



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 12, 2021 – 11:03 am BST

PDB ID : 7NPE
Title : Vibrio cholerae ParA2-ADP
Authors : Parker, A.V.; Bergeron, J.R.C.
Deposited on : 2021-02-26
Resolution : 3.18 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
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)	:	2.22

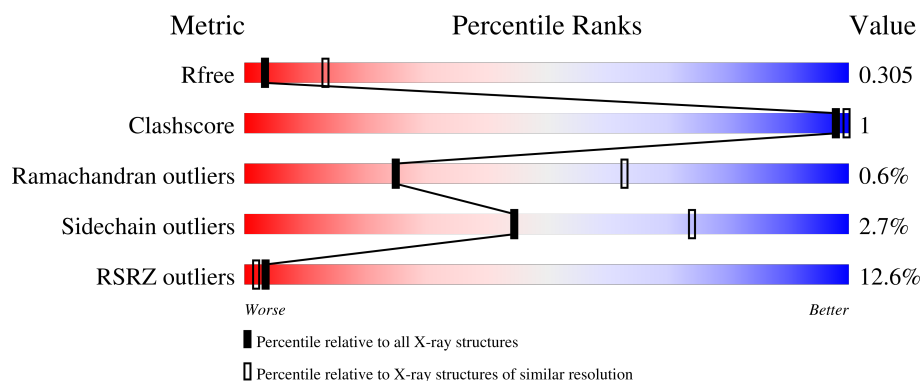
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	407	<div> <div>11%</div> <div>90%</div> <div>8%</div> </div>
1	B	407	<div> <div>11%</div> <div>93%</div> <div>5%</div> </div>
1	C	407	<div> <div>14%</div> <div>92%</div> <div>6%</div> </div>
1	D	407	<div> <div>13%</div> <div>93%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	501	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23125 atoms, of which 11064 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.

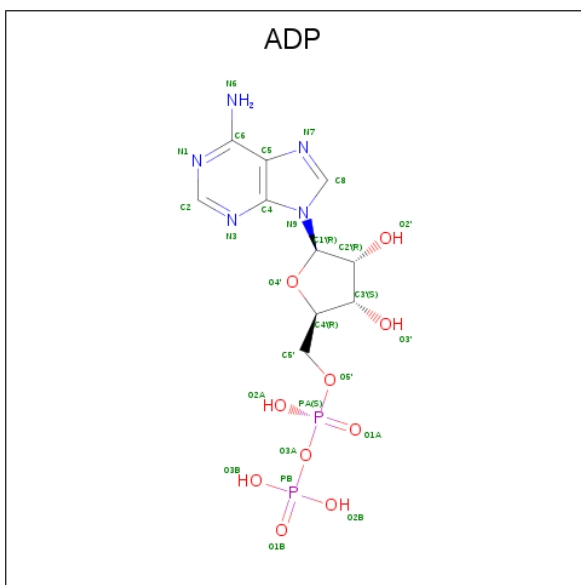
- Molecule 1 is a protein called AAA family ATPase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	397	Total	C	H	N	O	S	0	2	0
			5855	1915	2831	509	580	20			
1	B	402	Total	C	H	N	O	S	0	2	0
			5865	1913	2836	512	584	20			
1	C	400	Total	C	H	N	O	S	0	2	0
			5579	1855	2652	483	570	19			
1	D	402	Total	C	H	N	O	S	0	2	0
			5638	1870	2681	496	574	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A085S0Z4
A	2	ALA	-	expression tag	UNP A0A085S0Z4
B	1	MET	-	initiating methionine	UNP A0A085S0Z4
B	2	ALA	-	expression tag	UNP A0A085S0Z4
C	1	MET	-	initiating methionine	UNP A0A085S0Z4
C	2	ALA	-	expression tag	UNP A0A085S0Z4
D	1	MET	-	initiating methionine	UNP A0A085S0Z4
D	2	ALA	-	expression tag	UNP A0A085S0Z4

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0
2	B	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0
2	C	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0
2	D	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

