



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:12 pm BST

PDB ID : 4E4K
Title : Crystal Structure of PPARgamma with the ligand JO21
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Deposited on : 2012-03-13
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

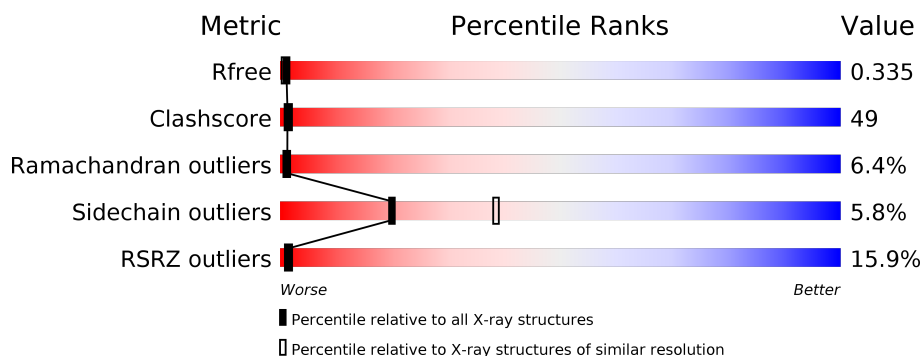
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	287	
1	B	287	

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	RRG	A	501	-	-	X	-
2	RRG	A	502	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4486 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.

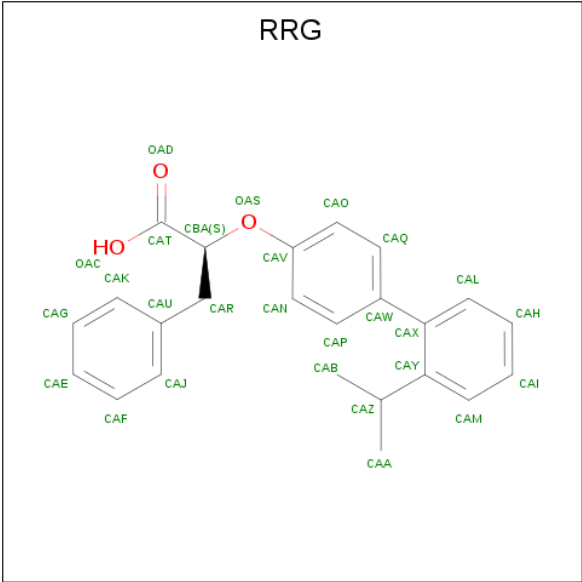
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2149	1387	352	400	10			
1	B	268	Total	C	N	O	S	28	0	0
			2149	1387	352	400	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 (2S)-3-phenyl-2-{[2'-(propan-2-yl)biphenyl-4-yl]oxy}propanoic acid (three-letter code: RRG) (formula: C₂₄H₂₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			27	24	3		
2	A	1	Total	C	O	0	0
			27	24	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total	O	0	0
			65	65		
3	B	69	Total	O	0	0
			69	69		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.01Å 62.12Å 118.98Å 90.00° 102.42° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 24.62 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 99.9 (24.62-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.265 , 0.335 0.263 , 0.335	Depositor DCC
R_{free} test set	1117 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.744	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 75.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4486	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/2186	0.63	0/2945
1	B	0.52	0/2186	0.69	1/2945 (0.0%)
All	All	0.48	0/4372	0.66	1/5890 (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	B	257	MET	C-N-CA	-5.27	111.22	122.30

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	2149	0	2217	263	0
1	B	2149	0	2217	151	0
2	A	54	0	46	77	0
3	A	65	0	0	22	0
3	B	69	0	0	25	0
All	All	4486	0	4480	434	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 49.

