



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:19 PM UTC

PDB ID : 1TF2 / pdb_00001tf2
Title : Crystal structure of SecA:ADP in an open conformation from Bacillus Subtilis
Authors : Osborne, A.R.; Clemons Jr., W.M.; Rapoport, T.A.
Deposited on : 2004-05-26
Resolution : 2.90 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

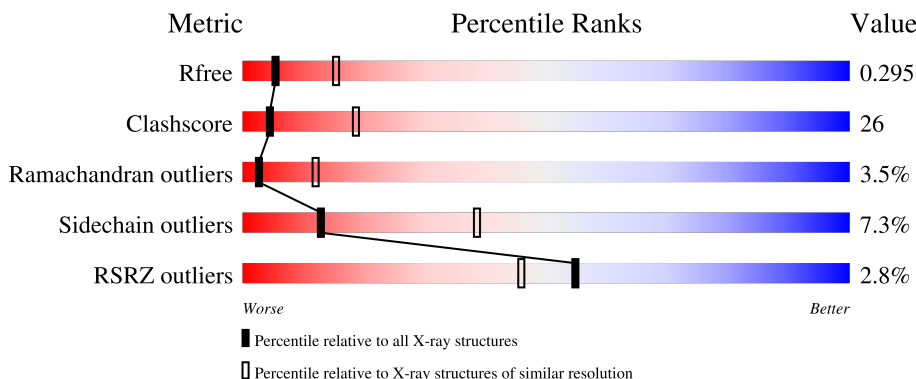
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	844	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6217 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 Preprotein translocase secA subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	772	Total	C	N	O	S	0	0	0
			6163	3856	1077	1196	34			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P28366
A	-1	PRO	-	cloning artifact	UNP P28366
A	0	HIS	-	cloning artifact	UNP P28366

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- 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	0	0
			27	10	5	10	2		

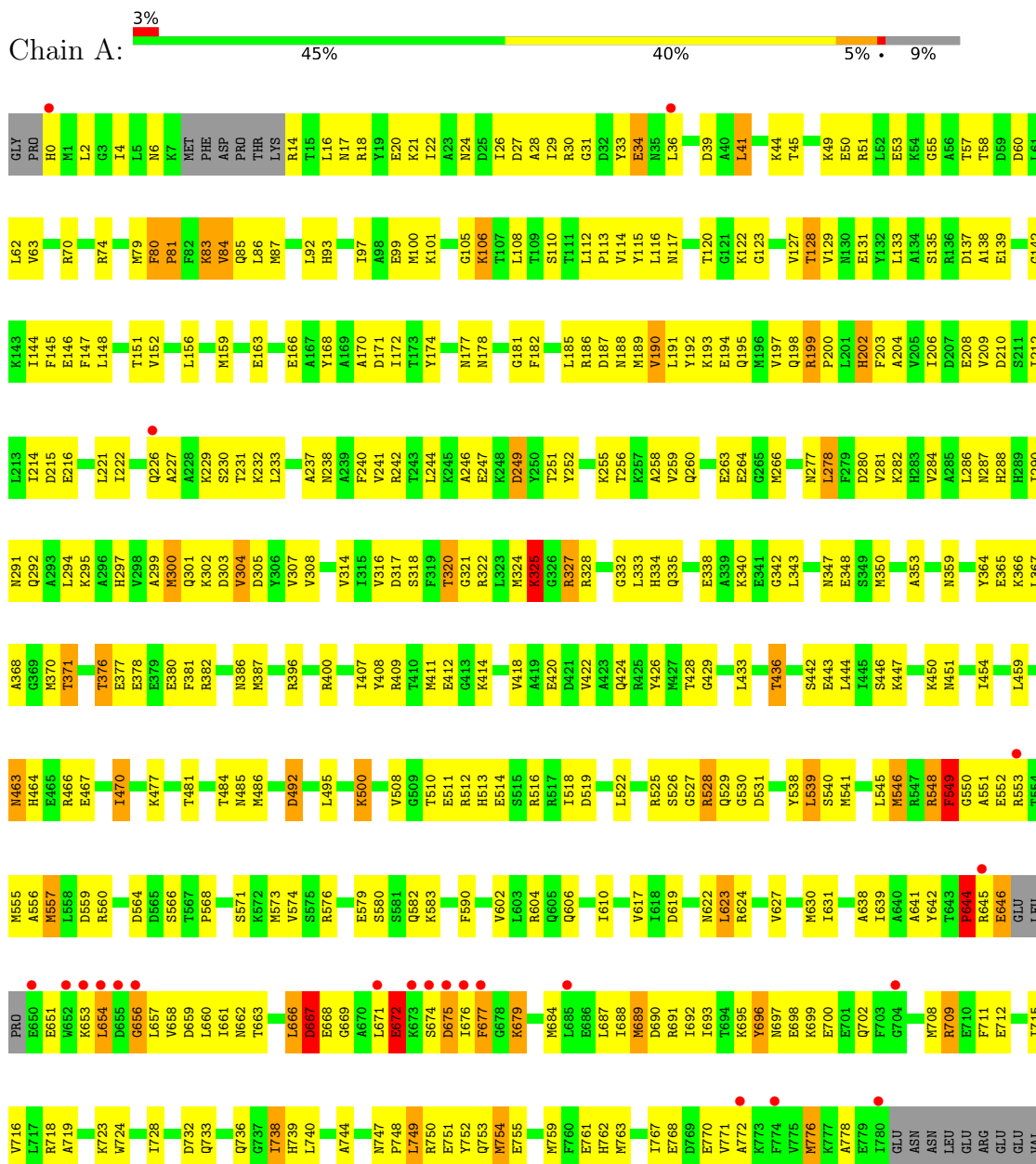
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		

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: Preprotein translocase secA subunit



VAL	GLN	GLY	GLN	THR	ALA	HIS	GLN	PRO	GLN	GLU	GLY	ASP	ASP	ASN	LYS	LYS	ALA	LYS	LYS	ALA	PRO	VAL	ARG	LYS	VAL	VAL	ASP	ILE	GLY	ARG	ASN	ALA	PRO	CYS	HIS	CYS	GLY	SER	GLY	GLY	LYS	LYS	TYR	LYS	ASN	CYS	CYS	GLY	ARG	THR	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.23Å 107.19Å 72.05Å 90.00° 94.96° 90.00°	Depositor
Resolution (Å)	44.98 – 2.90 44.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.3 (44.98-2.90) 97.6 (44.98-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.292 0.236 , 0.295	Depositor DCC
R_{free} test set	3265 reflections (5.69%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6217	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.50	0/6247	1.01	22/8396 (0.3%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	LEU	N-CA-C	10.79	124.56	111.40
1	A	246	ALA	N-CA-C	8.53	120.58	111.28
1	A	33	TYR	N-CA-C	-7.44	105.11	114.56
1	A	199	ARG	N-CA-C	-7.08	101.13	110.40
1	A	711	PHE	N-CA-C	-6.59	104.10	111.28
1	A	127	VAL	N-CA-C	6.50	118.76	108.87
1	A	222	ILE	N-CA-C	6.37	117.65	108.48
1	A	325	LYS	N-CA-C	6.36	124.35	110.80
1	A	761	GLU	N-CA-C	-6.36	104.27	111.07
1	A	212	ILE	N-CA-C	6.14	116.93	110.72
1	A	80	PHE	CA-C-N	6.03	127.38	119.84
1	A	80	PHE	C-N-CA	6.03	127.38	119.84
1	A	481	THR	N-CA-C	6.02	118.21	108.34
1	A	667	ASP	N-CA-C	-5.99	98.03	110.80
1	A	206	ILE	N-CA-C	5.99	117.39	108.23
1	A	209	VAL	N-CA-C	5.90	119.31	111.17
