Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 12:21 am GMT

PDB ID	:	5NBD
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 (i) 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 (i)) were used in the production of this report:

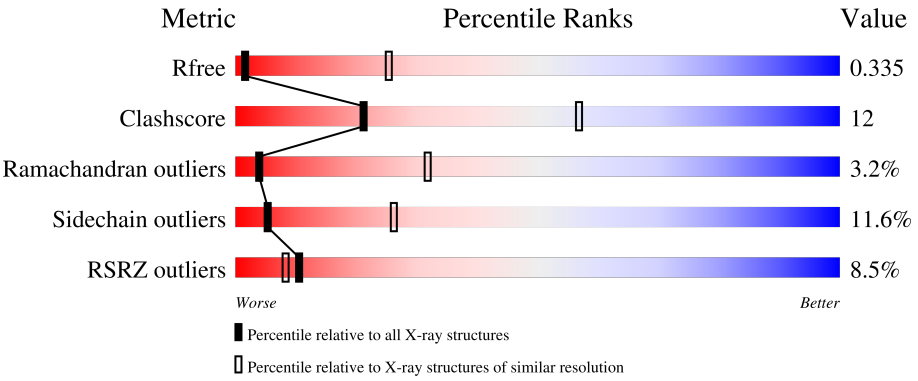
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 <=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	9% 65% 31% .
1	B	564	7% 59% 34% 7%
2	C	123	11% 59% 30% 9% .

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
3	ADP	A	601	-	-	-	X

2 Entry composition (i)

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			

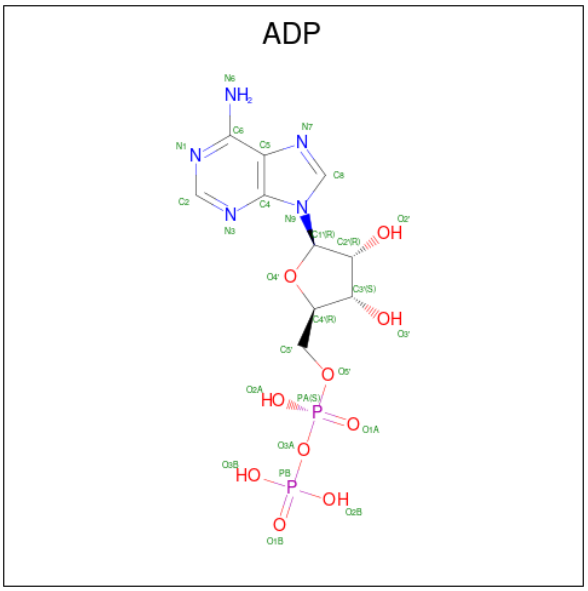
There are 6 discrepancies between the modelled and reference sequences:

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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