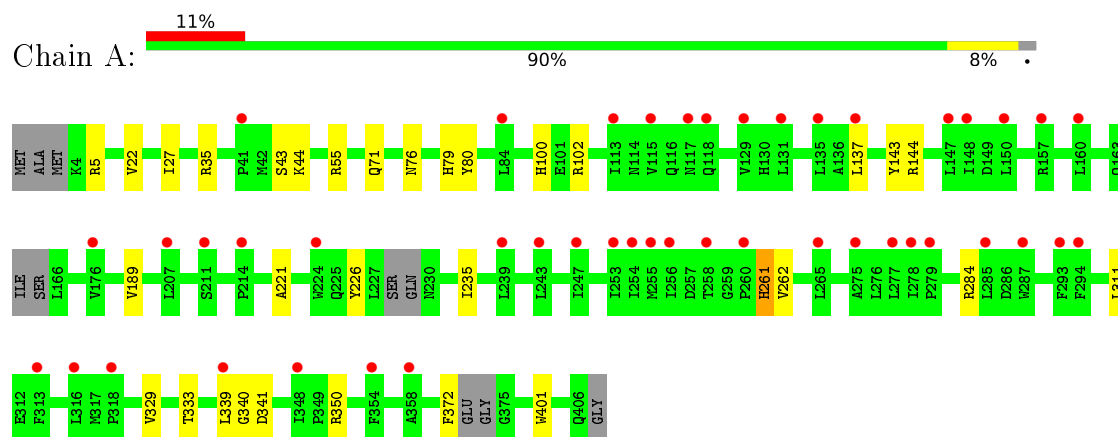


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		

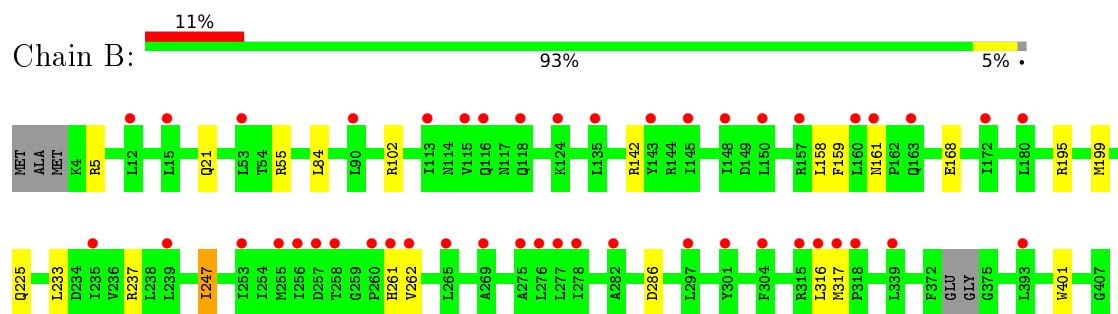
3 Residue-property plots [i](#)

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.

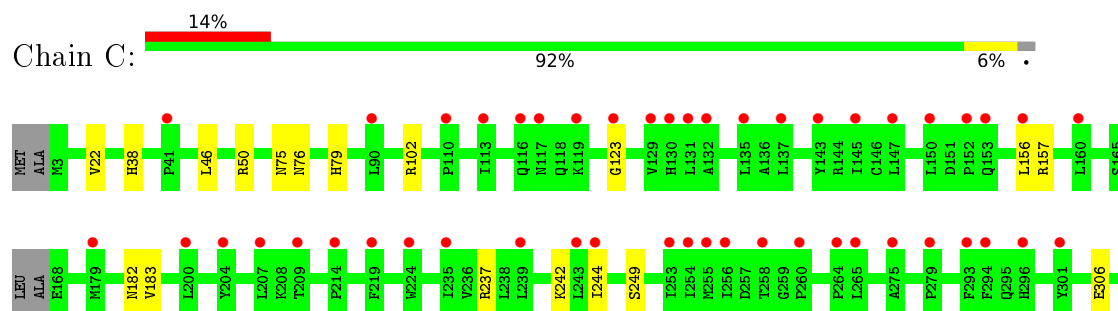
• Molecule 1: AAA family ATPase

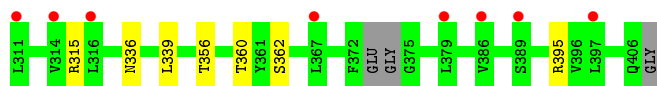


• Molecule 1: AAA family ATPase

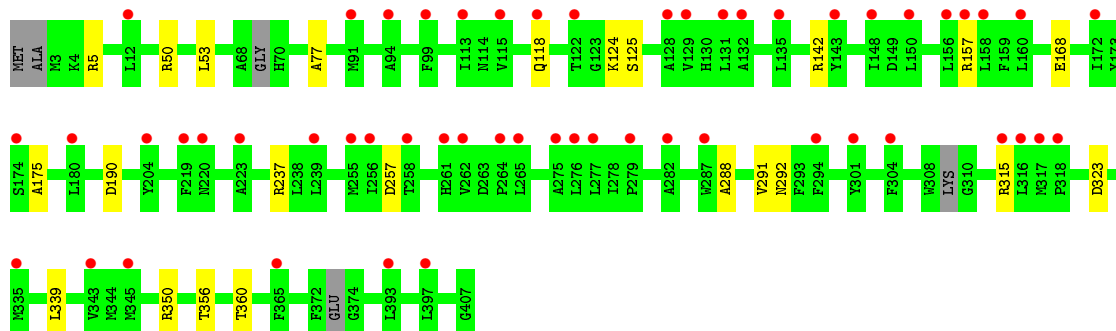


• Molecule 1: AAA family ATPase





- Molecule 1: AAA family ATPase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	199.21Å 199.21Å 260.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.59 – 3.18 172.52 – 3.18	Depositor EDS
% Data completeness (in resolution range)	96.4 (52.59-3.18) 96.5 (172.52-3.18)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.15.2	Depositor
R, R_{free}	0.262 , 0.308 0.261 , 0.305	Depositor DCC
R_{free} test set	2457 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	134.1	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 110.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23125	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.18% 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: ADP, GOL, MG

