WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:22 PM GMT

PDB ID : 1GWX
Title : MOLECULAR RECOGNITION OF FATTY ACIDS BY PEROXISOME PR OLIFERATOR-ACTIVATEDRECEPTORS
Authors : Xu, H.E.; Lambert, M.H.; Montana, V.G.; Park, D.J.; Blanchard, S.; Brown, P.; Sternbach, D.; Lehmann, J.; Bruce, G.W.; Willson, T.M.; Kliewer, S.A.; Milburn, M.V.
Deposited on : 1999-03-17
Resolution : 2.50 Å(reported)

1 Overall quality at a glance (i)

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.306
Clashscore		48
Ramachandran outliers		7.2%
Sidechain outliers		17.4%
RSRZ outliers		9.4%

Worse　　　　　Better

∎ Percentile relative to all X-ray structures

⬚ Percentile relative to X-ray structures of similar resolution
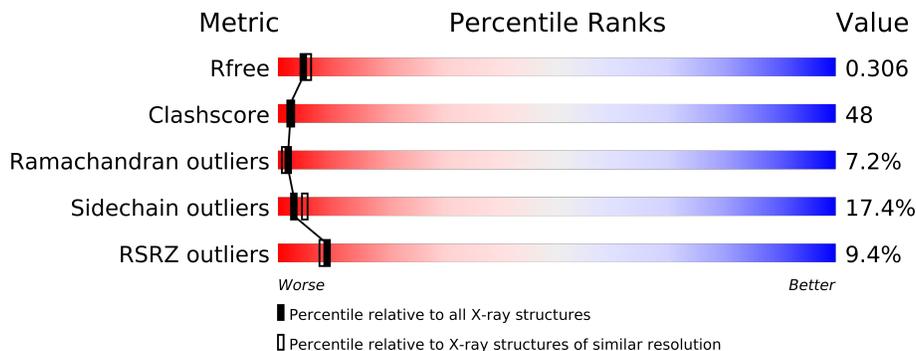
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol	Chain	Length	Quality of chain
1	A	271	
1	B	271	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4493 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN (PPAR-DELTA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	1
			2172	1405	368	389	10			
1	B	271	Total	C	N	O	S	0	0	0
			2158	1396	362	390	10			

- Molecule 2 is 2-(4-{3-[1-[2-(2-CHLORO-6-FLUORO-PHENYL)-ETHYL]-3-(2,3-DICH LORO-PHENYL)-UREIDO]-PROPYL}-PHENOXY)-2-METHYL-PROPIONICACID (three-letter code: 433) (formula: $C_{28}H_{28}Cl_3FN_2O_4$).
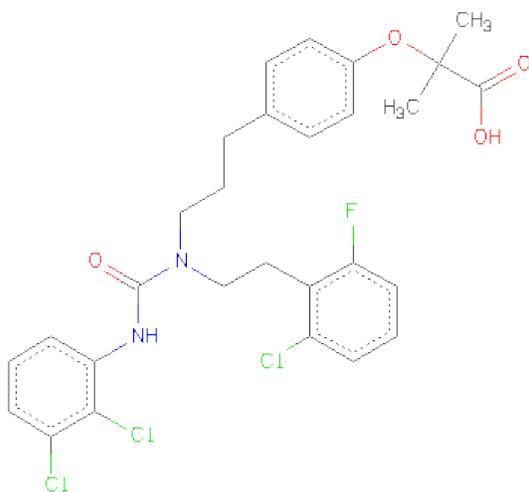
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			38	28	3	1	2	4		
2	B	1	Total	C	Cl	F	N	O	0	0
			38	28	3	1	2	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total 51	O 51	0	0
3	B	36	Total 36	O 36	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 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: PROTEIN (PPAR-DELTA)

Chain A:
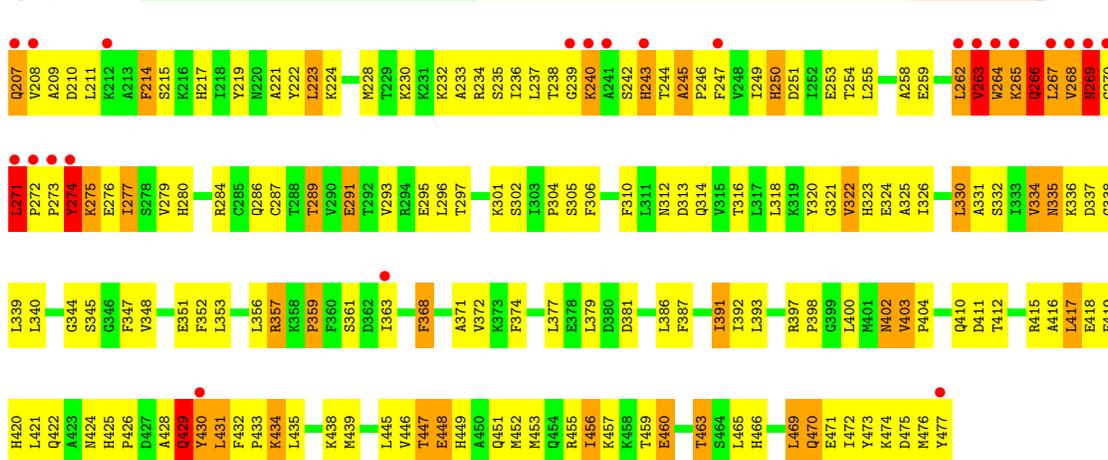
- Molecule 1: PROTEIN (PPAR-DELTA)

Chain B:
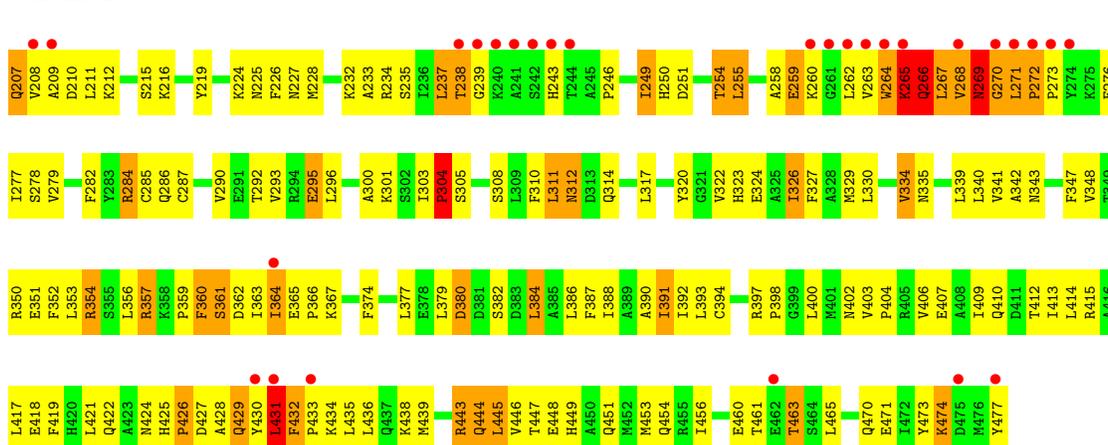
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	39.25Å 94.90Å 96.20Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 13.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	73.4 (8.00-2.50) 73.1 (13.18-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.50Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.246 , 0.303 0.251 , 0.306	Depositor DCC
R_{free} test set	1786 reflections (11.32%)	DCC
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 64.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.46, < L^2 > = 0.30$	Xtriage
Outliers	0 of 17557 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4493	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
433

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	0.47	0/2219	0.68	0/3001
1	B	0.42	0/2205	0.66	0/2986
All	All	0.44	0/4424	0.67	0/5987

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2172	0	2218	209	0
1	B	2158	0	2173	220	0
2	A	38	0	27	7	0
2	B	38	0	27	9	0
3	A	51	0	0	1	0
3	B	36	0	0	1	0
All	All	4493	0	4445	426	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 48.

