wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:16 PM GMT

PDB ID	:	1EQ2
Title	:	THE CRYSTAL STRUCTURE OF ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE
Authors	:	Deacon, A.M.; Ni, Y.S.; Coleman Jr., W.G.; Ealick, S.E.
Deposited on	:	2000-03-31
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

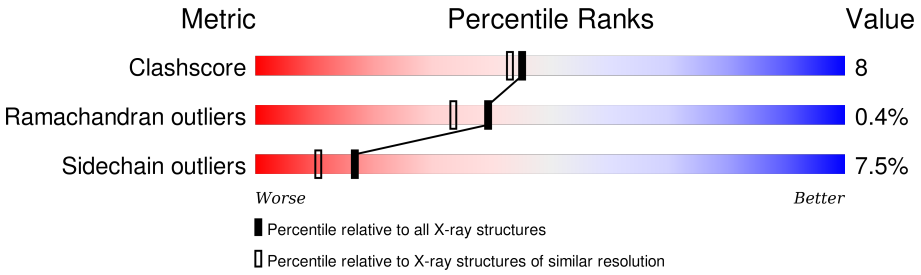
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	69% 16% • 12%
1	B	310	79% 15% • • •
1	C	310	69% 17% • 12%
1	D	310	77% 19% • •
1	E	310	76% 17% • •
1	F	310	75% 22% • •
1	G	310	83% 14% • •

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Mol	Chain	Length	Quality of chain
1	H	310	
1	I	310	
1	J	310	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAP	G	2406	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25435 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 ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2150	1375	349	417	9			
1	B	300	Total	C	N	O	S	0	0	0
			2386	1531	384	462	9			
1	C	272	Total	C	N	O	S	0	0	0
			2160	1385	348	418	9			
1	D	307	Total	C	N	O	S	0	0	0
			2442	1566	396	471	9			
1	E	300	Total	C	N	O	S	0	0	0
			2386	1531	384	462	9			
1	F	307	Total	C	N	O	S	0	0	0
			2442	1566	396	471	9			
1	G	307	Total	C	N	O	S	0	0	0
			2442	1566	396	471	9			
1	H	297	Total	C	N	O	S	0	0	0
			2360	1511	381	459	9			
1	I	307	Total	C	N	O	S	0	0	0
			2442	1566	396	471	9			
1	J	300	Total	C	N	O	S	0	0	0
			2386	1531	384	462	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
B	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
C	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
D	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
E	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
F	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
G	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
H	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
I	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910

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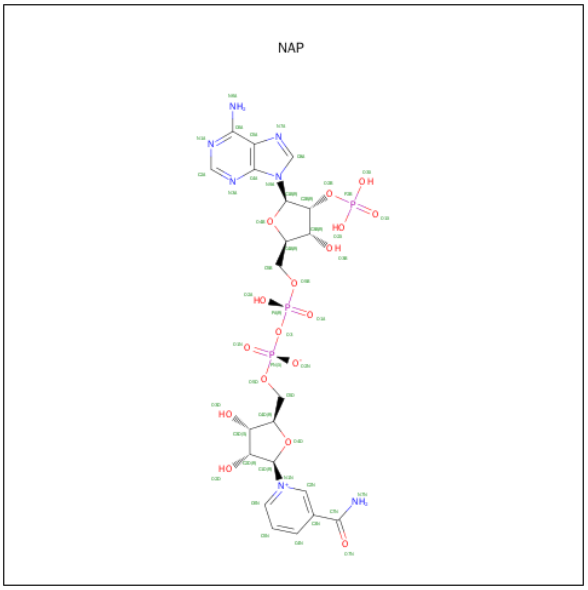
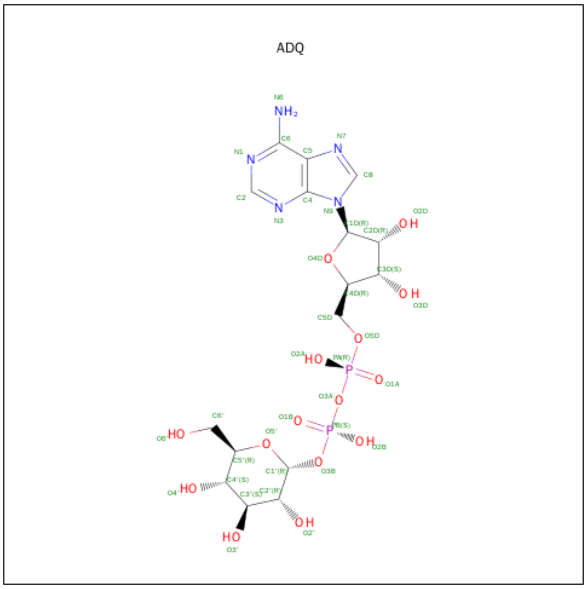
Chain	Residue	Modelled	Actual	Comment	Reference
J	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: ADQ) (formula: $C_{16}H_{25}N_5O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	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	70	Total O 70 70	0	0
4	B	119	Total O 119 119	0	0
4	C	82	Total O 82 82	0	0
4	D	118	Total O 118 118	0	0
4	E	105	Total O 105 105	0	0
4	F	106	Total O 106 106	0	0
4	G	118	Total O 118 118	0	0
4	H	114	Total O 114 114	0	0
4	I	123	Total O 123 123	0	0
4	J	101	Total O 101 101	0	0

