



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:43 PM EDT

PDB ID : 5NBD / pdb_00005nbd
Title : PglK flippase in complex with inhibitory nanobody
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Deposited on : 2017-03-01
Resolution : 3.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

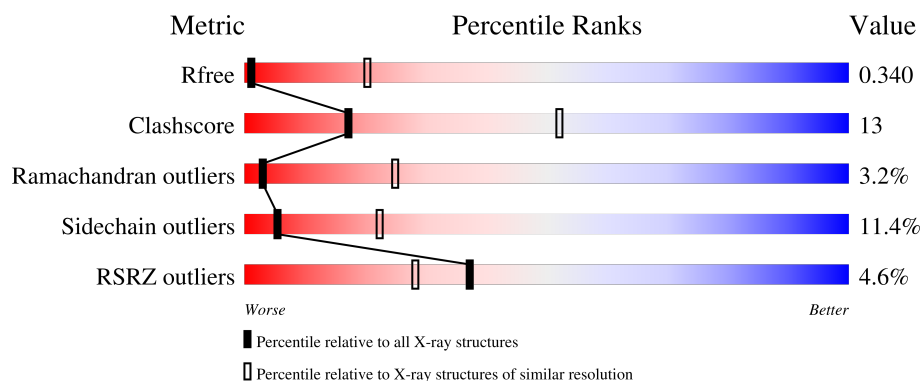
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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 of 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	564	4% 66% 30% .
1	B	564	5% 59% 33% 7%
2	C	123	7% 59% 29% 10% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10091 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 WlaB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			
1	B	564	Total	C	N	O	S	0	0	0
			4557	3000	732	811	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	conflict	UNP O86150
A	105	LYS	TYR	conflict	UNP O86150
A	510	GLN	GLU	engineered mutation	UNP O86150
B	2	VAL	LEU	conflict	UNP O86150
B	105	LYS	TYR	conflict	UNP O86150
B	510	GLN	GLU	engineered mutation	UNP O86150

- Molecule 2 is a protein called Nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	123	Total	C	N	O	S	0	0	0
			923	578	154	187	4			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

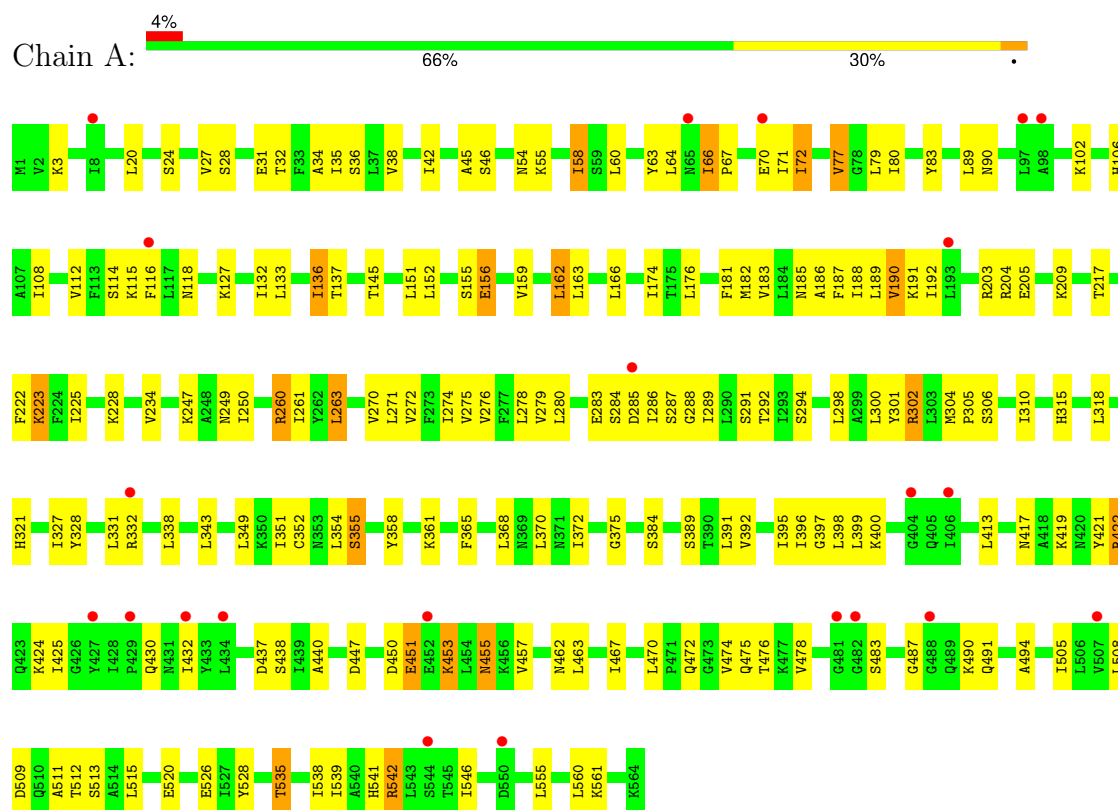


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	11	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	4	0
			27	10	5	10	2		