All (426) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:266:GLN:CD	1:A:267:LEU:H	1.59	1.04
1:B:363:ILE:HD11	1:B:453:MET:HE2	1.42	1.00
1:B:249:ILE:O	1:B:254:THR:HG21	1.62	0.98
1:B:322:VAL:O	1:B:326:ILE:HG22	1.63	0.97
1:A:236:ILE:HA	1:A:243:HIS:NE2	1.81	0.95
1:B:310:PHE:HB3	1:B:312:ASN:HD21	1.32	0.94
1:B:431:LEU:O	1:B:433:PRO:HD2	1.69	0.92
1:B:312:ASN:H	1:B:312:ASN:HD22	1.11	0.92
1:A:245:ALA:HB3	1:B:209:ALA:HB3	1.50	0.90
1:A:455:ARG:O	1:A:459:THR:HG22	1.72	0.90
1:A:271:LEU:O	1:A:276:GLU:HA	1.74	0.87
1:B:310:PHE:HB3	1:B:312:ASN:ND2	1.90	0.86
1:B:421:LEU:HB3	1:B:431:LEU:HD23	1.59	0.85
1:B:465:LEU:HD23	1:B:470:GLN:HE21	1.43	0.84
1:A:297:THR:O	1:A:301:LYS:HG3	1.78	0.84
1:B:277:ILE:HG23	1:B:278:SER:H	1.44	0.83
1:A:348:VAL:HG11	2:A:1:433:CL3F	2.15	0.83
1:A:270:GLY:O	1:A:271:LEU:HD13	1.78	0.83
1:A:275:LYS:HE3	1:A:280:HIS:HA	1.62	0.82
1:B:430:TYR:HA	1:B:434:LYS:HD3	1.59	0.82
1:B:431:LEU:H	1:B:431:LEU:HD12	1.45	0.81
1:B:250:HIS:HA	1:B:352:PHE:HB2	1.61	0.81
1:B:312:ASN:N	1:B:312:ASN:HD22	1.80	0.80
1:A:268:VAL:HG22	1:A:269:ASN:H	1.47	0.79
1:B:418:GLU:HA	1:B:432:PHE:CZ	2.17	0.79
1:A:296:LEU:HD22	1:A:392:ILE:HD11	1.64	0.78
1:A:215:SER:OG	1:A:386:LEU:HD11	1.83	0.78
1:B:251:ASP:OD1	1:B:254:THR:HG22	1.84	0.76
1:B:424:ASN:HD22	1:B:425:HIS:CE1	2.03	0.76
1:B:286:GLN:O	1:B:290:VAL:HG23	1.86	0.76
1:A:357:ARG:HH12	1:A:460:GLU:CD	1.90	0.76
1:B:269:ASN:ND2	1:B:271:LEU:HD21	2.02	0.74
1:A:465:LEU:HD23	1:A:470:GLN:HG2	1.68	0.74
1:B:269:ASN:HD21	1:B:271:LEU:HD21	1.50	0.74
1:B:460:GLU:HB3	1:B:463:THR:HG23	1.70	0.73
1:A:430:TYR:O	1:A:434:LYS:HB2	1.89	0.73
1:B:430:TYR:HA	1:B:434:LYS:CD	2.20	0.72
1:A:391:ILE:HD12	1:A:391:ILE:O	1.90	0.72
1:B:460:GLU:HB3	1:B:463:THR:CG2	2.20	0.72
1:B:305:SER:O	1:B:308:SER:HB2	1.90	0.72
1:B:339:LEU:HG	1:B:340:LEU:N	2.04	0.71
1:B:238:THR:HG22	1:B:239:GLY:N	2.05	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:267:LEU:HD11	1:A:284:ARG:HG2	1.72	0.70
1:A:275:LYS:HG2	1:A:279:VAL:HG12	1.74	0.70
1:A:321:GLY:O	1:A:391:ILE:HD11	1.90	0.70
1:B:334:VAL:HG13	1:B:335:ASN:H	1.56	0.70
1:A:271:LEU:HB3	1:A:277:ILE:N	2.07	0.70
1:B:330:LEU:HD13	2:B:2:433:CL2F	2.28	0.70
1:A:266:GLN:NE2	1:A:267:LEU:H	1.88	0.70
1:A:351:GLU:HG3	1:A:352:PHE:N	2.05	0.70
1:A:320:TYR:HB2	1:A:397:ARG:HD2	1.74	0.70
1:B:473:TYR:O	1:B:474:LYS:HB3	1.92	0.70
1:B:320:TYR:HB3	1:B:397:ARG:HD2	1.73	0.70
1:A:271:LEU:CA	1:A:276:GLU:HA	2.21	0.69
1:A:266:GLN:HB3	1:A:267:LEU:HD23	1.75	0.69
1:B:387:PHE:O	1:B:391:ILE:HG22	1.93	0.69
1:B:260:LYS:HE2	1:B:268:VAL:HB	1.74	0.69
1:A:266:GLN:CD	1:A:267:LEU:N	2.42	0.68
1:B:207:GLN:HG3	1:B:210:ASP:HB3	1.74	0.68
1:B:272:PRO:HB2	1:B:273:PRO:CD	2.24	0.68
1:B:323:HIS:HA	1:B:326:ILE:CG2	2.23	0.68
1:B:268:VAL:O	1:B:269:ASN:HB2	1.94	0.68
1:B:310:PHE:CB	1:B:312:ASN:HD21	2.05	0.68
1:B:259:GLU:OE2	1:B:284:ARG:NH1	2.27	0.67
1:B:334:VAL:CG1	1:B:335:ASN:N	2.57	0.67
1:B:312:ASN:H	1:B:312:ASN:ND2	1.89	0.67
1:B:430:TYR:O	1:B:434:LYS:HB2	1.93	0.67
1:A:236:ILE:HA	1:A:243:HIS:CE1	2.29	0.67
1:A:267:LEU:O	1:A:268:VAL:HG12	1.95	0.67
1:B:266:GLN:HG2	1:B:284:ARG:NH2	2.09	0.67
1:A:268:VAL:HA	1:A:280:HIS:HE1	1.59	0.67
1:B:377:LEU:HD11	1:B:438:LYS:HD2	1.77	0.67
1:A:387:PHE:O	1:A:391:ILE:HG23	1.95	0.66
1:B:354:ARG:HB3	1:B:354:ARG:NH1	2.10	0.66
1:B:271:LEU:HD13	1:B:277:ILE:HA	1.77	0.66
1:A:271:LEU:C	1:A:276:GLU:HA	2.14	0.66
1:A:258:ALA:HA	1:A:262:LEU:HD13	1.76	0.66
1:A:233:ALA:O	1:A:237:LEU:HD12	1.96	0.66
1:B:334:VAL:HG13	1:B:335:ASN:N	2.11	0.65
1:B:215:SER:HA	1:B:386:LEU:HD21	1.78	0.65
1:B:415:ARG:O	1:B:418:GLU:HB3	1.97	0.65
1:B:265:LYS:HE2	1:B:265:LYS:O	1.97	0.65
1:A:452:MET:O	1:A:456:ILE:HG22	1.97	0.64
1:B:233:ALA:O	1:B:237:LEU:HD23	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:249:ILE:HD12	1:A:348:VAL:HG22	1.78	0.64
1:B:300:ALA:HA	1:B:303:ILE:HD13	1.78	0.64
1:B:356:LEU:HB2	1:B:361:SER:HB3	1.79	0.64
1:A:259:GLU:OE2	1:A:284:ARG:NH1	2.31	0.64
1:B:431:LEU:H	1:B:431:LEU:CD1	2.04	0.64
1:B:324:GLU:HB2	1:B:391:ILE:CD1	2.27	0.64
1:A:320:TYR:CB	1:A:397:ARG:HD2	2.27	0.64
1:A:267:LEU:CD1	1:A:284:ARG:HG2	2.27	0.64
1:A:374:PHE:O	1:A:377:LEU:HD13	1.98	0.63
1:A:228:MET:HE1	1:A:232:LYS:HG2	1.81	0.63
1:A:259:GLU:CD	1:A:284:ARG:HH12	2.01	0.63
1:A:271:LEU:O	1:A:276:GLU:CA	2.47	0.63
1:A:207:GLN:HB2	1:A:209:ALA:O	1.98	0.63
1:B:431:LEU:O	1:B:432:PHE:HB2	1.97	0.63
1:A:244:THR:HA	1:B:208:VAL:HG23	1.81	0.62
1:B:418:GLU:HA	1:B:432:PHE:HZ	1.64	0.62
1:A:425:HIS:HB3	1:A:428:ALA:HB2	1.82	0.62
1:B:249:ILE:O	1:B:250:HIS:ND1	2.31	0.62
1:A:402:ASN:HD22	1:A:404:PRO:HD2	1.64	0.61
1:B:282:PHE:HE1	1:B:453:MET:HE1	1.65	0.61
1:A:312:ASN:O	1:A:316:THR:HG23	1.99	0.61
1:B:432:PHE:O	1:B:436:LEU:HB2	2.01	0.61
1:B:471:GLU:OE1	1:B:474:LYS:HE2	2.00	0.61