1	A	41	LEU	N-CA-C	-5.87	104.79	111.07
1	A	327	ARG	N-CA-C	5.51	118.27	110.50
1	A	215	ASP	N-CA-C	5.49	117.07	111.14
1	A	654	LEU	N-CA-C	-5.27	103.74	110.53
1	A	739	HIS	N-CA-C	-5.16	106.24	112.54
1	A	407	ILE	N-CA-C	5.01	115.06	107.75

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	6163	0	6159	325	0
2	A	1	0	0	0	0
3	A	27	0	12	1	0
4	A	26	0	0	6	0
All	All	6217	0	6171	325	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 26.

All (325) 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:31:GLY:HA2	1:A:34:GLU:HB2	1.43	0.97
1:A:738:ILE:HD12	1:A:752:TYR:HB2	1.48	0.92
1:A:84:VAL:HA	1:A:87:MET:HE3	1.55	0.88
1:A:436:THR:HG22	1:A:484:THR:HA	1.56	0.86
1:A:159:MET:HE2	1:A:163:GLU:HG2	1.57	0.85
1:A:238:ASN:OD1	1:A:297:HIS:HE1	1.61	0.84
1:A:676:ILE:HG23	1:A:684:MET:HE2	1.60	0.83
1:A:83:LYS:HD3	1:A:83:LYS:N	1.96	0.80
1:A:301:GLN:HB2	1:A:304:VAL:HG13	1.62	0.80
1:A:622:ASN:HA	1:A:709:ARG:HD2	1.64	0.80
1:A:693:ILE:HG22	1:A:697:ASN:HD21	1.46	0.79
1:A:409:ARG:HG3	1:A:541:MET:SD	2.23	0.78
1:A:380:GLU:HB2	1:A:590:PHE:HE1	1.48	0.78
1:A:128:THR:HG22	1:A:129:VAL:H	1.46	0.78
1:A:83:LYS:HD3	1:A:83:LYS:H	1.47	0.78
1:A:675:ASP:HB3	1:A:687:LEU:HD13	1.66	0.77
1:A:676:ILE:HG23	1:A:684:MET:CE	2.14	0.77
1:A:486:MET:HA	1:A:486:MET:HE2	1.68	0.75
1:A:671:LEU:HD11	1:A:691:ARG:HG3	1.67	0.75
1:A:463:ASN:HD22	1:A:463:ASN:C	1.93	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:VAL:HG11	1:A:672:GLU:HG2	1.68	0.74
1:A:83:LYS:H	1:A:83:LYS:CD	1.95	0.73
1:A:237:ALA:O	1:A:241:VAL:HG23	1.88	0.73
1:A:193:LYS:HE2	1:A:619:ASP:OD1	1.88	0.72
1:A:260:GLN:HE21	1:A:740:LEU:HD22	1.54	0.72
1:A:420:GLU:O	1:A:424:GLN:HG2	1.89	0.72
1:A:715:ILE:HA	1:A:718:ARG:HD3	1.69	0.72
1:A:190:VAL:HG22	1:A:195:GLN:HB2	1.72	0.72
1:A:624:ARG:NH2	1:A:696:TYR:HB2	2.05	0.70
1:A:301:GLN:HB2	1:A:304:VAL:CG1	2.20	0.70
1:A:747:ASN:HD22	1:A:748:PRO:HD2	1.57	0.70
1:A:100:MET:O	1:A:106:LYS:HE3	1.92	0.70
1:A:617:VAL:HG13	1:A:623:LEU:HD21	1.75	0.69
1:A:693:ILE:HG22	1:A:697:ASN:ND2	2.07	0.68
1:A:204:ALA:HB2	1:A:364:TYR:CE2	2.28	0.68
1:A:332:GLY:HA2	1:A:335:GLN:OE1	1.94	0.68
1:A:418:VAL:O	1:A:422:VAL:HG23	1.94	0.68
1:A:627:VAL:O	1:A:631:ILE:HG13	1.94	0.68
1:A:359:ASN:OD1	1:A:604:ARG:HD3	1.95	0.67
1:A:142:GLY:HA2	1:A:152:VAL:HG21	1.75	0.67
1:A:549:PHE:HD1	1:A:549:PHE:H	1.41	0.67
1:A:624:ARG:HD3	1:A:712:GLU:OE2	1.93	0.67
1:A:675:ASP:O	1:A:679:LYS:HG3	1.95	0.67
1:A:112:LEU:HB2	1:A:113:PRO:CD	2.25	0.66
1:A:378:GLU:HB3	4:A:2028:HOH:O	1.95	0.66
1:A:31:GLY:CA	1:A:34:GLU:HB2	2.22	0.65
1:A:571:SER:HB3	1:A:574:VAL:HG23	1.78	0.65