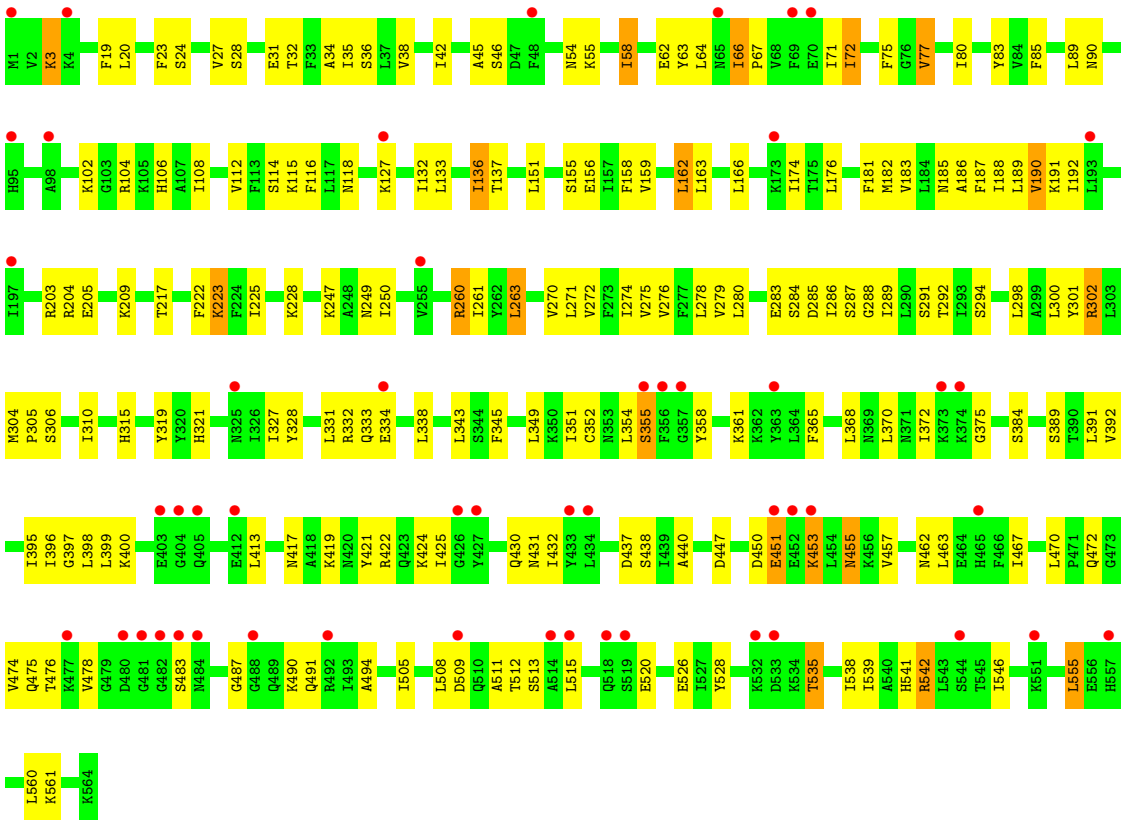
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	11	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	4	0
			27	10	5	10	2		

3 Residue-property plots (i)

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.

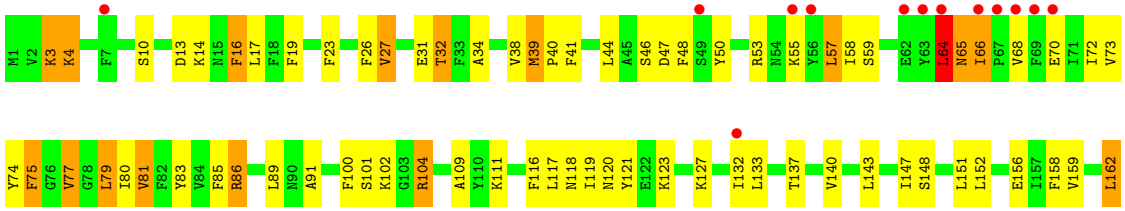
• Molecule 1: WlaB protein

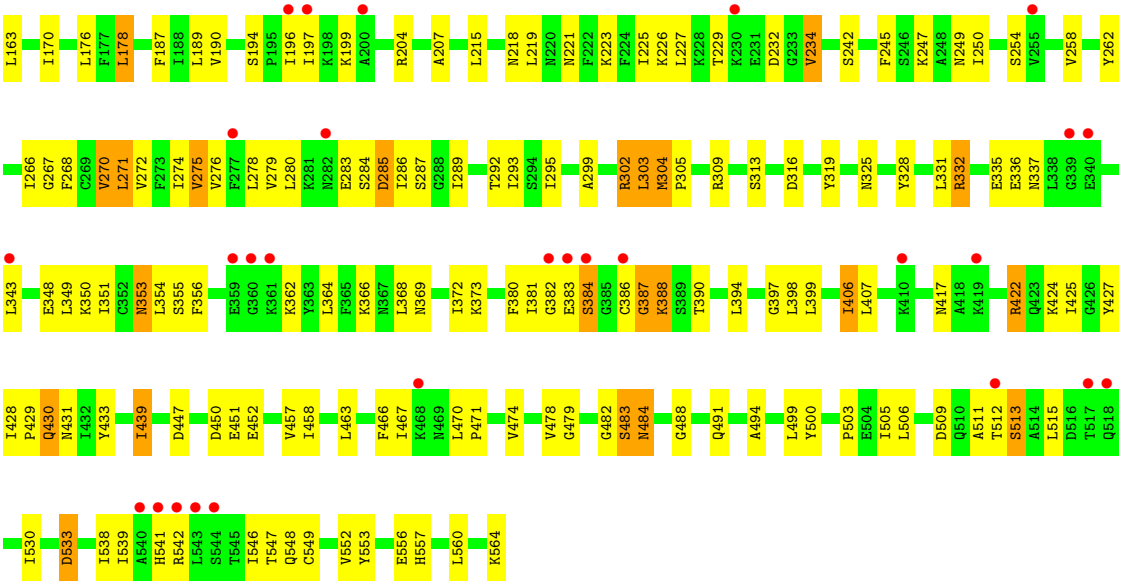
Chain A:



