



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:52 PM GMT

PDB ID : 4JL4  
Title : Crystal structure of the complex between PPARgamma LBD and the ligand LJ570 [(2S)-3-(biphenyl-4-yl)-2-(biphenyl-4-yloxy)propanoic acid]  
Authors : Pochetti, G.; Montanari, R.; Capelli, D.  
Deposited on : 2013-03-12  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

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

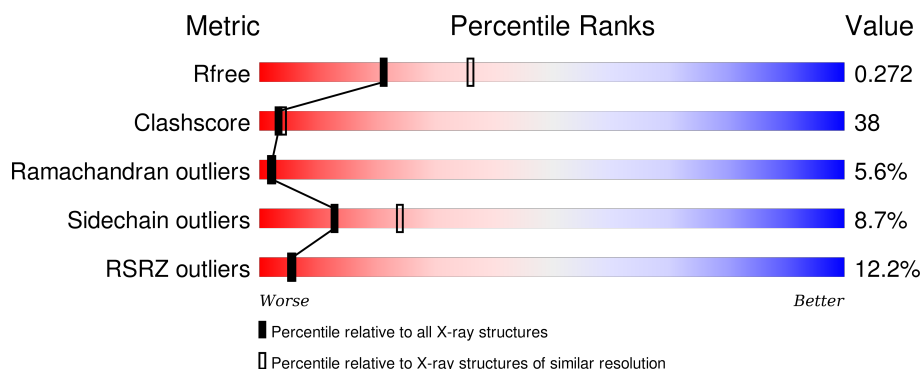
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	287	<div> <div>11%</div> <div>38%</div> <div>49%</div> <div>6%</div> <div>7%</div> </div>
1	B	287	<div> <div>11%</div> <div>35%</div> <div>47%</div> <div>10%</div> <div>7%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AXY	A	501	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4505 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.

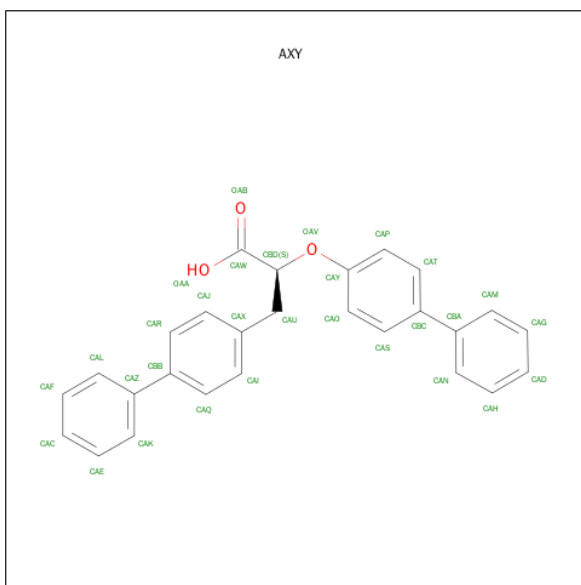
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

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	267	Total	C	N	O	S	33	0	0
			2140	1381	350	399	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-(BIPHENYL-4-YL)-2-(BIPHENYL-4-YLOXY)PROPANOIC ACID (three-letter code: AXY) (formula: C<sub>27</sub>H<sub>22</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			30	27	3		

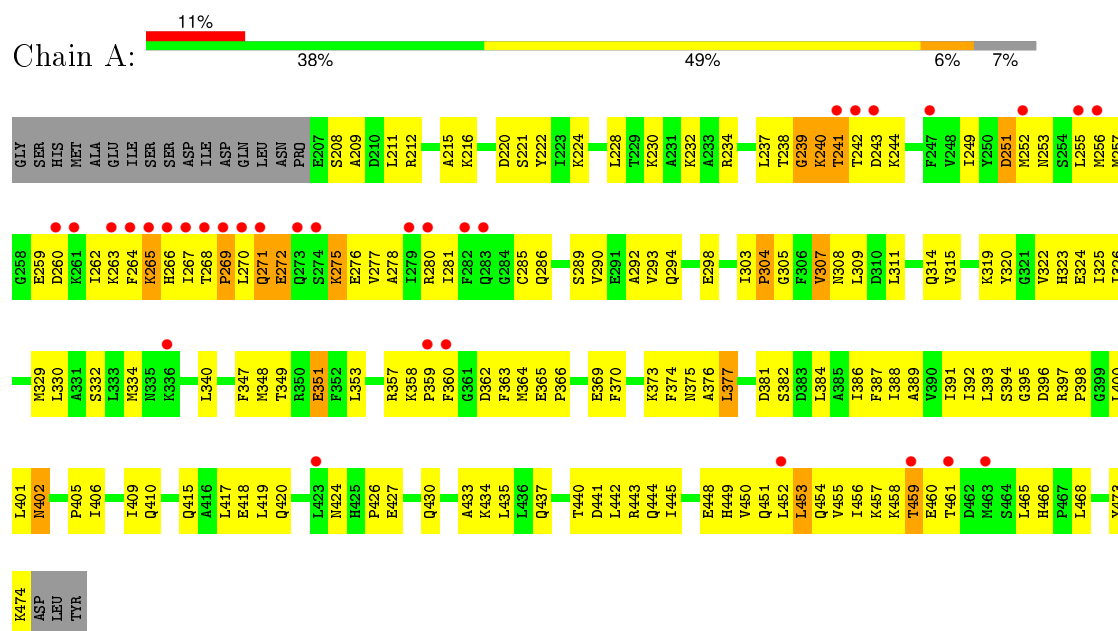
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	92	Total O 92 92	0	0
3	B	94	Total O 94 94	0	0