1:A:243:HIS:O	1:B:207:GLN:HA	2.00	0.60
1:A:289:THR:O	1:A:293:VAL:HG23	2.00	0.60
1:A:262:LEU:HD12	1:A:262:LEU:N	2.16	0.60
1:B:348:VAL:HG11	2:B:2:433:CL3F	2.38	0.60
1:B:277:ILE:HG23	1:B:278:SER:N	2.13	0.60
1:A:449:HIS:O	1:A:453:MET:HG2	2.01	0.60
1:A:228:MET:SD	1:A:232:LYS:HE3	2.41	0.60
1:B:237:LEU:HD21	1:B:340:LEU:HD13	1.82	0.60
1:A:403:VAL:HG13	1:A:404:PRO:HD3	1.82	0.60
1:B:354:ARG:HB3	1:B:354:ARG:HH11	1.65	0.60
1:B:266:GLN:CG	1:B:284:ARG:HH22	2.14	0.60
1:B:249:ILE:HG22	1:B:250:HIS:N	2.15	0.59
1:A:324:GLU:CB	1:A:391:ILE:HD13	2.32	0.59
1:A:445:LEU:O	1:A:448:GLU:HG3	2.01	0.59
1:A:435:LEU:O	1:A:439:MET:HG3	2.02	0.59
1:B:431:LEU:N	1:B:431:LEU:HD12	2.15	0.59
1:B:424:ASN:HD22	1:B:425:HIS:HE1	1.50	0.59
1:B:397:ARG:HB2	1:B:400:LEU:HD22	1.84	0.59
1:A:268:VAL:O	1:A:269:ASN:CB	2.50	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:363:ILE:CD1	1:B:453:MET:HE2	2.26	0.59
1:B:377:LEU:HD22	1:B:430:TYR:HB2	1.84	0.58
1:B:226:PHE:HZ	1:B:296:LEU:HD23	1.66	0.58
1:A:243:HIS:C	1:B:207:GLN:HB3	2.23	0.58
1:A:264:TRP:HB3	1:A:284:ARG:NH2	2.18	0.58
1:B:271:LEU:HB3	1:B:276:GLU:C	2.24	0.58
1:B:473:TYR:O	1:B:474:LYS:CB	2.52	0.57
1:B:279:VAL:HG22	1:B:360:PHE:CZ	2.40	0.57
1:A:270:GLY:C	1:A:271:LEU:HD13	2.25	0.57
1:B:249:ILE:C	1:B:254:THR:HG21	2.24	0.57
1:A:273:PRO:O	1:A:275:LYS:N	2.37	0.57
1:B:388:ILE:O	1:B:391:ILE:HG23	2.04	0.57
1:B:357:ARG:NH2	1:B:460:GLU:OE2	2.36	0.57
1:B:228:MET:HE3	1:B:233:ALA:HA	1.85	0.57
1:B:379:LEU:HD11	1:B:435:LEU:HD11	1.87	0.57
1:B:384:LEU:O	1:B:388:ILE:HG12	2.04	0.57
1:B:451:GLN:O	1:B:454:GLN:HG2	2.04	0.57
1:A:411:ASP:CG	1:A:415:ARG:HH21	2.08	0.57
1:B:208:VAL:O	1:B:208:VAL:HG12	2.03	0.57
1:A:259:GLU:O	1:A:263:VAL:HA	2.06	0.56
1:A:272:PRO:N	1:A:273:PRO:HD2	2.21	0.56
1:B:250:HIS:NE2	1:B:251:ASP:OD2	2.38	0.56
1:B:387:PHE:CE2	1:B:435:LEU:HG	2.39	0.56
1:A:266:GLN:C	1:A:267:LEU:HD23	2.25	0.56
1:B:403:VAL:HB	1:B:404:PRO:HD3	1.87	0.56
1:A:447:THR:O	1:A:451:GLN:HG3	2.05	0.56
1:A:324:GLU:HB2	1:A:391:ILE:HD13	1.87	0.56
1:A:387:PHE:CE1	1:A:435:LEU:HD22	2.40	0.56
1:A:271:LEU:HD22	1:A:271:LEU:N	2.21	0.56
1:B:430:TYR:CE2	1:B:431:LEU:HG	2.41	0.56
1:A:208:VAL:HG23	1:A:419:PHE:CE2	2.41	0.56
1:B:465:LEU:HD23	1:B:470:GLN:HG2	1.87	0.55
1:A:425:HIS:HB3	1:A:428:ALA:CB	2.36	0.55
1:B:410:GLN:O	1:B:413:ILE:HB	2.07	0.55
1:A:268:VAL:HA	1:A:280:HIS:CE1	2.41	0.55
1:B:312:ASN:N	1:B:312:ASN:ND2	2.50	0.55
1:A:211:LEU:HD11	1:A:412:THR:HG23	1.87	0.55
1:A:466:HIS:HB3	1:A:469:LEU:HD22	1.87	0.55
1:B:465:LEU:CD2	1:B:470:GLN:HE21	2.17	0.55
1:A:230:LYS:HB2	1:A:332:SER:HB3	1.89	0.55
2:A:1:433:H1G1	2:A:1:433:C1A	2.37	0.54
1:A:276:GLU:OE2	1:A:357:ARG:NH2	2.32	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:232:LYS:O	1:B:235:SER:HB3	2.07	0.54
1:B:430:TYR:HA	1:B:434:LYS:CG	2.37	0.54
1:B:324:GLU:HB2	1:B:391:ILE:HD11	1.89	0.54
1:B:209:ALA:HA	1:B:212:LYS:HB2	1.88	0.54
1:B:259:GLU:HG2	1:B:269:ASN:HA	1.90	0.54
1:A:379:LEU:HD11	1:A:435:LEU:HD21	1.90	0.54
1:B:360:PHE:O	1:B:362:ASP:N	2.34	0.54
1:A:271:LEU:HA	1:A:276:GLU:HA	1.90	0.54
1:B:264:TRP:HB3	1:B:284:ARG:HH22	1.73	0.54
1:B:419:PHE:O	1:B:422:GLN:HB2	2.08	0.54
1:B:292:THR:HA	1:B:295:GLU:HG3	1.90	0.54
1:B:365:GLU:N	1:B:366:PRO:HD2	2.21	0.53
1:B:324:GLU:HB2	1:B:391:ILE:HD13	1.91	0.53
1:A:306:PHE:CE2	1:A:314:GLN:HG2	2.44	0.53
1:A:429:GLN:HE21	1:A:429:GLN:C	2.11	0.53
1:A:476:MET:HG2	1:A:477:TYR:N	2.24	0.53
1:B:387:PHE:CD2	1:B:435:LEU:HG	2.44	0.53
1:B:209:ALA:HA	1:B:212:LYS:CB	2.38	0.53
1:B:418:GLU:CA	1:B:432:PHE:HZ	2.21	0.53
1:A:432:PHE:HB3	1:A:433:PRO:CD	2.39	0.53
1:B:268:VAL:O	1:B:269:ASN:CB	2.58	0.52
1:A:353:LEU:HD21	2:A:1:433:CL3F	2.46	0.52
1:B:320:TYR:CB	1:B:397:ARG:HD2	2.37	0.52
1:A:214:PHE:CZ	1:A:412:THR:HG22	2.45	0.52
1:B:340:LEU:HD12	1:B:347:PHE:HD1	1.73	0.52
1:A:217:HIS:HE1	1:A:302:SER:O	1.92	0.52
1:A:330:LEU:O	1:A:330:LEU:HD22	2.09	0.52
1:B:456:ILE:O	1:B:460:GLU:HB2	2.10	0.52
1:B:430:TYR:CA	1:B:434:LYS:HD3	2.34	0.52
1:A:250:HIS:CE1	1:A:251:ASP:OD2	2.63	0.52
1:B:271:LEU:HD13	1:B:277:ILE:CA	2.40	0.52
1:A:280:HIS:HE2	1:A:284:ARG:NH1	2.08	0.51
1:B:225:ASN:O	1:B:295:GLU:HB3	2.10	0.51
1:B:435:LEU:O	1:B:439:MET:HG3	2.10	0.51
1:B:421:LEU:HD22	1:B:430:TYR:OH	2.10	0.51
1:B:418:GLU:HA	1:B:432:PHE:CE1	2.45	0.51
1:A:247:PHE:CD2	1:A:262:LEU:HG	2.46	0.51
1:B:264:TRP:CZ2	1:B:342:ALA:HB2	2.46	0.51
1:A:474:LYS:HG2	1:A:474:LYS:O	2.09	0.51
1:A:271:LEU:HD12	1:A:276:GLU:O	2.11	0.51
1:B:284:ARG:HG2	2:B:2:433:C3E	2.40	0.51
1:B:266:GLN:O	1:B:267:LEU:HB3	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:421:LEU:HD12	1:B:431:LEU:HB3	1.93	0.51
1:B:303:ILE:HG23	1:B:304:PRO:HD2	1.92	0.51
1:A:393:LEU:O	1:A:410:GLN:HB2	2.10	0.51
1:B:470:GLN:O	1:B:473:TYR:O	2.29	0.51