• Molecule 1: WlaB protein

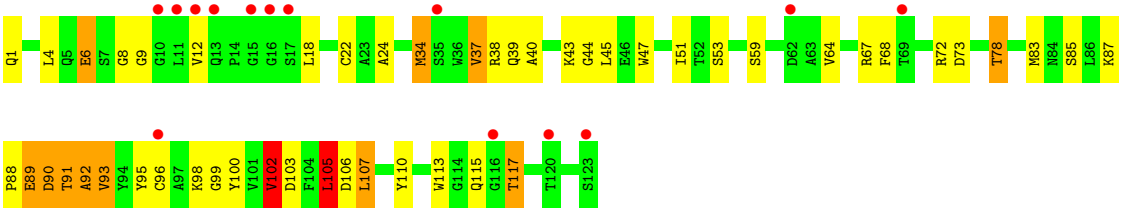
Chain B:





- Molecule 2: Nanobody

Chain C:



4 Data and refinement statistics (i)

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 29.45 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.35-3.90) 92.2 (29.45-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.70 (at 3.86Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.311 , 0.335 0.311 , 0.335	Depositor DCC
R_{free} test set	1999 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)	0.20 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.25	0/4641	0.41	0/6246
1	B	0.25	0/4641	0.42	1/6246 (0.0%)
2	C	0.26	0/942	0.48	0/1275
All	All	0.26	0/10224	0.42	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(^{o})	Ideal(^{o})
1	B	64	LEU	CA-CB-CG	5.55	128.07	115.30

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	4557	0	4764	100	0
1	B	4557	0	4764	143	0
2	C	923	0	883	24	0
3	A	27	0	12	0	0
3	B	27	0	12	3	0
All	All	10091	0	10435	249	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 12.

All (249) 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:B:111:LYS:HB2	1:B:332:ARG:HH22	1.69	0.58
1:A:66:ILE:HB	1:A:67:PRO:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:278:LEU:HG	1:A:289:ILE:HD12	1.90	0.53
1:A:285:ASP:C	1:A:287:SER:H	2.12	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:291:SER:O	1:A:294:SER:OG	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:GLN:C	2:C:92:ALA:HB1	2.36	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:VAL:O	1:B:163:LEU:HB2	2.17	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: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:20:LEU:HB3	1:A:151:LEU:HD13	2.00	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	6 38
1	B	562/564 (100%)	493 (88%)	55 (10%)	14 (2%)	5 36
2	C	121/123 (98%)	88 (73%)	20 (16%)	13 (11%)	0 8
All	All	1245/1251 (100%)	1071 (86%)	134 (11%)	40 (3%)	4 32

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	ILE
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

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Mol	Chain	Res	Type
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 (i)

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%)	450 (89%)	55 (11%)	6 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	505/505 (100%)	445 (88%)	60 (12%)	5 25
2	C	98/98 (100%)	84 (86%)	14 (14%)	3 20
All	All	1108/1108 (100%)	979 (88%)	129 (12%)	5 26

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	19	PHE
1	A	23	PHE
1	A	27	VAL
1	A	32	THR
1	A	55	LYS
1	A	58	ILE
1	A	62	GLU
1	A	63	TYR
1	A	64	LEU
1	A	71	ILE
1	A	72	ILE
1	A	75	PHE
1	A	77	VAL
1	A	85	PHE
1	A	89	LEU
1	A	104	ARG
1	A	115	LYS
1	A	136	ILE
1	A	158	PHE
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
1	A	260	ARG
1	A	263	LEU
1	A	271	LEU
1	A	272	VAL
1	A	275	VAL
1	A	279	VAL