All (434) 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)
2:A:501:RRG:H15	2:A:501:RRG:H19	1.36	1.07
2:A:502:RRG:H14	2:A:502:RRG:H4	1.19	1.07
2:A:501:RRG:H4	2:A:502:RRG:CAF	1.86	1.06
1:A:460:GLU:HB3	1:A:463:MET:HB2	1.38	1.05
1:A:364:MET:SD	2:A:501:RRG:H7	1.97	1.05
2:A:501:RRG:CAZ	2:A:502:RRG:H21	1.88	1.03
1:B:258:GLY:O	1:B:262:ILE:HG22	1.57	1.03
2:A:501:RRG:H12	2:A:502:RRG:H21	1.39	1.01
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.46	0.96
1:A:268:THR:H	1:A:269:PRO:HD2	1.31	0.95
1:A:293:VAL:HG22	1:A:322:VAL:HG21	1.47	0.95
2:A:502:RRG:CAZ	2:A:502:RRG:H14	1.98	0.94
1:A:267:ILE:HD12	1:A:280:ARG:HD2	1.51	0.92
1:A:440:THR:HB	1:B:440:THR:HG22	1.50	0.92
1:A:326:ILE:HD13	2:A:502:RRG:H24	1.50	0.92
1:A:330:LEU:HD21	2:A:501:RRG:H6	1.50	0.92
2:A:501:RRG:H4	2:A:502:RRG:H21	0.94	0.91
1:A:282:PHE:CE2	2:A:501:RRG:H10	2.05	0.91
1:A:288:ARG:HH21	1:A:291:GLU:HB2	1.36	0.90
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.53	0.89
1:B:298:GLU:HG3	3:B:521:HOH:O	1.73	0.88
1:A:271:GLN:HB2	1:A:276:GLU:HA	1.56	0.88
1:A:449:HIS:CE1	2:A:502:RRG:H15	2.09	0.87
1:A:292:ALA:O	1:A:296:ILE:HG13	1.75	0.86
1:A:419:LEU:HA	1:A:422:LYS:HE2	1.57	0.85
2:A:501:RRG:H12	2:A:502:RRG:CAF	2.06	0.85
2:A:501:RRG:H12	2:A:501:RRG:H4	1.56	0.84
1:A:286:GLN:NE2	1:A:465:LEU:HD12	1.92	0.83
1:A:230:LYS:HE3	1:A:379:LEU:O	1.77	0.82
1:A:357:ARG:HG2	1:A:358:LYS:H	1.45	0.82
1:A:286:GLN:HE22	1:A:465:LEU:HA	1.43	0.81
1:A:460:GLU:HB3	1:A:463:MET:CB	2.09	0.81
1:A:293:VAL:HG11	1:A:468:LEU:HD11	1.61	0.81
1:A:282:PHE:HB3	2:A:502:RRG:H7	1.63	0.80
1:A:288:ARG:HH21	1:A:291:GLU:CB	1.94	0.80
2:A:502:RRG:CAP	2:A:502:RRG:H4	2.06	0.79
1:A:319:LYS:NZ	1:A:474:LYS:HD3	1.98	0.79
1:A:473:TYR:O	1:A:474:LYS:HD2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:THR:C	1:A:240:LYS:H	1.87	0.78
1:A:322:VAL:HG11	1:A:472:ILE:HD13	1.66	0.77
1:A:265:LYS:NZ	1:A:265:LYS:HB3	1.98	0.77
1:A:286:GLN:HB2	2:A:502:RRG:H12	1.66	0.77
1:A:286:GLN:HB2	2:A:502:RRG:H11	1.65	0.77
1:A:330:LEU:CD2	2:A:501:RRG:H6	2.15	0.77
1:A:363:PHE:HB3	2:A:501:RRG:H9	1.65	0.77
1:A:433:ALA:O	1:A:437:GLN:HG3	1.84	0.77
1:A:350:ARG:NH1	1:A:368:PHE:HB3	2.00	0.76
1:A:293:VAL:HG22	1:A:322:VAL:CG2	2.16	0.76
1:B:222:TYR:CE1	1:B:381:ASP:HB3	2.22	0.75
1:B:463:MET:HB2	3:B:511:HOH:O	1.86	0.73
1:B:293:VAL:HG22	1:B:322:VAL:HG11	1.71	0.73
1:A:270:LEU:HD11	1:A:273:GLN:H	1.53	0.72
1:A:271:GLN:HB3	1:A:280:ARG:NH1	2.03	0.72
1:A:430:GLN:O	1:A:434:LYS:HG2	1.89	0.72
1:A:262:ILE:HG22	1:A:263:LYS:H	1.53	0.72
1:A:238:THR:O	1:A:240:LYS:N	2.23	0.72
1:B:275:LYS:HE3	1:B:275:LYS:HA	1.72	0.72
1:B:271:GLN:HE21	1:B:271:GLN:HA	1.54	0.72
1:A:402:ASN:HD22	1:A:402:ASN:N	1.86	0.71
1:A:357:ARG:HG2	1:A:358:LYS:N	2.03	0.71
2:A:501:RRG:CAN	2:A:501:RRG:H19	2.18	0.71
1:A:270:LEU:HD22	1:A:271:GLN:H	1.54	0.71
1:A:406:ILE:HB	3:A:652:HOH:O	1.89	0.71
1:A:325:ILE:HD13	1:A:388:ILE:HG23	1.72	0.71
1:A:364:MET:CE	2:A:501:RRG:H7	2.21	0.70
1:B:222:TYR:HE1	1:B:381:ASP:HB3	1.54	0.70
1:B:264:PHE:CZ	1:B:266:HIS:HB3	2.27	0.70
1:B:449:HIS:HE1	1:B:453:LEU:HD22	1.56	0.70
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.56	0.70
1:A:286:GLN:CB	2:A:502:RRG:H12	2.22	0.70
1:B:466:HIS:HA	3:B:505:HOH:O	1.92	0.70
1:A:437:GLN:O	1:A:440:THR:HG22	1.92	0.70
1:B:264:PHE:CE2	1:B:266:HIS:HB3	2.27	0.70
1:A:319:LYS:HZ3	1:A:474:LYS:HD3	1.56	0.70
1:A:249:ILE:HD12	1:A:255:LEU:HA	1.75	0.69
1:A:364:MET:SD	2:A:501:RRG:CAB	2.79	0.69
1:B:220:ASP:O	1:B:224:LYS:HG2	1.93	0.69
1:A:395:GLY:C	1:A:397:ARG:H	1.95	0.69
1:A:282:PHE:HD2	2:A:502:RRG:CAB	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:PRO:HG2	1:A:360:PHE:H	1.58	0.68
1:B:350:ARG:HB3	3:B:525:HOH:O	1.94	0.68
1:A:268:THR:N	1:A:269:PRO:HD2	2.08	0.68
1:A:286:GLN:NE2	1:A:465:LEU:HA	2.09	0.68
2:A:502:RRG:CAZ	2:A:502:RRG:CAP	2.66	0.68
1:B:327:TYR:OH	1:B:449:HIS:HD2	1.76	0.67
1:B:392:ILE:HG23	3:B:543:HOH:O	1.94	0.67
2:A:501:RRG:H15	2:A:501:RRG:CAR	2.21	0.67
1:B:288:ARG:HD2	1:B:288:ARG:O	1.95	0.67
1:A:364:MET:HE1	2:A:501:RRG:H7	1.78	0.66
2:A:501:RRG:CAZ	2:A:501:RRG:H12	2.26	0.66
1:A:393:LEU:O	1:A:410:GLN:HB2	1.95	0.65
1:A:419:LEU:HA	1:A:422:LYS:CE	2.26	0.65
1:B:469:LEU:HB2	3:B:505:HOH:O	1.95	0.65
1:A:311:LEU:HD23	1:A:311:LEU:C	2.17	0.65
1:A:430:GLN:HA	3:A:639:HOH:O	1.96	0.65
1:A:289:SER:OG	2:A:502:RRG:H16	1.96	0.65
1:A:262:ILE:HG22	1:A:263:LYS:N	2.12	0.64
1:A:330:LEU:HD21	2:A:501:RRG:CAB	2.27	0.64
1:A:238:THR:C	1:A:240:LYS:N	2.51	0.64
1:A:326:ILE:HD13	2:A:502:RRG:CAK	2.26	0.64
1:B:236:ILE:HG21	3:B:567:HOH:O	1.97	0.63
1:A:270:LEU:HD13	1:A:271:GLN:N	2.13	0.63
1:A:249:ILE:HA	1:A:254:SER:HB3	1.80	0.63
1:B:459:THR:HG22	1:B:460:GLU:H	1.63	0.63
1:B:400:LEU:HD13	1:B:406:ILE:CD1	2.29	0.63
1:A:407:GLU:HG3	3:A:652:HOH:O	1.99	0.62
1:B:258:GLY:C	1:B:262:ILE:HG22	2.20	0.62
