



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 11:50 PM EDT

PDB ID : 2I4J
Title : Crystal structure of the complex between PPARgamma and the agonist LT160 (ureidofibrate derivative)
Authors : Pochetti, G.; Mazza, F.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

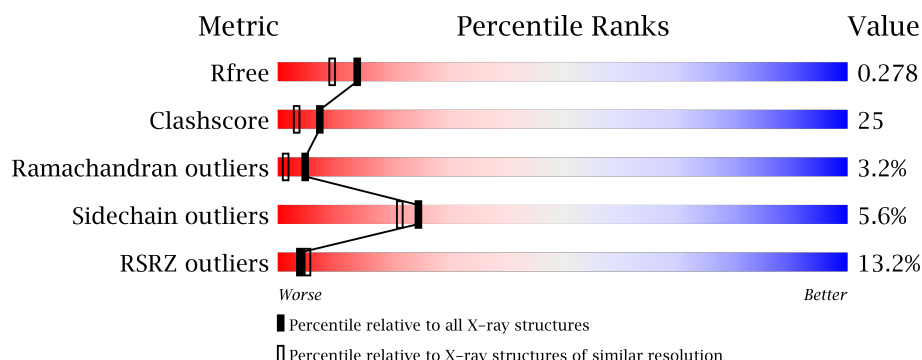
1 Overall quality at a glance

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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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. 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>31%</div> <div>• 6%</div> </div>
1	B	286	<div> <div>16%</div> <div>58%</div> <div>30%</div> <div>5% • 6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4552 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.

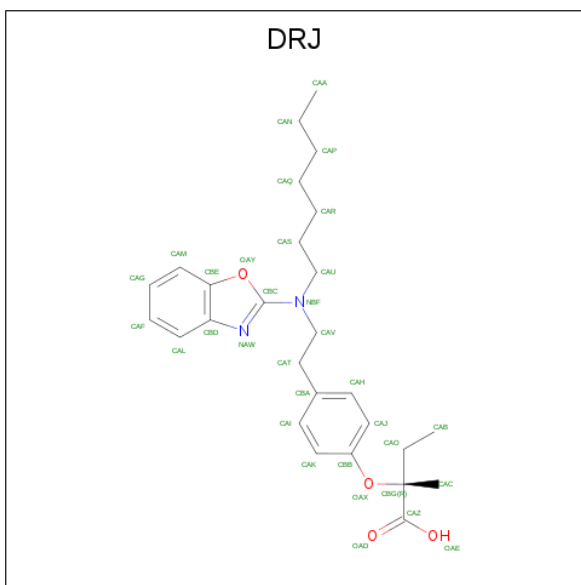
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	77	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	-	EXPRESSION TAG	UNP P37231
A	192	SER	-	EXPRESSION TAG	UNP P37231
A	193	HIS	-	EXPRESSION TAG	UNP P37231
A	194	MET	-	EXPRESSION TAG	UNP P37231
B	191	GLY	-	EXPRESSION TAG	UNP P37231
B	192	SER	-	EXPRESSION TAG	UNP P37231
B	193	HIS	-	EXPRESSION TAG	UNP P37231
B	194	MET	-	EXPRESSION TAG	UNP P37231

- Molecule 2 is (2R)-2-(4-{2-[1,3-BENZOXAZOL-2-YL(HEPTYL)AMINO]ETHYL}PHENOXY)-2-METHYLBUTANOIC ACID (three-letter code: DRJ) (formula: C₂₇H₃₆N₂O₄).



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

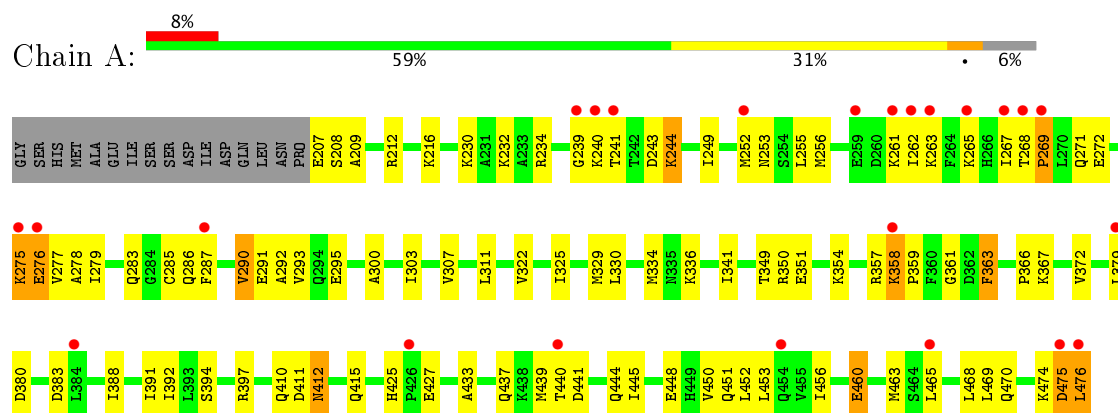
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	109	Total O 109 109	0	0
3	B	78	Total O 78 78	0	0