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	0.68	0/3091	1.08	7/4216 (0.2%)
1	B	0.61	0/3094	0.98	5/4225 (0.1%)
1	C	0.67	0/2991	1.03	4/4099 (0.1%)
1	D	0.68	0/3021	1.04	7/4135 (0.2%)
All	All	0.66	0/12197	1.03	23/16675 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	2
All	All	0	5

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	D	5	ARG	NE-CZ-NH2	8.15	124.37	120.30
1	A	350	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	B	195	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	B	55	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	D	350	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	5	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	C	315	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	D	157	ARG	NE-CZ-NH1	6.65	123.63	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	A	102	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	B	142	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	55	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	102	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	D	237	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	237	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	315	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	5	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	395	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	50	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	D	50	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	284	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	144	ARG	CD-NE-CZ	5.03	130.64	123.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	TYR	Sidechain
1	A	35	ARG	Sidechain
1	B	5	ARG	Sidechain
1	C	102	ARG	Sidechain
1	C	157	ARG	Sidechain

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	3024	2831	2821	9	40
1	B	3029	2836	2827	5	0
1	C	2927	2652	2642	4	40
1	D	2957	2681	2670	4	0
2	A	27	12	12	0	0
2	B	27	12	12	0	0
2	C	27	12	12	0	0
2	D	27	12	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	8	8	0	0
4	B	6	8	8	0	0
All	All	12061	11064	11024	17	40

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 1.

All (17) 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:D:125:SER:N	2:D:450:ADP:O1B	2.20	0.69
1:B:199:MET:SD	1:B:247:ILE:HD11	2.39	0.62
1:C:356:THR:O	1:C:360:THR:HG22	2.01	0.60
1:A:333:THR:HG21	1:C:336:ASN:HB3	1.91	0.53
1:A:221:ALA:HB2	1:B:262:VAL:CG1	2.42	0.49
1:A:221:ALA:HB2	1:B:262:VAL:HG13	1.95	0.48
1:A:329:VAL:O	1:A:333:THR:HG23	2.17	0.45
1:B:316:LEU:HD23	1:B:317:MET:N	2.34	0.43
1:C:360:THR:HG23	1:C:362:SER:OG	2.19	0.42
1:A:44:LYS:HE3	1:A:80:TYR:CE2	2.55	0.42
1:A:340:GLY:H	1:A:341:ASP:HA	1.84	0.42
1:C:22:VAL:HB	1:D:291:VAL:HG21	2.03	0.41
1:D:356:THR:O	1:D:360:THR:HG22	2.20	0.41
1:A:27:ILE:H	1:A:27:ILE:HD12	1.85	0.41
1:A:226:TYR:CE2	1:A:235:ILE:HD11	2.55	0.41
1:A:261:HIS:CE1	1:B:261:HIS:HE2	2.39	0.40
1:D:288:ALA:O	1:D:291:VAL:HG22	2.22	0.40

All (40) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:HIS:CD2	1:C:79:HIS:CD2[12_565]	0.42	1.78
1:A:79:HIS:NE2	1:C:79:HIS:NE2[12_565]	0.43	1.77
1:A:79:HIS:CE1	1:C:79:HIS:HE2[12_565]	0.19	1.41
1:A:79:HIS:HE2	1:C:79:HIS:CE1[12_565]	0.30	1.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:HIS:HD2	1:C:79:HIS:CG[12_565]	0.30	1.30
1:A:79:HIS:NE2	1:C:79:HIS:CE1[12_565]	0.93	1.27
1:A:79:HIS:CG	1:C:79:HIS:CD2[12_565]	0.96	1.24
1:A:79:HIS:CG	1:C:79:HIS:HD2[12_565]	0.38	1.22
1:A:79:HIS:CE1	1:C:79:HIS:NE2[12_565]	1.02	1.18
1:A:79:HIS:CD2	1:C:79:HIS:CG[12_565]	1.07	1.13
1:A:79:HIS:CD2	1:C:79:HIS:NE2[12_565]	1.32	0.88
1:A:76:ASN:HD21	1:C:46:LEU:HD22[12_565]	0.77	0.83
1:A:79:HIS:HE2	1:C:79:HIS:HE1[12_565]	0.85	0.75
1:A:79:HIS:NE2	1:C:79:HIS:CD2[12_565]	1.54	0.66
1:A:79:HIS:HE1	1:C:79:HIS:HE2[12_565]	1.05	0.55
1:A:76:ASN:HD22	1:C:46:LEU:HB2[12_565]	1.06	0.54
1:A:79:HIS:CB	1:C:79:HIS:HD2[12_565]	1.18	0.42
1:A:79:HIS:ND1	1:C:79:HIS:NE2[12_565]	1.79	0.41
1:A:43:SER:HB3	1:C:75:ASN:HD22[12_565]	1.24	0.36
1:A:79:HIS:NE2	1:C:79:HIS:ND1[12_565]	1.85	0.35
1:A:79:HIS:CD2	1:C:79:HIS:ND1[12_565]	1.87	0.33
1:A:76:ASN:HD21	1:C:46:LEU:CD2[12_565]	1.28	0.32
1:A:79:HIS:CG	1:C:79:HIS:NE2[12_565]	1.88	0.32
1:A:79:HIS:NE2	1:C:79:HIS:HE2[12_565]	1.30	0.30
1:A:79:HIS:ND1	1:C:79:HIS:CD2[12_565]	1.91	0.29
1:A:79:HIS:CD2	1:C:79:HIS:CE1[12_565]	1.93	0.27
1:A:79:HIS:HD2	1:C:79:HIS:CD2[12_565]	1.37	0.23
1:A:79:HIS:HD2	1:C:79:HIS:CB[12_565]	1.39	0.21
1:A:43:SER:N	1:C:75:ASN:OD1[12_565]	2.00	0.20
1:A:79:HIS:HE2	1:C:79:HIS:NE2[12_565]	1.42	0.18
1:A:71:GLN:OE1	1:C:38:HIS:H[12_565]	1.46	0.14
1:A:79:HIS:CD2	1:C:79:HIS:HD2[12_565]	1.46	0.14
1:A:79:HIS:ND1	1:C:79:HIS:HE2[12_565]	1.47	0.13
1:A:79:HIS:NE2	1:C:79:HIS:CG[12_565]	2.07	0.13
1:A:79:HIS:CE1	1:C:79:HIS:CD2[12_565]	2.09	0.11
1:A:76:ASN:ND2	1:C:46:LEU:HD22[12_565]	1.54	0.06
1:A:79:HIS:CE1	1:C:79:HIS:CE1[12_565]	2.14	0.06
1:A:79:HIS:HE2	1:C:79:HIS:ND1[12_565]	1.59	0.01
1:A:79:HIS:CB	1:C:79:HIS:CD2[12_565]	2.19	0.01
1:A:79:HIS:HD2	1:C:79:HIS:ND1[12_565]	1.60	0.00