1:A:449:HIS:HE1	2:A:502:RRG:H15	1.65	0.62
1:A:348:MET:SD	1:A:353:LEU:HD21	2.39	0.62
1:B:290:VAL:HG21	1:B:473:TYR:CD1	2.35	0.62
1:A:404:LYS:N	1:A:405:PRO:HD2	2.15	0.61
1:B:449:HIS:CE1	1:B:453:LEU:HD22	2.35	0.61
1:A:265:LYS:HZ2	1:A:265:LYS:HB3	1.64	0.61
1:A:259:GLU:HA	1:A:264:PHE:HB2	1.82	0.61
1:A:463:MET:HE3	1:A:463:MET:HA	1.83	0.61
1:A:276:GLU:HG3	1:A:279:ILE:HG12	1.82	0.61
1:A:286:GLN:HB2	2:A:502:RRG:CAL	2.29	0.61
1:B:268:THR:HB	1:B:269:PRO:HD2	1.83	0.61
1:A:268:THR:H	1:A:269:PRO:CD	2.10	0.60
1:A:336:LYS:HG2	1:A:372:VAL:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:SER:HA	3:B:542:HOH:O	2.00	0.60
1:A:378:GLU:HG2	3:A:656:HOH:O	2.01	0.60
1:A:448:GLU:HA	1:A:451:GLN:HE21	1.67	0.60
1:B:455:VAL:HG22	3:B:541:HOH:O	2.01	0.60
1:B:269:PRO:O	1:B:270:LEU:HD23	2.02	0.60
1:A:463:MET:HG3	3:A:607:HOH:O	2.02	0.60
1:B:411:ASP:O	1:B:415:GLN:HG3	2.01	0.60
1:A:212:ARG:HD2	3:A:626:HOH:O	2.01	0.59
1:A:286:GLN:HE22	1:A:465:LEU:HD12	1.66	0.59
1:B:275:LYS:HG3	1:B:276:GLU:H	1.67	0.59
1:A:282:PHE:CD2	2:A:501:RRG:H10	2.38	0.59
1:A:367:LYS:HE2	2:A:501:RRG:CAA	2.33	0.59
1:A:414:LEU:HB3	1:B:430:GLN:HG2	1.84	0.59
1:A:364:MET:SD	2:A:501:RRG:CAY	2.90	0.59
1:A:357:ARG:HG2	1:A:359:PRO:HD2	1.83	0.59
1:B:290:VAL:HG21	1:B:473:TYR:HD1	1.68	0.59
1:B:447:THR:O	1:B:450:VAL:HG22	2.03	0.58
1:B:452:LEU:O	1:B:456:ILE:HG12	2.03	0.58
1:A:404:LYS:HB3	1:A:404:LYS:NZ	2.17	0.58
1:B:459:THR:HG22	1:B:460:GLU:N	2.18	0.58
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.84	0.58
1:A:359:PRO:HG2	1:A:360:PHE:CD1	2.38	0.58
1:A:286:GLN:CD	2:A:502:RRG:H11	2.23	0.58
1:A:320:TYR:CE2	1:A:398:PRO:HD2	2.39	0.58
1:A:397:ARG:HB2	1:A:400:LEU:HD11	1.86	0.58
1:A:441:ASP:O	1:A:445:ILE:HG13	2.02	0.58
1:B:321:GLY:O	1:B:325:ILE:HG12	2.04	0.58
1:B:212:ARG:HD2	3:B:517:HOH:O	2.02	0.57
1:A:357:ARG:CG	1:A:359:PRO:HD2	2.34	0.57
1:A:298:GLU:OE1	1:A:298:GLU:HA	2.04	0.57
1:A:367:LYS:HG2	2:A:501:RRG:H2	1.86	0.57
1:B:358:LYS:HB2	1:B:359:PRO:HD3	1.87	0.57
1:B:468:LEU:O	1:B:472:ILE:HG13	2.04	0.57
1:A:365:GLU:N	1:A:366:PRO:HD2	2.19	0.57
1:B:267:ILE:HG12	1:B:268:THR:N	2.19	0.57
1:A:341:ILE:HB	2:A:501:RRG:H18	1.86	0.56
1:B:275:LYS:HG3	1:B:276:GLU:N	2.20	0.56
1:A:403:VAL:C	1:A:405:PRO:HD2	2.25	0.56
1:A:450:VAL:HG22	1:A:473:TYR:CE1	2.40	0.56
1:B:450:VAL:HG23	1:B:451:GLN:N	2.20	0.56
1:A:336:LYS:HG2	1:A:372:VAL:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:SER:O	1:A:465:LEU:HB2	2.05	0.56
1:A:323:HIS:NE2	2:A:502:RRG:OAC	2.38	0.56
1:B:257:MET:HG3	3:B:569:HOH:O	2.06	0.56
1:A:402:ASN:N	1:A:402:ASN:ND2	2.54	0.56
1:A:274:SER:O	1:A:275:LYS:HB2	2.06	0.56
1:B:374:PHE:HD1	1:B:438:LYS:HG2	1.70	0.56
1:A:287:PHE:HA	1:A:290:VAL:HG12	1.88	0.56
1:A:250:TYR:HA	1:A:349:THR:OG1	2.05	0.55
1:B:342:SER:O	1:B:345:GLN:HG2	2.06	0.55
1:B:320:TYR:HB2	1:B:397:ARG:HD2	1.87	0.55
1:A:242:THR:HG22	1:A:245:SER:OG	2.06	0.55
1:B:273:GLN:OE1	1:B:273:GLN:N	2.39	0.55
1:A:394:SER:CB	1:A:397:ARG:HE	2.20	0.55
1:B:393:LEU:O	1:B:410:GLN:HB2	2.05	0.55
1:A:419:LEU:HD12	1:A:422:LYS:HE3	1.88	0.55
1:B:421:LEU:HD12	1:B:432:PHE:HA	1.88	0.55
2:A:501:RRG:CAT	2:A:501:RRG:H20	2.37	0.55
1:B:340:LEU:HD22	3:B:567:HOH:O	2.07	0.55
1:B:256:MET:HB2	3:B:569:HOH:O	2.07	0.55
1:A:394:SER:HA	1:A:410:GLN:OE1	2.07	0.55
1:A:435:LEU:O	1:A:438:LYS:HB2	2.07	0.55
1:A:414:LEU:CB	1:B:430:GLN:HG2	2.36	0.55
2:A:501:RRG:CAQ	2:A:501:RRG:H5	2.37	0.55
1:B:465:LEU:C	1:B:467:PRO:HD2	2.27	0.55
2:A:501:RRG:CAQ	2:A:501:RRG:CAZ	2.83	0.55
1:B:368:PHE:HD1	3:B:549:HOH:O	1.90	0.54
1:A:223:ILE:HA	3:A:653:HOH:O	2.07	0.54
1:B:222:TYR:HB2	1:B:299:TYR:CE1	2.43	0.54
1:B:355:SER:O	1:B:356:LEU:HG	2.07	0.54
1:A:271:GLN:OE1	1:A:272:GLU:HG2	2.07	0.54
1:A:407:GLU:N	3:A:652:HOH:O	2.41	0.54
1:B:293:VAL:CG2	1:B:322:VAL:HG11	2.37	0.54
1:B:400:LEU:HD13	1:B:406:ILE:HD12	1.89	0.54
1:A:220:ASP:O	1:A:224:LYS:HG3	2.09	0.53
1:A:255:LEU:O	1:A:255:LEU:HD23	2.07	0.53
1:B:212:ARG:HB3	1:B:212:ARG:CZ	2.38	0.53
1:B:295:GLU:HG2	3:B:509:HOH:O	2.08	0.53
1:B:309:LEU:O	1:B:314:GLN:NE2	2.38	0.53
1:A:257:MET:O	1:A:261:LYS:HG2	2.09	0.53
1:B:308:ASN:HB2	3:B:540:HOH:O	2.08	0.53
1:A:310:ASP:OD2	1:A:312:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:PHE:HB3	2:A:501:RRG:CAI	2.35	0.53
1:A:449:HIS:NE2	2:A:502:RRG:H15	2.24	0.52
1:A:386:ILE:HD12	1:A:420:GLN:HG2	1.90	0.52
1:B:419:LEU:HD11	1:B:423:LEU:HD11	1.91	0.52
1:A:264:PHE:CE2	2:A:501:RRG:H22	2.44	0.52
1:A:288:ARG:HG3	2:A:501:RRG:CAT	2.39	0.52
1:B:336:LYS:HA	3:B:549:HOH:O	2.09	0.52
1:A:271:GLN:HB2	1:A:276:GLU:CA	2.36	0.52
1:A:311:LEU:O	1:A:311:LEU:HD23	2.09	0.52
1:A:282:PHE:CD2	2:A:502:RRG:CAB	2.90	0.52
1:A:336:LYS:HB2	3:A:622:HOH:O	2.09	0.52
1:A:440:THR:O	1:A:444:GLN:HG2	2.10	0.52
1:A:282:PHE:CD2	2:A:502:RRG:H7	2.45	0.52
1:A:271:GLN:NE2	1:A:272:GLU:N	2.57	0.51
1:A:364:MET:C	1:A:366:PRO:HD2	2.30	0.51