1:A:644:PRO:C	1:A:646:GLU:H	2.04	0.65
1:A:238:ASN:OD1	1:A:297:HIS:CE1	2.48	0.65
1:A:380:GLU:HB2	1:A:590:PHE:CE1	2.32	0.65
1:A:747:ASN:HD22	1:A:748:PRO:CD	2.08	0.65
1:A:676:ILE:O	1:A:677:PHE:HB2	1.97	0.65
1:A:657:LEU:HD23	1:A:661:ILE:HG12	1.80	0.64
1:A:166:GLU:OE2	1:A:166:GLU:HA	1.98	0.64
1:A:426:TYR:CD2	1:A:454:ILE:HD12	2.32	0.64
1:A:433:LEU:HD21	1:A:525:ARG:HD3	1.80	0.64
1:A:548:ARG:HB3	1:A:549:PHE:HD1	1.61	0.64
1:A:602:VAL:O	1:A:606:GLN:HG3	1.98	0.63
1:A:408:TYR:CE2	1:A:568:PRO:HG3	2.33	0.63
1:A:516:ARG:NH1	1:A:583:LYS:HG2	2.13	0.62
1:A:698:GLU:O	1:A:702:GLN:HB2	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:MET:HE3	1:A:108:LEU:HD22	1.80	0.62
1:A:216:GLU:HG2	4:A:2022:HOH:O	1.99	0.62
1:A:324:MET:HE2	1:A:327:ARG:HD3	1.81	0.62
1:A:252:TYR:HD2	1:A:259:VAL:HG22	1.64	0.62
1:A:292:GLN:OE1	1:A:292:GLN:HA	2.00	0.62
1:A:278:LEU:HD22	1:A:287:ASN:HB2	1.80	0.61
1:A:671:LEU:O	1:A:672:GLU:HB2	2.00	0.61
1:A:396:ARG:HB2	1:A:529:GLN:O	2.01	0.61
1:A:495:LEU:HD11	1:A:531:ASP:HB3	1.82	0.60
1:A:513:HIS:CD2	1:A:518:ILE:HG13	2.35	0.60
1:A:288:HIS:CD2	1:A:733:GLN:HE21	2.19	0.60
1:A:548:ARG:HB3	1:A:549:PHE:CD1	2.36	0.59
1:A:83:LYS:HA	1:A:86:LEU:HG	1.84	0.59
1:A:93:HIS:CD2	1:A:117:ASN:HD21	2.21	0.59
1:A:675:ASP:CB	1:A:687:LEU:HD13	2.31	0.59
1:A:549:PHE:CD1	1:A:549:PHE:N	2.71	0.59
1:A:300:MET:HE2	1:A:300:MET:HA	1.84	0.59
1:A:252:TYR:CD2	1:A:259:VAL:HG22	2.38	0.58
1:A:110:SER:O	1:A:114:VAL:HG23	2.02	0.58
1:A:128:THR:HG22	1:A:129:VAL:N	2.18	0.58
1:A:666:LEU:O	1:A:695:LYS:NZ	2.36	0.58
1:A:463:ASN:O	1:A:467:GLU:HG3	2.04	0.58
1:A:334:HIS:O	1:A:338:GLU:HG3	2.02	0.58
1:A:642:TYR:C	1:A:644:PRO:HD3	2.29	0.58
1:A:484:THR:O	1:A:486:MET:N	2.37	0.58
1:A:564:ASP:HB2	1:A:566:SER:OG	2.05	0.57
1:A:763:MET:O	1:A:767:ILE:HG13	2.04	0.57
1:A:187:ASP:OD1	1:A:197:VAL:HG22	2.05	0.56
1:A:18:ARG:HG3	1:A:18:ARG:HH11	1.70	0.56
1:A:178:ASN:H	1:A:178:ASN:HD22	1.51	0.56
1:A:512:ARG:HH12	1:A:582:GLN:HG2	1.70	0.56
1:A:277:ASN:HD22	1:A:278:LEU:N	2.03	0.56
1:A:463:ASN:C	1:A:463:ASN:ND2	2.62	0.56
1:A:522:LEU:O	1:A:525:ARG:HG3	2.06	0.55
1:A:738:ILE:CD1	1:A:752:TYR:HB2	2.29	0.55
1:A:400:ARG:HD3	1:A:526:SER:O	2.05	0.55
1:A:142:GLY:O	1:A:146:GLU:HG3	2.05	0.55
1:A:623:LEU:O	1:A:627:VAL:HG23	2.06	0.55
1:A:738:ILE:HG12	1:A:738:ILE:O	2.06	0.55
1:A:190:VAL:HG22	1:A:195:GLN:CB	2.37	0.55
1:A:181:GLY:HA3	1:A:221:LEU:CD1	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:THR:O	1:A:170:ALA:HB1	2.07	0.54
1:A:412:GLU:CD	1:A:412:GLU:H	2.14	0.54
1:A:443:GLU:O	1:A:447:LYS:HG3	2.07	0.54
1:A:657:LEU:O	1:A:661:ILE:HG12	2.06	0.54