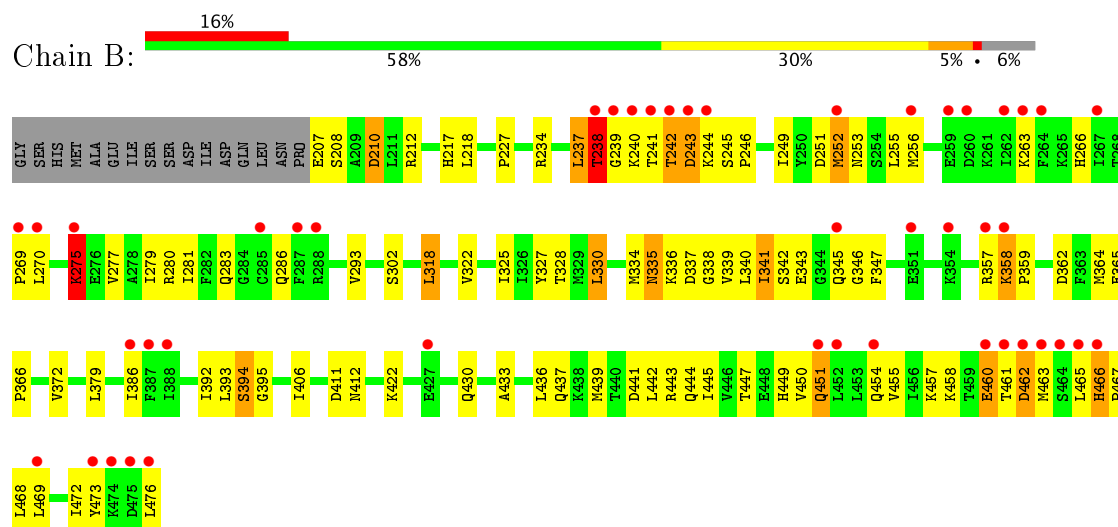
3 Residue-property plots

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: 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	93.14Å 60.95Å 118.11Å 90.00° 103.26° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10 19.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	85.1 (8.00-2.10) 85.9 (19.97-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.278 0.246 , 0.278	Depositor DCC
R_{free} test set	1576 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 58.9	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	0.93	EDS
Total number of atoms	4552	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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: DRJ

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	0/2203	0.61	1/2967 (0.0%)
1	B	0.33	0/2203	0.58	0/2967
All	All	0.36	0/4406	0.59	1/5934 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	ASP	CA-C-N	-5.01	106.17	117.20

