A:1000:HOH:O	1.85	0.60
1:A:296:ILE:HD11	2:A:999:DRH:HAA1	1.84	0.59
1:A:291:GLU:O	1:A:295:GLU:HG3	2.02	0.59
1:B:335:ASN:ND2	1:B:337:ASP:N	2.50	0.59
1:A:253:ASN:HA	1:A:256:MET:CE	2.33	0.59
1:B:358:LYS:HB2	1:B:359:PRO:HD3	1.84	0.59
1:A:363:PHE:CD1	1:A:452:LEU:HD23	2.38	0.59
1:B:343:GLU:HG3	1:B:343:GLU:O	2.04	0.58
1:B:348:MET:SD	1:B:353:LEU:HD21	2.44	0.58
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.33	0.58
1:A:474:LYS:O	1:A:475:ASP:CB	2.51	0.58
1:A:475:ASP:O	1:A:476[B]:LEU:HG	2.04	0.58
1:A:268:THR:N	1:A:269:PRO:HD2	2.19	0.58
1:A:259:GLU:HB3	1:A:268:THR:OG1	2.02	0.58
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.85	0.58
1:B:259:GLU:CD	1:B:280:ARG:HH21	2.07	0.57
1:B:212:ARG:CB	1:B:212:ARG:HH11	2.09	0.57
1:A:286:GLN:CA	2:A:999:DRH:HAB1	2.34	0.57
1:A:452:LEU:O	1:A:456:ILE:HG12	2.05	0.57
1:A:475:ASP:O	1:A:476[A]:LEU:HD23	2.04	0.57
2:A:999:DRH:HAC2	3:A:1000:HOH:O	2.05	0.57
1:A:450:VAL:HG21	1:A:476[B]:LEU:CD1	2.35	0.57
1:A:336:LYS:NZ	1:A:350:ARG:HH12	2.02	0.57
1:A:383:ASP:OD2	1:A:425:HIS:HE1	1.87	0.57
1:A:460:GLU:HB3	1:A:463:MET:HB2	1.87	0.56
1:A:286:GLN:HA	2:A:999:DRH:CAO	2.36	0.56
1:B:466:HIS:N	1:B:467:PRO:CD	2.68	0.56
1:A:475:ASP:O	1:A:476[A]:LEU:CB	2.53	0.55
1:A:336:LYS:HD3	1:A:350:ARG:NH1	2.21	0.55
1:B:259:GLU:OE2	1:B:280:ARG:NH2	2.38	0.55
1:A:286:GLN:N	2:A:999:DRH:HAB1	2.22	0.55
1:B:228:LEU:HD22	1:B:233:ALA:HB2	1.88	0.54
1:A:474:LYS:O	1:A:474:LYS:HG2	2.06	0.54
1:A:434:LYS:NZ	1:B:410:GLN:HE21	2.06	0.54
1:A:414:LEU:HB3	1:B:430:GLN:HG2	1.89	0.53
1:A:319:LYS:CE	1:A:475:ASP:HB3	2.39	0.53
1:B:335:ASN:ND2	1:B:335:ASN:C	2.60	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:VAL:O	1:B:281:ILE:HG12	2.09	0.53
1:A:443:ARG:NE	3:A:1014:HOH:O	2.30	0.53
1:A:276:GLU:OE2	1:A:357:ARG:NH2	2.42	0.53
1:B:232:LYS:HG3	3:B:540:HOH:O	2.09	0.53
1:A:433:ALA:O	1:A:437:GLN:HG3	2.08	0.53
1:B:256:MET:CE	1:B:280:ARG:HH22	2.23	0.52
1:A:402:ASN:HB2	3:A:1039:HOH:O	2.10	0.52