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/407 (96%)	374 (96%)	16 (4%)	1 (0%)	41	73
1	B	400/407 (98%)	370 (92%)	28 (7%)	2 (0%)	29	66
1	C	396/407 (97%)	368 (93%)	25 (6%)	3 (1%)	19	56
1	D	396/407 (97%)	362 (91%)	30 (8%)	4 (1%)	15	52
All	All	1583/1628 (97%)	1474 (93%)	99 (6%)	10 (1%)	25	63

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	306	GLU
1	C	123	GLY
1	C	249	SER
1	B	161	ASN
1	D	77	ALA
1	D	168	GLU
1	D	175	ALA
1	B	233	LEU
1	D	257	ASP
1	A	189	VAL

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	311/358 (87%)	302 (97%)	9 (3%)	42	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	311/358 (87%)	302 (97%)	9 (3%)	42	72
1	C	288/358 (80%)	281 (98%)	7 (2%)	49	76
1	D	290/358 (81%)	283 (98%)	7 (2%)	49	76
All	All	1200/1432 (84%)	1168 (97%)	32 (3%)	44	74

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	100	HIS
1	A	137	LEU
1	A	261	HIS
1	A	262	VAL
1	A	311	LEU
1	A	339	LEU
1	A	372	PHE
1	A	401	TRP
1	B	21	GLN
1	B	84	LEU
1	B	158	LEU
1	B	159	PHE
1	B	168	GLU
1	B	225	GLN
1	B	247	ILE
1	B	286	ASP
1	B	401	TRP
1	C	76	ASN
1	C	156	LEU
1	C	182	ASN
1	C	183	VAL
1	C	242	LYS
1	C	244	ILE
1	C	339	LEU
1	D	53	LEU
1	D	118	GLN
1	D	124	LYS
1	D	190	ASP
1	D	292	ASN
1	D	323	ASP
1	D	339	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	292	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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$
2	ADP	D	450	3	24,29,29	1.28	4 (16%)	29,45,45	1.69	6 (20%)
4	GOL	A	501	-	5,5,5	0.61	0	5,5,5	0.61	0
2	ADP	A	450	3	24,29,29	1.25	4 (16%)	29,45,45	1.59	6 (20%)
4	GOL	B	500	-	5,5,5	0.57	0	5,5,5	0.08	0
2	ADP	B	450	3	24,29,29	1.23	3 (12%)	29,45,45	1.64	5 (17%)
2	ADP	C	450	3	24,29,29	1.35	4 (16%)	29,45,45	1.54	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	D	450	3	-	1/12/32/32	0/3/3/3
4	GOL	A	501	-	-	0/4/4/4	-
2	ADP	A	450	3	-	1/12/32/32	0/3/3/3
4	GOL	B	500	-	-	0/4/4/4	-
2	ADP	B	450	3	-	1/12/32/32	0/3/3/3
2	ADP	C	450	3	-	0/12/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	450	ADP	C5-C4	-2.67	1.33	1.40
2	C	450	ADP	PB-O3B	-2.49	1.45	1.54
2	B	450	ADP	C5-C4	-2.46	1.34	1.40
2	A	450	ADP	C5-C4	-2.42	1.34	1.40
2	D	450	ADP	O4'-C1'	2.38	1.44	1.41
2	C	450	ADP	PB-O2B	-2.37	1.45	1.54
2	A	450	ADP	C4-N3	-2.29	1.32	1.35
2	B	450	ADP	PB-O3B	-2.25	1.46	1.54
2	D	450	ADP	PB-O3B	-2.24	1.46	1.54
2	A	450	ADP	PB-O2B	-2.18	1.46	1.54
2	D	450	ADP	C5-C4	-2.17	1.35	1.40
2	C	450	ADP	O4'-C1'	2.15	1.44	1.41
2	D	450	ADP	PB-O2B	-2.14	1.46	1.54
2	A	450	ADP	PB-O3B	-2.13	1.46	1.54
2	B	450	ADP	PB-O2B	-2.11	1.46	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	450	ADP	C4-C5-N7	5.18	114.80	109.40
2	B	450	ADP	C4-C5-N7	4.72	114.31	109.40
2	A	450	ADP	C4-C5-N7	4.63	114.22	109.40
2	B	450	ADP	PA-O3A-PB	-3.84	119.66	132.83
2	D	450	ADP	PA-O3A-PB	-3.80	119.80	132.83
2	C	450	ADP	C4-C5-N7	3.65	113.20	109.40
2	A	450	ADP	PA-O3A-PB	-3.33	121.40	132.83
2	C	450	ADP	O2B-PB-O3A	3.07	114.92	104.64
2	C	450	ADP	O3B-PB-O2B	-2.95	96.38	107.64
2	C	450	ADP	O3B-PB-O3A	2.94	114.49	104.64
2	C	450	ADP	PA-O3A-PB	-2.80	123.22	132.83
2	D	450	ADP	O2B-PB-O3A	2.72	113.76	104.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	450	ADP	O2B-PB-O3A	2.72	113.75	104.64
2	B	450	ADP	O3B-PB-O3A	2.66	113.55	104.64
2	A	450	ADP	O3B-PB-O2B	-2.66	97.49	107.64
2	A	450	ADP	O3B-PB-O3A	2.62	113.44	104.64
2	B	450	ADP	O3B-PB-O1B	-2.57	100.63	110.68
2	D	450	ADP	O2B-PB-O1B	-2.48	100.98	110.68
2	D	450	ADP	O3B-PB-O3A	2.27	112.25	104.64
2	A	450	ADP	C2-N1-C6	-2.05	115.25	118.75
2	A	450	ADP	N6-C6-N1	-2.03	114.37	118.57
2	D	450	ADP	N6-C6-N1	-2.00	114.42	118.57