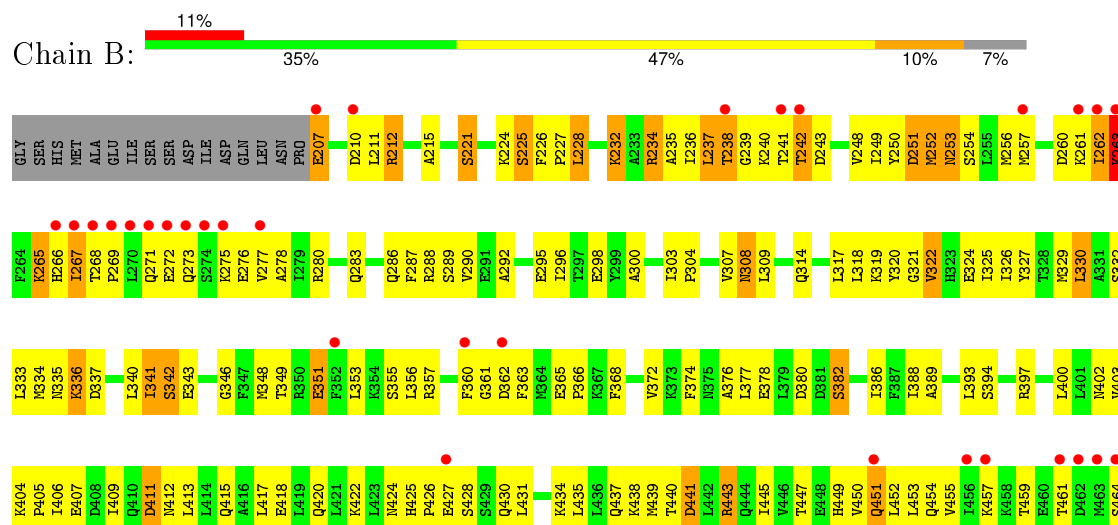
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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



L465	L468	L469	L470	L471	L472	L473	LYS	ASP	LEU	TYR

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.04Å 62.53Å 119.05Å 90.00° 102.31° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 45.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 80.1 (45.77-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.241 , 0.287 0.271 , 0.272	Depositor DCC
$R_{free}$ test set	837 reflections (4.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.995	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 65.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 18724 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	4505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

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	0.40	0/2177	0.62	0/2934
All	All	0.41	0/4363	0.62	0/5879

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2149	0	2217	157	0
1	B	2140	0	2204	166	0
2	A	30	0	21	8	0
3	A	92	0	0	14	0
3	B	94	0	0	18	0
All	All	4505	0	4442	326	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 38.

All (326) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:HIS:H	1:B:467:PRO:HD2	1.19	1.06
1:A:448:GLU:HA	1:A:451:GLN:HE21	1.21	1.01
1:B:466:HIS:H	1:B:467:PRO:CD	1.73	1.00
1:A:281:ILE:HG23	2:A:501:AXY:H17	1.48	0.96
1:A:357:ARG:HD2	1:A:359:PRO:HD2	1.46	0.95
1:B:343:GLU:HB2	3:B:581:HOH:O	1.67	0.93
1:A:401:LEU:C	1:A:402:ASN:HD22	1.74	0.91
1:A:437:GLN:O	1:A:440:THR:HG22	1.71	0.90
1:B:434:LYS:HA	1:B:437:GLN:HE21	1.36	0.88
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.59	0.84
1:A:293:VAL:HG22	1:A:322:VAL:HG21	1.59	0.82
1:B:377:LEU:HD11	1:B:438:LYS:HE3	1.61	0.82
1:B:455:VAL:HG21	3:B:550:HOH:O	1.80	0.80
1:A:265:LYS:NZ	1:A:265:LYS:HB3	1.98	0.79
1:B:212:ARG:NH1	1:B:212:ARG:HB3	1.98	0.79
1:A:392:ILE:HG22	1:A:393:LEU:HD23	1.62	0.78
1:A:267:ILE:H	1:A:280:ARG:HD2	1.47	0.78
1:B:321:GLY:O	1:B:325:ILE:HG12	1.85	0.76
1:B:466:HIS:N	1:B:467:PRO:CD	2.50	0.75
1:A:271:GLN:HB2	1:A:276:GLU:HA	1.68	0.74
1:B:238:THR:HG23	1:B:335:ASN:ND2	2.03	0.74
2:A:501:AXY:H14	2:A:501:AXY:CAW	2.16	0.74
1:B:425:HIS:O	1:B:428:SER:HB3	1.88	0.74
1:A:265:LYS:HZ3	1:A:265:LYS:HB3	1.52	0.73
1:A:402:ASN:HD22	1:A:402:ASN:N	1.84	0.73
1:A:434:LYS:HE3	3:B:563:HOH:O	1.89	0.73
1:A:330:LEU:HD11	2:A:501:AXY:H10	1.71	0.72
1:A:294:GLN:HB2	3:A:666:HOH:O	1.88	0.72
1:A:329:MET:HG3	3:A:649:HOH:O	1.90	0.72
1:B:469:LEU:HD22	1:B:472:ILE:HD12	1.70	0.72
1:A:322:VAL:HG13	1:A:323:HIS:HD2	1.54	0.71
1:B:351:GLU:HG2	3:B:512:HOH:O	1.90	0.71
1:B:271:GLN:HB2	1:B:280:ARG:HH12	1.55	0.70
1:B:425:HIS:HB3	1:B:428:SER:HB3	1.73	0.70
1:A:373:LYS:O	1:A:376:ALA:HB3	1.91	0.70
1:B:351:GLU:HG3	3:B:521:HOH:O	1.92	0.70
1:A:234:ARG:HH11	1:A:237:LEU:HD12	1.56	0.70
1:B:273:GLN:HA	3:B:570:HOH:O	1.91	0.70
1:A:270:LEU:HD13	1:A:271:GLN:N	2.07	0.70
1:A:293:VAL:HG22	1:A:322:VAL:CG2	2.22	0.70
1:A:320:TYR:HB2	1:A:397:ARG:HD2	1.75	0.69
1:A:363:PHE:CE2	1:A:456:ILE:HD11	2.28	0.69