1:A:449:HIS:NE2	2:A:1:433:O1C	2.43	0.51
1:A:240:LYS:HG2	1:A:240:LYS:O	2.09	0.51
1:B:351:GLU:HA	1:B:354:ARG:HG3	1.92	0.51
1:A:230:LYS:CB	1:A:332:SER:HB3	2.40	0.51
1:B:270:GLY:C	1:B:271:LEU:HD23	2.31	0.50
1:A:296:LEU:HD13	1:A:322:VAL:HG22	1.93	0.50
1:A:334:VAL:HG13	1:A:335:ASN:N	2.27	0.50
1:A:269:ASN:CG	1:A:270:GLY:N	2.64	0.50
1:B:271:LEU:N	1:B:271:LEU:HD23	2.27	0.50
1:B:323:HIS:HE2	2:B:2:433:C1A	2.23	0.50
1:A:245:ALA:CB	1:B:209:ALA:HB3	2.32	0.50
1:B:429:GLN:C	1:B:431:LEU:HD12	2.31	0.50
1:B:359:PRO:HG2	1:B:360:PHE:CD1	2.46	0.50
1:B:410:GLN:O	1:B:413:ILE:N	2.44	0.50
1:B:353:LEU:HD21	2:B:2:433:CL3D	2.49	0.50
1:A:209:ALA:O	1:A:210:ASP:CB	2.60	0.50
1:A:222:TYR:CE1	1:A:381:ASP:HB3	2.46	0.50
1:B:266:GLN:HG2	1:B:284:ARG:HH22	1.72	0.50
1:A:247:PHE:HD2	1:A:262:LEU:HG	1.75	0.50
1:B:348:VAL:HG13	1:B:352:PHE:HD2	1.76	0.50
1:A:268:VAL:HG22	1:A:269:ASN:N	2.24	0.50
1:A:236:ILE:O	1:A:243:HIS:HE1	1.95	0.50
1:A:368:PHE:O	1:A:372:VAL:HG23	2.12	0.49
1:A:275:LYS:HG2	1:A:279:VAL:CG1	2.41	0.49
1:B:417:LEU:O	1:B:421:LEU:HG	2.13	0.49
1:B:226:PHE:CE1	1:B:295:GLU:HB2	2.46	0.49
1:B:403:VAL:O	1:B:407:GLU:HG3	2.12	0.49
1:A:277:ILE:O	1:A:280:HIS:HB3	2.12	0.49
1:A:357:ARG:NH1	1:A:460:GLU:OE2	2.39	0.49
1:B:267:LEU:O	1:B:269:ASN:N	2.40	0.49
1:B:350:ARG:O	1:B:354:ARG:HG2	2.12	0.49
1:B:249:ILE:N	1:B:249:ILE:HD12	2.27	0.49
1:A:268:VAL:CA	1:A:280:HIS:HE1	2.24	0.49
1:A:263:VAL:O	1:A:264:TRP:CB	2.61	0.49
1:A:335:ASN:HD22	1:A:347:PHE:HZ	1.61	0.49
1:A:284:ARG:HG3	1:A:284:ARG:HH11	1.78	0.48
1:B:304:PRO:HA	3:B:509:HOH:O	2.13	0.48
1:B:323:HIS:HA	1:B:326:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:417:LEU:O	1:A:421:LEU:HG	2.14	0.48
1:A:411:ASP:O	1:A:415:ARG:HB2	2.14	0.48
1:B:414:LEU:HD22	1:B:436:LEU:HD21	1.95	0.48
1:A:476:MET:CG	1:A:477:TYR:N	2.76	0.48
1:B:237:LEU:HD22	1:B:237:LEU:N	2.27	0.48
1:B:374:PHE:HD2	1:B:438:LYS:HD3	1.79	0.48
1:A:271:LEU:O	1:A:275:LYS:O	2.31	0.48
1:A:472:ILE:HG22	1:A:476:MET:CE	2.44	0.48
1:B:380:ASP:C	1:B:380:ASP:OD1	2.52	0.48
1:B:323:HIS:HA	1:B:326:ILE:HG23	1.96	0.48
1:A:419:PHE:O	1:A:422:GLN:HB2	2.13	0.48
1:A:377:LEU:N	1:A:377:LEU:HD12	2.28	0.48
1:B:390:ALA:HA	1:B:413:ILE:HG21	1.96	0.48
1:A:270:GLY:C	1:A:271:LEU:HD22	2.34	0.47
1:A:324:GLU:HB3	1:A:391:ILE:HD13	1.95	0.47
1:A:418:GLU:HB2	1:A:432:PHE:CD1	2.49	0.47
1:A:306:PHE:HD1	1:A:393:LEU:HD21	1.78	0.47
1:A:335:ASN:OD1	1:A:336:LYS:N	2.47	0.47
1:B:296:LEU:HD12	1:B:322:VAL:HG22	1.96	0.47
1:A:208:VAL:HG13	1:A:209:ALA:N	2.29	0.47
1:A:235:SER:O	1:A:238:THR:HG22	2.14	0.47
1:A:247:PHE:CZ	1:B:212:LYS:NZ	2.82	0.47
1:A:374:PHE:CD1	1:A:438:LYS:HG2	2.49	0.47
1:A:250:HIS:CD2	1:A:254:THR:HG21	2.49	0.47
1:A:267:LEU:HD11	1:A:284:ARG:CG	2.43	0.47
1:B:265:LYS:C	1:B:265:LYS:HE2	2.33	0.47
1:B:394:CYS:O	1:B:397:ARG:HG2	2.15	0.47
1:A:268:VAL:O	1:A:269:ASN:HB3	2.13	0.47
1:B:430:TYR:CD2	1:B:431:LEU:HG	2.50	0.47
1:A:326:ILE:HG23	2:A:1:433:CL2F	2.52	0.47
1:A:472:ILE:O	1:A:476:MET:HE2	2.14	0.47
1:B:246:PRO:HB2	1:B:347:PHE:HB2	1.96	0.47
1:B:238:THR:HG22	1:B:239:GLY:H	1.78	0.47
1:A:418:GLU:HB2	1:A:432:PHE:CE1	2.50	0.47
1:A:411:ASP:OD2	1:A:415:ARG:NH2	2.40	0.47
1:B:301:LYS:NZ	1:B:314:GLN:HE22	2.12	0.47
1:A:419:PHE:HA	1:A:422:GLN:CG	2.45	0.47
1:A:217:HIS:CE1	1:A:302:SER:O	2.67	0.47
1:A:331:ALA:HA	1:A:371:ALA:HB1	1.95	0.47
1:B:264:TRP:HB3	1:B:284:ARG:NH2	2.30	0.47
1:B:432:PHE:O	1:B:436:LEU:N	2.42	0.47
1:B:207:GLN:N	1:B:211:LEU:HD22	2.29	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:276:GLU:OE2	1:B:357:ARG:NH1	2.43	0.46
1:A:425:HIS:N	1:A:426:PRO:HD3	2.31	0.46
1:B:216:LYS:O	1:B:219:TYR:HB3	2.15	0.46
1:A:271:LEU:HD12	1:A:276:GLU:C	2.35	0.46
1:A:258:ALA:CA	1:A:262:LEU:HD13	2.46	0.46
1:A:264:TRP:CB	1:A:284:ARG:NH2	2.77	0.46
1:A:219:TYR:CE1	1:A:223:LEU:HD11	2.50	0.46
1:A:247:PHE:HD2	1:A:262:LEU:CG	2.28	0.46
1:A:297:THR:OG1	1:A:318:LEU:HD13	2.15	0.46
1:A:291:GLU:O	1:A:295:GLU:HG3	2.15	0.46
1:A:228:MET:HE3	1:A:233:ALA:N	2.31	0.46
1:B:421:LEU:CD1	1:B:431:LEU:HB3	2.45	0.46
1:A:334:VAL:CG1	1:A:335:ASN:N	2.79	0.46
1:A:264:TRP:HB3	1:A:284:ARG:HH21	1.80	0.46
1:A:271:LEU:HB3	1:A:276:GLU:C	2.36	0.46
1:A:419:PHE:HA	1:A:422:GLN:HG3	1.98	0.45
1:A:240:LYS:HD3	1:A:240:LYS:H	1.80	0.45
1:B:285:CYS:SG	2:B:2:433:H1N1	2.56	0.45
1:B:431:LEU:O	1:B:432:PHE:CB	2.65	0.45
1:B:418:GLU:CA	1:B:432:PHE:CZ	2.94	0.45
1:B:300:ALA:O	1:B:303:ILE:HB	2.15	0.45
1:A:263:VAL:O	1:A:264:TRP:CG	2.70	0.45
1:B:219:TYR:CD2	1:B:382:SER:HA	2.52	0.45
1:A:258:ALA:HA	1:A:262:LEU:CD1	2.44	0.45
1:B:255:LEU:HD12	1:B:277:ILE:HD11	1.98	0.45
1:A:324:GLU:HG3	1:A:446:VAL:HG21	1.98	0.45
1:B:324:GLU:CG	1:B:446:VAL:HG21	2.47	0.45
1:A:275:LYS:HD3	1:A:276:GLU:O	2.16	0.45
1:B:260:LYS:HE2	1:B:268:VAL:CB	2.45	0.45