1:A:233:LEU:HD11	1:A:286:LEU:HD13	1.88	0.54
1:A:229:LYS:O	1:A:347:ASN:ND2	2.41	0.54
1:A:290:ILE:O	1:A:294:LEU:HB2	2.07	0.54
1:A:74:ARG:HB2	1:A:80:PHE:HD1	1.72	0.54
1:A:284:VAL:HG21	1:A:759:MET:HE1	1.90	0.54
1:A:299:ALA:O	1:A:300:MET:HE3	2.08	0.53
1:A:414:LYS:O	1:A:418:VAL:HG23	2.08	0.53
1:A:242:ARG:HG2	1:A:242:ARG:HH11	1.73	0.53
1:A:264:GLU:H	1:A:264:GLU:CD	2.16	0.53
1:A:436:THR:HG21	1:A:442:SER:OG	2.08	0.53
1:A:677:PHE:C	1:A:679:LYS:H	2.16	0.53
1:A:123:GLY:O	1:A:202:HIS:HD2	1.91	0.53
1:A:112:LEU:HB2	1:A:113:PRO:HD3	1.91	0.53
1:A:516:ARG:HH12	1:A:583:LYS:HG2	1.73	0.53
1:A:368:ALA:HA	1:A:387:MET:HE3	1.90	0.53
1:A:2:LEU:O	1:A:6:ASN:ND2	2.43	0.52
1:A:144:ILE:O	1:A:147:PHE:HB3	2.10	0.52
1:A:444:LEU:C	1:A:444:LEU:HD13	2.35	0.52
1:A:247:GLU:OE2	1:A:247:GLU:HA	2.10	0.52
1:A:424:GLN:HE21	1:A:424:GLN:HA	1.75	0.52
1:A:447:LYS:O	1:A:451:ASN:ND2	2.42	0.52
1:A:688:ILE:O	1:A:692:ILE:HG12	2.09	0.52
1:A:418:VAL:HG13	1:A:508:VAL:HG11	1.91	0.52
1:A:414:LYS:HG3	1:A:538:TYR:HB3	1.92	0.52
1:A:123:GLY:HA2	1:A:171:ASP:O	2.10	0.52
1:A:226:GLN:HE21	1:A:227:ALA:H	1.58	0.51
1:A:230:SER:OG	1:A:232:LYS:HG2	2.10	0.51
1:A:538:TYR:O	1:A:539:LEU:HD23	2.09	0.51
1:A:700:GLU:HA	1:A:708:MET:HE3	1.91	0.51
1:A:317:ASP:OD2	1:A:320:THR:HG23	2.09	0.51
1:A:546:MET:HG3	1:A:555:MET:SD	2.50	0.51
1:A:208:GLU:HA	1:A:208:GLU:OE1	2.10	0.51
1:A:492:ASP:OD2	1:A:528:ARG:NH1	2.43	0.51
1:A:199:ARG:O	1:A:200:PRO:C	2.53	0.51
1:A:252:TYR:HE2	1:A:299:ALA:HB2	1.76	0.51
1:A:553:ARG:O	1:A:556:ALA:HB3	2.10	0.51
1:A:624:ARG:HH21	1:A:696:TYR:HB2	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ILE:HA	1:A:657:LEU:HD11	1.92	0.51
1:A:79:MET:CE	1:A:108:LEU:HD22	2.41	0.50
1:A:512:ARG:HH11	1:A:512:ARG:HB3	1.76	0.50
1:A:571:SER:HB3	1:A:574:VAL:CG2	2.40	0.50
1:A:771:VAL:HG12	1:A:771:VAL:O	2.10	0.50
1:A:93:HIS:HD2	1:A:117:ASN:HD21	1.59	0.50
1:A:644:PRO:C	1:A:646:GLU:N	2.70	0.50
1:A:36:LEU:HD21	1:A:44:LYS:HE2	1.93	0.50
1:A:202:HIS:HB3	4:A:2029:HOH:O	2.11	0.50
1:A:307:VAL:HG13	1:A:316:VAL:CG2	2.42	0.50
1:A:320:THR:C	1:A:322:ARG:H	2.20	0.50
1:A:302:LYS:O	1:A:303:ASP:HB2	2.12	0.50
1:A:376:THR:HG21	1:A:516:ARG:HH21	1.76	0.49
1:A:610:ILE:HD11	1:A:763:MET:CE	2.41	0.49
1:A:510:THR:C	1:A:511:GLU:HG3	2.37	0.49
1:A:185:LEU:HD22	1:A:353:ALA:HB1	1.94	0.49
1:A:190:VAL:CG2	1:A:195:GLN:HB2	2.41	0.49
1:A:684:MET:HA	1:A:687:LEU:HD12	1.93	0.49
1:A:776:MET:HE3	1:A:776:MET:HA	1.94	0.49
1:A:556:ALA:HB1	1:A:560:ARG:HH12	1.78	0.49
1:A:692:ILE:HG23	1:A:776:MET:SD	2.53	0.49
1:A:62:LEU:C	1:A:62:LEU:HD23	2.37	0.49