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:GLU:OE2	1:B:443:ARG:HD2	1.93	0.69
1:B:212:ARG:HB3	1:B:212:ARG:HH11	1.58	0.68
1:A:320:TYR:CB	1:A:397:ARG:HD2	2.23	0.68
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.74	0.68
1:B:210:ASP:HB3	3:B:510:HOH:O	1.93	0.67
1:A:332:SER:HA	3:A:667:HOH:O	1.94	0.67
1:B:447:THR:O	1:B:450:VAL:HG22	1.95	0.67
1:B:256:MET:O	1:B:257:MET:HB2	1.94	0.67
1:B:465:LEU:O	1:B:466:HIS:HB2	1.93	0.67
1:B:397:ARG:HB2	1:B:400:LEU:HD11	1.76	0.67
1:B:333:LEU:HB3	1:B:340:LEU:HB2	1.77	0.66
1:A:230:LYS:HG3	3:A:667:HOH:O	1.96	0.66
1:A:322:VAL:HG13	1:A:323:HIS:CD2	2.31	0.66
1:A:369:GLU:O	1:A:373:LYS:HG2	1.95	0.66
2:A:501:AXY:CAP	2:A:501:AXY:CAW	2.72	0.65
1:A:220:ASP:HB2	3:A:653:HOH:O	1.96	0.65
1:A:430:GLN:HG3	1:A:433:ALA:HB3	1.79	0.65
1:B:237:LEU:O	1:B:239:GLY:N	2.30	0.64
1:B:348:MET:SD	1:B:353:LEU:HD21	2.36	0.64
1:A:241:THR:HG22	1:A:243:ASP:OD2	1.97	0.64
1:B:441:ASP:O	1:B:445:ILE:HG12	1.97	0.64
1:B:253:ASN:N	1:B:253:ASN:HD22	1.93	0.64
1:A:238:THR:O	1:A:240:LYS:N	2.30	0.64
1:A:211:LEU:HD11	1:A:415:GLN:HE21	1.63	0.63
1:A:271:GLN:CG	1:A:272:GLU:H	2.11	0.63
1:A:402:ASN:ND2	1:A:402:ASN:N	2.44	0.63
1:B:212:ARG:CB	1:B:212:ARG:HH11	2.11	0.63
1:B:457:LYS:HD2	1:B:461:THR:HG21	1.79	0.62
1:A:263:LYS:C	1:A:264:PHE:HD1	2.04	0.61
1:B:289:SER:O	1:B:292:ALA:HB3	1.99	0.61
1:A:259:GLU:HA	1:A:264:PHE:HB2	1.81	0.61
1:A:319:LYS:HZ1	1:A:474:LYS:HB2	1.65	0.61
1:B:457:LYS:HG3	3:B:538:HOH:O	2.00	0.61
1:A:370:PHE:CZ	1:A:442:LEU:HD21	2.36	0.60
1:A:393:LEU:HD12	1:A:409:ILE:HB	1.84	0.60
1:A:268:THR:N	1:A:269:PRO:HD2	2.16	0.60
1:B:265:LYS:HD2	1:B:265:LYS:N	2.17	0.59
1:B:428:SER:OG	1:B:431:LEU:HB2	2.01	0.59
1:B:210:ASP:OD2	1:B:211:LEU:N	2.36	0.59
1:B:439:MET:HE3	3:B:507:HOH:O	2.03	0.59
1:A:311:LEU:O	1:A:315:VAL:HG23	2.03	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLY:O	1:A:240:LYS:C	2.41	0.59
1:A:290:VAL:HG21	1:A:466:HIS:CD2	2.37	0.58
1:A:234:ARG:NH2	1:A:375:ASN:ND2	2.50	0.58
1:B:307:VAL:C	1:B:309:LEU:H	2.06	0.58
1:A:393:LEU:CD1	1:A:409:ILE:HB	2.33	0.58
1:A:230:LYS:HE3	3:A:667:HOH:O	2.04	0.58
1:B:322:VAL:O	1:B:326:ILE:HG13	2.03	0.58
1:A:363:PHE:CZ	1:A:456:ILE:HD11	2.37	0.57
1:A:473:TYR:O	1:A:474:LYS:HG3	2.04	0.57
1:B:261:LYS:O	1:B:262:ILE:HB	2.04	0.57
1:B:263:LYS:H	1:B:263:LYS:HD3	1.70	0.57
1:A:395:GLY:HA2	1:A:400:LEU:CD1	2.35	0.57
1:B:368:PHE:O	1:B:372:VAL:HG23	2.05	0.57
1:A:364:MET:SD	2:A:501:AXY:H9	2.45	0.56
1:A:249:ILE:HD12	1:A:255:LEU:HA	1.87	0.56
1:A:211:LEU:HD11	1:A:415:GLN:NE2	2.21	0.56
1:A:374:PHE:O	1:A:377:LEU:HG	2.05	0.56
1:A:259:GLU:OE2	1:A:268:THR:HA	2.05	0.56
1:A:285:CYS:SG	2:A:501:AXY:CAQ	2.93	0.56
1:B:397:ARG:HB2	1:B:400:LEU:CD1	2.35	0.56
1:B:243:ASP:HB3	3:B:548:HOH:O	2.05	0.56
1:A:277:VAL:HG13	1:A:278:ALA:H	1.71	0.56
1:B:241:THR:HG22	1:B:241:THR:O	2.06	0.56
1:A:228:LEU:HD12	1:A:232:LYS:HB3	1.88	0.56
1:B:263:LYS:N	1:B:263:LYS:HD3	2.22	0.55
1:A:322:VAL:HG13	1:A:323:HIS:H	1.72	0.55
1:B:271:GLN:CD	1:B:277:VAL:HG23	2.27	0.55
1:B:365:GLU:HB3	3:B:556:HOH:O	2.05	0.55
1:B:267:ILE:HG13	1:B:268:THR:N	2.21	0.55
1:A:444:GLN:O	1:A:448:GLU:HG3	2.07	0.55