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Mol	Chain	Res	Type
1	A	302	ARG
1	A	315	HIS
1	A	319	TYR
1	A	333	GLN
1	A	334	GLU
1	A	338	LEU
1	A	345	PHE
1	A	354	LEU
1	A	368	LEU
1	A	384	SER
1	A	400	LYS
1	A	431	ASN
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	A	555	LEU
1	B	3	LYS
1	B	4	LYS
1	B	16	PHE
1	B	19	PHE
1	B	23	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	53	ARG
1	B	57	LEU
1	B	64	LEU
1	B	68	VAL
1	B	70	GLU
1	B	72	ILE
1	B	74	TYR
1	B	75	PHE
1	B	77	VAL
1	B	79	LEU

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Mol	Chain	Res	Type
1	B	81	VAL
1	B	85	PHE
1	B	86	ARG
1	B	104	ARG
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	219	LEU
1	B	232	ASP
1	B	234	VAL
1	B	270	VAL
1	B	271	LEU
1	B	275	VAL
1	B	285	ASP
1	B	287	SER
1	B	302	ARG
1	B	303	LEU
1	B	304	MET
1	B	319	TYR
1	B	325	ASN
1	B	328	TYR
1	B	332	ARG
1	B	335	GLU
1	B	353	ASN
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	439	ILE
1	B	447	ASP
1	B	474	VAL
1	B	484	ASN
1	B	533	ASP
1	B	541	HIS
2	C	1	GLN
2	C	6	GLU
2	C	34	MET

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Mol	Chain	Res	Type
2	C	37	VAL
2	C	53	SER
2	C	78	THR
2	C	90	ASP
2	C	102	VAL
2	C	103	ASP
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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	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 monosaccharides 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	$\#\|Z\|>2$
3	ADP	A	601	-	24,29,29	0.91	1 (4%)	29,45,45	1.43	4 (13%)
3	ADP	B	601	-	24,29,29	0.90	1 (4%)	29,45,45	1.49	4 (13%)

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	A	601	-	-	3/12/32/32	0/3/3/3
3	ADP	B	601	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ADP	C5-C4	2.34	1.47	1.40
3	B	601	ADP	C5-C4	2.32	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	ADP	PA-O3A-PB	-3.93	119.34	132.83
3	A	601	ADP	C3'-C2'-C1'	3.62	106.42	100.98
3	B	601	ADP	C3'-C2'-C1'	3.41	106.12	100.98
3	A	601	ADP	PA-O3A-PB	-3.39	121.21	132.83
3	B	601	ADP	C4-C5-N7	-2.81	106.47	109.40
3	A	601	ADP	C4-C5-N7	-2.80	106.48	109.40
3	B	601	ADP	N3-C2-N1	-2.60	124.62	128.68
3	A	601	ADP	N3-C2-N1	-2.56	124.68	128.68

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-O3A
3	A	601	ADP	C5'-O5'-PA-O1A