1:A:448:GLU:HB3	3:A:481:HOH:O	2.16	0.45
1:B:277:ILE:CG2	1:B:278:SER:H	2.22	0.45
1:A:386:LEU:HD13	1:A:417:LEU:HA	1.99	0.45
1:B:254:THR:O	1:B:258:ALA:HB2	2.17	0.45
1:B:377:LEU:HD11	1:B:438:LYS:CD	2.47	0.45
1:A:473:TYR:CD1	1:A:476:MET:HE3	2.51	0.45
1:A:221:ALA:HB1	1:A:302:SER:HB2	1.99	0.45
1:A:335:ASN:ND2	1:A:338:GLY:H	2.14	0.45
1:A:267:LEU:O	1:A:268:VAL:CG1	2.62	0.45
1:B:432:PHE:HB2	1:B:433:PRO:CD	2.47	0.45
1:A:262:LEU:O	1:A:263:VAL:HG23	2.17	0.44
1:B:363:ILE:HG12	1:B:363:ILE:O	2.16	0.44
1:B:391:ILE:HD12	1:B:397:ARG:NH2	2.31	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:418:GLU:O	1:A:422:GLN:HG2	2.18	0.44
1:A:246:PRO:HA	1:A:345:SER:O	2.17	0.44
1:B:272:PRO:CB	1:B:273:PRO:CD	2.95	0.44
1:B:390:ALA:CA	1:B:413:ILE:HG21	2.47	0.44
1:A:340:LEU:HD22	1:A:344:GLY:HA2	1.98	0.44
1:B:327:PHE:CD2	1:B:445:LEU:HD13	2.52	0.44
1:A:232:LYS:O	1:A:236:ILE:HG13	2.17	0.44
1:B:258:ALA:C	1:B:260:LYS:H	2.21	0.44
1:A:276:GLU:H	1:A:279:VAL:HB	1.82	0.44
1:A:460:GLU:HG3	1:A:463:THR:CG2	2.48	0.44
1:A:214:PHE:HE1	1:A:416:ALA:HB2	1.83	0.43
1:A:236:ILE:O	1:A:243:HIS:CE1	2.72	0.43
1:B:432:PHE:O	1:B:433:PRO:C	2.53	0.43
1:A:403:VAL:N	1:A:404:PRO:CD	2.81	0.43
1:B:380:ASP:OD1	1:B:382:SER:N	2.47	0.43
1:B:228:MET:HE1	1:B:340:LEU:HD23	2.00	0.43
1:B:249:ILE:O	1:B:250:HIS:CG	2.71	0.43
2:A:1:433:HN31	2:A:1:433:H1N1	1.60	0.43
1:A:445:LEU:HD23	1:A:445:LEU:C	2.39	0.43
1:A:335:ASN:ND2	1:A:337:ASP:H	2.16	0.43
1:A:234:ARG:HG2	1:A:234:ARG:NH1	2.34	0.43
1:A:268:VAL:O	1:A:269:ASN:CG	2.57	0.43
1:A:357:ARG:C	1:A:359:PRO:HD2	2.39	0.43
1:A:243:HIS:CG	1:A:244:THR:H	2.37	0.43
1:B:228:MET:CE	1:B:340:LEU:HD23	2.49	0.43
1:A:320:TYR:HB3	1:A:397:ARG:HD2	1.99	0.43
1:A:391:ILE:C	1:A:391:ILE:HD12	2.39	0.43
1:B:447:THR:HG23	1:B:477:TYR:OXT	2.19	0.43
1:B:397:ARG:HA	1:B:398:PRO:HD3	1.85	0.42
1:B:430:TYR:CG	1:B:431:LEU:N	2.87	0.42
1:B:209:ALA:C	1:B:212:LYS:H	2.22	0.42
1:B:393:LEU:HD13	1:B:409:ILE:CG2	2.49	0.42
1:B:449:HIS:NE2	2:B:2:433:O1C	2.42	0.42
1:B:339:LEU:HD23	1:B:341:VAL:CG1	2.50	0.42
1:A:240:LYS:N	1:A:240:LYS:HD3	2.33	0.42
1:B:434:LYS:O	1:B:438:LYS:HG3	2.20	0.42
1:A:296:LEU:HD11	1:A:325:ALA:HB3	2.01	0.42
1:A:296:LEU:HD22	1:A:392:ILE:CD1	2.43	0.42
1:A:457:LYS:O	1:A:457:LYS:HG2	2.19	0.42
1:B:249:ILE:HA	1:B:254:THR:OG1	2.20	0.42
1:B:444:GLN:HB3	1:B:444:GLN:HE21	1.60	0.42
1:A:263:VAL:O	1:A:264:TRP:HB2	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:251:ASP:O	1:B:254:THR:HG23	2.20	0.42
1:A:296:LEU:CD1	1:A:322:VAL:HG22	2.50	0.42
1:B:324:GLU:HG2	1:B:446:VAL:HG21	2.02	0.42
1:A:215:SER:OG	1:A:386:LEU:HD21	2.20	0.41
1:A:435:LEU:HD23	1:A:435:LEU:HA	1.68	0.41
1:B:391:ILE:HD12	1:B:397:ARG:HH21	1.84	0.41
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.92	0.41
1:B:435:LEU:HA	1:B:435:LEU:HD12	1.81	0.41
1:A:266:GLN:NE2	1:A:267:LEU:N	2.61	0.41
1:A:271:LEU:HA	1:A:275:LYS:O	2.19	0.41
1:A:359:PRO:O	1:A:363:ILE:HG23	2.20	0.41
2:B:2:433:HN31	2:B:2:433:H1N1	1.69	0.41
1:A:471:GLU:OE1	1:A:471:GLU:HA	2.21	0.41
1:A:255:LEU:O	1:A:259:GLU:HG2	2.21	0.41
1:B:296:LEU:HD12	1:B:322:VAL:CG2	2.50	0.41
1:B:356:LEU:HB2	1:B:361:SER:CB	2.48	0.41
1:A:267:LEU:N	1:A:267:LEU:HD23	2.36	0.41
1:A:429:GLN:O	1:A:431:LEU:N	2.48	0.41
1:A:284:ARG:CG	1:A:284:ARG:HH11	2.34	0.41
1:A:363:ILE:HA	1:A:452:MET:SD	2.61	0.41
1:B:353:LEU:HD21	2:B:2:433:CL3F	2.58	0.41
1:B:269:ASN:CG	1:B:270:GLY:H	2.24	0.41
1:B:386:LEU:HD13	1:B:417:LEU:HA	2.03	0.41
1:A:323:HIS:CE1	1:A:472:ILE:HG21	2.56	0.41
1:A:397:ARG:HA	1:A:398:PRO:HD3	1.86	0.41
1:B:303:ILE:HG21	1:B:393:LEU:HD11	2.02	0.41
1:B:364:ILE:HG12	1:B:364:ILE:H	1.71	0.41
1:A:472:ILE:HG22	1:A:476:MET:HE1	2.02	0.41
1:B:329:MET:O	1:B:330:LEU:C	2.59	0.40
1:B:207:GLN:CG	1:B:210:ASP:HB3	2.46	0.40
1:A:323:HIS:HA	1:A:326:ILE:HB	2.02	0.40
1:B:324:GLU:OE2	1:B:443:ARG:CD	2.69	0.40
1:A:416:ALA:O	1:A:420:HIS:N	2.53	0.40
1:B:402:ASN:O	1:B:406:VAL:HG23	2.22	0.40
1:A:310:PHE:O	1:A:313:ASP:N	2.52	0.40
1:A:267:LEU:C	1:A:268:VAL:O	2.59	0.40
1:B:293:VAL:HG13	1:B:322:VAL:HG21	2.02	0.40
1:B:465:LEU:HD23	1:B:470:GLN:NE2	2.23	0.40
1:A:286:GLN:HB3	2:A:1:433:H1Y1	2.03	0.40
1:A:351:GLU:HG3	1:A:352:PHE:H	1.79	0.40
1:B:224:LYS:HG3	1:B:224:LYS:O	2.20	0.40
1:A:255:LEU:HD13	1:A:277:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:317:LEU:HD22	1:B:392:ILE:O	2.21	0.40
1:A:274:TYR:CD2	1:A:274:TYR:N	2.87	0.40
1:A:268:VAL:HG13	1:A:269:ASN:N	2.37	0.40
1:B:238:THR:CG2	1:B:239:GLY:N	2.72	0.40
1:B:311:LEU:HD23	1:B:311:LEU:HA	1.93	0.40
1:B:367:LYS:HG2	1:B:367:LYS:H	1.66	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	269/271 (99%)	230 (86%)	23 (9%)	16 (6%)	2	2
1	B	269/271 (99%)	218 (81%)	28 (10%)	23 (9%)	1	1
All	All	538/542 (99%)	448 (83%)	51 (10%)	39 (7%)	2	1