1:A:440:THR:HB	1:B:440:THR:HG22	1.88	0.54
1:B:466:HIS:N	1:B:467:PRO:HD2	2.03	0.54
1:A:448:GLU:HA	1:A:451:GLN:NE2	2.06	0.54
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.37	0.54
1:B:265:LYS:HD2	1:B:265:LYS:H	1.73	0.54
1:B:451:GLN:NE2	1:B:452:LEU:HG	2.23	0.54
1:A:430:GLN:HE21	1:A:433:ALA:HB2	1.72	0.53
1:A:322:VAL:HG13	1:A:323:HIS:N	2.21	0.53
1:A:267:ILE:O	1:A:280:ARG:CZ	2.56	0.53
1:B:425:HIS:HB3	1:B:428:SER:CB	2.39	0.53
1:A:393:LEU:O	1:A:410:GLN:HB2	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASP:O	1:A:224:LYS:HG3	2.09	0.53
1:A:400:LEU:HD13	1:A:406:ILE:HD12	1.90	0.53
1:B:271:GLN:HE22	1:B:276:GLU:HA	1.73	0.53
1:B:234:ARG:NH2	1:B:334:MET:O	2.33	0.53
1:B:451:GLN:O	1:B:454:GLN:HG2	2.09	0.53
1:B:365:GLU:N	1:B:366:PRO:HD2	2.24	0.53
1:A:257:MET:O	1:A:260:ASP:HB3	2.09	0.52
1:A:387:PHE:CE2	1:A:391:ILE:HD11	2.44	0.52
1:B:380:ASP:OD1	1:B:382:SER:N	2.42	0.52
1:B:237:LEU:C	1:B:239:GLY:N	2.63	0.52
1:A:468:LEU:O	1:A:468:LEU:HD13	2.10	0.52
1:B:341:ILE:HG22	1:B:346:GLY:HA3	1.92	0.52
1:A:435:LEU:O	1:A:435:LEU:HD12	2.09	0.52
1:B:341:ILE:HG23	1:B:342:SER:N	2.25	0.52
1:A:449:HIS:O	1:A:453:LEU:HB2	2.10	0.52
1:A:289:SER:O	1:A:292:ALA:HB3	2.09	0.52
1:B:253:ASN:N	1:B:253:ASN:ND2	2.57	0.52
1:A:271:GLN:HG3	1:A:272:GLU:H	1.74	0.51
1:A:234:ARG:HH22	1:A:375:ASN:ND2	2.09	0.51
1:B:236:ILE:O	1:B:237:LEU:O	2.28	0.51
1:A:322:VAL:HG22	1:A:326:ILE:HD12	1.91	0.51
1:B:232:LYS:HG3	3:B:534:HOH:O	2.11	0.51
1:A:349:THR:HG22	1:A:351:GLU:H	1.75	0.51
1:B:405:PRO:O	1:B:409:ILE:HG13	2.11	0.51
1:B:425:HIS:N	1:B:426:PRO:CD	2.74	0.51
1:B:250:TYR:HA	1:B:349:THR:OG1	2.11	0.51
1:A:365:GLU:N	1:A:366:PRO:HD2	2.26	0.51
1:A:286:GLN:NE2	1:A:465:LEU:HD12	2.26	0.51
1:A:208:SER:O	1:A:211:LEU:N	2.44	0.50
1:A:363:PHE:HE2	1:A:456:ILE:HD11	1.77	0.50
1:B:212:ARG:CA	1:B:212:ARG:HH11	2.24	0.50
1:B:374:PHE:HD1	1:B:438:LYS:HG2	1.77	0.50
1:B:351:GLU:OE2	1:B:355:SER:HB3	2.12	0.50
1:A:325:ILE:O	1:A:329:MET:HG2	2.12	0.49
1:A:433:ALA:O	1:A:437:GLN:HG3	2.12	0.49
1:A:220:ASP:HA	3:A:642:HOH:O	2.10	0.49
1:B:290:VAL:HG21	1:B:473:TYR:CE1	2.47	0.49
1:A:320:TYR:HB3	1:A:397:ARG:NH1	2.27	0.49
1:A:453:LEU:HD21	3:A:689:HOH:O	2.11	0.49
1:B:250:TYR:CD1	1:B:251:ASP:HB2	2.48	0.49
1:B:329:MET:O	1:B:332:SER:HB2	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:VAL:HG12	1:B:249:ILE:N	2.28	0.49
1:A:262:ILE:HG22	1:A:263:LYS:N	2.28	0.49
1:B:263:LYS:H	1:B:263:LYS:CD	2.25	0.49
1:A:349:THR:HG22	1:A:351:GLU:N	2.27	0.49
1:A:420:GLN:NE2	1:A:424:ASN:HB2	2.28	0.48
1:A:286:GLN:NE2	1:A:465:LEU:HA	2.28	0.48
1:A:303:ILE:HD11	1:A:392:ILE:HD12	1.95	0.48
1:B:300:ALA:HA	1:B:303:ILE:HD12	1.95	0.48
1:A:266:HIS:HB3	1:A:280:ARG:HG2	1.95	0.48
1:B:298:GLU:HB2	3:B:513:HOH:O	2.13	0.48
1:B:434:LYS:HA	1:B:437:GLN:NE2	2.18	0.48
1:B:319:LYS:HE3	1:B:320:TYR:CZ	2.49	0.48
1:A:319:LYS:NZ	1:A:474:LYS:HD2	2.28	0.48
1:A:277:VAL:HG13	1:A:278:ALA:N	2.29	0.48
1:B:290:VAL:HG21	1:B:473:TYR:CD1	2.49	0.47
1:B:403:VAL:HG12	1:B:407:GLU:HG3	1.95	0.47
1:B:417:LEU:HD21	1:B:435:LEU:HD23	1.96	0.47
1:B:276:GLU:O	1:B:280:ARG:HD3	2.15	0.47
1:B:330:LEU:O	1:B:334:MET:HG3	2.15	0.47
1:A:262:ILE:HB	1:A:264:PHE:CE1	2.50	0.47