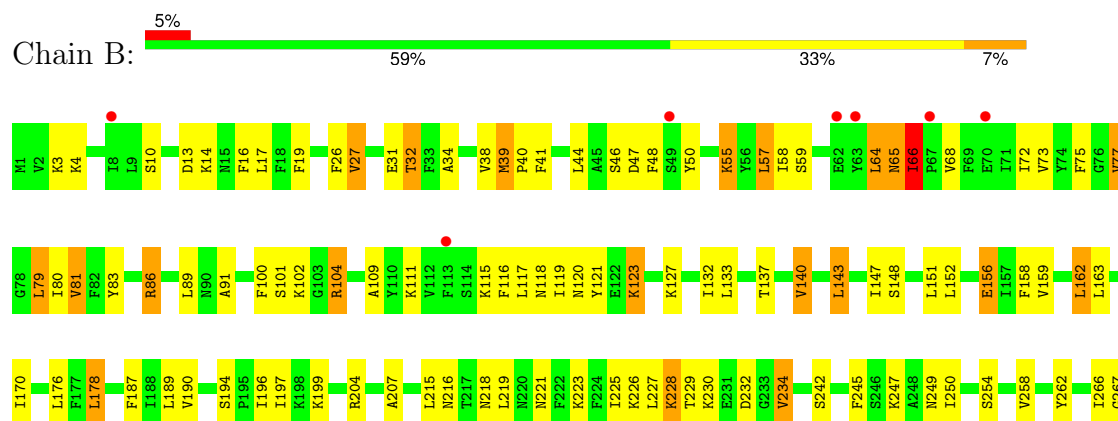
3 Residue-property plots

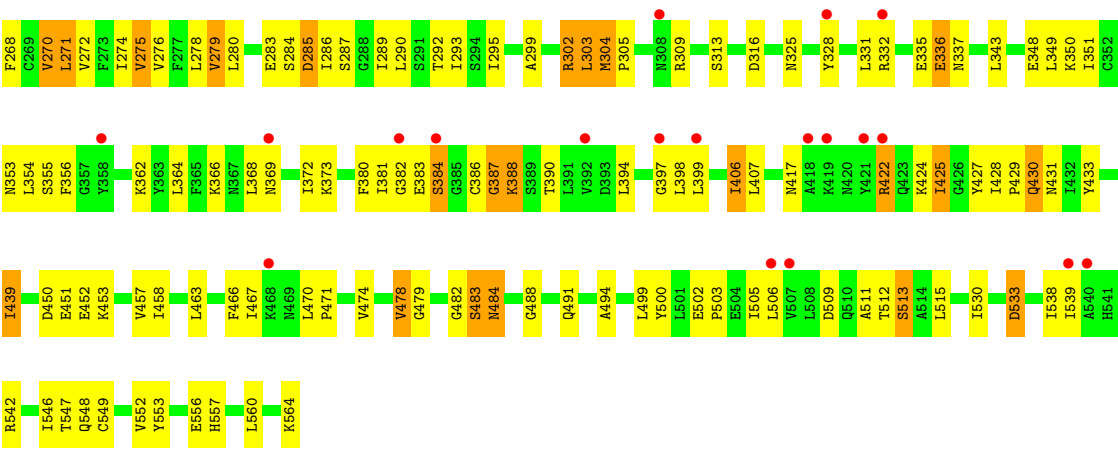
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: WlaB protein

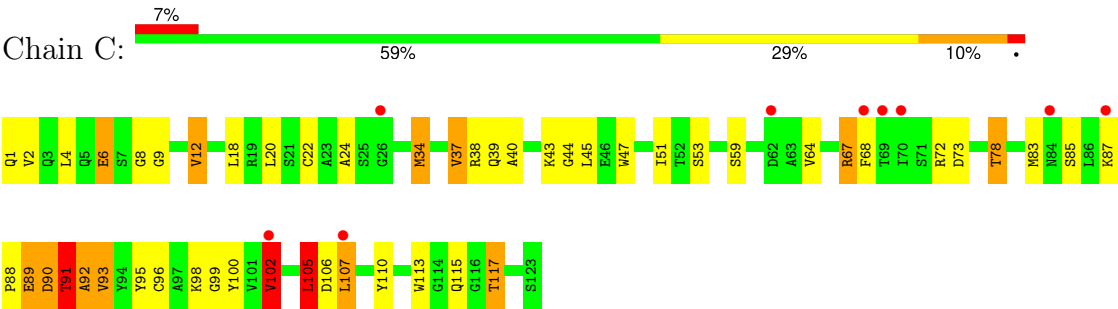


• Molecule 1: WlaB protein





● Molecule 2: Nanobody



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.34Å 142.66Å 199.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.35 – 3.90 29.35 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.35-3.90) 91.9 (29.35-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.70 (at 3.86Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.311 , 0.335 0.313 , 0.340	Depositor DCC
R_{free} test set	2000 reflections (8.87%)	wwPDB-VP
Wilson B-factor (Å ²)	162.8	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10091	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: ADP

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	0.14	0/4641	0.33	0/6246
1	B	0.12	0/4641	0.33	0/6246
2	C	0.13	0/942	0.41	1/1275 (0.1%)
All	All	0.13	0/10224	0.34	1/13767 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	67	ARG	N-CA-C	-5.48	108.37	114.62

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	4557	0	4764	104	0
1	B	4557	0	4764	147	0
2	C	923	0	883	26	0
3	A	27	0	12	0	0
3	B	27	0	12	3	0
All	All	10091	0	10435	258	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 13.