1:A:264:PHE:CE2	2:A:501:RRG:CAE	2.93	0.51
1:A:353:LEU:HD13	1:A:364:MET:HG3	1.92	0.51
1:A:271:GLN:HB3	1:A:280:ARG:HH11	1.72	0.51
1:B:454:GLN:HG3	1:B:455:VAL:N	2.25	0.51
1:B:448:GLU:HA	1:B:451:GLN:NE2	2.26	0.51
1:A:323:HIS:NE2	2:A:502:RRG:CAT	2.74	0.51
2:A:501:RRG:CAW	2:A:501:RRG:H5	2.41	0.51
1:A:259:GLU:OE1	1:A:264:PHE:HB3	2.10	0.51
1:A:468:LEU:O	1:A:472:ILE:HG13	2.10	0.51
1:B:250:TYR:CE1	1:B:251:ASP:HB2	2.46	0.50
1:B:461:THR:HG22	3:B:535:HOH:O	2.11	0.50
1:A:255:LEU:HD23	1:A:255:LEU:C	2.31	0.50
1:A:286:GLN:HE21	1:A:465:LEU:HD12	1.74	0.50
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.46	0.50
1:B:467:PRO:HG2	1:B:468:LEU:H	1.76	0.50
1:A:326:ILE:HG21	2:A:502:RRG:CAK	2.41	0.50
1:A:330:LEU:O	1:A:334:MET:HG3	2.11	0.50
1:B:340:LEU:HD13	3:B:567:HOH:O	2.11	0.50
1:B:267:ILE:HG12	1:B:268:THR:H	1.76	0.50
1:A:319:LYS:HD3	1:A:320:TYR:CE1	2.47	0.50
2:A:501:RRG:H20	2:A:501:RRG:OAC	2.11	0.50
1:A:286:GLN:CB	2:A:502:RRG:H11	2.39	0.50
1:B:334:MET:HG2	1:B:339:VAL:HB	1.94	0.50
1:A:360:PHE:HA	1:A:363:PHE:HD2	1.77	0.49
1:B:457:LYS:O	1:B:457:LYS:HG3	2.11	0.49
1:B:266:HIS:CG	1:B:267:ILE:N	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:HZ3	1:A:265:LYS:HB3	1.74	0.49
1:A:285:CYS:SG	2:A:501:RRG:CAX	3.00	0.49
1:A:267:ILE:HB	1:A:280:ARG:CZ	2.42	0.49
1:A:250:TYR:HB2	3:A:630:HOH:O	2.12	0.49
1:A:367:LYS:HG2	2:A:501:RRG:CAA	2.42	0.49
1:B:228:LEU:HD23	1:B:232:LYS:HD3	1.94	0.49
1:A:367:LYS:HE2	2:A:501:RRG:H1	1.94	0.49
1:A:378:GLU:HA	3:A:610:HOH:O	2.13	0.49
1:A:438:LYS:O	1:A:441:ASP:HB2	2.13	0.49
1:A:333:LEU:HB3	1:A:340:LEU:HB2	1.95	0.49
1:B:214:LEU:HD21	1:B:413:LEU:HD23	1.95	0.49
1:B:275:LYS:CE	1:B:275:LYS:HA	2.41	0.49
1:A:440:THR:CB	1:B:440:THR:HG22	2.32	0.49
1:B:320:TYR:CB	1:B:397:ARG:HD2	2.42	0.49
1:A:442:LEU:O	1:A:446:VAL:HG23	2.13	0.48
1:B:364:MET:C	1:B:366:PRO:HD2	2.33	0.48
1:A:252:MET:O	1:A:256:MET:HB2	2.13	0.48
1:A:397:ARG:HB2	1:A:400:LEU:CD1	2.43	0.48
1:B:454:GLN:HG3	1:B:455:VAL:H	1.78	0.48
1:A:283:GLN:O	1:A:286:GLN:HB3	2.13	0.48
1:A:394:SER:HB2	1:A:397:ARG:HE	1.77	0.48
1:A:363:PHE:CZ	1:A:452:LEU:HD22	2.49	0.48
1:A:282:PHE:CB	2:A:502:RRG:H7	2.39	0.48
1:A:259:GLU:OE2	1:A:264:PHE:CD2	2.67	0.48
1:B:327:TYR:OH	1:B:449:HIS:CD2	2.62	0.48
1:A:271:GLN:HE22	1:A:272:GLU:CD	2.17	0.48
1:A:460:GLU:CB	1:A:463:MET:HB2	2.27	0.48
1:A:350:ARG:NH2	1:A:365:GLU:OE2	2.46	0.48
1:B:272:GLU:HG2	1:B:272:GLU:O	2.14	0.48
1:B:287:PHE:CD2	1:B:473:TYR:OH	2.64	0.48
1:B:402:ASN:OD1	1:B:405:PRO:CD	2.61	0.47
1:B:404:LYS:N	1:B:405:PRO:HD2	2.29	0.47
1:A:285:CYS:SG	2:A:501:RRG:CAQ	3.03	0.47
1:B:269:PRO:HA	1:B:280:ARG:HH22	1.79	0.47
1:A:270:LEU:HD22	1:A:271:GLN:N	2.27	0.47
1:A:286:GLN:CA	2:A:502:RRG:H12	2.44	0.47
1:B:267:ILE:HD13	1:B:280:ARG:HD2	1.96	0.47
1:A:370:PHE:HA	1:A:373:LYS:NZ	2.29	0.47
1:A:395:GLY:C	1:A:397:ARG:N	2.64	0.47
1:B:450:VAL:HA	1:B:453:LEU:HB3	1.95	0.47
1:A:259:GLU:HG3	1:A:268:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ILE:HD12	1:A:456:ILE:N	2.30	0.47
1:B:402:ASN:OD1	1:B:405:PRO:HD2	2.15	0.47
1:B:240:LYS:O	1:B:241:THR:C	2.53	0.47
1:B:335:ASN:OD1	1:B:337:ASP:N	2.37	0.47
1:B:450:VAL:CG2	1:B:451:GLN:N	2.78	0.47
3:A:648:HOH:O	1:B:430:GLN:HB2	2.15	0.47
1:A:363:PHE:CE2	2:A:502:RRG:H3	2.50	0.47
1:B:262:ILE:HD11	1:B:345:GLN:HB2	1.97	0.47
1:A:393:LEU:HD12	1:A:409:ILE:HB	1.97	0.46
1:B:257:MET:HB3	3:B:506:HOH:O	2.15	0.46
1:B:339:VAL:O	1:B:341:ILE:HD13	2.15	0.46
1:B:430:GLN:HG3	1:B:433:ALA:HB3	1.97	0.46
1:A:323:HIS:CD2	2:A:502:RRG:H19	2.50	0.46
1:B:352:PHE:O	1:B:355:SER:O	2.34	0.46
1:A:319:LYS:O	1:A:472:ILE:HG23	2.15	0.46
1:A:349:THR:HB	1:A:352:PHE:H	1.81	0.46
1:A:464:SER:HB2	1:A:465:LEU:H	1.58	0.46
1:A:287:PHE:O	1:A:291:GLU:HG3	2.16	0.46
1:A:436:LEU:O	1:A:439:MET:HG3	2.16	0.46
1:A:243:ASP:HB2	3:A:609:HOH:O	2.15	0.45
1:A:363:PHE:CE2	1:A:452:LEU:HD22	2.51	0.45
1:A:393:LEU:O	1:A:410:GLN:OE1	2.33	0.45
1:B:340:LEU:O	1:B:341:ILE:HD12	2.16	0.45
1:B:272:GLU:C	1:B:274:SER:H	2.20	0.45
1:B:404:LYS:HB3	1:B:405:PRO:HD3	1.99	0.45
1:A:282:PHE:HB3	2:A:502:RRG:CAB	2.38	0.45
1:A:335:ASN:O	1:A:337:ASP:N	2.50	0.45
1:A:430:GLN:HG3	3:A:639:HOH:O	2.16	0.45
1:A:373:LYS:O	1:A:376:ALA:HB3	2.17	0.45
1:A:319:LYS:HZ1	1:A:474:LYS:HD3	1.81	0.45
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.78	0.45
1:A:305:GLY:HA2	1:A:308:ASN:ND2	2.28	0.45
1:A:424:ASN:HB3	1:A:425:HIS:CD2	2.51	0.45
1:A:465:LEU:HD11	3:A:625:HOH:O	2.17	0.45
1:A:277:VAL:O	1:A:281:ILE:HG13	2.15	0.45
1:A:249:ILE:CG2	1:A:255:LEU:HB2	2.46	0.45
1:A:317:LEU:HD21	1:A:406:ILE:HD13	1.99	0.45
1:A:359:PRO:O	1:A:360:PHE:C	2.55	0.45
1:A:259:GLU:OE2	1:A:264:PHE:HD2	2.00	0.45
1:A:320:TYR:HB3	1:A:397:ARG:HH11	1.82	0.45
1:A:364:MET:SD	2:A:501:RRG:CAM	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ARG:HG3	3:A:638:HOH:O	2.17	0.44
1:A:255:LEU:HD13	1:A:352:PHE:HZ	1.82	0.44