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	A	264	TRP
1	A	266	GLN
1	A	268	VAL
1	A	269	ASN
1	A	429	GLN
1	B	238	THR
1	B	263	VAL
1	B	266	GLN
1	B	269	ASN
1	B	304	PRO
1	B	360	PHE
1	B	361	SER
1	B	426	PRO

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Mol	Chain	Res	Type
1	B	432	PHE
1	B	474	LYS
1	A	263	VAL
1	A	265	LYS
1	A	274	TYR
1	B	237	LEU
1	B	268	VAL
1	B	343	ASN
1	B	428	ALA
1	B	429	GLN
1	B	461	THR
1	A	243	HIS
1	A	245	ALA
1	A	475	ASP
1	B	265	LYS
1	B	270	GLY
1	B	357	ARG
1	A	271	LEU
1	B	431	LEU
1	A	242	SER
1	A	430	TYR
1	B	427	ASP
1	B	272	PRO
1	B	249	ILE
1	A	359	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	238/239 (100%)	191 (80%)	47 (20%)	2	3
1	B	233/239 (98%)	198 (85%)	35 (15%)	4	7
All	All	471/478 (98%)	389 (83%)	82 (17%)	3	5

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	214	PHE
1	A	223	LEU
1	A	224	LYS
1	A	240	LYS
1	A	250	HIS
1	A	253	GLU
1	A	262	LEU
1	A	263	VAL
1	A	265	LYS
1	A	266	GLN
1	A	267	LEU
1	A	269	ASN
1	A	271	LEU
1	A	274	TYR
1	A	275	LYS
1	A	277	ILE
1	A	287	CYS
1	A	289	THR
1	A	291	GLU
1	A	304	PRO
1	A	305	SER
1	A	322	VAL
1	A	330	LEU
1	A	334	VAL
1	A	335	ASN
1	A	339	LEU
1	A	356	LEU
1	A	357	ARG
1	A	361	SER
1	A	368	PHE
1	A	391	ILE
1	A	400	LEU
1	A	402	ASN
1	A	403	VAL
1	A	417	LEU
1	A	424	ASN
1	A	429	GLN
1	A	431	LEU
1	A	434	LYS
1	A	447	THR
1	A	448	GLU
1	A	456	ILE