1:B:411:ASP:O	1:B:415:GLN:HG3	2.14	0.47
1:B:361:GLY:C	1:B:363:PHE:H	2.16	0.47
1:B:271:GLN:HE21	1:B:280:ARG:NH1	2.12	0.47
1:B:266:HIS:O	1:B:267:ILE:HB	2.15	0.47
1:B:469:LEU:O	1:B:469:LEU:HD13	2.15	0.47
1:A:256:MET:HG2	1:A:268:THR:O	2.15	0.47
1:A:253:ASN:O	1:A:257:MET:HG2	2.14	0.47
1:A:303:ILE:O	1:A:304:PRO:C	2.53	0.46
1:B:288:ARG:HD2	1:B:288:ARG:O	2.15	0.46
1:B:273:GLN:HG2	3:B:570:HOH:O	2.14	0.46
1:B:427:GLU:HA	1:B:427:GLU:OE2	2.14	0.46
1:B:271:GLN:NE2	1:B:277:VAL:HG23	2.31	0.46
1:A:340:LEU:HD23	1:A:347:PHE:HD1	1.81	0.46
1:A:309:LEU:HD13	1:A:406:ILE:HG12	1.98	0.46
1:B:286:GLN:O	1:B:287:PHE:C	2.53	0.46
1:B:234:ARG:O	1:B:235:ALA:C	2.52	0.46
1:B:320:TYR:HB2	1:B:397:ARG:HD2	1.97	0.46
1:B:252:MET:C	1:B:253:ASN:HD22	2.18	0.46
1:A:473:TYR:HE2	3:A:689:HOH:O	1.99	0.46
1:B:277:VAL:HG22	1:B:280:ARG:NH1	2.31	0.46
1:B:287:PHE:CD1	1:B:287:PHE:C	2.90	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.80	0.46
1:A:457:LYS:NZ	1:A:461:THR:HG22	2.30	0.46
2:A:501:AXY:H14	2:A:501:AXY:OAB	2.16	0.46
1:B:250:TYR:CE1	1:B:251:ASP:HB2	2.52	0.46
1:B:221:SER:O	1:B:225:SER:OG	2.33	0.46
1:B:319:LYS:HE3	1:B:320:TYR:CE1	2.51	0.45
1:B:449:HIS:O	1:B:453:LEU:HB2	2.16	0.45
1:B:237:LEU:C	1:B:239:GLY:H	2.19	0.45
1:B:215:ALA:CB	1:B:386:ILE:HD11	2.46	0.45
1:B:240:LYS:HG2	1:B:242:THR:HG22	1.99	0.45
1:A:374:PHE:C	1:A:376:ALA:N	2.69	0.45
1:A:370:PHE:CB	1:A:445:ILE:HD11	2.47	0.45
1:A:293:VAL:HG11	1:A:468:LEU:HD11	1.99	0.45
1:B:273:GLN:HG3	3:B:539:HOH:O	2.15	0.45
1:B:207:GLU:O	1:B:210:ASP:OD2	2.35	0.45
1:A:251:ASP:OD2	1:A:253:ASN:CB	2.65	0.45
1:B:402:ASN:O	1:B:405:PRO:HD2	2.16	0.45
1:B:265:LYS:CD	1:B:265:LYS:H	2.30	0.45
1:B:207:GLU:HA	1:B:207:GLU:OE1	2.17	0.45
1:B:241:THR:O	1:B:243:ASP:N	2.50	0.45
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.99	0.45
1:A:212:ARG:O	1:A:216:LYS:HD3	2.17	0.45
1:A:450:VAL:O	1:A:454:GLN:HG3	2.17	0.45
1:B:376:ALA:O	1:B:378:GLU:HG3	2.17	0.45
1:A:402:ASN:O	1:A:405:PRO:HG2	2.16	0.45
1:B:353:LEU:HA	1:B:356:LEU:HG	1.99	0.45
1:A:239:GLY:O	1:A:241:THR:N	2.49	0.45
1:A:271:GLN:NE2	1:A:272:GLU:OE2	2.50	0.44
1:A:319:LYS:NZ	1:A:474:LYS:HB2	2.31	0.44
1:A:212:ARG:HD2	3:A:679:HOH:O	2.17	0.44
1:B:418:GLU:HG2	1:B:422:LYS:HE2	2.00	0.44
1:B:283:GLN:HB3	3:B:502:HOH:O	2.17	0.44
1:B:228:LEU:HD23	1:B:232:LYS:HB3	1.99	0.44
1:B:353:LEU:O	1:B:356:LEU:HG	2.17	0.44
1:B:265:LYS:CD	1:B:265:LYS:N	2.79	0.44
1:B:307:VAL:C	1:B:309:LEU:N	2.71	0.44
1:A:263:LYS:O	1:A:264:PHE:HD1	2.01	0.44
1:A:395:GLY:HA2	1:A:400:LEU:HD12	1.99	0.44
1:A:286:GLN:HE21	1:A:465:LEU:HD12	1.82	0.44
1:A:455:VAL:O	1:A:459:THR:HG23	2.17	0.44
1:A:259:GLU:O	1:A:262:ILE:O	2.36	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:PRO:HG2	1:B:427:GLU:H	1.82	0.44
1:B:309:LEU:O	1:B:314:GLN:NE2	2.49	0.44
1:B:418:GLU:O	1:B:422:LYS:HG3	2.18	0.44
1:B:261:LYS:HG3	1:B:262:ILE:N	2.32	0.44
1:B:317:LEU:HD21	1:B:406:ILE:HD13	1.99	0.44
1:B:251:ASP:C	1:B:253:ASN:N	2.71	0.44
1:A:222:TYR:CE2	1:A:381:ASP:HB3	2.53	0.44
1:B:228:LEU:HD13	1:B:333:LEU:CD2	2.48	0.43
1:A:384:LEU:O	1:A:388:ILE:HG12	2.18	0.43
1:B:307:VAL:HG23	1:B:308:ASN:N	2.33	0.43