1:A:414:LEU:CB	1:B:430:GLN:HG2	2.40	0.52
1:B:467:PRO:O	1:B:469:LEU:N	2.39	0.52
1:B:241:THR:HG22	1:B:243:ASP:OD1	2.10	0.51
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.41	0.51
1:A:253:ASN:HA	1:A:256:MET:HE2	1.93	0.51
1:A:330:LEU:HD22	2:A:999:DRH:HAT1	1.93	0.51
1:B:334:MET:HG2	1:B:339:VAL:HB	1.93	0.50
1:B:448:GLU:O	1:B:451:GLN:HB3	2.12	0.50
1:B:212:ARG:NH1	1:B:212:ARG:HB3	2.11	0.50
1:B:430:GLN:HG3	1:B:433:ALA:CB	2.39	0.50
1:A:450:VAL:HG21	1:A:476[A]:LEU:HD13	1.94	0.50
1:A:261:LYS:C	1:A:261:LYS:HD3	2.32	0.50
1:B:255:LEU:CD2	1:B:281:ILE:HD11	2.40	0.50
1:A:354:LYS:HA	1:A:361:GLY:O	2.12	0.50
1:A:276:GLU:O	1:A:280:ARG:HB2	2.12	0.49
1:A:249:ILE:HD12	1:A:255:LEU:HA	1.94	0.49
1:A:329:MET:HB2	2:A:999:DRH:HAA3	1.95	0.49
1:B:252:MET:O	1:B:256:MET:HG2	2.12	0.48
1:A:475:ASP:O	1:A:476[B]:LEU:CB	2.54	0.48
1:B:335:ASN:ND2	1:B:338:GLY:N	2.58	0.48
1:B:324:GLU:OE2	1:B:443:ARG:HD2	2.13	0.48
1:B:341:ILE:CD1	1:B:342:SER:H	2.21	0.48
1:B:256:MET:HE1	1:B:280:ARG:HH22	1.78	0.48
1:A:329:MET:SD	2:A:999:DRH:CAA	3.00	0.48
1:A:288:ARG:NH1	1:A:292:ALA:HB2	2.29	0.48
1:A:256:MET:O	1:A:268:THR:HG23	2.14	0.48
1:B:435:LEU:O	1:B:438:LYS:HB2	2.13	0.48
1:A:239:GLY:C	1:A:241:THR:N	2.64	0.48
1:A:475:ASP:O	1:A:476[B]:LEU:CG	2.62	0.48
1:A:453:LEU:HD11	2:A:999:DRH:CAC	2.44	0.47
1:A:261:LYS:O	1:A:261:LYS:HD3	2.14	0.47
1:A:330:LEU:HD13	2:A:999:DRH:NBF	2.28	0.47
1:A:277:VAL:HG13	1:A:278:ALA:N	2.29	0.47
1:B:447:THR:O	1:B:450:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:HA	1:A:256:MET:HE3	1.97	0.47
1:A:454[B]:GLN:NE2	3:A:1076:HOH:O	2.47	0.47
1:A:453:LEU:HD11	2:A:999:DRH:HAC1	1.96	0.47
1:A:330:LEU:HD13	2:A:999:DRH:CAU	2.44	0.47
1:A:288:ARG:HH12	1:A:292:ALA:HB2	1.80	0.47
1:B:328:THR:OG1	1:B:442:LEU:HD11	2.14	0.47
1:B:293:VAL:HG22	1:B:322:VAL:CG2	2.35	0.47
1:A:460:GLU:O	1:A:463:MET:HB2	2.15	0.47
1:A:475:ASP:O	1:A:476[A]:LEU:CD2	2.63	0.46
1:A:473:TYR:CD2	1:A:476[B]:LEU:HD11	2.44	0.46