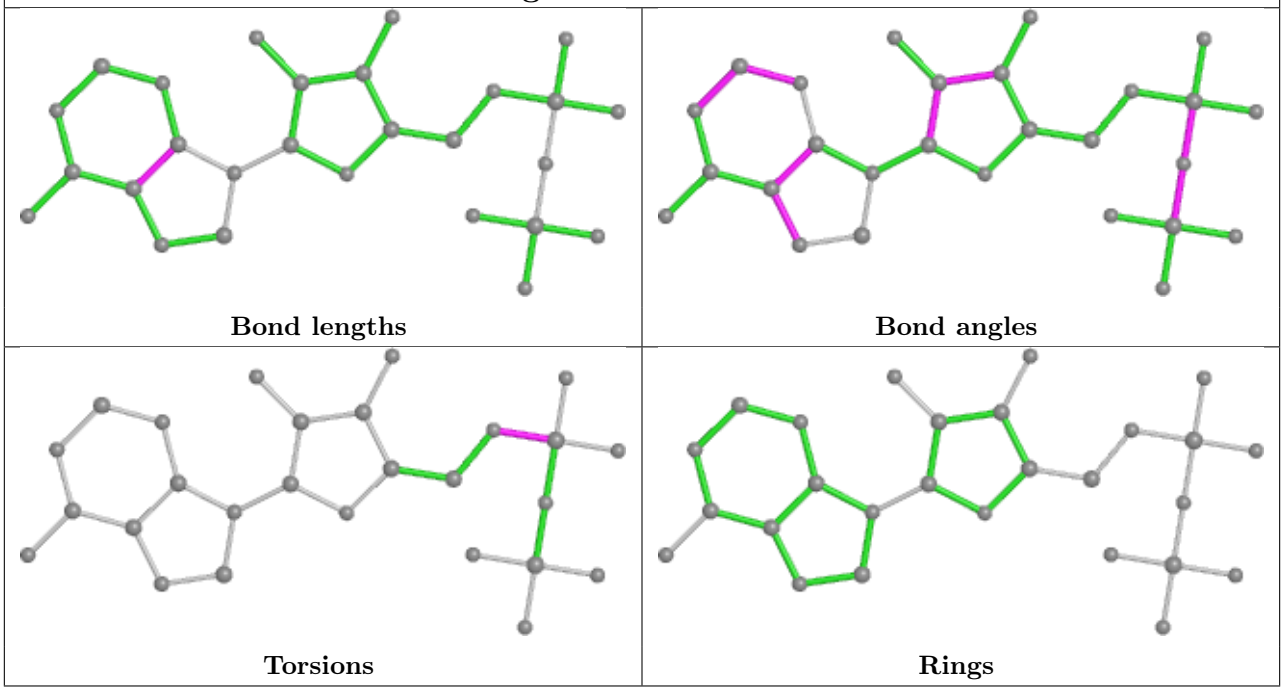
There are no ring outliers.

1 monomer is involved in 3 short contacts:

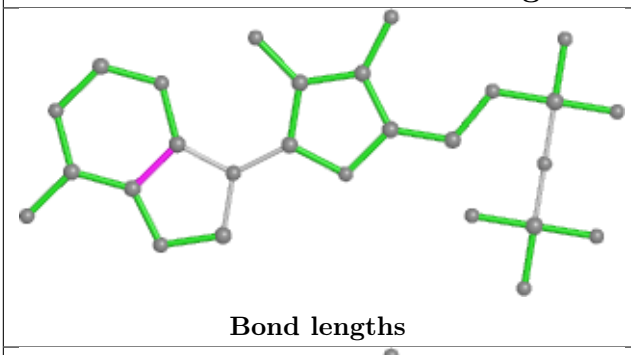
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	ADP	3	0

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 then 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.