1:A:330:LEU:O	1:A:334:MET:HG3	2.18	0.43
1:A:267:ILE:HD12	1:A:275:LYS:HB2	1.99	0.43
1:A:459:THR:OG1	1:A:460:GLU:N	2.51	0.43
1:A:363:PHE:CZ	1:A:452:LEU:HD22	2.53	0.43
1:A:265:LYS:NZ	1:A:265:LYS:CB	2.78	0.43
1:B:251:ASP:O	1:B:253:ASN:N	2.51	0.43
1:B:250:TYR:HB3	1:B:349:THR:HG21	2.01	0.43
1:A:359:PRO:HG2	1:A:360:PHE:CD1	2.54	0.43
1:B:307:VAL:O	1:B:309:LEU:N	2.51	0.43
1:A:255:LEU:HD21	1:A:277:VAL:HG23	2.01	0.43
1:B:237:LEU:HA	1:B:237:LEU:HD23	1.84	0.43
1:A:243:ASP:O	1:A:244:LYS:HG2	2.19	0.43
1:B:393:LEU:HD13	1:B:393:LEU:HA	1.80	0.43
1:A:452:LEU:O	1:A:452:LEU:HD23	2.19	0.42
1:B:248:VAL:CG1	1:B:249:ILE:N	2.82	0.42
1:B:292:ALA:O	1:B:296:ILE:HG13	2.19	0.42
1:B:336:LYS:HE2	1:B:337:ASP:OD2	2.19	0.42
1:A:271:GLN:CG	1:A:272:GLU:N	2.80	0.42
1:B:438:LYS:HE2	1:B:438:LYS:HB2	1.85	0.42
1:A:220:ASP:OD2	1:A:224:LYS:HE3	2.18	0.42
1:A:228:LEU:HD13	1:A:232:LYS:HD3	2.01	0.42
1:B:389:ALA:HB1	1:B:413:LEU:HD13	2.00	0.42
1:A:237:LEU:HG	1:A:340:LEU:HD11	2.02	0.42
1:A:286:GLN:HE22	1:A:465:LEU:HA	1.83	0.42
1:B:327:TYR:N	1:B:327:TYR:CD1	2.87	0.42
1:B:227:PRO:CD	1:B:295:GLU:OE2	2.67	0.42
1:A:348:MET:SD	1:A:353:LEU:HD21	2.60	0.42
1:B:256:MET:O	1:B:257:MET:CB	2.66	0.42
1:B:286:GLN:O	1:B:289:SER:N	2.52	0.42
1:B:307:VAL:O	1:B:314:GLN:NE2	2.53	0.42
1:A:365:GLU:OE1	1:A:365:GLU:HA	2.20	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ILE:O	1:B:304:PRO:C	2.57	0.42
1:A:234:ARG:HD2	3:A:624:HOH:O	2.20	0.42
1:B:403:VAL:O	1:B:404:LYS:C	2.58	0.42
1:A:271:GLN:HG3	1:A:272:GLU:N	2.35	0.42
1:A:442:LEU:O	1:A:443:ARG:C	2.57	0.42
1:B:226:PHE:HA	1:B:227:PRO:HD3	1.77	0.41
1:B:380:ASP:C	1:B:380:ASP:OD1	2.57	0.41
1:B:451:GLN:HE22	1:B:452:LEU:HG	1.84	0.41
1:B:434:LYS:HA	1:B:437:GLN:HG2	2.03	0.41
2:A:501:AXY:H15	3:A:687:HOH:O	2.21	0.41
1:A:401:LEU:C	1:A:402:ASN:ND2	2.57	0.41
1:B:443:ARG:NH1	3:B:507:HOH:O	2.53	0.41
1:B:335:ASN:C	1:B:335:ASN:OD1	2.59	0.41
1:B:271:GLN:HE21	1:B:271:GLN:HA	1.85	0.41
1:B:251:ASP:C	1:B:253:ASN:H	2.23	0.41
1:B:267:ILE:CG1	1:B:268:THR:N	2.83	0.41
1:A:212:ARG:HD3	1:A:419:LEU:CD2	2.51	0.41
1:A:323:HIS:HA	1:A:326:ILE:HB	2.02	0.41
1:B:451:GLN:HB3	1:B:451:GLN:HE21	1.61	0.41
1:A:324:GLU:HB3	1:A:442:LEU:HD13	2.03	0.41
1:B:215:ALA:HB1	1:B:386:ILE:HD11	2.03	0.41
1:B:224:LYS:HA	1:B:224:LYS:HD3	1.91	0.41
1:B:278:ALA:HB1	1:B:360:PHE:CD2	2.55	0.41
1:B:261:LYS:O	1:B:262:ILE:CB	2.68	0.41
1:A:212:ARG:O	1:A:215:ALA:HB3	2.21	0.41
1:B:269:PRO:HA	3:B:564:HOH:O	2.21	0.41
1:B:343:GLU:HG3	1:B:343:GLU:O	2.20	0.40
1:B:386:ILE:HD12	1:B:420:GLN:HG2	2.02	0.40
1:A:381:ASP:O	1:A:382:SER:C	2.59	0.40
1:A:373:LYS:HG2	1:A:373:LYS:H	1.68	0.40
1:A:397:ARG:HA	1:A:398:PRO:HD3	1.83	0.40
1:A:386:ILE:O	1:A:389:ALA:HB3	2.21	0.40
1:A:230:LYS:CE	3:A:667:HOH:O	2.67	0.40
1:A:362:ASP:HB2	3:A:625:HOH:O	2.20	0.40
1:B:251:ASP:O	1:B:254:SER:N	2.53	0.40
1:B:340:LEU:O	1:B:341:ILE:HD12	2.22	0.40
1:A:417:LEU:O	1:A:418:GLU:C	2.59	0.40
1:A:307:VAL:HA	1:A:314:GLN:OE1	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	266/287 (93%)	228 (86%)	28 (10%)	10 (4%)	4	5
1	B	265/287 (92%)	215 (81%)	30 (11%)	20 (8%)	1	1
All	All	531/574 (92%)	443 (83%)	58 (11%)	30 (6%)	2	2