There are no chirality outliers.

All (3) torsion outliers are listed below:

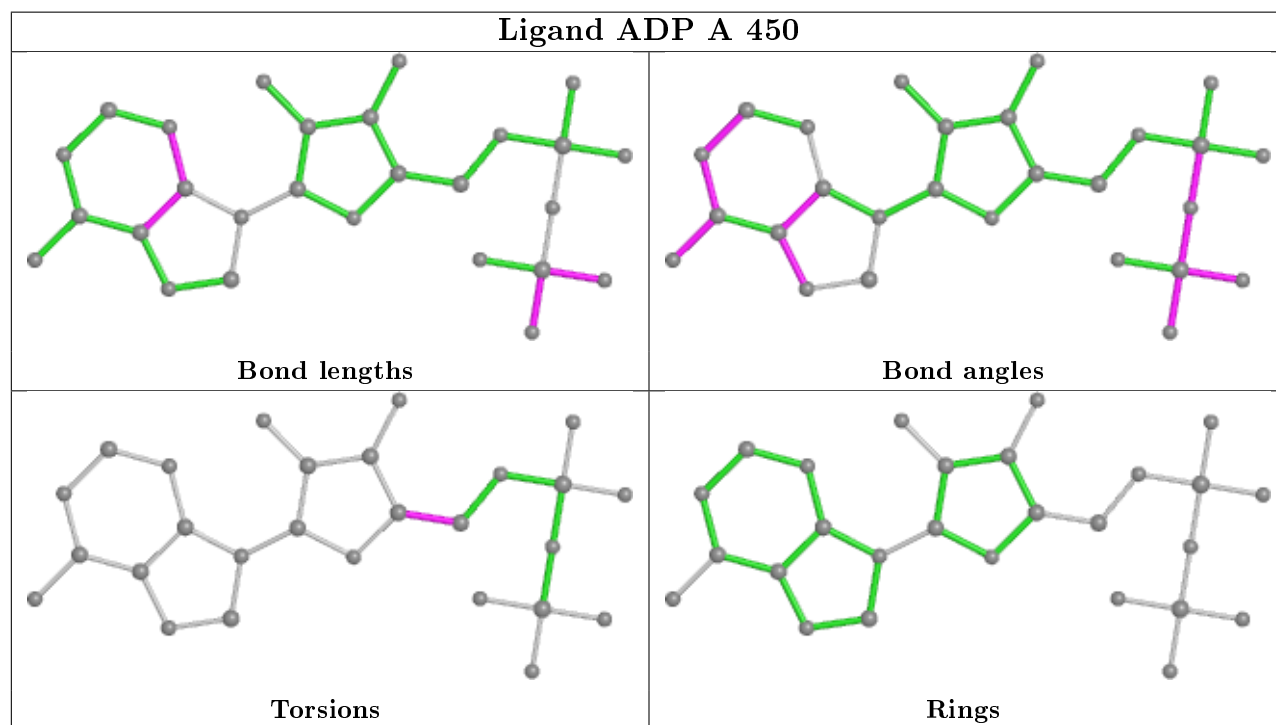
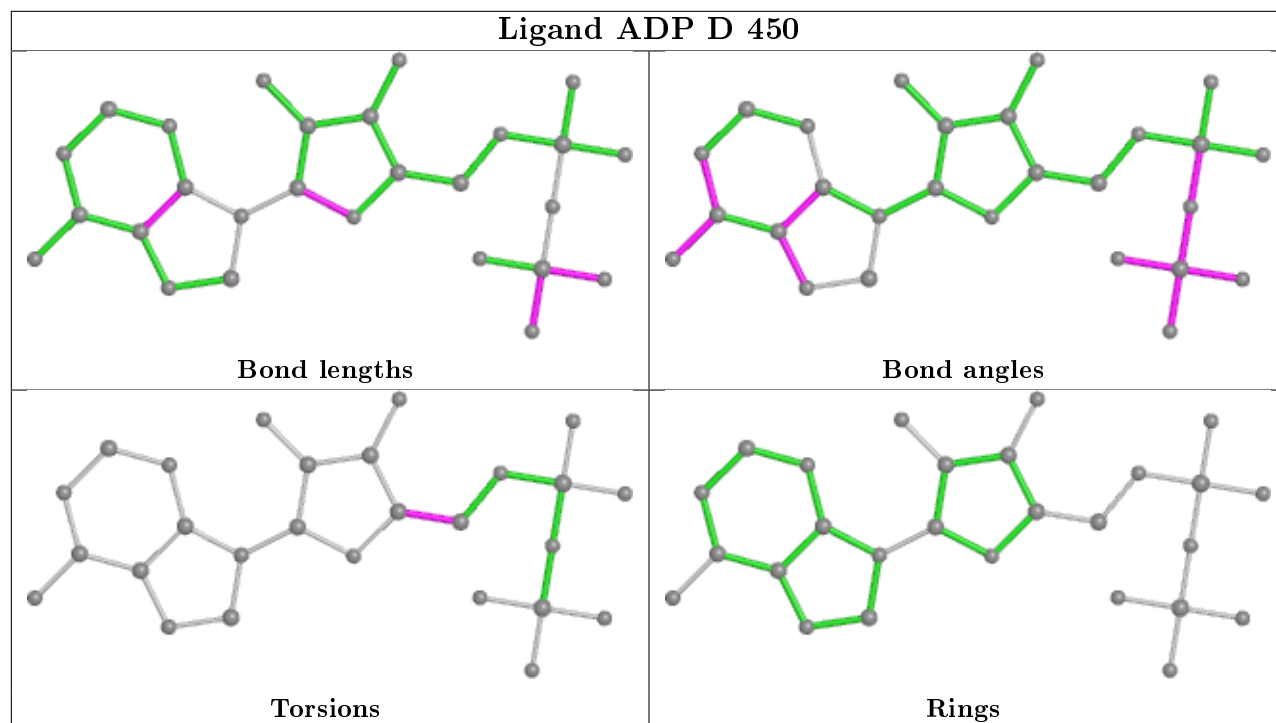
Mol	Chain	Res	Type	Atoms
2	A	450	ADP	O4'-C4'-C5'-O5'
2	B	450	ADP	O4'-C4'-C5'-O5'
2	D	450	ADP	O4'-C4'-C5'-O5'