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	2166	0	2232	112	0
1	B	2166	0	2232	98	0
2	A	33	0	35	13	0
3	A	109	0	0	13	0
3	B	78	0	0	12	0
All	All	4552	0	4499	211	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 (211) 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:329:MET:SD	2:A:999:DRJ:HAA2	1.86	1.13
1:B:293:VAL:HG22	1:B:322:VAL:HG21	1.35	1.08
1:A:292:ALA:HB1	2:A:999:DRJ:HAN1	1.35	1.04
1:A:275:LYS:HE2	1:A:283:GLN:HE22	1.26	1.01
1:B:335:ASN:ND2	1:B:337:ASP:H	1.60	0.98
1:A:474:LYS:C	1:A:476:LEU:H	1.62	0.94
1:B:293:VAL:HG21	1:B:476:LEU:HD11	1.50	0.90
1:A:437:GLN:O	1:A:440:THR:HG22	1.77	0.85
1:B:335:ASN:HD22	1:B:335:ASN:C	1.80	0.85
1:A:474:LYS:C	1:A:476:LEU:N	2.29	0.84
1:A:476:LEU:HA	3:A:1046:HOH:O	1.78	0.84
1:B:240:LYS:HG3	1:B:241:THR:H	1.45	0.82
1:B:430:GLN:HG3	1:B:433:ALA:HB3	1.60	0.81
1:A:300:ALA:HA	1:A:303:ILE:HD13	1.61	0.81
1:B:451:GLN:O	1:B:454:GLN:HG2	1.81	0.81
1:A:444:GLN:HB3	3:A:1077:HOH:O	1.79	0.81
1:A:253:ASN:HA	1:A:256:MET:HE3	1.65	0.78
1:B:455:VAL:HA	1:B:458:LYS:HE2	1.64	0.78
1:B:275:LYS:HE3	1:B:275:LYS:HA	1.66	0.78
1:B:335:ASN:HD22	1:B:337:ASP:H	1.29	0.78
1:B:269:PRO:HA	1:B:280:ARG:NH2	1.99	0.77
1:B:212:ARG:NH1	1:B:212:ARG:HB3	2.00	0.76
1:B:411:ASP:HB2	3:B:527:HOH:O	1.86	0.74
1:B:239:GLY:HA3	3:B:522:HOH:O	1.86	0.73
1:B:358:LYS:N	1:B:358:LYS:HE3	2.05	0.72
1:B:466:HIS:N	1:B:467:PRO:HD2	2.05	0.72
2:A:999:DRJ:CAZ	2:A:999:DRJ:HAK	2.21	0.70
1:A:341:ILE:HG22	2:A:999:DRJ:HAL	1.73	0.69
1:B:335:ASN:ND2	1:B:337:ASP:N	2.39	0.69
1:A:329:MET:SD	2:A:999:DRJ:CAA	2.74	0.68
1:A:341:ILE:HG22	2:A:999:DRJ:CAL	2.24	0.68
1:B:466:HIS:N	1:B:467:PRO:CD	2.58	0.66
1:A:291:GLU:O	1:A:295:GLU:HG3	1.96	0.65
1:A:433:ALA:O	1:A:437:GLN:HG3	1.97	0.65
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.78	0.65
1:A:363:PHE:CZ	1:A:452:LEU:HG	2.31	0.65
1:B:279:ILE:O	1:B:283:GLN:HG3	1.97	0.64
1:B:358:LYS:HB2	1:B:359:PRO:HD3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:THR:H	1:A:269:PRO:HD2	1.63	0.64
1:B:336:LYS:HG3	3:B:492:HOH:O	1.97	0.64
1:B:217:HIS:HE1	1:B:302:SER:O	1.81	0.64
1:A:476:LEU:HD12	3:A:1005:HOH:O	1.98	0.63
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.81	0.63
1:B:207:GLU:HB3	3:B:529:HOH:O	1.99	0.63
1:A:383:ASP:OD2	1:A:425:HIS:HE1	1.82	0.63
1:B:249:ILE:HD12	1:B:255:LEU:HA	1.80	0.62
1:B:252:MET:O	1:B:256:MET:HG2	1.99	0.62
1:B:343:GLU:HG3	1:B:343:GLU:O	2.00	0.62
1:A:349:THR:HG22	1:A:351:GLU:H	1.64	0.61