1:B:276:GLU:O	1:B:280:ARG:HD3	2.17	0.44
1:B:319:LYS:HE3	1:B:320:TYR:OH	2.17	0.44
1:B:358:LYS:HE2	3:B:534:HOH:O	2.16	0.44
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.82	0.44
1:B:448:GLU:HB2	3:B:531:HOH:O	2.18	0.44
1:A:325:ILE:O	1:A:329:MET:HG3	2.17	0.44
1:A:289:SER:O	1:A:293:VAL:HG23	2.16	0.44
1:B:404:LYS:HB3	1:B:405:PRO:CD	2.47	0.44
1:A:323:HIS:CD2	2:A:502:RRG:CAR	3.01	0.44
1:B:459:THR:CG2	1:B:460:GLU:H	2.28	0.44
1:A:268:THR:N	1:A:269:PRO:CD	2.77	0.44
1:A:271:GLN:C	1:A:276:GLU:HA	2.37	0.44
1:A:288:ARG:HH21	1:A:291:GLU:HB3	1.78	0.44
1:A:336:LYS:HE3	3:A:660:HOH:O	2.17	0.44
1:A:413:LEU:O	1:A:416:ALA:N	2.51	0.44
1:B:319:LYS:HE3	1:B:320:TYR:CZ	2.53	0.44
1:A:393:LEU:CD1	1:A:409:ILE:HG21	2.48	0.44
1:B:237:LEU:HB3	1:B:238:THR:H	1.52	0.44
1:B:364:MET:O	1:B:367:LYS:HG2	2.18	0.43
1:A:426:PRO:C	1:A:428:SER:H	2.21	0.43
1:B:228:LEU:HD23	1:B:232:LYS:CG	2.48	0.43
1:B:456:ILE:O	1:B:456:ILE:HG22	2.18	0.43
1:A:319:LYS:HD3	1:A:320:TYR:HE1	1.83	0.43
1:B:235:ALA:HB1	1:B:241:THR:HG21	1.99	0.43
1:A:270:LEU:C	1:A:270:LEU:HD13	2.39	0.43
1:A:358:LYS:N	1:A:359:PRO:HD2	2.33	0.43
1:A:364:MET:HB2	3:A:641:HOH:O	2.17	0.43
1:B:474:LYS:HE2	1:B:474:LYS:HB2	1.78	0.43
1:A:262:ILE:CG2	1:A:263:LYS:H	2.29	0.43
1:A:285:CYS:SG	2:A:501:RRG:CAW	3.07	0.43
1:B:262:ILE:O	1:B:264:PHE:N	2.51	0.43
1:B:348:MET:SD	1:B:353:LEU:HD21	2.58	0.43
1:A:448:GLU:HA	1:A:451:GLN:NE2	2.32	0.43
1:A:320:TYR:OH	1:A:398:PRO:HB2	2.19	0.43
1:B:466:HIS:N	1:B:467:PRO:CD	2.82	0.43
1:A:317:LEU:HD22	1:A:392:ILE:O	2.18	0.43
1:A:449:HIS:CD2	1:A:473:TYR:OH	2.71	0.43
2:A:501:RRG:CAQ	2:A:501:RRG:H4	2.36	0.43
1:B:313:ASP:O	1:B:317:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:O	1:A:218:LEU:HG	2.19	0.43
1:A:375:ASN:HA	3:A:616:HOH:O	2.19	0.43
1:A:323:HIS:NE2	2:A:502:RRG:H18	2.34	0.43
1:B:336:LYS:O	1:B:350:ARG:HD2	2.19	0.43
1:A:271:GLN:CB	1:A:276:GLU:HA	2.38	0.42
1:A:419:LEU:O	1:A:423:LEU:HG	2.18	0.42
2:A:501:RRG:CAJ	2:A:501:RRG:CAT	2.96	0.42
1:B:278:ALA:HB1	1:B:360:PHE:CD2	2.54	0.42
1:A:286:GLN:OE1	2:A:502:RRG:H10	2.19	0.42
1:B:288:ARG:CD	1:B:288:ARG:O	2.65	0.42
1:A:307:VAL:HG22	3:A:601:HOH:O	2.17	0.42
1:B:465:LEU:C	1:B:467:PRO:CD	2.87	0.42
1:A:335:ASN:C	1:A:337:ASP:H	2.23	0.42
1:B:450:VAL:O	1:B:453:LEU:N	2.50	0.42
1:A:270:LEU:CD1	1:A:273:GLN:H	2.27	0.42
1:A:350:ARG:NH2	3:A:660:HOH:O	2.49	0.42
1:A:411:ASP:O	1:A:415:GLN:HG3	2.19	0.42
1:B:237:LEU:O	1:B:239:GLY:O	2.37	0.42
1:A:359:PRO:CG	1:A:360:PHE:H	2.28	0.42
1:A:286:GLN:HA	2:A:502:RRG:H12	2.02	0.42
1:A:456:ILE:H	1:A:456:ILE:HD12	1.85	0.42
2:A:501:RRG:CAQ	2:A:501:RRG:CAB	2.98	0.42
1:B:230:LYS:O	1:B:230:LYS:HG2	2.19	0.41
1:B:392:ILE:HG12	3:B:543:HOH:O	2.19	0.41
1:A:360:PHE:O	1:A:362:ASP:N	2.53	0.41
1:A:456:ILE:O	1:A:460:GLU:HB2	2.20	0.41
1:B:226:PHE:HA	1:B:227:PRO:HD3	1.89	0.41
1:A:337:ASP:N	3:A:620:HOH:O	2.53	0.41
1:A:452:LEU:O	1:A:452:LEU:HD23	2.21	0.41
2:A:502:RRG:H13	2:A:502:RRG:H16	1.77	0.41
1:B:212:ARG:NH1	1:B:212:ARG:HB3	2.35	0.41
1:B:265:LYS:HG3	1:B:287:PHE:CE1	2.55	0.41
1:A:268:THR:HB	1:A:269:PRO:CD	2.50	0.41
1:A:267:ILE:HG22	1:A:268:THR:N	2.35	0.41
1:A:271:GLN:NE2	1:A:272:GLU:OE2	2.53	0.41
1:A:395:GLY:O	1:A:397:ARG:N	2.52	0.41
1:B:472:ILE:HG22	1:B:472:ILE:O	2.20	0.41
1:A:311:LEU:CD2	1:A:311:LEU:C	2.88	0.41
1:B:457:LYS:HZ3	1:B:461:THR:HB	1.86	0.41
1:A:427:GLU:CD	1:A:427:GLU:N	2.74	0.41
1:B:250:TYR:HE1	1:B:251:ASP:OD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:PHE:CD1	1:B:438:LYS:HG2	2.54	0.41
1:B:466:HIS:CD2	3:B:511:HOH:O	2.73	0.41
1:A:380:ASP:C	1:A:380:ASP:OD1	2.59	0.41
2:A:501:RRG:CAJ	2:A:501:RRG:OAC	2.68	0.41
1:B:293:VAL:HG22	1:B:322:VAL:CG1	2.44	0.41
1:B:451:GLN:O	1:B:454:GLN:HG2	2.20	0.41
1:B:457:LYS:HD2	3:B:535:HOH:O	2.20	0.41
1:A:357:ARG:CD	1:A:359:PRO:HD2	2.50	0.41
1:A:287:PHE:O	1:A:290:VAL:HG12	2.20	0.40
1:B:271:GLN:HE21	1:B:271:GLN:CA	2.20	0.40
1:A:262:ILE:HG23	1:A:345:GLN:CD	2.41	0.40
1:B:265:LYS:HG3	1:B:287:PHE:HE1	1.85	0.40
1:B:426:PRO:HG2	1:B:427:GLU:H	1.85	0.40
1:A:413:LEU:O	1:A:416:ALA:HB3	2.21	0.40
1:A:427:GLU:H	1:A:427:GLU:CD	2.25	0.40
1:A:438:LYS:HD3	1:A:441:ASP:OD2	2.21	0.40
1:A:463:MET:SD	2:A:502:RRG:H9	2.61	0.40
1:B:273:GLN:N	1:B:273:GLN:CD	2.74	0.40
1:B:353:LEU:C	1:B:355:SER:H	2.24	0.40
1:B:380:ASP:C	1:B:380:ASP:OD1	2.60	0.40
1:A:467:PRO:O	1:A:471:GLU:HB2	2.21	0.40
1:B:392:ILE:HG22	1:B:393:LEU:HD22	2.03	0.40
1:A:212:ARG:HA	1:A:212:ARG:HD2	1.89	0.40
1:A:267:ILE:HG22	1:A:268:THR:H	1.87	0.40
1:A:326:ILE:HG22	1:A:327:TYR:N	2.36	0.40
1:A:450:VAL:HG22	1:A:473:TYR:HE1	1.85	0.40
1:B:469:LEU:HA	1:B:469:LEU:HD22	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	266/287 (93%)	234 (88%)	16 (6%)	16 (6%)	1	1
1	B	266/287 (93%)	218 (82%)	30 (11%)	18 (7%)	1	1
All	All	532/574 (93%)	452 (85%)	46 (9%)	34 (6%)	1	1