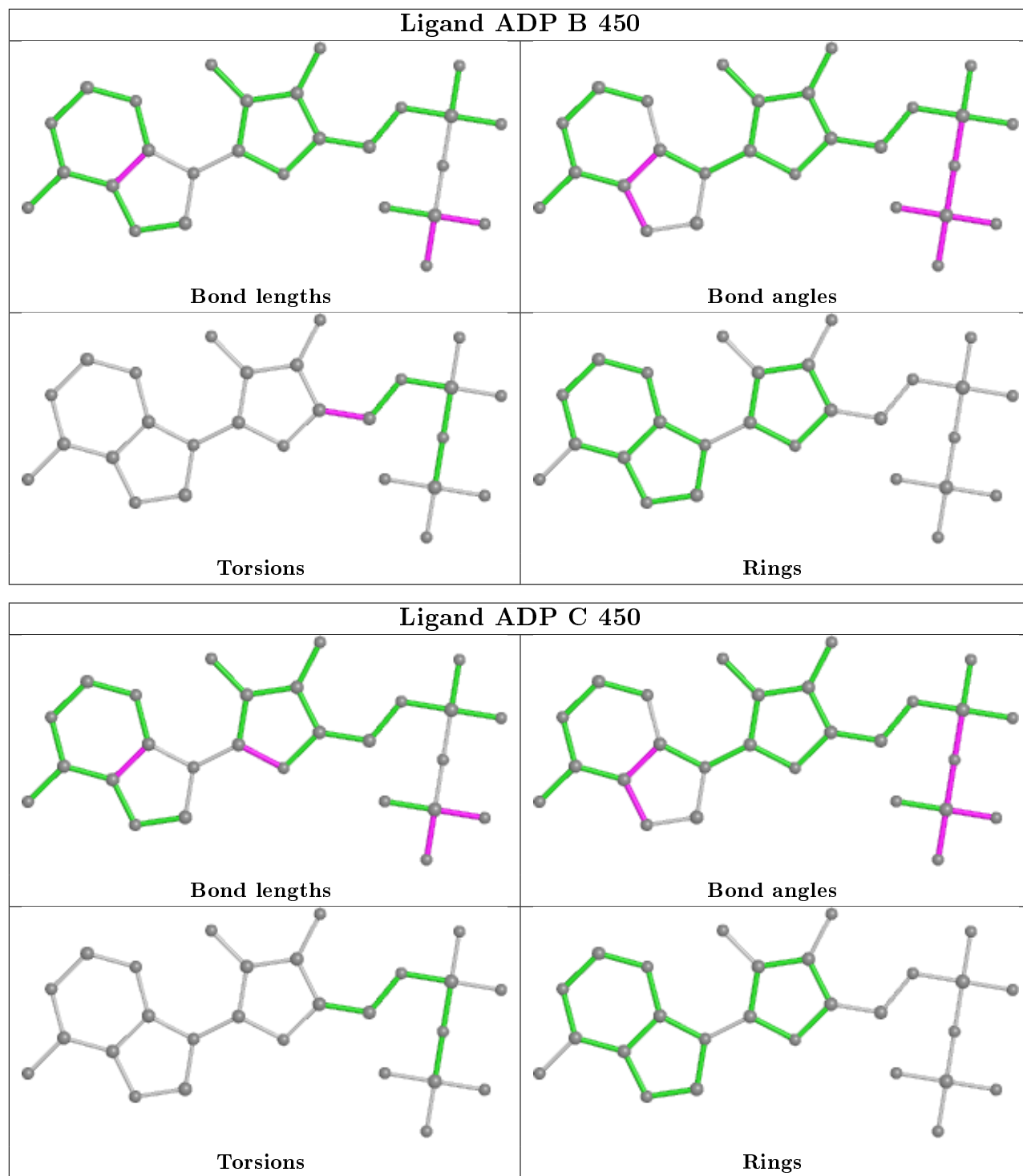
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	450	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 ⓘ