1:A:240:PHE:CZ	1:A:244:LEU:HD21	2.47	0.49
1:A:97:ILE:HG13	1:A:387:MET:HE2	1.95	0.49
1:A:277:ASN:O	1:A:280:ASP:HB2	2.13	0.48
1:A:610:ILE:HD11	1:A:763:MET:HE3	1.93	0.48
1:A:671:LEU:HD22	1:A:674:SER:CB	2.43	0.48
1:A:724:TRP:NE1	1:A:728:ILE:HD11	2.28	0.48
1:A:657:LEU:HD23	1:A:661:ILE:CG1	2.42	0.48
1:A:260:GLN:HE21	1:A:740:LEU:CD2	2.21	0.48
1:A:624:ARG:HG2	1:A:696:TYR:CE1	2.48	0.48
1:A:99:GLU:HA	1:A:371:THR:O	2.13	0.48
1:A:376:THR:HB	1:A:377:GLU:OE2	2.13	0.48
1:A:382:ARG:O	1:A:386:ASN:HA	2.14	0.48
1:A:754:MET:HE2	1:A:755:GLU:N	2.29	0.48
1:A:624:ARG:CD	1:A:712:GLU:OE2	2.61	0.48
1:A:644:PRO:O	1:A:646:GLU:N	2.45	0.48
1:A:51:ARG:HB3	4:A:2017:HOH:O	2.12	0.48
1:A:651:GLU:OE1	1:A:654:LEU:HD13	2.13	0.48
1:A:17:ASN:ND2	1:A:20:GLU:HG3	2.28	0.48
1:A:131:GLU:CD	1:A:156:LEU:HD22	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:GLY:O	1:A:551:ALA:C	2.56	0.47
1:A:242:ARG:HG2	1:A:242:ARG:NH1	2.28	0.47
1:A:576:ARG:HH11	1:A:576:ARG:HG3	1.78	0.47
1:A:698:GLU:HG3	1:A:702:GLN:CD	2.39	0.47
1:A:307:VAL:HG13	1:A:316:VAL:HG21	1.96	0.47
1:A:630:MET:HE3	1:A:768:GLU:HA	1.97	0.47
1:A:129:VAL:CG2	1:A:133:LEU:HD12	2.44	0.47
1:A:696:TYR:CD1	1:A:696:TYR:C	2.93	0.47
1:A:698:GLU:HG3	1:A:702:GLN:OE1	2.14	0.47
1:A:178:ASN:H	1:A:178:ASN:ND2	2.12	0.47
1:A:328:ARG:HB3	1:A:334:HIS:ND1	2.30	0.47
1:A:145:PHE:CD2	1:A:172:ILE:CD1	2.98	0.47
1:A:28:ALA:C	1:A:30:ARG:H	2.23	0.47
1:A:671:LEU:HD22	1:A:674:SER:HB2	1.97	0.47
1:A:115:TYR:C	1:A:115:TYR:CD2	2.93	0.46
1:A:92:LEU:HB2	1:A:113:PRO:HG3	1.98	0.46
1:A:168:TYR:CE2	1:A:198:GLN:HG2	2.51	0.46
1:A:424:GLN:HA	1:A:424:GLN:NE2	2.31	0.46
1:A:576:ARG:HG3	1:A:576:ARG:NH1	2.31	0.46
1:A:31:GLY:HA2	1:A:34:GLU:CB	2.29	0.46
1:A:557:MET:HE2	1:A:557:MET:O	2.16	0.46
1:A:571:SER:CB	1:A:574:VAL:HG23	2.44	0.46
1:A:676:ILE:O	1:A:677:PHE:CB	2.64	0.46
1:A:308:VAL:HG13	1:A:343:LEU:HD11	1.98	0.46
1:A:2:LEU:HA	1:A:2:LEU:HD23	1.74	0.46
1:A:408:TYR:CZ	1:A:568:PRO:HG3	2.51	0.46
1:A:251:THR:CG2	1:A:260:GLN:HB2	2.46	0.46
1:A:70:ARG:HG3	1:A:81:PRO:HB2	1.98	0.46
1:A:27:ASP:O	1:A:30:ARG:HB3	2.16	0.45
1:A:74:ARG:NH2	1:A:80:PHE:CE1	2.84	0.45
1:A:185:LEU:O	1:A:189:MET:HG3	2.16	0.45
1:A:79:MET:HB3	3:A:843:ADP:C6	2.51	0.45
1:A:738:ILE:HD13	1:A:748:PRO:HB3	1.98	0.45
1:A:656:GLY:C	1:A:658:VAL:N	2.74	0.45
1:A:21:LYS:O	1:A:24:ASN:N	2.46	0.45
1:A:314:VAL:HA	4:A:2004:HOH:O	2.16	0.45
1:A:759:MET:O	1:A:762:HIS:HB3	2.16	0.45
1:A:14:ARG:HD3	1:A:14:ARG:N	2.31	0.45
1:A:41:LEU:O	1:A:44:LYS:HB2	2.17	0.45
1:A:408:TYR:O	1:A:540:SER:HA	2.17	0.45