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	PRO
1	A	309	LEU
1	A	359	PRO
1	B	237	LEU
1	B	263	LYS
1	B	266	HIS
1	B	272	GLU
1	A	239	GLY
1	A	276	GLU
1	A	336	LYS
1	A	357	ARG
1	A	361	GLY
1	A	465	LEU
1	B	257	MET
1	B	261	LYS
1	B	357	ARG
1	B	394	SER
1	A	396	ASP
1	B	227	PRO
1	B	364	MET
1	B	365	GLU
1	B	467	PRO
1	A	244	LYS
1	A	268	THR
1	A	427	GLU
1	B	241	THR
1	B	244	LYS
1	A	240	LYS
1	A	401	LEU
1	B	275	LYS
1	A	360	PHE
1	B	240	LYS
1	B	466	HIS
1	B	358	LYS

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	241/258 (93%)	227 (94%)	14 (6%)	20	38
1	B	241/258 (93%)	227 (94%)	14 (6%)	20	38
All	All	482/516 (93%)	454 (94%)	28 (6%)	20	38

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	SER
1	A	271	GLN
1	A	287	PHE
1	A	288	ARG
1	A	349	THR
1	A	362	ASP
1	A	363	PHE
1	A	393	LEU
1	A	402	ASN
1	A	404	LYS
1	A	427	GLU
1	A	460	GLU
1	A	464	SER
1	A	474	LYS
1	B	210	ASP
1	B	221	SER
1	B	228	LEU
1	B	251	ASP
1	B	271	GLN
1	B	272	GLU
1	B	273	GLN
1	B	318	LEU
1	B	351	GLU
1	B	430	GLN
1	B	438	LYS
1	B	443	ARG
1	B	451	GLN