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, 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	397/407 (97%)	0.64	45 (11%) 5 3	72, 116, 171, 200	0
1	B	402/407 (98%)	0.60	46 (11%) 5 2	74, 113, 177, 206	0
1	C	400/407 (98%)	0.65	56 (14%) 2 1	76, 126, 177, 222	0
1	D	402/407 (98%)	0.64	54 (13%) 3 2	87, 126, 183, 253	0
All	All	1601/1628 (98%)	0.63	201 (12%) 3 2	72, 120, 177, 253	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	174	SER	8.7
1	D	316	LEU	6.1
1	B	150	LEU	5.0
1	D	255	MET	4.8
1	A	150	LEU	4.6
1	D	118	GLN	4.6
1	C	254	ILE	4.5
1	A	224	TRP	4.4
1	C	207	LEU	4.3
1	A	207	LEU	4.2
1	D	277	LEU	4.2
1	D	279	PRO	4.1
1	A	118	GLN	3.9
1	D	256	ILE	3.9
1	A	113	ILE	3.9
1	B	258	THR	3.8
1	B	301	TYR	3.7
1	C	256	ILE	3.7
1	D	301	TYR	3.7
1	D	122	THR	3.7
1	C	150	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	172	ILE	3.6
1	C	311	LEU	3.6
1	B	143	TYR	3.6
1	B	282	ALA	3.5
1	B	115	VAL	3.5
1	C	224	TRP	3.4
1	D	135	LEU	3.3
1	C	113	ILE	3.3
1	A	160	LEU	3.3
1	B	262	VAL	3.3
1	A	214	PRO	3.2
1	A	84	LEU	3.2
1	D	113	ILE	3.2
1	B	277	LEU	3.1
1	B	124	LYS	3.1
1	D	143	TYR	3.1
1	C	258	THR	3.1
1	C	253	ILE	3.1
1	C	243	LEU	3.1
1	C	219	PHE	3.0
1	B	276	LEU	3.0
1	A	254	ILE	3.0
1	D	129	VAL	3.0
1	A	287	TRP	3.0
1	C	294	PHE	3.0
1	B	118	GLN	3.0
1	A	258	THR	3.0
1	D	317	MET	3.0
1	C	293	PHE	2.9
1	D	156	LEU	2.9
1	D	345	MET	2.9
1	A	243	LEU	2.9
1	D	91	MET	2.9
1	D	276	LEU	2.9
1	D	393	LEU	2.9
1	A	275	ALA	2.9
1	B	253	ILE	2.9
1	C	264	PRO	2.8
1	D	148	ILE	2.8
1	D	131	LEU	2.8
1	D	335	MET	2.8
1	C	301	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	158	LEU	2.8
1	C	296	HIS	2.8
1	B	113	ILE	2.8
1	A	255	MET	2.8
1	C	239	LEU	2.8
1	C	145	ILE	2.8
1	C	260	PRO	2.8
1	A	293	PHE	2.8
1	D	294	PHE	2.7
1	D	128	ALA	2.7
1	B	255	MET	2.7
1	C	147	LEU	2.7
1	B	256	ILE	2.7
1	A	256	ILE	2.7
1	B	275	ALA	2.7
1	A	147	LEU	2.7
1	D	282	ALA	2.7
1	C	137	LEU	2.7
1	C	179	MET	2.7
1	D	219	PHE	2.7
1	B	260	PRO	2.6
1	A	279	PRO	2.6
1	C	397	LEU	2.6
1	B	278	ILE	2.6
1	C	41	PRO	2.6
1	D	94	ALA	2.6
1	D	115	VAL	2.6
1	C	204	TYR	2.6
1	D	397	LEU	2.6
1	C	275	ALA	2.6
1	C	90	LEU	2.6
1	B	339	LEU	2.6
1	D	157	ARG	2.6
1	D	261	HIS	2.6
1	D	265	LEU	2.6
1	B	304	PHE	2.5
1	A	316	LEU	2.5
1	C	135	LEU	2.5
1	A	278	ILE	2.5
1	C	110	PRO	2.5
1	C	153	GLN	2.5