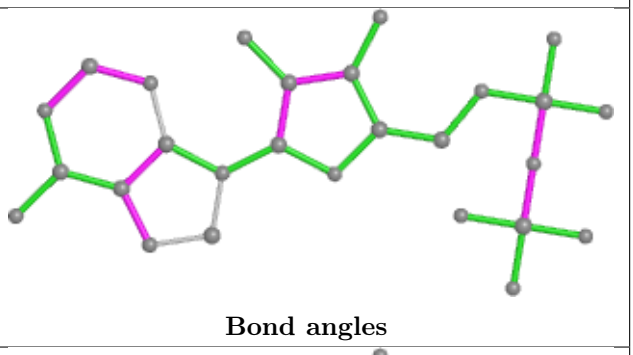
Ligand ADP A 601



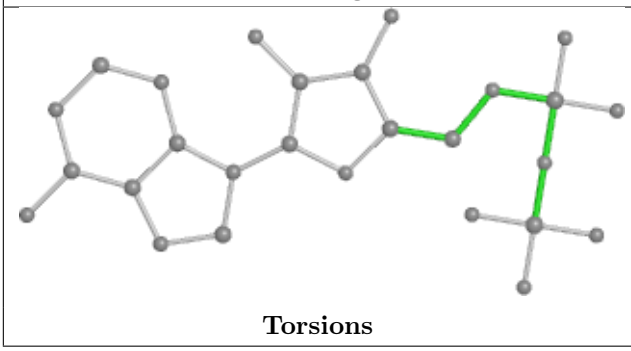
Ligand ADP B 601



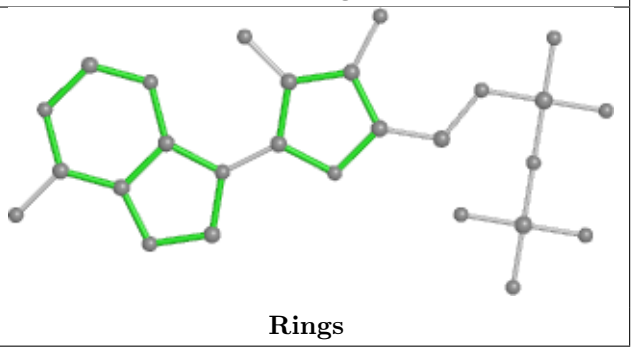
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.23	51 (9%) 9 7	93, 167, 223, 257	0
1	B	564/564 (100%)	0.05	41 (7%) 15 11	98, 156, 212, 258	0
2	C	123/123 (100%)	0.49	14 (11%) 5 4	110, 162, 200, 227	0
All	All	1251/1251 (100%)	0.17	106 (8%) 10 8	93, 161, 218, 258	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	ASN	7.3
1	A	404	GLY	6.2
1	B	382	GLY	6.1
1	B	282	ASN	5.7
1	B	67	PRO	5.5
1	A	426	GLY	5.4
1	B	66	ILE	5.4
1	A	70	GLU	5.4
1	A	482	GLY	5.3
1	B	517	THR	5.3
1	B	70	GLU	5.2
1	B	540	ALA	5.2
1	A	481	GLY	5.1
1	A	515	LEU	4.8
2	C	11	LEU	4.7
1	A	452	GLU	4.7
1	A	405	GLN	4.5
2	C	13	GLN	4.3
1	A	357	GLY	4.3
1	B	63	TYR	4.1
1	A	356	PHE	4.1
1	A	427	TYR	4.0
2	C	62	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	255	VAL	4.0
1	A	544	SER	3.9
1	A	1	MET	3.9
2	C	16	GLY	3.9
2	C	12	VAL	3.8
2	C	10	GLY	3.8
1	A	373	LYS	3.7
1	B	468	LYS	3.7
1	B	62	GLU	3.7
1	A	403	GLU	3.6
1	B	383	GLU	3.6
2	C	123	SER	3.5
1	B	49	SER	3.4
1	B	518	GLN	3.4
1	A	193	LEU	3.3
1	A	433	TYR	3.3
1	A	197	ILE	3.3
1	B	544	SER	3.2
1	A	325	ASN	3.1
2	C	96	CYS	3.1
1	B	340	GLU	3.0
1	B	541	HIS	3.0
1	A	483	SER	2.9
1	B	359	GLU	2.9
1	A	533	ASP	2.9
1	B	360	GLY	2.8
2	C	120	THR	2.8
1	A	95	HIS	2.7
1	A	334	GLU	2.7
1	A	4	LYS	2.7
1	A	518	GLN	2.7
1	B	277	PHE	2.7
2	C	116	GLY	2.7
1	B	343	LEU	2.7
1	A	465	HIS	2.7
1	B	339	GLY	2.6
1	B	196	ILE	2.6
2	C	15	GLY	2.6
1	B	56	TYR	2.5
1	A	557	HIS	2.5
1	B	68	VAL	2.5
1	A	355	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	488	GLY	2.5
1	A	453	LYS	2.5
1	A	363	TYR	2.5
1	A	374	LYS	2.5
1	A	412	GLU	2.5
2	C	69	THR	2.4
1	B	384	SER	2.4
1	B	55	LYS	2.4
1	B	69	PHE	2.4
1	A	480	ASP	2.4
1	B	512	THR	2.4
1	A	492	ARG	2.4
1	B	7	PHE	2.3
1	B	543	LEU	2.3
1	B	230	LYS	2.3
1	A	434	LEU	2.3
1	B	410	LYS	2.3
2	C	17	SER	2.3
1	A	551	LYS	2.3
1	A	519	SER	2.2
1	B	542	ARG	2.2
1	A	255	VAL	2.2
1	A	514	ALA	2.2
1	B	197	ILE	2.2
1	B	419	LYS	2.2
1	B	132	ILE	2.2
1	A	98	ALA	2.1
1	A	532	LYS	2.1
1	A	69	PHE	2.1
1	A	127	LYS	2.1
1	B	200	ALA	2.1
1	A	48	PHE	2.1
1	B	361	LYS	2.1
1	A	509	ASP	2.1
2	C	35	SER	2.1
1	B	64	LEU	2.1
1	B	386	CYS	2.1
1	A	451	GLU	2.0
1	A	173	LYS	2.0
1	A	477	LYS	2.0
1	A	484	ASN	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 monosaccharides in this entry.