1:A:771:VAL:O	1:A:771:VAL:CG1	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:ARG:HH22	1:A:776:MET:HE1	1.82	0.45
1:A:698:GLU:HG2	1:A:699:LYS:N	2.32	0.45
1:A:241:VAL:HG13	1:A:294:LEU:HD12	1.99	0.44
1:A:429:GLY:O	1:A:477:LYS:HG3	2.18	0.44
1:A:463:ASN:HD22	1:A:464:HIS:N	2.16	0.44
1:A:666:LEU:O	1:A:667:ASP:CB	2.64	0.44
1:A:693:ILE:O	1:A:697:ASN:ND2	2.50	0.44
1:A:137:ASP:HB3	1:A:174:TYR:HE2	1.82	0.44
1:A:630:MET:CE	1:A:771:VAL:HB	2.48	0.44
1:A:244:LEU:HB3	1:A:249:ASP:HB3	1.98	0.44
1:A:662:ASN:HB3	1:A:668:GLU:HA	1.99	0.44
1:A:16:LEU:HB3	1:A:20:GLU:HB2	1.99	0.44
1:A:231:THR:HG23	1:A:347:ASN:ND2	2.32	0.44
1:A:281:VAL:O	1:A:759:MET:HE2	2.18	0.44
1:A:516:ARG:HD2	1:A:579:GLU:OE1	2.17	0.44
1:A:657:LEU:HD23	1:A:657:LEU:O	2.17	0.44
1:A:159:MET:CE	1:A:163:GLU:HG2	2.39	0.44
1:A:754:MET:HE2	1:A:754:MET:C	2.43	0.44
1:A:26:ILE:HG13	1:A:63:VAL:HG13	1.99	0.44
1:A:295:LYS:HD3	1:A:333:LEU:HD13	2.00	0.44
1:A:320:THR:C	1:A:322:ARG:N	2.76	0.44
1:A:623:LEU:HA	4:A:2002:HOH:O	2.17	0.44
1:A:692:ILE:O	1:A:695:LYS:HB3	2.17	0.44
1:A:320:THR:O	1:A:322:ARG:N	2.51	0.44
1:A:57:THR:O	1:A:60:ASP:HB2	2.18	0.43
1:A:186:ARG:C	1:A:188:ASN:N	2.75	0.43
1:A:638:ALA:O	1:A:641:ALA:HB3	2.17	0.43
1:A:659:ASP:O	1:A:663:THR:HB	2.18	0.43
1:A:690:ASP:O	1:A:691:ARG:C	2.61	0.43
1:A:463:ASN:ND2	1:A:466:ARG:H	2.16	0.43
1:A:516:ARG:NH1	1:A:583:LYS:CG	2.81	0.43
1:A:630:MET:CE	1:A:768:GLU:HA	2.49	0.43
1:A:630:MET:HE2	1:A:771:VAL:HB	1.99	0.43
1:A:231:THR:CG2	1:A:347:ASN:ND2	2.82	0.43
1:A:191:LEU:HD23	1:A:192:TYR:CE1	2.54	0.43
1:A:500:LYS:H	1:A:500:LYS:CE	2.32	0.43
1:A:233:LEU:HD11	1:A:286:LEU:CD1	2.48	0.43
1:A:529:GLN:OE1	1:A:529:GLN:HA	2.18	0.43
1:A:45:THR:O	1:A:49:LYS:HG3	2.19	0.43
1:A:444:LEU:HD13	1:A:444:LEU:O	2.18	0.43
1:A:513:HIS:CG	1:A:514:GLU:N	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASP:O	1:A:214:ILE:HB	2.19	0.43
1:A:527:GLY:HA2	1:A:531:ASP:O	2.19	0.43
1:A:719:ALA:O	1:A:723:LYS:HG2	2.19	0.42
1:A:340:LYS:C	1:A:342:GLY:H	2.27	0.42
1:A:557:MET:HE2	1:A:557:MET:C	2.44	0.42
1:A:20:GLU:O	1:A:24:ASN:ND2	2.52	0.42
1:A:202:HIS:O	1:A:365:GLU:HB3	2.18	0.42
1:A:610:ILE:HG13	1:A:763:MET:HE1	2.01	0.42
1:A:622:ASN:ND2	1:A:709:ARG:HE	2.17	0.42
1:A:259:VAL:HG12	1:A:294:LEU:HD23	2.02	0.42
1:A:147:PHE:HD2	1:A:148:LEU:HD23	1.83	0.42
1:A:287:ASN:O	1:A:291:ASN:ND2	2.52	0.42
1:A:324:MET:HE2	1:A:327:ARG:CD	2.49	0.42
1:A:182:PHE:HB3	1:A:186:ARG:HH21	1.85	0.42
1:A:671:LEU:CD1	1:A:691:ARG:HG3	2.45	0.42
1:A:715:ILE:HD13	1:A:718:ARG:HD3	2.01	0.42
1:A:203:PHE:HB2	1:A:366:LYS:HB3	2.02	0.42
1:A:264:GLU:CD	1:A:264:GLU:N	2.78	0.42
1:A:277:ASN:HB3	1:A:280:ASP:HB2	2.01	0.42