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	A	240	LYS
1	A	269	PRO
1	A	272	GLU
1	A	394	SER
1	B	237	LEU
1	B	242	THR
1	B	466	HIS
1	B	238	THR
1	B	308	ASN
1	B	342	SER
1	B	394	SER
1	B	424	ASN
1	A	209	ALA
1	A	275	LYS
1	B	263	LYS
1	B	362	ASP
1	B	459	THR
1	B	464	SER
1	A	242	THR
1	A	459	THR
1	B	252	MET
1	B	275	LYS
1	B	357	ARG
1	B	232	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	260	ASP
1	B	262	ILE
1	B	272	GLU
1	A	426	PRO
1	B	267	ILE

### 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%)	224 (93%)	17 (7%)	18	34
1	B	240/258 (93%)	215 (90%)	25 (10%)	9	16
All	All	481/516 (93%)	439 (91%)	42 (9%)	13	24

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	SER
1	A	241	THR
1	A	251	ASP
1	A	252	MET
1	A	265	LYS
1	A	271	GLN
1	A	298	GLU
1	A	304	PRO
1	A	307	VAL
1	A	351	GLU
1	A	377	LEU
1	A	396	ASP
1	A	402	ASN
1	A	427	GLU
1	A	441	ASP
1	A	453	LEU
1	A	458	LYS
1	B	207	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	212	ARG
1	B	221	SER
1	B	225	SER
1	B	228	LEU
1	B	234	ARG
1	B	251	ASP
1	B	253	ASN
1	B	263	LYS
1	B	265	LYS
1	B	318	LEU
1	B	322	VAL
1	B	330	LEU
1	B	336	LYS
1	B	341	ILE
1	B	351	GLU
1	B	382	SER
1	B	411	ASP
1	B	412	ASN
1	B	430	GLN
1	B	441	ASP
1	B	443	ARG
1	B	451	GLN
1	B	469	LEU
1	B	471	GLU