All (258) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:SER:HB3	1:A:166:LEU:HD11	1.63	0.80
1:A:425:ILE:HG22	1:A:505:ILE:HB	1.68	0.74
1:B:512:THR:O	1:B:542:ARG:NH1	2.20	0.73
2:C:87:LYS:HG2	2:C:88:PRO:HD2	1.69	0.72
1:A:283:GLU:HB3	1:A:289:ILE:HD13	1.72	0.71
1:B:152:LEU:HD11	1:B:309:ARG:HD2	1.73	0.71
1:A:512:THR:HG22	1:A:542:ARG:HH11	1.56	0.70
1:A:349:LEU:HB2	1:A:372:ILE:HB	1.73	0.70
1:A:509:ASP:HA	1:A:539:ILE:HB	1.75	0.69
2:C:51:ILE:HD13	2:C:72:ARG:HG3	1.74	0.68
1:A:35:ILE:HD12	1:A:298:LEU:HB3	1.75	0.68
1:A:24:SER:HB3	1:A:155:SER:HB2	1.74	0.68
1:B:278:LEU:HD22	1:B:293:ILE:HD12	1.76	0.68
1:B:429:PRO:O	1:B:431:ASN:N	2.27	0.67
1:B:278:LEU:HD23	1:B:289:ILE:HD12	1.76	0.67
1:A:343:LEU:HB2	1:A:417:ASN:HB2	1.76	0.66
1:B:39:MET:HG3	1:B:295:ILE:HG13	1.78	0.65
1:A:487:GLY:HA2	1:A:490:LYS:HE3	1.77	0.64
1:A:419:LYS:HG3	1:B:229:THR:HG21	1.80	0.64
1:A:260:ARG:HA	1:A:263:LEU:HB2	1.80	0.64
1:B:207:ALA:HB1	1:B:245:PHE:HA	1.79	0.63
1:B:270:VAL:O	1:B:274:ILE:HG12	1.99	0.63
1:B:390:THR:OG1	3:B:601:ADP:O1A	2.16	0.63
1:B:430:GLN:HG2	1:B:431:ASN:H	1.64	0.63
1:B:156:GLU:OE2	1:B:302:ARG:NH1	2.33	0.62
1:A:174:ILE:HG23	1:A:274:ILE:HD12	1.81	0.61
1:A:396:ILE:HB	1:A:425:ILE:HD12	1.82	0.61
1:B:196:ILE:HA	1:B:199:LYS:HB3	1.81	0.61
1:B:450:ASP:O	1:B:452:GLU:N	2.32	0.61
1:A:392:VAL:HG21	1:A:539:ILE:HG12	1.83	0.61
1:B:397:GLY:HA3	1:B:422:ARG:HD2	1.82	0.60
1:A:261:ILE:HD13	1:B:91:ALA:HA	1.84	0.59
2:C:37:VAL:HG11	2:C:107:LEU:HD11	1.84	0.59
1:B:64:LEU:HD13	1:B:65:ASN:H	1.66	0.59
1:B:279:VAL:HG22	1:B:280:LEU:HD22	1.86	0.58
1:A:285:ASP:C	1:A:287:SER:H	2.12	0.58
1:B:111:LYS:HB2	1:B:332:ARG:HH22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:HB	1:A:67:PRO:HD3	1.84	0.58
1:B:118:ASN:HB3	1:B:336:GLU:HB3	1.85	0.57
1:A:355:SER:HA	1:A:365:PHE:HB2	1.85	0.57
1:A:440:ALA:HB2	1:A:474:VAL:HG12	1.87	0.57
1:A:77:VAL:HA	1:A:80:ILE:HG12	1.86	0.57
2:C:6:GLU:OE1	2:C:117:THR:OG1	2.21	0.57
1:A:270:VAL:O	1:A:274:ILE:HG12	2.04	0.57
1:A:358:TYR:HB2	1:A:361:LYS:HG3	1.86	0.56
1:A:28:SER:HB3	1:A:162:LEU:HD11	1.87	0.56
1:B:381:ILE:HD11	1:B:546:ILE:HD13	1.88	0.56
1:B:546:ILE:O	1:B:548:GLN:N	2.39	0.56
1:A:451:GLU:O	1:A:455:ASN:HB2	2.04	0.56
1:B:10:SER:O	1:B:14:LYS:N	2.29	0.56
1:A:188:ILE:HG23	1:A:192:ILE:HD12	1.86	0.56
1:B:353:ASN:N	1:B:369:ASN:OD1	2.37	0.55
1:B:127:LYS:HG3	1:B:132:ILE:HD11	1.87	0.55
1:A:34:ALA:HB1	1:A:83:TYR:CE1	2.41	0.54
1:A:304:MET:HB2	1:A:305:PRO:HD3	1.88	0.54
2:C:4:LEU:HG	2:C:24:ALA:HA	1.89	0.54
1:A:462:ASN:ND2	1:A:526:GLU:OE1	2.40	0.54
1:A:291:SER:O	1:A:294:SER:OG	2.24	0.54
1:A:278:LEU:HG	1:A:289:ILE:HD12	1.90	0.53
1:B:34:ALA:HB1	1:B:83:TYR:CE1	2.44	0.53
1:B:109:ALA:HB2	1:B:140:VAL:HG21	1.89	0.53
1:B:119:ILE:HD12	1:B:123:LYS:HG2	1.90	0.53
1:A:472:GLN:HB2	1:A:476:THR:HA	1.89	0.53
2:C:91:THR:O	2:C:93:VAL:N	2.41	0.53
1:A:222:PHE:HE1	1:B:117:LEU:HA	1.74	0.53
1:B:218:ASN:HD21	1:B:234:VAL:HG13	1.74	0.53
1:A:217:THR:HG23	1:B:433:TYR:HD2	1.73	0.53
1:B:430:GLN:HB3	1:B:511:ALA:HA	1.91	0.53
1:A:46:SER:OG	1:A:287:SER:OG	2.25	0.53
1:B:26:PHE:HE1	1:B:89:LEU:HD11	1.73	0.53
1:B:120:ASN:HA	1:B:337:ASN:HD21	1.74	0.53
1:B:390:THR:N	3:B:601:ADP:O2B	2.34	0.53
1:B:482:GLY:O	1:B:484:ASN:N	2.43	0.53
1:B:77:VAL:HA	1:B:80:ILE:HG12	1.91	0.52
2:C:6:GLU:HB2	2:C:22:CYS:HA	1.90	0.52
1:A:204:ARG:NH2	1:A:249:ASN:OD1	2.43	0.52
1:A:289:ILE:O	1:A:292:THR:OG1	2.23	0.52
1:B:247:LYS:HA	1:B:250:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLU:OE2	1:A:90:ASN:ND2	2.43	0.52
1:B:546:ILE:O	1:B:549:CYS:N	2.35	0.52
1:A:3:LYS:H	1:A:3:LYS:HD3	1.74	0.51
1:A:127:LYS:HG3	1:A:132:ILE:HD11	1.92	0.51
1:B:204:ARG:HG3	1:B:249:ASN:HA	1.91	0.51
2:C:45:LEU:HG	2:C:107:LEU:HD12	1.90	0.51
1:A:187:PHE:O	1:A:189:LEU:N	2.41	0.51
1:B:34:ALA:HB1	1:B:83:TYR:HE1	1.76	0.51
1:B:553:TYR:HB3	1:B:560:LEU:HD11	1.93	0.51