1:A:657:LEU:O	1:A:660:LEU:HB3	2.19	0.42
1:A:747:ASN:ND2	1:A:748:PRO:HD2	2.30	0.42
1:A:112:LEU:CB	1:A:113:PRO:CD	2.97	0.42
1:A:659:ASP:O	1:A:663:THR:HG22	2.19	0.42
1:A:280:ASP:OD2	1:A:282:LYS:HD2	2.20	0.41
1:A:689:MET:O	1:A:693:ILE:HG12	2.20	0.41
1:A:241:VAL:O	1:A:241:VAL:HG12	2.19	0.41
1:A:277:ASN:HD22	1:A:277:ASN:C	2.28	0.41
1:A:545:LEU:O	1:A:545:LEU:HD12	2.19	0.41
1:A:751:GLU:OE1	1:A:755:GLU:OE2	2.38	0.41
1:A:135:SER:O	1:A:139:GLU:HB3	2.20	0.41
1:A:459:LEU:HD21	1:A:470:ILE:HG21	2.03	0.41
1:A:546:MET:HA	1:A:551:ALA:HB1	2.02	0.41
1:A:668:GLU:OE2	1:A:669:GLY:N	2.54	0.41
1:A:709:ARG:N	1:A:709:ARG:HH11	2.18	0.41
1:A:214:ILE:HD11	1:A:381:PHE:CE2	2.55	0.41
1:A:256:THR:C	1:A:258:ALA:H	2.29	0.41
1:A:446:SER:O	1:A:450:LYS:HG3	2.21	0.41
1:A:573:MET:HE2	1:A:573:MET:HB3	1.86	0.41
1:A:138:ALA:HB2	1:A:174:TYR:CG	2.56	0.41
1:A:763:MET:O	1:A:763:MET:HG2	2.19	0.41
1:A:50:GLU:O	1:A:53:GLU:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLN:NE2	1:A:105:GLY:HA3	2.36	0.41
1:A:716:VAL:O	1:A:719:ALA:HB3	2.21	0.41
1:A:749:LEU:HD13	1:A:753:GLN:CD	2.44	0.41
1:A:137:ASP:O	1:A:138:ALA:C	2.63	0.41
1:A:226:GLN:NE2	1:A:227:ALA:H	2.19	0.41
1:A:294:LEU:HD12	1:A:294:LEU:HA	1.89	0.41
1:A:301:GLN:O	1:A:305:ASP:HB2	2.21	0.41
1:A:93:HIS:HD2	1:A:117:ASN:ND2	2.19	0.41
1:A:657:LEU:HD23	1:A:657:LEU:C	2.45	0.40
1:A:120:THR:OG1	1:A:122:LYS:HG3	2.20	0.40
1:A:512:ARG:HD2	1:A:519:ASP:OD1	2.21	0.40
1:A:0:HIS:O	1:A:4:ILE:HG13	2.20	0.40
1:A:292:GLN:OE1	1:A:292:GLN:CA	2.69	0.40
1:A:93:HIS:CD2	1:A:116:LEU:HD23	2.56	0.40
1:A:541:MET:HE1	1:A:559:ASP:HB2	2.04	0.40
1:A:639:ILE:HA	1:A:657:LEU:CD1	2.52	0.40
1:A:732:ASP:OD2	1:A:736:GLN:NE2	2.54	0.40
1:A:770:GLU:C	1:A:772:ALA:N	2.79	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	766/844 (91%)	678 (88%)	61 (8%)	27 (4%)	3 12

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	SER
1	A	485	ASN
1	A	528	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	549	PHE
1	A	667	ASP
1	A	672	GLU
1	A	677	PHE
1	A	679	LYS
1	A	778	ALA
1	A	29	ILE
1	A	249	ASP
1	A	325	LYS
1	A	548	ARG
1	A	645	ARG
1	A	675	ASP
1	A	744	ALA
1	A	55	GLY
1	A	101	LYS
1	A	255	LYS
1	A	81	PRO
1	A	202	HIS
1	A	530	GLY
1	A	653	LYS
1	A	656	GLY
1	A	321	GLY
1	A	552	GLU
1	A	644	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	662/723 (92%)	614 (93%)	48 (7%)	13	38

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	34	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	39	ASP
1	A	58	THR
1	A	83	LYS
1	A	84	VAL
1	A	106	LYS
1	A	128	THR
1	A	177	ASN
1	A	190	VAL
1	A	194	GLU
1	A	263	GLU