1:B:207:GLU:HB2	1:B:210:ASP:OD1	2.00	0.61
1:B:212:ARG:HB3	1:B:212:ARG:HH11	1.64	0.61
1:B:457:LYS:NZ	1:B:461:THR:HG22	2.15	0.61
1:A:249:ILE:HD12	1:A:255:LEU:HA	1.82	0.61
1:B:335:ASN:ND2	1:B:335:ASN:C	2.54	0.61
1:A:276:GLU:OE2	1:A:279:ILE:HG13	2.01	0.61
1:A:411:ASP:O	1:A:415:GLN:HG3	2.01	0.61
1:A:311:LEU:HD23	1:A:311:LEU:C	2.22	0.60
1:A:286:GLN:NE2	1:A:465:LEU:HD12	2.17	0.60
1:B:275:LYS:HA	1:B:275:LYS:CE	2.32	0.60
1:A:475:ASP:O	1:A:476:LEU:O	2.20	0.60
1:A:207:GLU:HA	3:A:1025:HOH:O	2.02	0.60
1:B:335:ASN:HD22	1:B:337:ASP:N	2.00	0.60
1:A:212:ARG:O	1:A:216:LYS:HD3	2.02	0.59
1:A:261:LYS:HE2	1:A:262:ILE:CD1	2.30	0.59
1:A:262:ILE:N	1:A:262:ILE:HD12	2.17	0.59
1:A:285:CYS:SG	2:A:999:DRJ:HAM	2.42	0.59
1:A:275:LYS:HE2	1:A:283:GLN:NE2	2.08	0.58
1:B:467:PRO:C	1:B:469:LEU:H	2.06	0.58
1:B:286:GLN:HG3	3:B:526:HOH:O	2.04	0.58
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.33	0.58
1:A:394:SER:O	1:A:397:ARG:HG2	2.04	0.58
1:B:255:LEU:HD21	1:B:281:ILE:HD11	1.86	0.58
1:A:475:ASP:HB3	3:A:1079:HOH:O	2.04	0.57
1:B:468:LEU:O	1:B:472:ILE:HG13	2.04	0.57
1:A:469:LEU:HD13	2:A:999:DRJ:HAC3	1.87	0.56
1:B:465:LEU:O	1:B:466:HIS:CB	2.53	0.56
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.86	0.56
1:A:256:MET:HG2	1:A:268:THR:O	2.04	0.56
1:A:293:VAL:HG11	1:A:468:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:GLN:HE22	1:B:437:GLN:HE22	1.54	0.55
1:A:440:THR:HB	3:B:525:HOH:O	2.05	0.55
1:B:336:LYS:HG2	1:B:372:VAL:HG22	1.88	0.55
1:A:239:GLY:HA2	1:A:241:THR:HG22	1.89	0.55
1:B:255:LEU:CD2	1:B:281:ILE:HD11	2.37	0.55
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.37	0.55
1:B:208:SER:O	1:B:212:ARG:HG2	2.06	0.55
1:B:227:PRO:HD2	3:B:516:HOH:O	2.06	0.54
1:B:335:ASN:ND2	1:B:338:GLY:H	2.05	0.54
1:A:268:THR:N	1:A:269:PRO:HD2	2.20	0.54
1:B:212:ARG:CB	1:B:212:ARG:HH11	2.20	0.54
1:B:218:LEU:HD12	1:B:386:ILE:HD12	1.89	0.54
1:A:208:SER:O	1:A:212:ARG:HG2	2.07	0.54
1:A:450:VAL:CG1	1:A:475:ASP:HA	2.38	0.54
1:A:476:LEU:CD1	3:A:1005:HOH:O	2.56	0.54
1:B:330:LEU:HD11	1:B:364:MET:HE1	1.88	0.54
1:A:391:ILE:HD13	1:A:439:MET:CE	2.38	0.53
1:A:448:GLU:O	1:A:451:GLN:HG2	2.09	0.53
1:A:276:GLU:CD	1:A:357:ARG:NH2	2.62	0.53
1:A:240:LYS:HG2	1:A:240:LYS:O	2.08	0.53
1:A:325:ILE:CD1	1:A:388:ILE:HG23	2.38	0.53
1:B:394:SER:O	1:B:406:ILE:HG22	2.10	0.52
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.39	0.52
1:B:441:ASP:O	1:B:445:ILE:HG12	2.10	0.52
1:A:303:ILE:HD12	1:A:303:ILE:N	2.25	0.52