2:C:40:ALA:HB3	2:C:43:LYS:HB2	1.93	0.51
1:A:250:ILE:HG22	1:B:102:LYS:HB2	1.92	0.51
2:C:39:GLN:C	2:C:92:ALA:HB1	2.36	0.51
1:B:509:ASP:HA	1:B:539:ILE:HD12	1.93	0.51
1:A:421:TYR:HA	1:A:424:LYS:HD3	1.93	0.51
1:B:499:LEU:HD21	1:B:530:ILE:HD12	1.93	0.50
1:B:380:PHE:N	1:B:538:ILE:O	2.44	0.50
1:B:266:ILE:O	1:B:270:VAL:HG13	2.11	0.50
1:B:427:TYR:CE2	1:B:429:PRO:HB3	2.46	0.50
1:B:430:GLN:HG2	1:B:431:ASN:N	2.26	0.50
1:A:430:GLN:HB3	1:A:511:ALA:HA	1.93	0.50
1:A:225:ILE:HG21	1:B:117:LEU:HD22	1.92	0.50
1:B:31:GLU:OE1	1:B:86:ARG:NH2	2.45	0.50
1:A:45:ALA:HA	1:A:72:ILE:HG13	1.93	0.50
1:A:112:VAL:HG12	1:A:136:ILE:HG22	1.94	0.49
1:B:382:GLY:HA3	1:B:388:LYS:HD2	1.95	0.49
1:B:457:VAL:HG21	1:B:500:TYR:HA	1.95	0.49
1:A:181:PHE:O	1:A:185:ASN:ND2	2.46	0.49
1:B:187:PHE:O	1:B:189:LEU:N	2.43	0.49
1:B:488:GLY:N	1:B:515:LEU:HD21	2.27	0.49
1:B:65:ASN:HB3	1:B:66:ILE:HG23	1.94	0.49
1:B:425:ILE:HG22	1:B:505:ILE:HB	1.94	0.49
1:A:515:LEU:HB3	1:A:520:GLU:HG3	1.95	0.48
1:B:283:GLU:O	1:B:285:ASP:N	2.45	0.48
1:B:348:GLU:HA	1:B:373:LYS:HA	1.95	0.48
1:B:354:LEU:HD13	1:B:394:LEU:HD13	1.95	0.48
1:B:65:ASN:O	1:B:66:ILE:HG12	2.13	0.48
1:B:479:GLY:O	1:B:483:SER:OG	2.28	0.48
2:C:12:VAL:HG13	2:C:18:LEU:HD11	1.96	0.48
1:A:66:ILE:HB	1:A:67:PRO:CD	2.44	0.48
1:A:112:VAL:HG21	1:A:328:TYR:HE1	1.79	0.48
1:A:343:LEU:HD23	1:A:421:TYR:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LEU:HB2	1:B:372:ILE:HB	1.96	0.48
2:C:105:LEU:HD13	2:C:106:ASP:H	1.78	0.48
1:A:159:VAL:O	1:A:163:LEU:HB2	2.12	0.48
1:B:41:PHE:HB2	1:B:75:PHE:CD2	2.49	0.48
1:B:313:SER:HA	1:B:316:ASP:HB2	1.96	0.48
1:B:348:GLU:HB3	1:B:373:LYS:HG3	1.94	0.48
1:A:351:ILE:HD11	1:A:395:ILE:HG12	1.96	0.48
1:A:397:GLY:HA2	1:A:413:LEU:HD21	1.96	0.48
2:C:34:MET:HA	2:C:98:LYS:O	2.14	0.48
1:A:391:LEU:HD12	1:A:555:LEU:HD13	1.94	0.48
1:B:55:LYS:HA	1:B:59:SER:HB3	1.95	0.47
1:B:77:VAL:O	1:B:81:VAL:HG22	2.14	0.47
2:C:87:LYS:O	2:C:89:GLU:N	2.41	0.47
2:C:90:ASP:N	2:C:90:ASP:OD1	2.44	0.47
1:A:389:SER:HA	1:A:539:ILE:HD13	1.95	0.47
1:B:104:ARG:HD3	1:B:104:ARG:HA	1.75	0.47
1:B:484:ASN:N	1:B:484:ASN:OD1	2.48	0.47
1:B:387:GLY:N	3:B:601:ADP:O3B	2.48	0.47
1:B:513:SER:HA	1:B:542:ARG:HH22	1.80	0.47
1:A:114:SER:O	1:A:118:ASN:ND2	2.44	0.47
1:A:285:ASP:HB3	1:A:288:GLY:H	1.80	0.47
1:B:484:ASN:O	2:C:100:TYR:HB2	2.15	0.47
2:C:64:VAL:HA	2:C:67:ARG:HD3	1.96	0.47
1:A:156:GLU:OE1	1:A:306:SER:OG	2.22	0.46
1:A:430:GLN:HB2	1:A:491:GLN:HE22	1.80	0.46
1:A:467:ILE:HD13	1:A:470:LEU:HD12	1.95	0.46
1:A:438:SER:HB2	1:A:475:GLN:HA	1.98	0.46
1:B:3:LYS:H	1:B:3:LYS:HD3	1.80	0.46
2:C:47:TRP:CE2	2:C:102:VAL:HG23	2.50	0.46
1:A:375:GLY:H	1:A:535:THR:HB	1.81	0.46
1:B:428:ILE:HA	1:B:494:ALA:HB1	1.96	0.46
2:C:9:GLY:H	2:C:117:THR:HG21	1.80	0.46
1:A:106:HIS:ND1	1:B:242:SER:HB3	2.31	0.46
1:A:83:TYR:CE1	1:B:268:PHE:HD2	2.34	0.46
1:A:304:MET:HE1	1:B:304:MET:HE1	1.97	0.46
1:B:10:SER:H	1:B:13:ASP:HB2	1.80	0.46
1:A:182:MET:O	1:A:186:ALA:N	2.36	0.46
1:B:121:TYR:HB2	1:B:398:LEU:HD22	1.98	0.45
1:A:300:LEU:O	1:A:304:MET:HG3	2.16	0.45
1:B:272:VAL:O	1:B:276:VAL:HG23	2.16	0.45
1:B:386:CYS:SG	1:B:387:GLY:N	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ASP:H	1:B:289:ILE:HG12	1.81	0.45
1:B:178:LEU:HD23	1:B:274:ILE:HD11	1.98	0.45
1:B:159:VAL:O	1:B:163:LEU:HB2	2.17	0.45
2:C:91:THR:C	2:C:93:VAL:H	2.24	0.45
1:A:463:LEU:O	1:A:467:ILE:HG12	2.17	0.45
1:B:16:PHE:CD2	1:B:100:PHE:HB2	2.52	0.45
1:B:38:VAL:HG22	1:B:79:LEU:HD11	1.99	0.45
1:A:561:LYS:HD2	1:A:561:LYS:HA	1.87	0.45
1:B:121:TYR:CG	1:B:398:LEU:HD13	2.52	0.45
1:B:533:ASP:N	1:B:533:ASP:OD1	2.49	0.45
1:B:466:PHE:CE2	1:B:470:LEU:HD11	2.52	0.44
1:B:3:LYS:HG2	1:B:4:LYS:HD2	1.99	0.44
1:B:170:ILE:HG21	1:B:292:THR:HB	1.97	0.44
1:B:356:PHE:CG	1:B:394:LEU:HD21	2.52	0.44
1:B:458:ILE:HG23	1:B:463:LEU:HB2	1.99	0.44
1:B:343:LEU:HB2	1:B:417:ASN:HB2	2.00	0.44