1	A	266	MET
1	A	278	LEU
1	A	300	MET
1	A	304	VAL
1	A	320	THR
1	A	325	LYS
1	A	348	GLU
1	A	350	MET
1	A	367	LEU
1	A	370	MET
1	A	371	THR
1	A	376	THR
1	A	411	MET
1	A	428	THR
1	A	436	THR
1	A	463	ASN
1	A	470	ILE
1	A	492	ASP
1	A	500	LYS
1	A	539	LEU
1	A	546	MET
1	A	549	PHE
1	A	557	MET
1	A	580	SER
1	A	623	LEU
1	A	644	PRO
1	A	646	GLU
1	A	672	GLU
1	A	689	MET
1	A	696	TYR
1	A	709	ARG
1	A	738	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	749	LEU
1	A	750	ARG
1	A	754	MET
1	A	776	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	6	ASN
1	A	24	ASN
1	A	93	HIS
1	A	178	ASN
1	A	202	HIS
1	A	226	GLN
1	A	260	GLN
1	A	277	ASN
1	A	288	HIS
1	A	297	HIS
1	A	346	GLN
1	A	347	ASN
1	A	386	ASN
1	A	395	ASN
1	A	424	GLN
1	A	451	ASN
1	A	463	ASN
1	A	485	ASN
1	A	513	HIS
1	A	588	ASN
1	A	595	GLN
1	A	598	GLN
1	A	605	GLN
1	A	613	GLN
1	A	622	ASN
1	A	697	ASN
1	A	736	GLN
1	A	747	ASN
1	A	762	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	843	2	28,29,29	1.85	2 (7%)	43,45,45	1.84	6 (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	843	2	-	2/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	843	ADP	PA-O3A	-7.60	1.51	1.59
3	A	843	ADP	PA-O5'	-2.98	1.47	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	843	ADP	N3-C2-N1	-6.13	119.30	128.58
3	A	843	ADP	C5-C4-N3	-4.99	119.85	126.72
3	A	843	ADP	C2-N3-C4	4.37	122.51	111.83
3	A	843	ADP	N3-C4-N9	3.65	133.37	127.17
3	A	843	ADP	C5-N7-C8	2.65	107.62	103.45
3	A	843	ADP	C4-C5-N7	-2.49	107.74	110.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

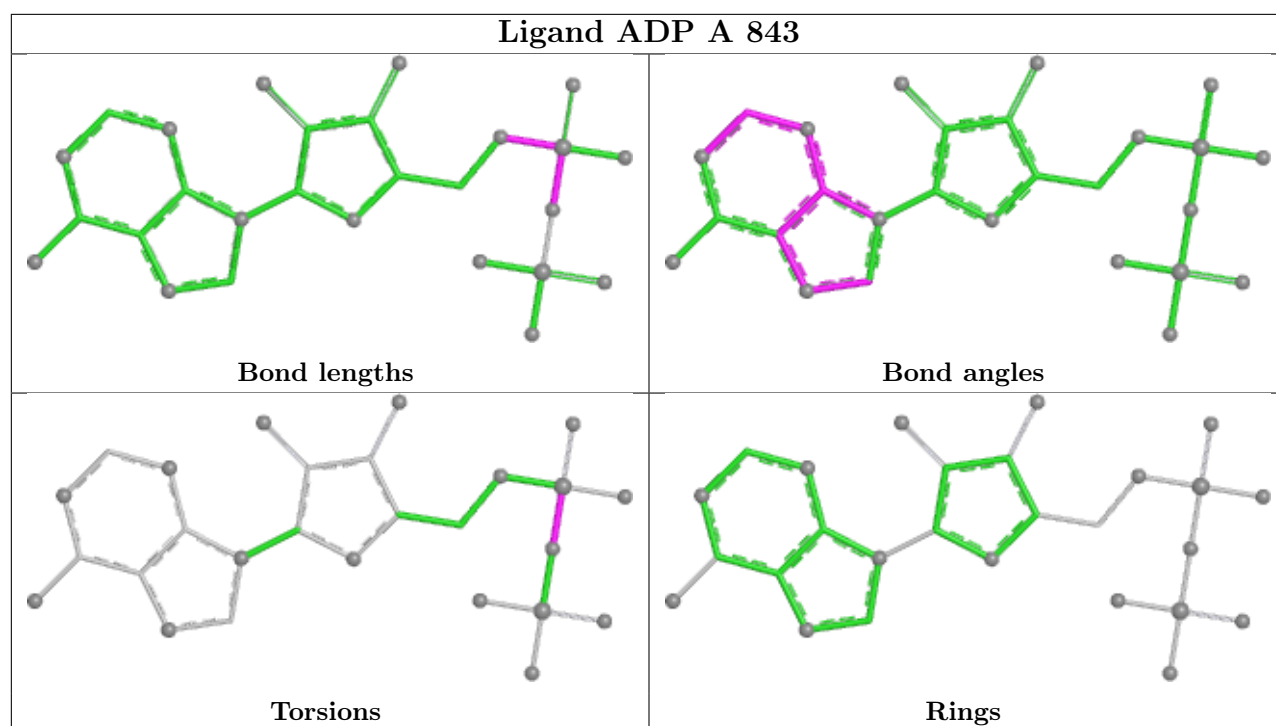
Mol	Chain	Res	Type	Atoms
3	A	843	ADP	PB-O3A-PA-O1A
3	A	843	ADP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	843	ADP	1	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	772/844 (91%)	0.10	22 (2%) 55 46	26, 54, 114, 140	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	671	LEU	4.1
1	A	676	ILE	3.2
1	A	780	ILE	3.2
1	A	652	TRP	3.0
1	A	0	HIS	2.9
1	A	654	LEU	2.9
1	A	673	LYS	2.7
1	A	674	SER	2.6
1	A	553	ARG	2.6
1	A	226	GLN	2.5
1	A	774	PHE	2.5
1	A	704	GLY	2.5
1	A	645	ARG	2.3
1	A	653	LYS	2.3
1	A	685	LEU	2.3
1	A	677	PHE	2.3
1	A	772	ALA	2.3
1	A	656	GLY	2.3
1	A	655	ASP	2.2
1	A	675	ASP	2.1
1	A	650	GLU	2.1
1	A	36	LEU	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](#)

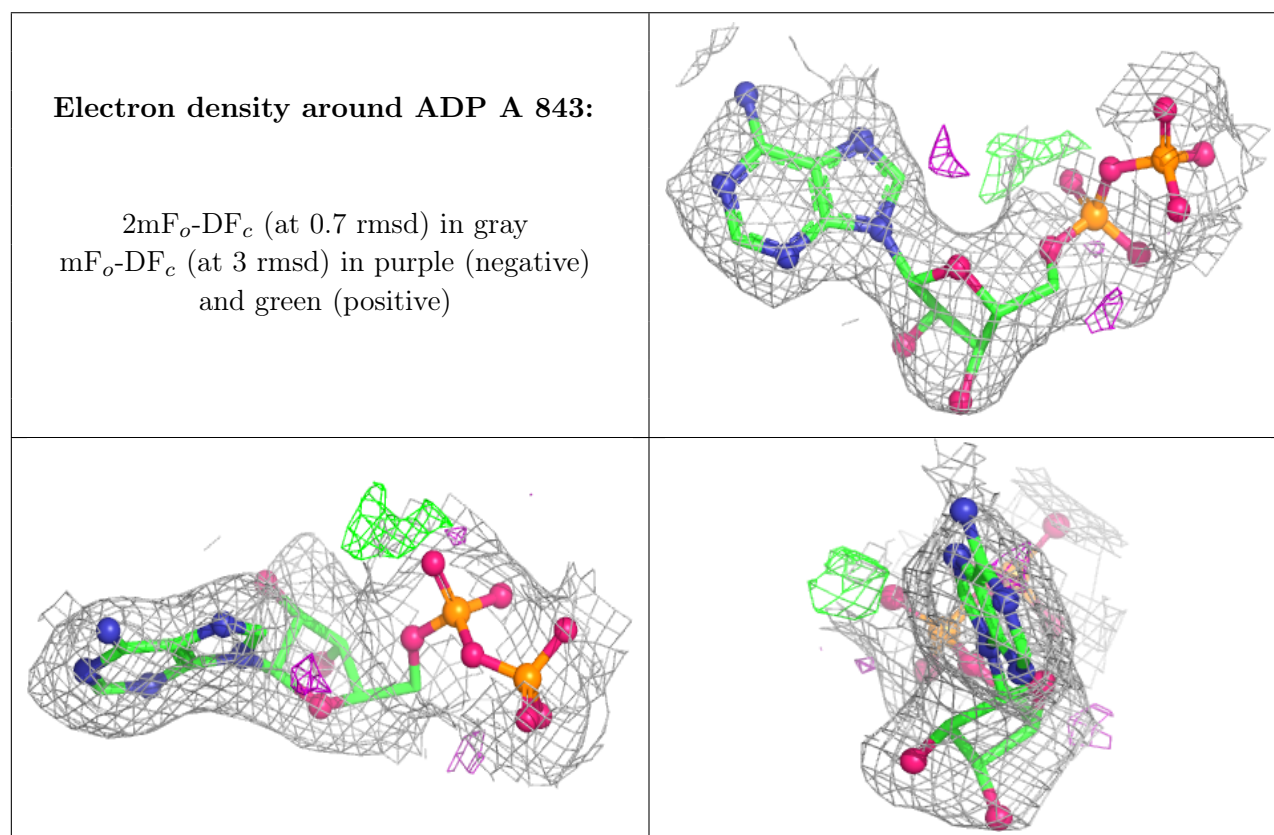
There are no oligosaccharides in this entry.

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
2	MG	A	842	1/1	0.89	0.11	41,41,41,41	0
3	ADP	A	843	27/27	0.90	0.10	65,69,74,75	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.