6.4 Ligands (i)

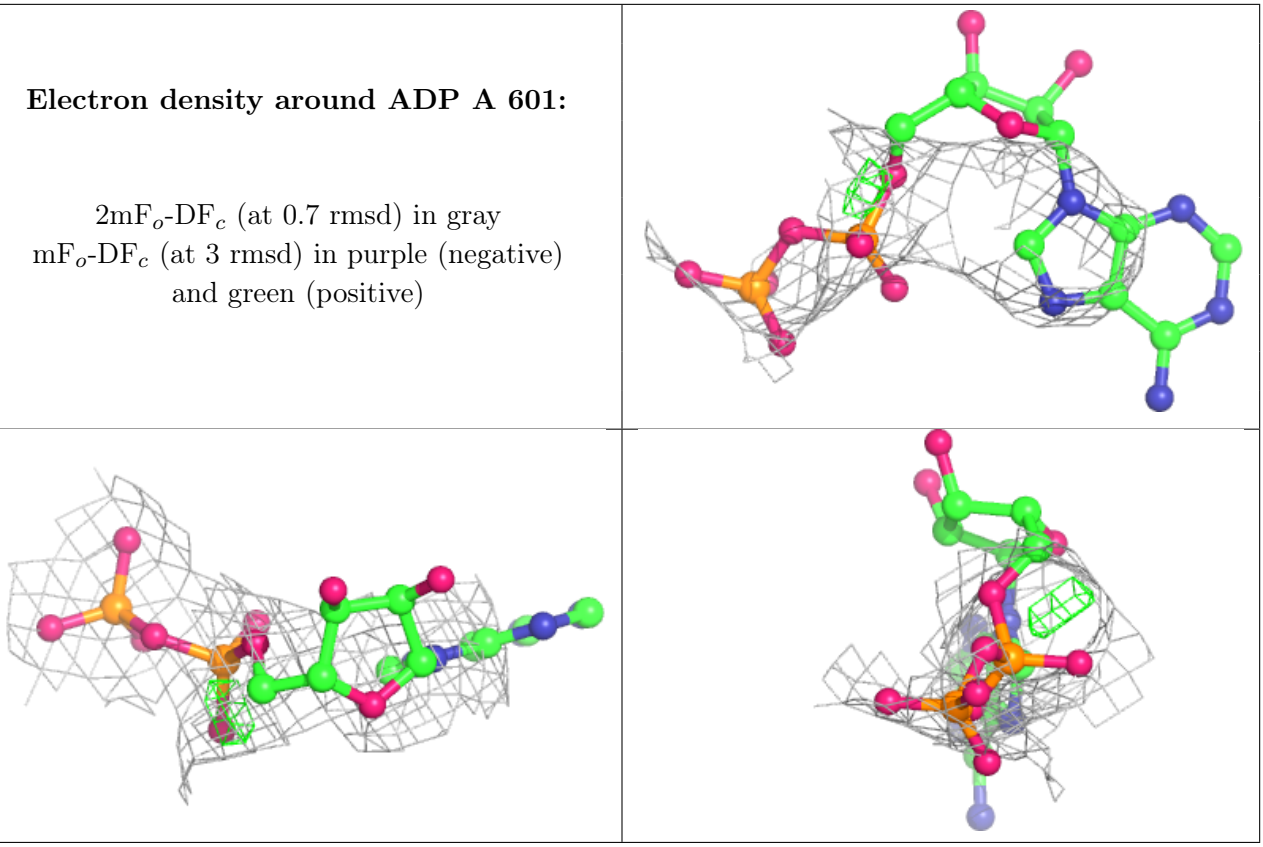
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	A	601	27/27	0.73	0.42	148,202,229,247	18
3	ADP	B	601	27/27	0.80	0.26	147,201,229,246	15

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.