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Mol	Chain	Res	Type
1	A	460	GLU
1	A	463	THR
1	A	469	LEU
1	A	470	GLN
1	B	207	GLN
1	B	227	ASN
1	B	234	ARG
1	B	243	HIS
1	B	254	THR
1	B	255	LEU
1	B	259	GLU
1	B	262	LEU
1	B	264	TRP
1	B	265	LYS
1	B	266	GLN
1	B	267	LEU
1	B	269	ASN
1	B	271	LEU
1	B	284	ARG
1	B	287	CYS
1	B	295	GLU
1	B	304	PRO
1	B	311	LEU
1	B	312	ASN
1	B	326	ILE
1	B	334	VAL
1	B	354	ARG
1	B	364	ILE
1	B	380	ASP
1	B	384	LEU
1	B	391	ILE
1	B	412	THR
1	B	426	PRO
1	B	431	LEU
1	B	443	ARG
1	B	444	GLN
1	B	445	LEU
1	B	448	GLU
1	B	463	THR

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	217	HIS
1	A	220	ASN
1	A	250	HIS
1	A	257	GLN
1	A	335	ASN
1	A	343	ASN
1	A	402	ASN
1	A	420	HIS
1	A	424	ASN
1	A	429	GLN
1	B	227	ASN
1	B	257	GLN
1	B	266	GLN
1	B	269	ASN
1	B	312	ASN
1	B	314	GLN
1	B	422	GLN
1	B	425	HIS
1	B	429	GLN
1	B	444	GLN
1	B	451	GLN
1	B	470	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	433	A	1	-	40,40,40	2.38	11 (27%)	56,56,56	3.17	24 (42%)
2	433	B	2	-	40,40,40	2.43	10 (25%)	56,56,56	3.19	24 (42%)