1:B:156:GLU:OE2	1:B:309:ARG:NH1	2.50	0.44
1:B:304:MET:HG3	1:B:305:PRO:HD3	1.98	0.44
1:A:528:TYR:OH	1:A:546:ILE:HA	2.18	0.44
1:B:57:LEU:HD12	1:B:58:ILE:HG12	1.99	0.44
1:B:73:VAL:O	1:B:77:VAL:HG13	2.18	0.44
1:A:156:GLU:O	1:A:159:VAL:HG12	2.18	0.44
2:C:73:ASP:HB3	2:C:78:THR:HG23	1.99	0.44
1:B:189:LEU:HD21	1:B:262:TYR:CD1	2.53	0.44
1:A:102:LYS:HB2	1:B:250:ILE:HG22	1.98	0.43
1:A:453:LYS:O	1:A:457:VAL:HG23	2.18	0.43
1:B:116:PHE:HZ	1:B:331:LEU:HD22	1.83	0.43
1:B:453:LYS:HD2	1:B:502:GLU:CD	2.43	0.43
1:B:46:SER:OG	1:B:286:ILE:O	2.36	0.43
1:B:79:LEU:HD22	1:B:79:LEU:HA	1.88	0.43
2:C:68:PHE:CD1	2:C:83:MET:HA	2.53	0.43
1:A:38:VAL:O	1:A:42:ILE:HG22	2.18	0.43
1:A:108:ILE:HG23	1:A:332:ARG:NH2	2.34	0.43
1:A:133:LEU:O	1:A:137:THR:HG22	2.19	0.43
1:B:267:GLY:O	1:B:271:LEU:HB2	2.19	0.43
1:A:398:LEU:HD23	1:A:422:ARG:HD2	2.01	0.43
1:A:432:ILE:HD12	1:A:494:ALA:HA	2.00	0.43
1:B:471:PRO:HA	2:C:59:SER:HB2	2.00	0.43
1:A:487:GLY:C	1:A:515:LEU:HD11	2.44	0.43
1:B:86:ARG:C	1:B:86:ARG:HD2	2.44	0.43
1:A:20:LEU:HB3	1:A:151:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LEU:HD23	1:B:143:LEU:HA	1.86	0.43
1:B:276:VAL:O	1:B:280:LEU:HD23	2.18	0.43
1:B:299:ALA:O	1:B:303:LEU:HB2	2.19	0.43
2:C:38:ARG:HD2	2:C:92:ALA:HB3	2.01	0.42
1:B:31:GLU:OE2	1:B:86:ARG:HD3	2.19	0.42
1:A:116:PHE:HZ	1:A:331:LEU:HD22	1.84	0.42
1:A:542:ARG:HH21	1:B:383:GLU:HB3	1.84	0.42
1:B:194:SER:HA	1:B:197:ILE:HD12	2.01	0.42
1:A:304:MET:HB2	1:A:304:MET:HE3	1.73	0.42
1:A:508:LEU:HD22	1:A:538:ILE:HG23	2.02	0.42
1:B:40:PRO:O	1:B:44:LEU:HG	2.19	0.42
1:B:384:SER:H	1:B:388:LYS:HE3	1.84	0.42
1:A:301:TYR:CD1	1:B:268:PHE:HE1	2.38	0.42
1:B:254:SER:O	1:B:258:VAL:HG23	2.20	0.42
1:B:354:LEU:HD21	1:B:406:ILE:HD11	2.00	0.42
1:B:463:LEU:O	1:B:467:ILE:HG12	2.20	0.42
1:B:471:PRO:CA	2:C:59:SER:HB2	2.50	0.42
1:B:101:SER:HB3	1:B:148:SER:HB2	2.02	0.42
1:A:42:ILE:CD1	1:B:275:VAL:HG11	2.49	0.42
1:A:425:ILE:HG13	1:B:227:LEU:HD22	2.02	0.42
1:B:143:LEU:O	1:B:147:ILE:HG13	2.20	0.42
1:B:221:ASN:O	1:B:225:ILE:N	2.49	0.42
1:B:351:ILE:HD13	1:B:406:ILE:HG23	2.02	0.42
1:B:552:VAL:HB	1:B:564:LYS:H	1.84	0.42
1:B:556:GLU:HB3	1:B:557:HIS:H	1.68	0.42
1:A:349:LEU:N	1:A:372:ILE:O	2.44	0.41
1:B:226:LYS:HD3	1:B:226:LYS:HA	1.87	0.41
2:C:20:LEU:HD11	2:C:83:MET:HE2	2.02	0.41
1:B:3:LYS:HE2	1:B:4:LYS:HE2	2.03	0.41
1:B:223:LYS:O	1:B:227:LEU:HG	2.20	0.41
1:B:491:GLN:HG3	1:B:515:LEU:HD11	2.01	0.41
1:A:247:LYS:HA	1:A:250:ILE:HG12	2.02	0.41
1:A:302:ARG:HA	1:A:302:ARG:HD2	1.83	0.41
1:B:228:LYS:C	1:B:230:LYS:H	2.27	0.41
1:B:503:PRO:HG2	1:B:506:LEU:HD21	2.02	0.41
1:A:190:VAL:HG13	1:A:191:LYS:HG2	2.02	0.41
1:A:437:ASP:OD2	1:A:438:SER:N	2.48	0.41
1:A:370:LEU:HD22	1:A:560:LEU:HD22	2.03	0.41
1:B:17:LEU:HD22	1:B:151:LEU:HD21	2.02	0.41
1:A:108:ILE:O	1:A:112:VAL:HG23	2.21	0.41
1:B:16:PHE:HD2	1:B:100:PHE:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LEU:HD22	1:B:178:LEU:HA	1.80	0.41
1:B:27:VAL:O	1:B:31:GLU:HG2	2.20	0.41
1:B:439:ILE:HG22	1:B:478:VAL:HG23	2.01	0.41
1:A:34:ALA:HB1	1:A:83:TYR:HE1	1.83	0.41
1:A:46:SER:HA	1:B:279:VAL:HG21	2.02	0.41
1:A:515:LEU:CB	1:A:520:GLU:HG3	2.50	0.41
1:B:350:LYS:HB2	1:B:407:LEU:HB2	2.03	0.41
1:A:276:VAL:O	1:A:280:LEU:HG	2.20	0.41
1:A:183:VAL:HA	1:A:186:ALA:HB3	2.02	0.40
1:B:283:GLU:HG2	1:B:289:ILE:HG21	2.03	0.40
1:B:32:THR:OG1	1:B:162:LEU:HD13	2.22	0.40
1:A:156:GLU:HB3	1:A:310:ILE:HG12	2.02	0.40
1:A:223:LYS:HE2	1:B:427:TYR:CZ	2.57	0.40
1:B:133:LEU:O	1:B:137:THR:HG22	2.21	0.40
1:A:422:ARG:HA	1:A:425:ILE:HD11	2.02	0.40
1:B:304:MET:HG3	1:B:305:PRO:CD	2.52	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	562/564 (100%)	490 (87%)	59 (10%)	13 (2%)	5	30
1	B	562/564 (100%)	493 (88%)	55 (10%)	14 (2%)	4	29
2	C	121/123 (98%)	88 (73%)	20 (16%)	13 (11%)	0	6
All	All	1245/1251 (100%)	1071 (86%)	134 (11%)	40 (3%)	3	25