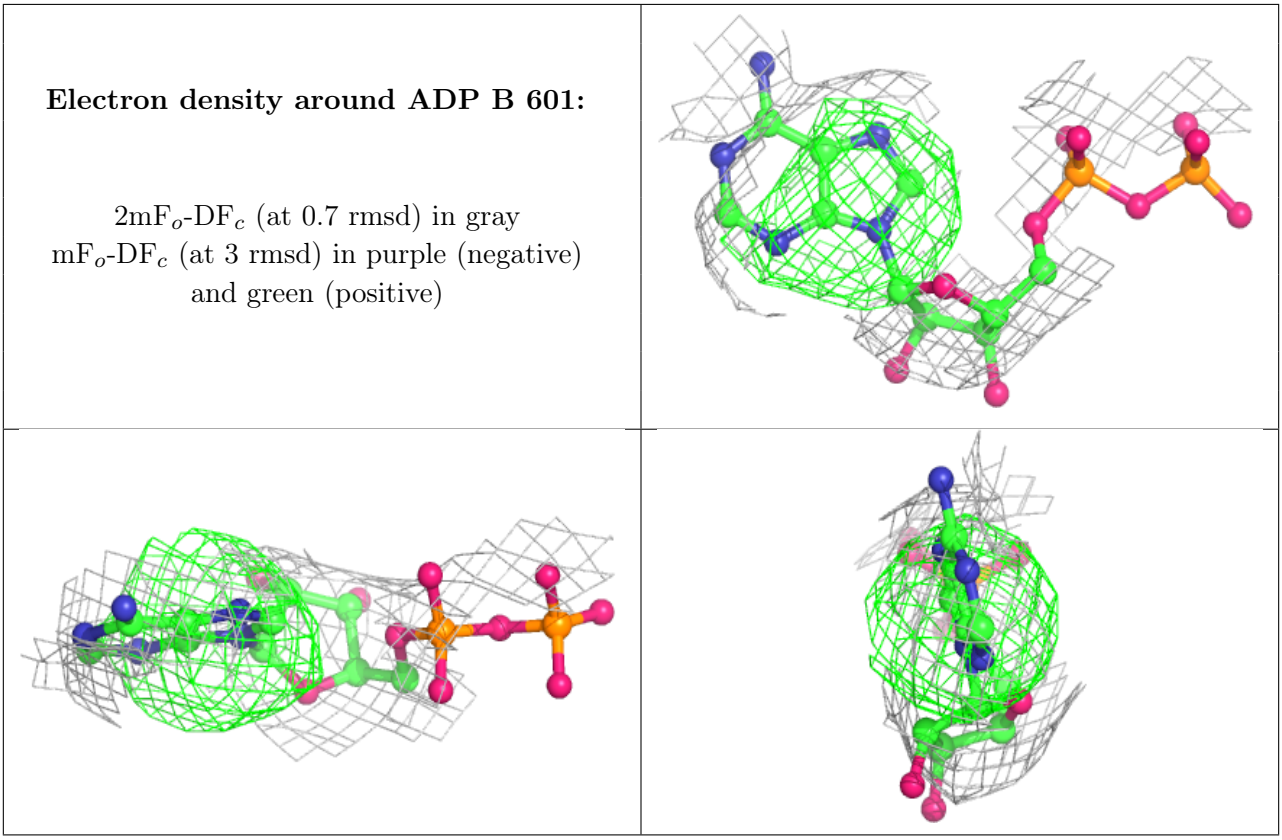
Electron density around ADP A 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ADP B 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.