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	323	HIS
1	A	402	ASN
1	A	415	GLN
1	A	430	GLN
1	A	451	GLN
1	A	454	GLN
1	B	217	HIS
1	B	253	ASN
1	B	271	GLN
1	B	345	GLN
1	B	412	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	424	ASN
1	B	437	GLN
1	B	444	GLN
1	B	451	GLN
1	B	470	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	AXY	A	501	-	28,33,33	1.39	3 (10%)	39,44,44	0.70	0

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	AXY	A	501	-	-	0/16/20/20	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	AXY	CAU-CAX	-4.82	1.39	1.51
2	A	501	AXY	CBC-CBA	-3.80	1.39	1.49
2	A	501	AXY	CAZ-CBB	-3.61	1.39	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AXY	8	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	268/287 (93%)	0.67	32 (11%) 6 6	22, 47, 113, 130	0
1	B	264/287 (91%)	0.92	33 (12%) 5 5	22, 47, 119, 135	1 (0%)
All	All	532/574 (92%)	0.80	65 (12%) 5 5	22, 47, 116, 135	1 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	PRO	12.1
1	B	268	THR	11.3
1	B	271	GLN	9.7
1	B	270	LEU	9.2
1	A	270	LEU	9.2
1	B	462	ASP	8.4
1	B	269	PRO	7.7
1	B	274	SER	7.4
1	A	268	THR	7.1
1	B	464	SER	7.0
1	B	465	LEU	6.7
1	A	274	SER	6.0
1	A	264	PHE	5.4
1	A	266	HIS	5.3
1	B	272	GLU	5.2
1	A	273	GLN	5.2
1	B	273	GLN	5.0
1	B	238	THR	4.8
1	B	267	ILE	4.5
1	B	241	THR	4.4
1	B	275	LYS	4.2
1	A	263	LYS	4.2
1	A	359	PRO	4.1
1	B	277	VAL	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	261	LYS	3.7
1	A	282	PHE	3.7
1	A	461	THR	3.6
1	B	427	GLU	3.6
1	A	271	GLN	3.4
1	B	463	MET	3.4
1	B	469	LEU	3.2
1	A	463	MET	3.2
1	A	459	THR	3.0
1	B	451	GLN	3.0
1	B	262	ILE	3.0
1	A	336	LYS	2.9
1	A	267	ILE	2.9
1	B	360	PHE	2.9
1	A	452	LEU	2.9
1	A	265	LYS	2.8
1	B	210	ASP	2.7
1	B	461	THR	2.6
1	B	457	LYS	2.5
1	A	423	LEU	2.4
1	B	207	GLU	2.4
1	B	362	ASP	2.4
1	B	242	THR	2.4
1	B	257	MET	2.4
1	A	283	GLN	2.4
1	B	352	PHE	2.3
1	A	252	MET	2.3
1	A	280	ARG	2.3
1	A	279	ILE	2.2
1	A	255	LEU	2.2
1	A	256	MET	2.2
1	A	260	ASP	2.2
1	A	360	PHE	2.1
1	B	263	LYS	2.1
1	A	241	THR	2.1
1	A	247	PHE	2.1
1	B	261	LYS	2.1
1	A	243	ASP	2.1
1	B	456	ILE	2.0
1	B	266	HIS	2.0
1	A	242	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	AXY	A	501	30/30	0.57	0.73	4.77	83,85,89,91	30

## 6.5 Other polymers [i](#)

There are no such residues in this entry.