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.96	0.46
1:A:441:ASP:O	1:A:445:ILE:HG12	2.15	0.46
1:A:468:LEU:O	1:A:472:ILE:HG23	2.14	0.46
1:B:244:LYS:HG3	1:B:244:LYS:O	2.15	0.46
1:A:268:THR:HB	1:A:269:PRO:HD3	1.96	0.46
1:A:239:GLY:C	1:A:241:THR:H	2.19	0.46
1:A:276:GLU:HG2	1:A:277:VAL:N	2.30	0.46
1:A:472:ILE:HD12	1:A:472:ILE:C	2.36	0.46
1:A:311:LEU:HD23	1:A:311:LEU:C	2.35	0.46
1:A:296:ILE:HD11	2:A:999:DRH:CAA	2.45	0.46
1:B:335:ASN:HD22	1:B:337:ASP:H	1.57	0.46
1:B:307:VAL:HG22	3:B:480:HOH:O	2.15	0.46
1:A:336:LYS:HZ3	1:A:350:ARG:HH12	1.64	0.46
1:B:335:ASN:HD21	1:B:338:GLY:N	2.14	0.46
1:A:262:ILE:HG22	1:A:263:LYS:N	2.29	0.46
1:A:259:GLU:OE1	1:A:268:THR:OG1	2.33	0.46
1:B:335:ASN:HD22	1:B:337:ASP:N	2.14	0.45
1:A:210:ASP:N	3:A:1086:HOH:O	2.44	0.45
1:B:327:TYR:OH	1:B:449:HIS:CD2	2.68	0.45
1:A:466:HIS:ND1	1:A:467:PRO:HD2	2.31	0.45
1:B:341:ILE:HD13	1:B:342:SER:N	2.26	0.45
1:A:471:GLU:O	1:A:474:LYS:HB3	2.17	0.45
1:A:207:GLU:HG3	1:A:209:ALA:H	1.82	0.45
1:B:228:LEU:HD23	1:B:232:LYS:HB3	1.99	0.45
1:A:341:ILE:HG22	2:A:999:DRH:CAL	2.47	0.45
1:A:341:ILE:HG22	2:A:999:DRH:HAL	1.99	0.45
1:A:268:THR:HB	1:A:269:PRO:CD	2.46	0.45
1:B:451:GLN:OE1	1:B:452:LEU:N	2.49	0.45
1:A:268:THR:H	1:A:269:PRO:HD2	1.81	0.45
1:A:446:VAL:HG11	3:A:1065:HOH:O	2.17	0.45
1:B:460:GLU:O	1:B:461:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LEU:HD22	2:A:999:DRH:CAT	2.48	0.44
1:B:466:HIS:CD2	1:B:469:LEU:HB3	2.53	0.44
1:B:249:ILE:HD12	1:B:255:LEU:HA	1.99	0.44
1:A:449:HIS:HE2	2:A:999:DRH:HAC1	1.83	0.44
1:A:289:SER:HG	2:A:999:DRH:HAK	1.81	0.44
1:B:249:ILE:HG23	1:B:255:LEU:HA	2.00	0.44
1:B:367:LYS:NZ	1:B:449:HIS:HB2	2.32	0.44
1:B:313:ASP:CB	3:B:510:HOH:O	2.65	0.44
1:B:467:PRO:C	1:B:469:LEU:H	2.19	0.43
1:A:476[A]:LEU:HG	1:A:476[A]:LEU:O	2.19	0.43
1:A:428:SER:OG	1:A:431:LEU:HB2	2.19	0.43
1:B:288:ARG:CZ	1:B:291:GLU:OE1	2.66	0.43
1:B:418:GLU:O	1:B:422[B]:LYS:HG3	2.19	0.43
1:B:466:HIS:N	1:B:467:PRO:HD2	2.32	0.43