1:A:311:LEU:O	1:A:311:LEU:HD23	2.10	0.52
1:B:436:LEU:HA	1:B:439:MET:CE	2.40	0.52
1:A:450:VAL:HG11	1:A:475:ASP:HA	1.91	0.51
1:A:380:ASP:HB2	3:A:1007:HOH:O	2.10	0.51
1:B:325:ILE:HD11	1:B:392:ILE:HG12	1.93	0.51
1:A:391:ILE:HD13	1:A:439:MET:HE3	1.92	0.51
1:A:474:LYS:O	1:A:475:ASP:HB2	2.11	0.51
1:A:276:GLU:OE1	1:A:357:ARG:NH2	2.44	0.51
1:A:256:MET:HA	1:A:268:THR:HG23	1.93	0.51
1:A:453:LEU:HD21	2:A:999:DRJ:HAB1	1.92	0.51
1:B:365:GLU:N	1:B:366:PRO:HD2	2.27	0.50
1:A:253:ASN:HA	1:A:256:MET:CE	2.40	0.50
1:A:325:ILE:HD13	1:A:388:ILE:HG23	1.93	0.50
1:A:336:LYS:HD3	1:A:350:ARG:HH12	1.76	0.50
1:B:341:ILE:HG22	1:B:346:GLY:HA3	1.94	0.49
1:A:465:LEU:HD23	1:A:470:GLN:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:PRO:HD2	3:B:531:HOH:O	2.11	0.49
1:B:334:MET:HG2	1:B:339:VAL:HB	1.92	0.49
1:A:239:GLY:C	1:A:241:THR:N	2.65	0.49
1:B:457:LYS:HZ2	1:B:461:THR:HG22	1.77	0.49
1:A:261:LYS:HB3	1:A:262:ILE:HD12	1.93	0.49
1:A:336:LYS:HD3	1:A:350:ARG:NH1	2.28	0.49
1:B:241:THR:O	1:B:243:ASP:OD1	2.30	0.48
1:B:279:ILE:N	1:B:279:ILE:HD12	2.28	0.48
1:A:267:ILE:HD12	1:A:275:LYS:HB3	1.95	0.48
1:A:357:ARG:HG2	1:A:358:LYS:N	2.28	0.48
1:B:240:LYS:HG3	1:B:241:THR:N	2.21	0.48
1:A:232:LYS:HE3	3:A:1000:HOH:O	2.14	0.48
2:A:999:DRJ:OAD	2:A:999:DRJ:HAK	2.13	0.48
1:B:457:LYS:HD2	1:B:457:LYS:O	2.14	0.48
1:B:447:THR:O	1:B:450:VAL:HG22	2.14	0.47
1:B:433:ALA:O	1:B:437:GLN:HG2	2.15	0.47
1:A:441:ASP:O	1:A:445:ILE:HG12	2.15	0.46
1:A:293:VAL:HG22	1:A:322:VAL:CG1	2.45	0.46
1:A:292:ALA:CB	2:A:999:DRJ:HAN1	2.24	0.46
1:A:287:PHE:O	1:A:290:VAL:HG13	2.16	0.46
1:B:444:GLN:HG3	3:B:539:HOH:O	2.16	0.46
1:B:393:LEU:O	1:B:394:SER:O	2.34	0.45
1:A:263:LYS:HZ3	1:A:265:LYS:HG3	1.80	0.45
1:B:255:LEU:CD2	1:B:277:VAL:HG13	2.47	0.45
1:B:439:MET:HG2	3:B:514:HOH:O	2.16	0.45
1:A:300:ALA:CA	1:A:303:ILE:HD13	2.39	0.45
1:A:268:THR:HB	1:A:269:PRO:CD	2.46	0.45
1:B:242:THR:O	1:B:243:ASP:HB3	2.16	0.45
1:B:342:SER:O	1:B:345:GLN:HG2	2.17	0.45
1:B:234:ARG:NH2	1:B:334:MET:O	2.35	0.45
1:A:207:GLU:HG3	1:A:209:ALA:H	1.82	0.45
1:B:255:LEU:HD23	1:B:277:VAL:HG13	1.98	0.45
1:B:237:LEU:HD21	1:B:340:LEU:HG	1.98	0.44
1:A:336:LYS:CD	1:A:372:VAL:HG21	2.47	0.44
1:A:357:ARG:HH12	1:A:460:GLU:CD	2.20	0.44
1:B:237:LEU:O	1:B:238:THR:C	2.56	0.44
1:A:474:LYS:HB2	3:A:1046:HOH:O	2.16	0.44
1:B:238:THR:HB	3:B:537:HOH:O	2.17	0.44
1:B:286:GLN:HB3	1:B:473:TYR:CD2	2.53	0.44
1:A:286:GLN:NE2	1:A:465:LEU:HA	2.33	0.44