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	ILE

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Mol	Chain	Res	Type
1	B	284	SER
1	B	430	GLN
1	B	451	GLU
1	B	547	THR
1	A	284	SER
1	A	286	ILE
1	A	483	SER
1	B	483	SER
2	C	44	GLY
2	C	92	ALA
1	A	355	SER
1	A	399	LEU
1	A	450	ASP
1	B	384	SER
1	B	387	GLY
1	B	399	LEU
2	C	89	GLU
2	C	95	TYR
2	C	96	CYS
2	C	105	LEU
1	A	513	SER
1	B	355	SER
2	C	85	SER
2	C	102	VAL
2	C	115	GLN
1	A	321	HIS
1	B	65	ASN
1	B	366	LYS
1	B	513	SER
2	C	91	THR
2	C	93	VAL
1	A	54	ASN
1	A	352	CYS
2	C	8	GLY
1	A	58	ILE
1	B	66	ILE
1	B	406	ILE
2	C	99	GLY
1	A	327	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	505/505 (100%)	455 (90%)	50 (10%)	7	28
1	B	505/505 (100%)	445 (88%)	60 (12%)	5	21
2	C	98/98 (100%)	82 (84%)	16 (16%)	2	14
All	All	1108/1108 (100%)	982 (89%)	126 (11%)	5	22

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	32	THR
1	A	55	LYS
1	A	58	ILE
1	A	60	LEU
1	A	63	TYR
1	A	64	LEU
1	A	70	GLU
1	A	71	ILE
1	A	72	ILE
1	A	77	VAL
1	A	79	LEU
1	A	89	LEU
1	A	115	LYS
1	A	136	ILE
1	A	145	THR
1	A	152	LEU
1	A	156	GLU
1	A	162	LEU
1	A	176	LEU
1	A	190	VAL
1	A	203	ARG
1	A	205	GLU
1	A	209	LYS
1	A	223	LYS
1	A	228	LYS

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Mol	Chain	Res	Type
1	A	234	VAL
1	A	260	ARG
1	A	263	LEU
1	A	271	LEU
1	A	272	VAL
1	A	275	VAL
1	A	279	VAL
1	A	302	ARG
1	A	315	HIS
1	A	318	LEU
1	A	338	LEU
1	A	354	LEU
1	A	368	LEU
1	A	384	SER
1	A	400	LYS
1	A	422	ARG
1	A	447	ASP
1	A	451	GLU
1	A	453	LYS
1	A	455	ASN
1	A	478	VAL
1	A	535	THR
1	A	541	HIS
1	A	542	ARG
1	B	19	PHE
1	B	27	VAL
1	B	32	THR
1	B	39	MET
1	B	47	ASP
1	B	48	PHE
1	B	50	TYR
1	B	55	LYS
1	B	57	LEU
1	B	64	LEU
1	B	66	ILE
1	B	68	VAL
1	B	72	ILE
1	B	77	VAL
1	B	79	LEU
1	B	81	VAL
1	B	86	ARG
1	B	104	ARG

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Mol	Chain	Res	Type
1	B	115	LYS
1	B	123	LYS
1	B	140	VAL
1	B	143	LEU
1	B	156	GLU
1	B	158	PHE
1	B	162	LEU
1	B	176	LEU
1	B	178	LEU
1	B	190	VAL
1	B	215	LEU
1	B	216	ASN
1	B	219	LEU
1	B	228	LYS
1	B	232	ASP
1	B	234	VAL
1	B	270	VAL
1	B	271	LEU
1	B	275	VAL
1	B	279	VAL
1	B	285	ASP
1	B	287	SER
1	B	290	LEU
1	B	302	ARG
1	B	303	LEU
1	B	304	MET
1	B	325	ASN
1	B	328	TYR
1	B	335	GLU
1	B	336	GLU
1	B	362	LYS
1	B	364	LEU
1	B	368	LEU
1	B	388	LYS
1	B	422	ARG
1	B	424	LYS
1	B	425	ILE
1	B	439	ILE
1	B	474	VAL
1	B	478	VAL
1	B	484	ASN
1	B	533	ASP

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Mol	Chain	Res	Type
2	C	1	GLN
2	C	2	VAL
2	C	6	GLU
2	C	12	VAL
2	C	34	MET
2	C	37	VAL
2	C	53	SER
2	C	78	THR
2	C	90	ASP
2	C	91	THR
2	C	102	VAL
2	C	105	LEU
2	C	107	LEU
2	C	110	TYR
2	C	113	TRP
2	C	117	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	325	ASN
1	A	346	ASN
1	A	420	ASN
1	B	120	ASN
1	B	129	GLN
1	B	142	ASN
1	B	325	ASN
1	B	337	ASN
1	B	420	ASN
1	B	472	GLN
2	C	84	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	ADP	B	601	-	28,29,29	1.35	3 (10%)	43,45,45	1.79	10 (23%)
3	ADP	A	601	-	28,29,29	1.36	3 (10%)	43,45,45	1.79	10 (23%)

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
3	ADP	B	601	-	-	0/16/32/32	0/3/3/3
3	ADP	A	601	-	-	3/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ADP	C5-C4	4.50	1.47	1.39
3	B	601	ADP	C5-C4	4.47	1.47	1.39
3	A	601	ADP	C5-C6	2.89	1.49	1.41
3	B	601	ADP	C5-C6	2.83	1.48	1.41
3	A	601	ADP	C8-N7	2.20	1.35	1.31
3	B	601	ADP	C8-N7	2.19	1.35	1.31