1:A:363:PHE:CE2	1:A:456:ILE:HG13	2.54	0.43
1:A:323:HIS:CE1	1:A:472:ILE:HD11	2.54	0.43
1:A:234[B]:ARG:HH11	1:A:234[B]:ARG:HG3	1.84	0.42
1:A:437:GLN:HG2	1:B:439:MET:CE	2.48	0.42
1:A:475:ASP:O	1:A:476[B]:LEU:HB2	2.17	0.42
1:A:435:LEU:O	1:A:438:LYS:HB2	2.19	0.42
1:A:336:LYS:HD3	1:A:350:ARG:HH12	1.82	0.42
1:B:286:GLN:HB3	1:B:473:TYR:CD2	2.54	0.42
1:A:262:ILE:CG2	1:A:263:LYS:H	2.27	0.42
1:B:386:ILE:HB	1:B:417:LEU:HD13	2.02	0.42
1:A:255:LEU:HD21	1:A:277:VAL:HG23	2.01	0.42
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.83	0.42
1:B:219:TYR:HB2	3:B:503:HOH:O	2.19	0.42
1:A:359:PRO:HB2	1:A:456:ILE:HD11	2.01	0.42
1:A:252:MET:HG2	3:A:1087:HOH:O	2.19	0.42
1:A:277:VAL:O	1:A:281:ILE:HG13	2.20	0.41
1:B:468:LEU:O	1:B:472:ILE:HG13	2.20	0.41
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.55	0.41
1:A:359:PRO:HB2	1:A:456:ILE:CD1	2.50	0.41
1:B:436:LEU:HA	1:B:439:MET:HE2	2.02	0.41
1:A:286:GLN:HA	2:A:999:DRH:HAO2	2.01	0.41
1:A:330:LEU:HD13	2:A:999:DRH:HAU1	2.02	0.41
1:B:325:ILE:HD11	1:B:392:ILE:HG13	2.02	0.41
1:B:310:ASP:HA	3:B:483:HOH:O	2.20	0.41
1:A:443:ARG:HD3	3:A:1004:HOH:O	2.21	0.41
1:A:363:PHE:CZ	1:A:452:LEU:HG	2.56	0.41
1:A:357:ARG:HH12	1:A:460:GLU:CD	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ILE:O	1:B:237:LEU:O	2.39	0.41
1:A:443:ARG:NH1	3:A:1016:HOH:O	2.54	0.41
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.90	0.41
1:B:215:ALA:HA	1:B:386:ILE:CD1	2.51	0.40
1:B:217:HIS:HE1	1:B:302:SER:O	2.04	0.40
1:B:467:PRO:C	1:B:469:LEU:N	2.75	0.40
1:A:276:GLU:HG2	1:A:277:VAL:H	1.86	0.40
1:B:436:LEU:CA	1:B:439:MET:HE2	2.51	0.40
1:A:364:MET:SD	2:A:999:DRH:HAM	2.62	0.40
2:A:999:DRH:HAV1	2:A:999:DRH:HAI	1.97	0.40
1:B:373:LYS:HB3	1:B:438:LYS:NZ	2.36	0.40
1:B:329:MET:HB3	3:B:511:HOH:O	2.22	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	273/286 (96%)	258 (94%)	9 (3%)	6 (2%)	8	4
1	B	270/286 (94%)	239 (88%)	22 (8%)	9 (3%)	5	2
All	All	543/572 (95%)	497 (92%)	31 (6%)	15 (3%)	6	3