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	433	A	1	-	-	0/30/30/30	0/3/3/3
2	433	B	2	-	-	0/30/30/30	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	433	C3B-N3A	6.80	1.55	1.41
2	B	2	433	C1D-C1A	-6.26	1.46	1.53
2	A	1	433	C1D-C1A	-6.24	1.46	1.53
2	B	2	433	C2A-N3A	5.31	1.45	1.36
2	A	1	433	C2C-N2B	5.09	1.61	1.47
2	A	1	433	C3B-C3D	4.93	1.44	1.40
2	B	2	433	C2D-C2E	4.92	1.60	1.52
2	A	1	433	C3B-N3A	4.91	1.51	1.41
2	A	1	433	C2D-C2E	4.74	1.60	1.52
2	B	2	433	C2C-N2B	4.12	1.58	1.47
2	A	1	433	O1E-C1D	3.93	1.49	1.45
2	B	2	433	C1X-C1D	3.85	1.60	1.52
2	B	2	433	C3B-C3D	3.48	1.43	1.40
2	A	1	433	C2A-N3A	3.47	1.42	1.36
2	A	1	433	C1X-C1D	3.23	1.59	1.52
2	B	2	433	C3F-C3D	2.98	1.44	1.39
2	A	1	433	C1N-N2B	2.85	1.55	1.47
2	A	1	433	C2A-N2B	2.81	1.42	1.36
2	B	2	433	O1E-C1D	2.46	1.48	1.45
2	A	1	433	C2C-C2D	2.43	1.60	1.52
2	B	2	433	C1H-C1J	-2.05	1.34	1.38

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All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	433	C2D-C2C-N2B	14.99	136.25	113.23
2	B	2	433	C2D-C2C-N2B	12.46	132.37	113.23
2	B	2	433	C3C-C3B-C3D	-6.62	113.84	118.78
2	B	2	433	C3B-N3A-C2A	6.58	141.86	126.10
2	A	1	433	C3C-C3B-C3D	-6.31	114.07	118.78
2	B	2	433	C3B-C3D-CL3D	-6.23	115.82	119.58
2	B	2	433	C3D-C3F-CL3F	6.18	127.66	120.52
2	A	1	433	C3B-N3A-C2A	5.19	138.53	126.10
2	B	2	433	N3A-C2A-N2B	5.09	121.64	115.88
2	A	1	433	N3A-C2A-N2B	5.08	121.63	115.88
2	B	2	433	C2C-C2D-C2E	5.00	124.02	112.87
2	B	2	433	C1M-C1L-C1K	4.90	132.92	113.77
2	A	1	433	C1M-C1N-N2B	4.85	129.15	112.18
2	A	1	433	C1M-C1L-C1K	4.65	131.97	113.77
2	B	2	433	C3G-C3F-CL3F	-4.31	108.79	118.37
2	A	1	433	C2C-C2D-C2E	4.30	122.45	112.87
2	A	1	433	C3D-C3F-CL3F	4.28	125.47	120.52
2	A	1	433	C1D-O1E-C1F	4.02	128.28	121.15
2	B	2	433	C1M-C1N-N2B	3.67	125.03	112.18
2	A	1	433	O1E-C1D-C1X	3.40	122.66	108.25
2	B	2	433	F2G-C2G-C2E	3.30	122.16	117.52
2	B	2	433	O1E-C1D-C1X	3.27	122.14	108.25
2	B	2	433	O2A-C2A-N2B	-3.24	117.03	121.73
2	A	1	433	C3G-C3F-CL3F	-3.16	111.34	118.37
2	A	1	433	O2A-C2A-N3A	-3.16	117.93	124.16
2	B	2	433	C1D-O1E-C1F	3.13	126.71	121.15
2	A	1	433	F2G-C2G-C2E	3.11	121.90	117.52
2	A	1	433	C2C-N2B-C1N	3.00	123.34	116.99
2	A	1	433	O1E-C1F-C1H	2.86	132.30	119.27
2	A	1	433	O1E-C1D-C1A	-2.85	105.67	109.86
2	B	2	433	C3F-C3D-CL3D	2.80	123.92	120.22
2	B	2	433	C2C-N2B-C1N	2.69	122.68	116.99
2	B	2	433	C2D-C2E-C2G	2.66	125.37	122.29
2	B	2	433	C1Y-C1D-C1X	-2.60	103.31	110.82
2	A	1	433	C1H-C1F-C1G	-2.57	115.81	120.21
2	A	1	433	C1J-C1H-C1F	2.52	123.13	119.76
2	A	1	433	C1I-C1G-C1F	2.48	123.08	119.76
2	B	2	433	C3E-C3C-C3B	2.46	123.78	118.53
2	B	2	433	O1E-C1F-C1H	2.44	130.39	119.27
2	B	2	433	C3G-C3F-C3D	2.36	123.55	120.51
2	A	1	433	C2E-C2F-CL2F	2.28	124.02	119.52
2	A	1	433	C2H-C2F-CL2F	-2.26	113.35	118.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	433	C3E-C3C-C3B	2.19	123.21	118.53
2	B	2	433	C1X-C1D-C1A	-2.17	102.06	109.75
2	B	2	433	C3C-C3B-N3A	2.10	126.78	121.85
2	B	2	433	C1H-C1F-C1G	-2.09	116.63	120.21
2	A	1	433	C3G-C3F-C3D	2.08	123.19	120.51
2	A	1	433	O1C-C1A-C1D	-2.03	115.88	122.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	271/271 (100%)	0.55	23 (8%)	11	10	25, 48, 103, 114	0
1	B	271/271 (100%)	0.69	28 (10%)	7	6	31, 57, 107, 113	0
All	All	542/542 (100%)	0.62	51 (9%)	9	8	25, 52, 105, 114	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	GLY	8.9
1	B	244	THR	7.4
1	A	274	TYR	6.9
1	A	265	LYS	6.6
1	B	241	ALA	6.5
1	B	274	TYR	6.4
1	A	269	ASN	6.1
1	A	207	GLN	5.5
1	B	240	LYS	5.4
1	B	273	PRO	5.2
1	A	247	PHE	5.1
1	A	208	VAL	5.1
1	A	270	GLY	5.0
1	B	264	TRP	4.9
1	B	268	VAL	4.8
1	A	241	ALA	4.8
1	B	209	ALA	4.6
1	B	263	VAL	4.6
1	B	242	SER	4.5
1	A	240	LYS	4.4
1	A	264	TRP	4.3
1	B	433	PRO	4.2
1	B	265	LYS	4.1
1	B	430	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	272	PRO	3.9
1	B	243	HIS	3.6
1	B	270	GLY	3.6
1	A	430	TYR	3.4
1	A	272	PRO	3.4
1	B	462	GLU	3.4
1	B	271	LEU	3.4
1	B	260	LYS	3.3
1	A	212	LYS	3.1
1	B	475	ASP	3.1
1	A	268	VAL	3.0
1	B	477	TYR	3.0
1	A	273	PRO	2.9
1	A	262	LEU	2.8
1	B	208	VAL	2.8
1	A	271	LEU	2.8
1	A	263	VAL	2.7
1	A	267	LEU	2.7
1	B	239	GLY	2.6
1	A	243	HIS	2.6
1	B	431	LEU	2.6
1	B	262	LEU	2.5
1	A	363	ILE	2.4
1	B	238	THR	2.4
1	A	477	TYR	2.4
1	B	364	ILE	2.3
1	B	261	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	433	A	1	38/38	0.17	-0.09	19,35,44,46	0
2	433	B	2	38/38	0.19	-0.10	36,45,54,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.