1:A:276:GLU:OE2	1:A:278:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:H	1:B:280:ARG:NH1	2.16	0.44
1:B:286:GLN:HB3	1:B:473:TYR:HD2	1.83	0.44
1:A:336:LYS:HE2	1:A:372:VAL:HG11	2.00	0.43
1:A:230:LYS:O	1:A:234:ARG:HG2	2.18	0.43
1:B:293:VAL:HG22	1:B:322:VAL:CG2	2.25	0.43
1:B:279:ILE:N	1:B:279:ILE:CD1	2.82	0.43
1:B:460:GLU:O	1:B:461:THR:HG23	2.19	0.43
1:A:239:GLY:O	1:A:240:LYS:HB3	2.19	0.43
1:A:465:LEU:HD11	2:A:999:DRJ:CAB	2.49	0.43
1:B:327:TYR:OH	1:B:449:HIS:CD2	2.72	0.43
1:B:256:MET:HA	1:B:269:PRO:HB3	2.01	0.42
1:A:256:MET:CA	1:A:268:THR:HG23	2.49	0.42
1:A:268:THR:HB	1:A:269:PRO:HD3	2.00	0.42
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.80	0.42
1:A:349:THR:HG23	3:A:1017:HOH:O	2.19	0.42
1:A:444:GLN:HG3	3:A:1095:HOH:O	2.19	0.42
1:A:354:LYS:HA	1:A:361:GLY:O	2.20	0.42
1:B:358:LYS:CD	1:B:358:LYS:H	2.32	0.42
1:B:467:PRO:C	1:B:469:LEU:N	2.72	0.42
1:A:252:MET:O	1:A:255:LEU:HB3	2.20	0.42
1:A:474:LYS:O	1:A:476:LEU:N	2.52	0.42
1:B:240:LYS:O	1:B:241:THR:HB	2.20	0.42
1:B:358:LYS:CE	1:B:358:LYS:H	2.33	0.42
1:A:363:PHE:CE2	1:A:452:LEU:HG	2.54	0.42
1:A:244:LYS:O	1:A:244:LYS:HG2	2.20	0.41
1:B:358:LYS:HE3	1:B:358:LYS:H	1.80	0.41
1:B:436:LEU:HA	1:B:439:MET:HE3	2.00	0.41
1:B:422:LYS:HE2	3:B:535:HOH:O	2.19	0.41
1:B:328:THR:OG1	1:B:442:LEU:HD11	2.21	0.41
1:B:341:ILE:HG23	1:B:342:SER:N	2.35	0.41
1:A:357:ARG:HG2	1:A:359:PRO:HD2	2.03	0.41
1:A:456:ILE:HG21	1:A:463:MET:HE1	2.01	0.41
1:B:436:LEU:HA	1:B:439:MET:HE2	2.03	0.41
1:A:412:ASN:HD22	1:A:412:ASN:HA	1.68	0.41
1:B:245:SER:HA	1:B:246:PRO:HD3	1.94	0.41
1:B:473:TYR:N	1:B:473:TYR:CD1	2.88	0.41
1:A:285:CYS:SG	2:A:999:DRJ:CAM	3.09	0.41
1:B:244:LYS:HG3	1:B:244:LYS:O	2.21	0.41
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.55	0.41
1:A:330:LEU:O	1:A:334:MET:HG3	2.22	0.40
1:B:469:LEU:O	1:B:473:TYR:HD1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ILE:HD11	1:A:439:MET:HG2	2.03	0.40
1:A:240:LYS:HE2	3:A:1049:HOH:O	2.21	0.40
1:A:243:ASP:OD2	1:A:244:LYS:HD2	2.21	0.40
1:A:239:GLY:C	1:A:241:THR:H	2.24	0.40
1:A:307:VAL:HG22	3:A:1008:HOH:O	2.21	0.40
1:A:366:PRO:HG2	1:A:367:LYS:HE3	2.03	0.40
1:B:454:GLN:HG3	1:B:455:VAL:N	2.36	0.40
1:A:255:LEU:HD21	1:A:277:VAL:HG23	2.04	0.40
1:A:230:LYS:HE3	1:A:379:LEU:O	2.21	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%)	249 (93%)	14 (5%)	5 (2%)	9	4
1	B	268/286 (94%)	241 (90%)	15 (6%)	12 (4%)	3	1
All	All	536/572 (94%)	490 (91%)	29 (5%)	17 (3%)	5	1