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ADP	C5-C4-N3	-5.35	119.34	126.72
3	B	601	ADP	C5-C4-N3	-5.15	119.63	126.72
3	A	601	ADP	N3-C4-N9	4.35	134.56	127.17
3	B	601	ADP	N3-C4-N9	4.19	134.30	127.17
3	B	601	ADP	C4-C5-N7	-3.59	106.47	110.58
3	A	601	ADP	C4-C5-N7	-3.58	106.48	110.58
3	A	601	ADP	C2-N3-C4	3.36	120.03	111.83
3	B	601	ADP	C2-N3-C4	3.29	119.87	111.83
3	B	601	ADP	C4-N9-C8	3.25	109.15	105.74
3	A	601	ADP	C4-N9-C8	3.17	109.06	105.74
3	A	601	ADP	C3'-C2'-C1'	2.62	106.42	101.46
3	B	601	ADP	N3-C2-N1	-2.62	124.62	128.58
3	B	601	ADP	C5-N7-C8	2.60	107.53	103.45
3	A	601	ADP	C5-N7-C8	2.58	107.51	103.45
3	A	601	ADP	N3-C2-N1	-2.58	124.68	128.58
3	B	601	ADP	C6-C5-N7	2.53	136.96	132.09
3	B	601	ADP	C3'-C2'-C1'	2.46	106.12	101.46
3	A	601	ADP	C6-C5-N7	2.44	136.79	132.09
3	B	601	ADP	N9-C8-N7	-2.23	110.78	113.94
3	A	601	ADP	N9-C8-N7	-2.18	110.84	113.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ADP	C5'-O5'-PA-O2A
3	A	601	ADP	C5'-O5'-PA-O1A
3	A	601	ADP	C5'-O5'-PA-O3A

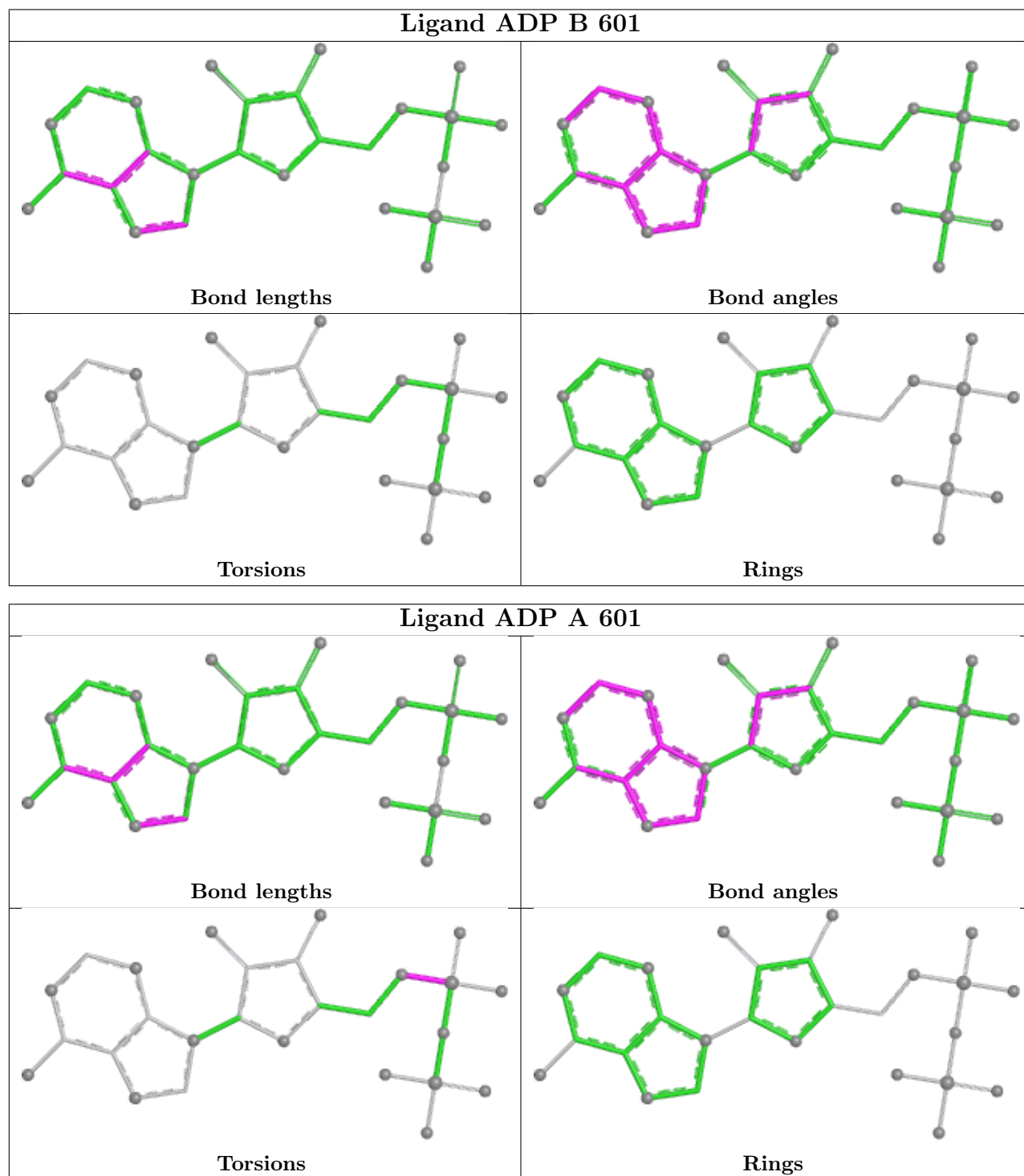
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	ADP	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	564/564 (100%)	0.11	22 (3%) 43 31	93, 167, 223, 257	0
1	B	564/564 (100%)	0.11	26 (4%) 37 28	98, 156, 212, 258	0
2	C	123/123 (100%)	0.40	9 (7%) 21 19	110, 162, 200, 227	0
All	All	1251/1251 (100%)	0.14	57 (4%) 37 28	93, 161, 218, 258	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	404	GLY	6.3
1	A	65	ASN	5.9
1	B	419	LYS	5.1
1	A	70	GLU	4.8
1	B	328	TYR	4.8
1	B	382	GLY	4.2
1	B	397	GLY	4.1
1	A	406	ILE	4.1
1	B	418	ALA	4.0
1	B	308	ASN	3.9
2	C	70	ILE	3.8
1	A	481	GLY	3.7
1	A	544	SER	3.5
1	B	540	ALA	3.5
1	A	8	ILE	3.3
1	A	482	GLY	3.2
2	C	84	ASN	3.1
1	B	421	TYR	3.1
1	A	116	PHE	3.0
1	A	332	ARG	2.8
2	C	69	THR	2.8
1	B	49	SER	2.7
2	C	107	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	392	VAL	2.6
1	B	62	GLU	2.6
1	B	369	ASN	2.5
2	C	26	GLY	2.5
1	B	507	VAL	2.5
1	B	422	ARG	2.5
1	B	506	LEU	2.4
2	C	68	PHE	2.4
1	B	113	PHE	2.4
1	A	427	TYR	2.4
1	B	358	TYR	2.4
1	B	539	ILE	2.4
1	A	488	GLY	2.3
1	B	63	TYR	2.3
1	A	97	LEU	2.3
2	C	62	ASP	2.3
1	B	67	PRO	2.3
1	A	98	ALA	2.2
2	C	102	VAL	2.2
1	B	8	ILE	2.1
1	A	429	PRO	2.1
1	B	384	SER	2.1
1	A	507	VAL	2.1
1	B	468	LYS	2.1
1	B	70	GLU	2.1
1	B	332	ARG	2.1
1	A	432	ILE	2.1
1	A	285	ASP	2.0
1	A	550	ASP	2.0
1	A	452	GLU	2.0
2	C	87	LYS	2.0
1	A	193	LEU	2.0
1	A	434	LEU	2.0
1	B	399	LEU	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 [i](#)