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Mol	Chain	Res	Type
1	B	469	LEU

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

Mol	Chain	Res	Type
1	A	271	GLN
1	A	286	GLN
1	A	308	ASN
1	A	314	GLN
1	A	402	ASN
1	A	410	GLN
1	A	415	GLN
1	A	451	GLN
1	A	454	GLN
1	A	470	GLN
1	B	217	HIS
1	B	266	HIS
1	B	271	GLN
1	B	308	ASN
1	B	444	GLN
1	B	449	HIS
1	B	451	GLN
1	B	466	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

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	RRG	A	501	-	26,29,29	1.15	1 (3%)	33,39,39	0.95	1 (3%)
2	RRG	A	502	-	26,29,29	1.14	1 (3%)	33,39,39	1.90	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	RRG	A	501	-	-	7/16/20/20	0/3/3/3
2	RRG	A	502	-	-	5/16/20/20	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	RRG	CAX-CAW	-5.37	1.39	1.49
2	A	502	RRG	CAX-CAW	-5.28	1.39	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	RRG	CAV-OAS-CBA	-10.33	111.73	118.62
2	A	501	RRG	CAV-OAS-CBA	-4.56	115.58	118.62

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	RRG	CAM-CAY-CAZ-CAA

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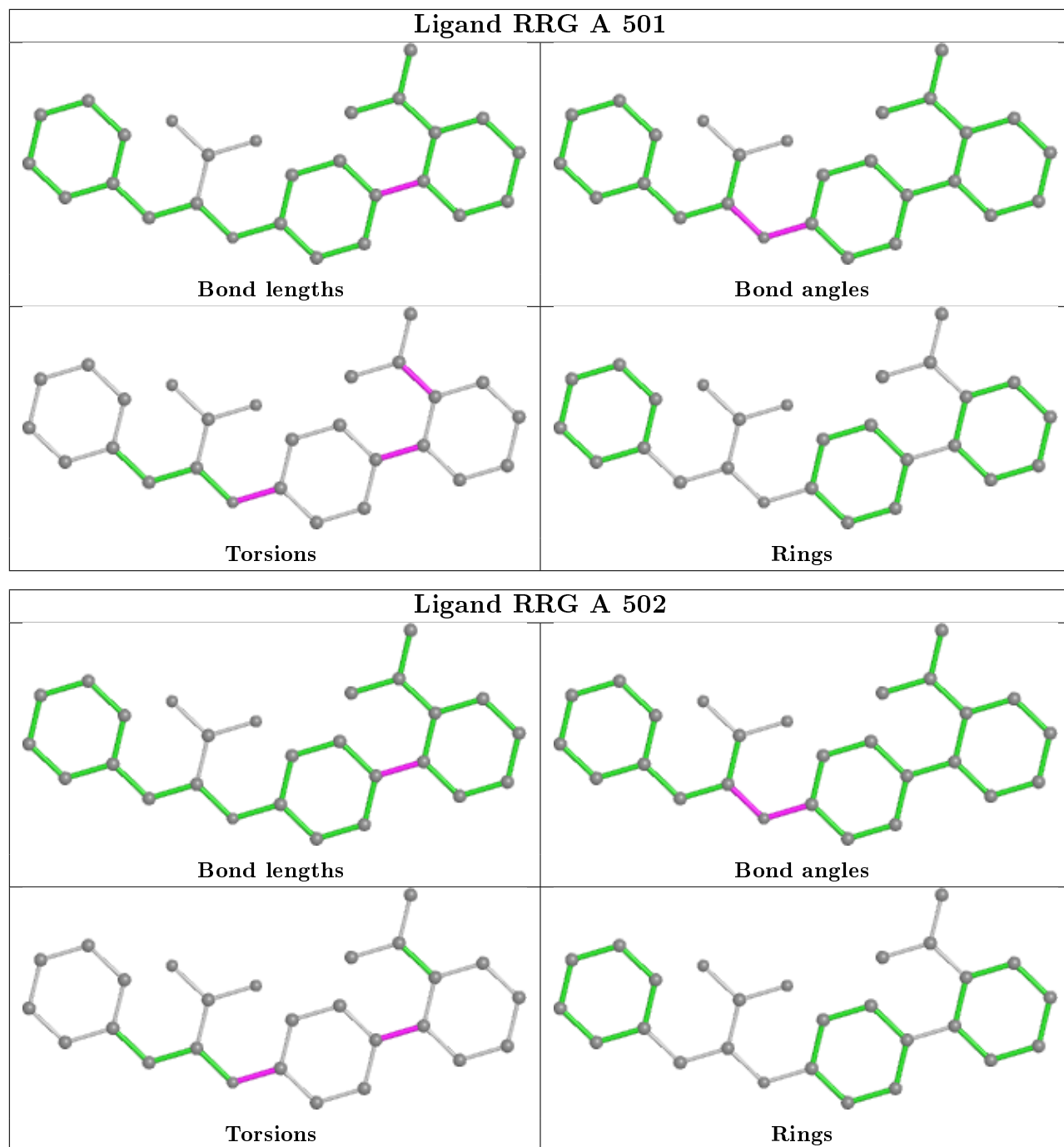
Mol	Chain	Res	Type	Atoms
2	A	501	RRG	CAX-CAY-CAZ-CAB
2	A	501	RRG	CAM-CAY-CAZ-CAB
2	A	501	RRG	CAX-CAY-CAZ-CAA
2	A	502	RRG	CAP-CAW-CAX-CAY
2	A	502	RRG	CAP-CAW-CAX-CAL
2	A	502	RRG	CAQ-CAW-CAX-CAL
2	A	502	RRG	CAQ-CAW-CAX-CAY
2	A	501	RRG	CAN-CAV-OAS-CBA
2	A	501	RRG	CAO-CAV-OAS-CBA
2	A	501	RRG	CAP-CAW-CAX-CAY
2	A	502	RRG	CAN-CAV-OAS-CBA

There are no ring outliers.

2 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	RRG	43	0
2	A	502	RRG	39	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	268/287 (93%)	0.94	43 (16%) 1 1	25, 61, 92, 97	0
1	B	265/287 (92%)	0.96	42 (15%) 2 1	26, 51, 93, 100	0
All	All	533/574 (92%)	0.95	85 (15%) 1 1	25, 57, 93, 100	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	THR	10.9
1	B	270	LEU	9.9
1	B	465	LEU	9.8
1	B	267	ILE	9.3
1	B	463	MET	9.3
1	A	269	PRO	9.2
1	B	462	ASP	8.8
1	B	464	SER	8.5
1	B	269	PRO	7.6
1	A	267	ILE	6.8
1	B	268	THR	6.5
1	B	474	LYS	6.2
1	A	239	GLY	6.1
1	A	264	PHE	6.0
1	B	271	GLN	5.9
1	B	273	GLN	5.8
1	A	270	LEU	5.8
1	A	274	SER	5.7
1	B	274	SER	5.6
1	A	240	LYS	5.0
1	B	207	GLU	4.9
1	A	266	HIS	4.8
1	B	272	GLU	4.8
1	A	242	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	263	LYS	4.5
1	B	235	ALA	4.3
1	B	261	LYS	4.3
1	B	264	PHE	4.2
1	B	356	LEU	4.2
1	A	398	PRO	4.1
1	B	275	LYS	4.1
1	A	282	PHE	4.0
1	B	279	ILE	3.9
1	B	287	PHE	3.9
1	A	273	GLN	3.8
1	B	241	THR	3.8
1	B	358	LYS	3.6
1	A	390	VAL	3.5
1	A	422	LYS	3.4
1	A	336	LYS	3.4
1	A	454	GLN	3.3
1	B	360	PHE	3.2
1	B	451	GLN	3.2
1	B	461	THR	3.2
1	B	276	GLU	3.1
1	B	265	LYS	3.1
1	A	265	LYS	3.1
1	B	455	VAL	3.1
1	A	463	MET	3.1
1	A	280	ARG	3.0
1	B	452	LEU	2.9
1	A	461	THR	2.9
1	A	451	GLN	2.9
1	A	388	ILE	2.9
1	B	232	LYS	2.9
1	B	238	THR	2.8
1	A	252	MET	2.8
1	B	288	ARG	2.8
1	A	473	TYR	2.8
1	B	266	HIS	2.7
1	B	240	LYS	2.6
1	B	454	GLN	2.6
1	A	358	LYS	2.6
1	A	447	THR	2.6
1	A	360	PHE	2.6
1	B	355	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	429	SER	2.5
1	A	243	ASP	2.5
1	A	261	LYS	2.4
1	A	397	ARG	2.4
1	A	408	ASP	2.3
1	A	262	ILE	2.3
1	A	387	PHE	2.3
1	A	275	LYS	2.3
1	A	241	THR	2.2
1	B	362	ASP	2.2
1	A	263	LYS	2.2
1	B	212	ARG	2.2
1	A	391	ILE	2.2
1	A	389	ALA	2.1
1	B	239	GLY	2.1
1	A	271	GLN	2.1
1	A	392	ILE	2.0
1	B	236	ILE	2.0
1	A	320	TYR	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. 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.