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	475	ASP
1	B	237	LEU
1	B	357	ARG
1	B	466	HIS
1	A	269	PRO
1	A	275	LYS

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Mol	Chain	Res	Type
1	B	263	LYS
1	B	462	ASP
1	A	272	GLU
1	A	358	LYS
1	B	244	LYS
1	B	275	LYS
1	A	262	ILE
1	B	463	MET
1	B	227	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/257 (97%)	234 (94%)	15 (6%)	24	23
1	B	245/257 (95%)	227 (93%)	18 (7%)	17	16
All	All	494/514 (96%)	461 (93%)	33 (7%)	22	19

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244[A]	LYS
1	A	244[B]	LYS
1	A	271	GLN
1	A	283	GLN
1	A	342	SER
1	A	363	PHE
1	A	410	GLN
1	A	412	ASN
1	A	427	GLU
1	A	460	GLU
1	A	463	MET
1	A	465	LEU
1	A	472	ILE
1	A	476[A]	LEU

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Mol	Chain	Res	Type
1	A	476[B]	LEU
1	B	212	ARG
1	B	228	LEU
1	B	238	THR
1	B	251	ASP
1	B	263	LYS
1	B	272	GLU
1	B	273	GLN
1	B	318	LEU
1	B	330	LEU
1	B	335	ASN
1	B	336	LYS
1	B	341	ILE
1	B	358	LYS
1	B	412	ASN
1	B	443	ARG
1	B	451	GLN
1	B	460	GLU
1	B	470	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
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	437	GLN
1	A	451	GLN
1	A	470	GLN
1	B	217	HIS
1	B	308	ASN
1	B	335	ASN
1	B	410	GLN
1	B	412	ASN
1	B	430	GLN
1	B	449	HIS
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 ⓘ

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	-	29,35,35	0.81	0	28,47,47	0.94	1 (3%)

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	1/22/30/30	0/2/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	DRH	CAU-NBF-CBC	-2.84	116.59	120.55

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	999	DRH	NBF

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	999	DRH	CAT-CAV-NBF-CBC

There are no ring outliers.

1 monomer is involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	DRH	28	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	262/286 (91%)	0.70	24 (9%) 11 12	23, 39, 66, 81	1 (0%)
1	B	261/286 (91%)	1.29	55 (21%) 1 1	25, 43, 88, 98	7 (2%)
All	All	523/572 (91%)	0.99	79 (15%) 3 3	23, 41, 78, 98	8 (1%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	242	THR	14.8
1	A	267	ILE	13.6
1	A	269	PRO	12.7
1	B	270	LEU	12.0
1	B	285	CYS	11.1
1	A	268	THR	10.4
1	B	463	MET	10.3
1	B	269	PRO	9.4
1	B	465	LEU	9.4
1	B	264	PHE	8.8
1	B	461	THR	8.1
1	B	241	THR	7.9
1	A	265	LYS	7.5
1	B	238	THR	7.4
1	B	464	SER	7.4
1	B	462	ASP	7.3
1	B	240	LYS	6.7
1	A	240	LYS	6.0
1	B	267	ILE	5.9
1	B	476	LEU	5.8
1	B	263	LYS	5.6
1	A	476[A]	LEU	5.4
1	B	475	ASP	5.3
1	B	243	ASP	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	263	LYS	5.1
1	B	358	LYS	5.0
1	B	256	MET	4.7
1	A	358	LYS	4.6
1	B	454	GLN	4.6
1	B	207	GLU	4.5
1	A	252	MET	4.3
1	A	262	ILE	4.2
1	B	244	LYS	4.0
1	B	473	TYR	3.9
1	B	275	LYS	3.9
1	B	469	LEU	3.7
1	B	451	GLN	3.6
1	B	452	LEU	3.4
1	A	261	LYS	3.4
1	B	459	THR	3.3
1	A	287	PHE	3.2
1	A	259	GLU	3.2
1	B	255	LEU	3.2
1	A	241	THR	3.1
1	B	455	VAL	3.0
1	B	341	ILE	2.9
1	B	427	GLU	2.9
1	A	404	LYS	2.9
1	B	262	ILE	2.9
1	B	474	LYS	2.8
1	A	427	GLU	2.7
1	A	422	LYS	2.7
1	B	361	GLY	2.7
1	B	470	GLN	2.6
1	B	247	PHE	2.5
1	B	456	ILE	2.5
1	B	466	HIS	2.4
1	B	363	PHE	2.4
1	B	339	VAL	2.4
1	A	362	ASP	2.3
1	B	208	SER	2.3
1	B	345	GLN	2.3
1	B	359	PRO	2.3
1	B	259	GLU	2.3
1	A	325	ILE	2.2
1	B	237	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	460	GLU	2.2
1	A	474	LYS	2.2
1	B	234	ARG	2.2
1	B	279	ILE	2.1
1	A	363	PHE	2.1
1	A	243	ASP	2.1
1	B	210	ASP	2.1
1	B	252	MET	2.1
1	B	280	ARG	2.1
1	B	360	PHE	2.1
1	A	401	LEU	2.1
1	B	336	LYS	2.1
1	A	239	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DRH	A	999	33/33	0.70	0.42	7.44	69,76,79,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.