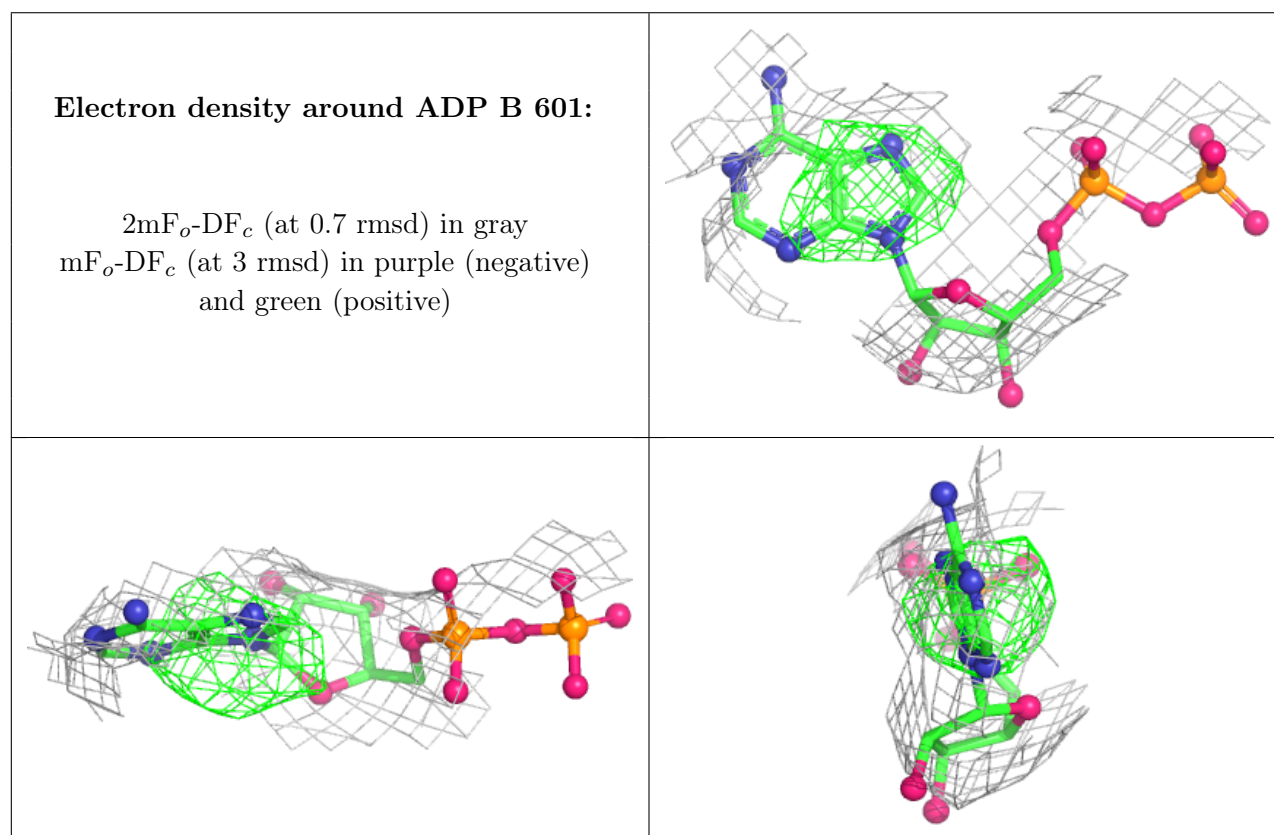
There are no oligosaccharides in this entry.

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.

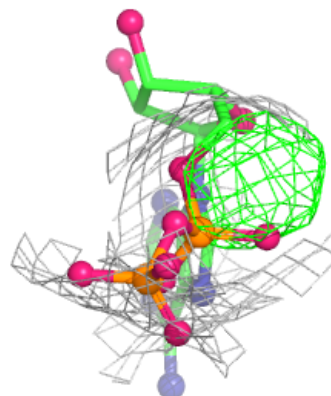
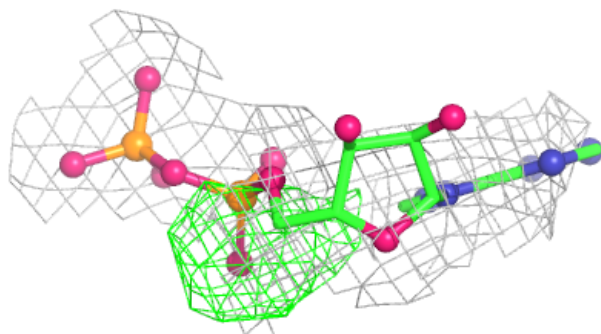
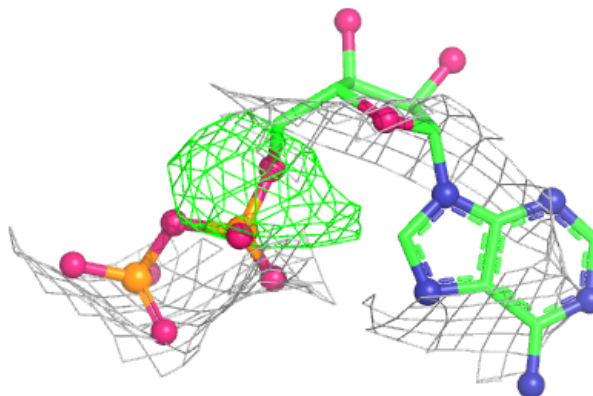
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	B	601	27/27	0.72	0.18	147,201,229,246	15
3	ADP	A	601	27/27	0.81	0.20	148,202,229,247	18

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 ADP A 601:

$2mF_o - DF_c$ (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.