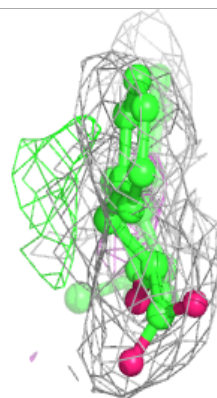
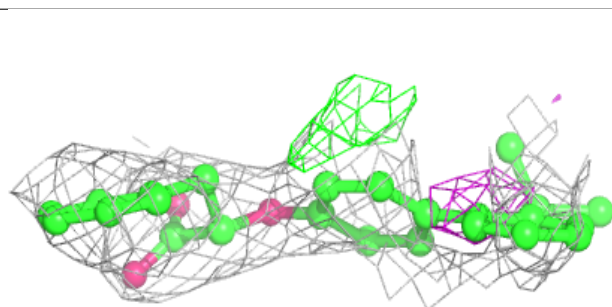
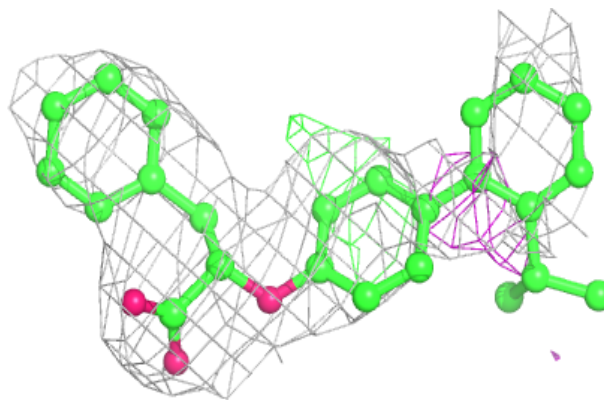
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	RRG	A	501	27/27	0.70	0.40	78,81,83,83	0
2	RRG	A	502	27/27	0.76	0.39	79,82,87,89	0

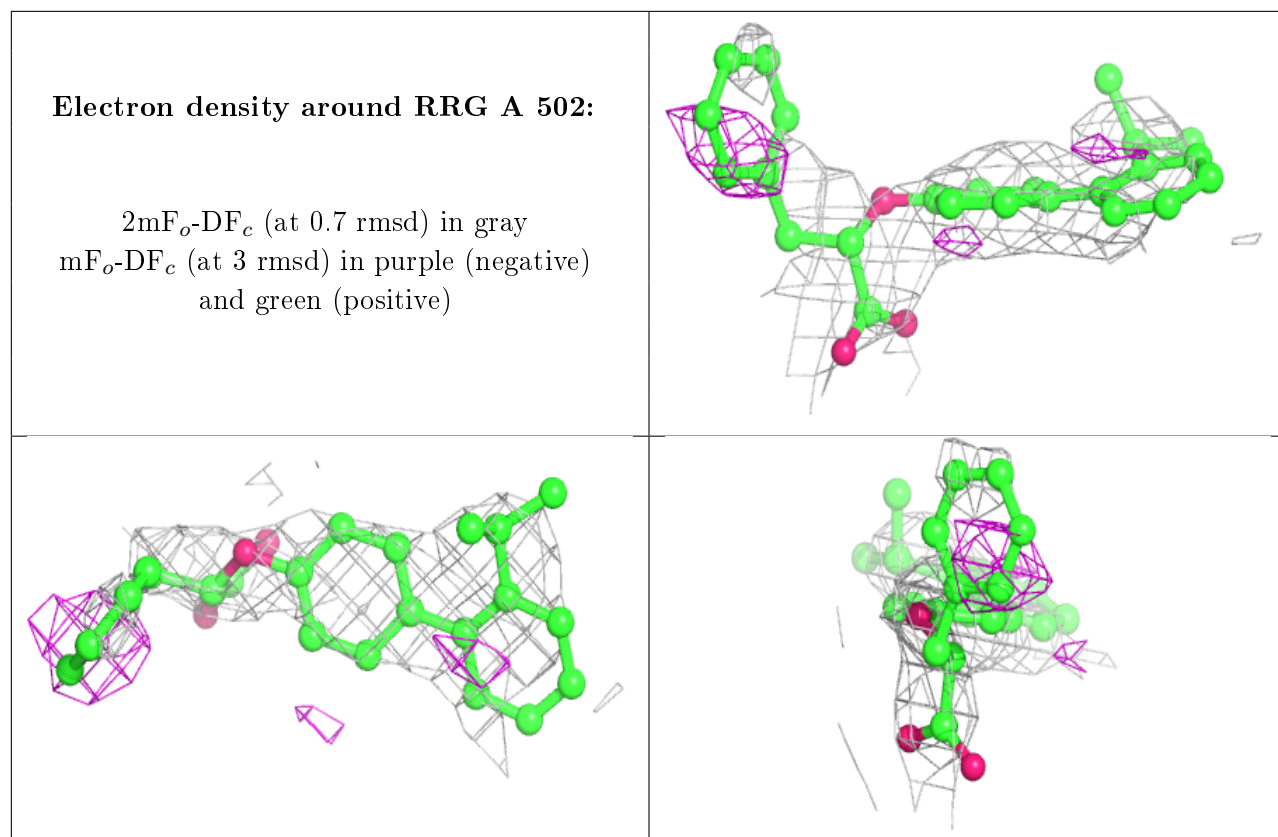
The following is a graphical depiction of the model fit to experimental electron density of all

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 RRG A 501:

$2mF_o-DF_c$ (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.