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	GLU
1	B	237	LEU
1	B	394	SER
1	B	462	ASP
1	B	466	HIS
1	A	269	PRO
1	B	243	ASP
1	B	357	ARG
1	A	358	LYS

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Mol	Chain	Res	Type
1	B	238	THR
1	B	266	HIS
1	B	275	LYS
1	A	276	GLU
1	B	242	THR
1	A	275	LYS
1	B	463	MET
1	B	395	GLY

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%)	235 (97%)	8 (3%)	43	45
1	B	243/257 (95%)	224 (92%)	19 (8%)	15	11
All	All	486/514 (95%)	459 (94%)	27 (6%)	25	21

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	LYS
1	A	271	GLN
1	A	290	VAL
1	A	363	PHE
1	A	412	ASN
1	A	427	GLU
1	A	460	GLU
1	A	476	LEU
1	B	210	ASP
1	B	238	THR
1	B	251	ASP
1	B	252	MET
1	B	253	ASN
1	B	263	LYS
1	B	275	LYS

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Mol	Chain	Res	Type
1	B	318	LEU
1	B	330	LEU
1	B	335	ASN
1	B	341	ILE
1	B	358	LYS
1	B	362	ASP
1	B	379	LEU
1	B	412	ASN
1	B	443	ARG
1	B	451	GLN
1	B	460	GLU
1	B	462	ASP

Some 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	415	GLN
1	A	425	HIS
1	A	451	GLN
1	A	470	GLN
1	B	217	HIS
1	B	253	ASN
1	B	294	GLN
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	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	DRJ	A	999	-	28,35,35	0.87	0	29,47,47	0.84	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	DRJ	A	999	-	-	0/22/30/30	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	DRJ	CAV-NBF-CBC	-2.61	117.16	120.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	DRJ	13	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, 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%)	0.66	24 (9%) 10 12	25, 38, 67, 88	2 (0%)
1	B	261/286 (91%)	1.18	45 (17%) 2 2	24, 44, 84, 95	7 (2%)
All	All	523/572 (91%)	0.92	69 (13%) 4 5	24, 41, 80, 95	9 (1%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	ILE	16.7
1	B	270	LEU	13.6
1	B	465	LEU	13.3
1	B	242	THR	11.9
1	B	463	MET	10.9
1	B	263	LYS	10.7
1	B	464	SER	10.7
1	A	475	ASP	8.9
1	B	269	PRO	8.1
1	A	465	LEU	8.0
1	B	285	CYS	7.6
1	B	461	THR	7.4
1	B	462	ASP	7.4
1	A	263	LYS	6.8
1	B	476	LEU	6.6
1	A	268	THR	6.6
1	A	240	LYS	6.5
1	A	265	LYS	6.4
1	A	269	PRO	6.3
1	A	476	LEU	6.0
1	B	241	THR	5.7
1	A	262	ILE	5.7
1	B	238	THR	5.3
1	B	264	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	358	LYS	4.6
1	A	261	LYS	4.4
1	B	262	ILE	4.1
1	B	240	LYS	4.0
1	B	451	GLN	3.9
1	B	275	LYS	3.8
1	B	244	LYS	3.8
1	B	475	ASP	3.7
1	B	243	ASP	3.6
1	B	466	HIS	3.6
1	B	460	GLU	3.3
1	B	474	LYS	3.3
1	B	473	TYR	3.2
1	B	454	GLN	3.1
1	A	275	LYS	3.1
1	A	267	ILE	3.1
1	B	239	GLY	3.0
1	B	259	GLU	2.9
1	B	354	LYS	2.9
1	B	260	ASP	2.9
1	B	288	ARG	2.8
1	B	256	MET	2.7
1	B	452	LEU	2.7
1	B	351	GLU	2.6
1	A	239	GLY	2.6
1	A	384	LEU	2.6
1	A	358	LYS	2.6
1	B	357	ARG	2.5
1	A	287	PHE	2.5
1	B	345	GLN	2.5
1	A	259	GLU	2.4
1	A	454	GLN	2.3
1	A	241	THR	2.3
1	B	386	ILE	2.3
1	B	427	GLU	2.3
1	B	388	ILE	2.3
1	A	276	GLU	2.2
1	B	469	LEU	2.1
1	B	387	PHE	2.1
1	A	252	MET	2.1
1	B	252	MET	2.1
1	B	287	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	426	PRO	2.0
1	A	379	LEU	2.0
1	A	440	THR	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	DRJ	A	999	33/33	0.81	0.23	0.98	57,63,65,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.