1	A	239	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	116	GLN	2.5
1	C	160	LEU	2.5
1	C	117	ASN	2.5
1	B	148	ILE	2.5
1	D	220	ASN	2.4
1	B	269	ALA	2.4
1	A	247	ILE	2.4
1	C	152	PRO	2.4
1	D	315	ARG	2.4
1	A	115	VAL	2.4
1	B	316	LEU	2.4
1	D	239	LEU	2.4
1	B	261	HIS	2.4
1	D	287	TRP	2.4
1	B	315	ARG	2.4
1	A	137	LEU	2.4
1	C	255	MET	2.4
1	C	265	LEU	2.4
1	C	386	VAL	2.4
1	B	161	ASN	2.4
1	B	239	LEU	2.4
1	D	12	LEU	2.4
1	A	294	PHE	2.4
1	B	265	LEU	2.4
1	B	12	LEU	2.4
1	D	150	LEU	2.4
1	D	262	VAL	2.3
1	A	277	LEU	2.3
1	D	318	PRO	2.3
1	A	129	VAL	2.3
1	B	172	ILE	2.3
1	D	365	PHE	2.3
1	A	117	ASN	2.3
1	B	163	GLN	2.3
1	A	354	PHE	2.3
1	A	318	PRO	2.3
1	B	317	MET	2.3
1	C	200	LEU	2.3
1	A	285	LEU	2.3
1	B	135	LEU	2.3
1	B	180	LEU	2.3
1	A	348	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	53	LEU	2.3
1	A	253	ILE	2.3
1	A	313	PHE	2.3
1	C	235	ILE	2.3
1	C	209	THR	2.2
1	B	145	ILE	2.2
1	C	316	LEU	2.2
1	A	260	PRO	2.2
1	C	367	LEU	2.2
1	C	129	VAL	2.2
1	C	123	GLY	2.2
1	B	157	ARG	2.2
1	C	132	ALA	2.2
1	D	304	PHE	2.2
1	C	379	LEU	2.2
1	D	264	PRO	2.2
1	D	343	VAL	2.2
1	B	15	LEU	2.1
1	C	116	GLN	2.1
1	C	314	VAL	2.1
1	A	339	LEU	2.1
1	C	130	HIS	2.1
1	C	389	SER	2.1
1	C	156	LEU	2.1
1	D	180	LEU	2.1
1	D	204	TYR	2.1
1	D	99	PHE	2.1
1	B	90	LEU	2.1
1	B	297	LEU	2.1
1	B	318	PRO	2.1
1	A	358	ALA	2.1
1	D	275	ALA	2.1
1	A	265	LEU	2.1
1	C	119	LYS	2.1
1	A	176	VAL	2.1
1	B	257	ASP	2.1
1	A	135	LEU	2.1
1	D	160	LEU	2.1
1	C	214	PRO	2.1
1	A	148	ILE	2.1
1	D	258	THR	2.1
1	A	131	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	41	PRO	2.0
1	B	235	ILE	2.0
1	A	211	SER	2.0
1	B	393	LEU	2.0
1	C	131	LEU	2.0
1	D	223	ALA	2.0
1	D	132	ALA	2.0
1	A	157	ARG	2.0
1	C	279	PRO	2.0
1	C	244	ILE	2.0
1	B	160	LEU	2.0
1	C	143	TYR	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
4	GOL	A	501	6/6	0.63	0.80	161,162,222,222	0
4	GOL	B	500	6/6	0.77	0.32	118,162,195,195	0
3	MG	D	451	1/1	0.80	0.12	74,74,74,74	0
3	MG	C	451	1/1	0.85	0.22	63,63,63,63	0
3	MG	A	451	1/1	0.88	0.10	56,56,56,56	0
2	ADP	D	450	27/27	0.92	0.20	73,76,76,76	0
2	ADP	B	450	27/27	0.93	0.21	67,75,75,75	0
3	MG	B	451	1/1	0.94	0.17	66,66,66,66	0
2	ADP	C	450	27/27	0.95	0.22	63,76,76,76	0
2	ADP	A	450	27/27	0.96	0.21	58,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.