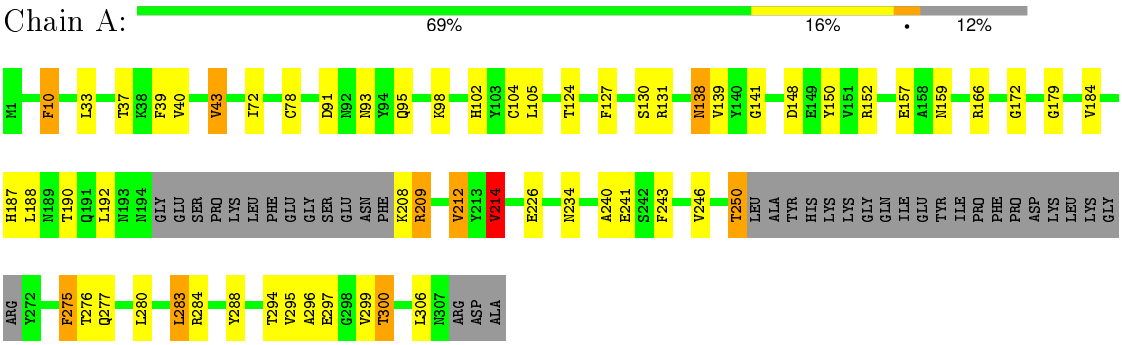
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

Note EDS was not executed.

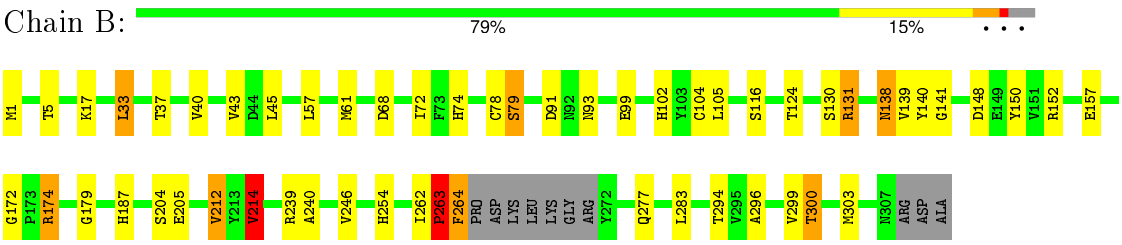
- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain A:



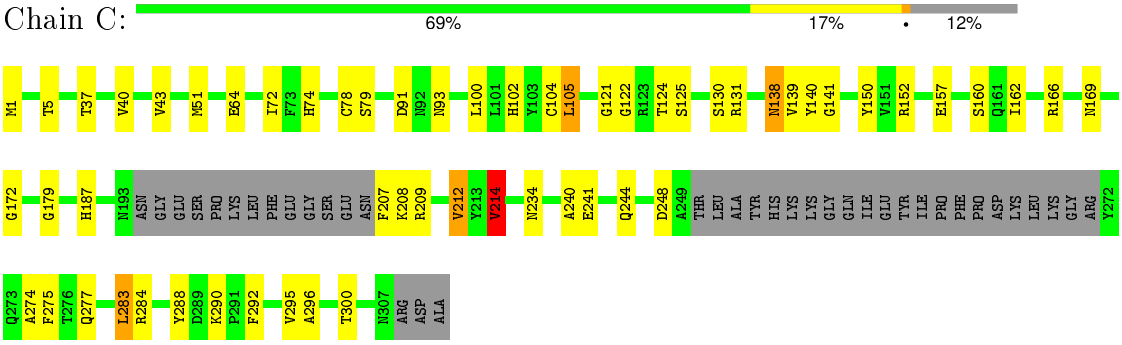
- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain B:



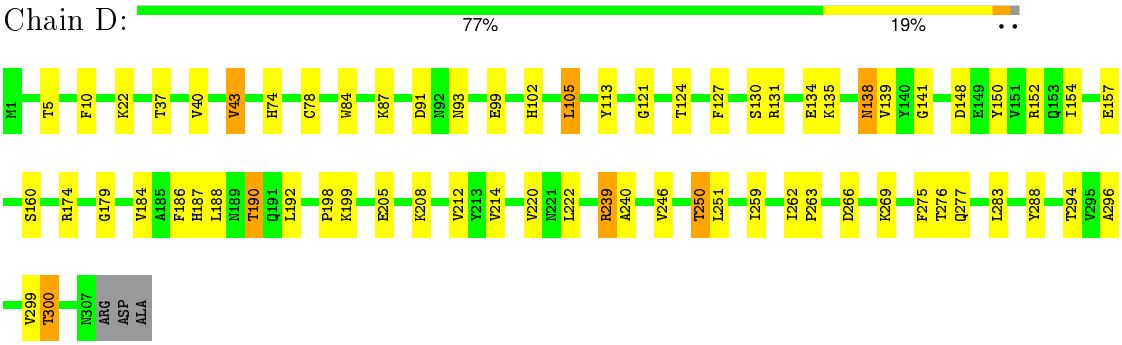
- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain C:



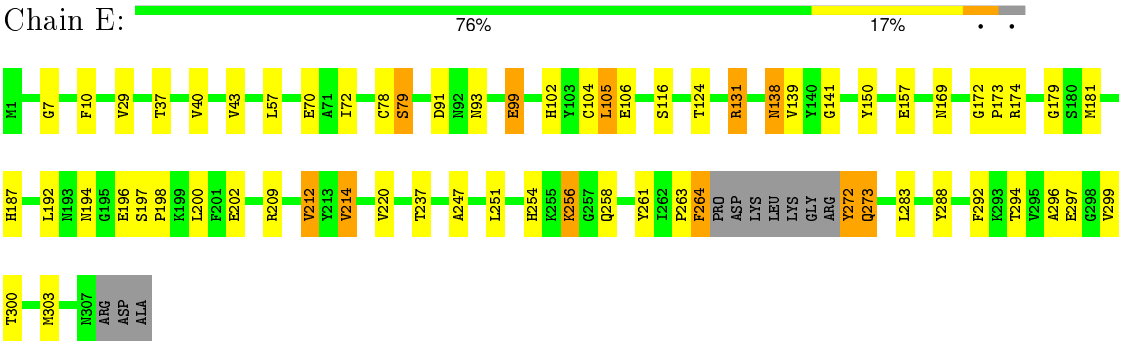
- Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain D:



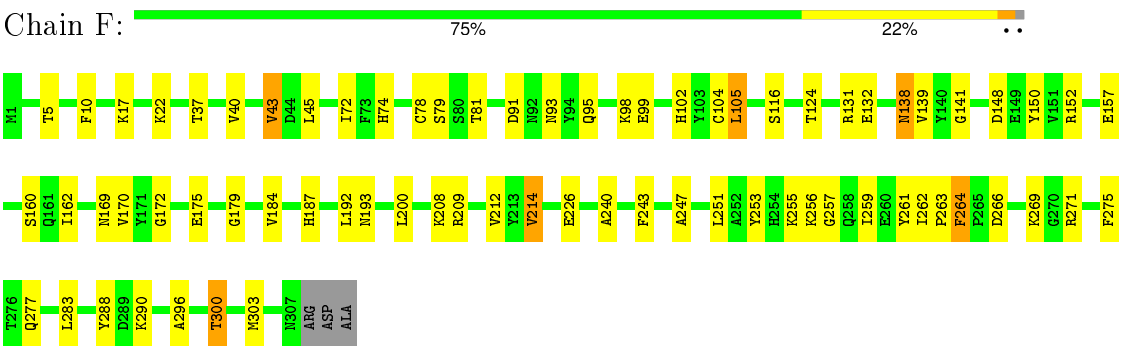
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain E:



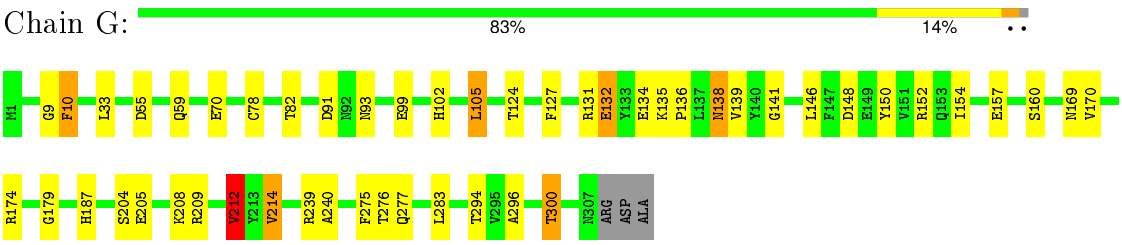
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain F:



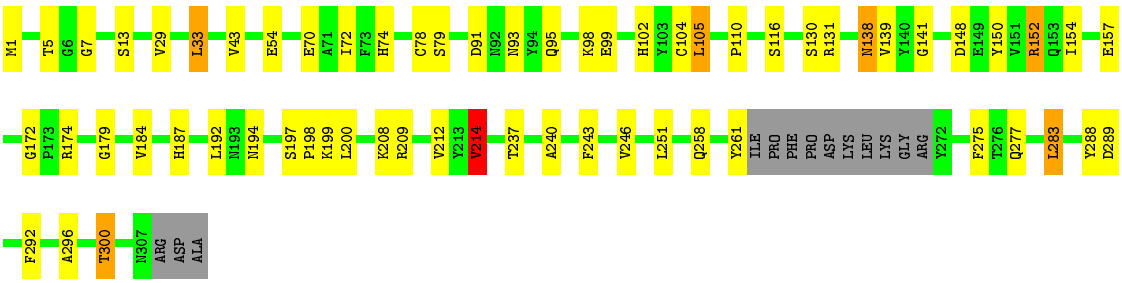
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain G:



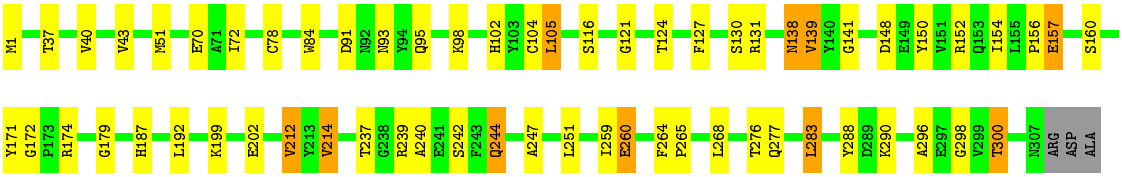
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain H:



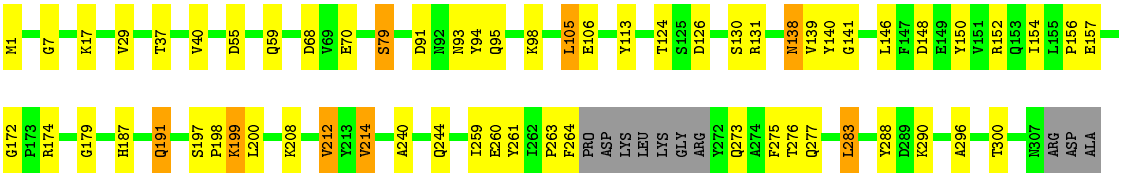
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain I:



• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain J:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.46Å 109.76Å 181.54Å 90.00° 91.04° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.3 (20.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.212 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25435	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, NAP, ADQ

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	0.59	0/2188	0.70	2/2958 (0.1%)
1	B	0.59	0/2434	0.73	4/3290 (0.1%)
1	C	0.63	0/2200	0.74	2/2973 (0.1%)
1	D	0.58	0/2492	0.74	0/3368
1	E	0.60	0/2434	0.74	2/3290 (0.1%)
1	F	0.59	0/2492	0.72	0/3368
1	G	0.59	0/2492	0.73	1/3368 (0.0%)
1	H	0.61	0/2406	0.73	2/3251 (0.1%)
1	I	0.60	0/2492	0.73	1/3368 (0.0%)
1	J	0.59	0/2434	0.73	2/3290 (0.1%)
All	All	0.60	0/24064	0.73	16/32524 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	205	GLU	N-CA-C	-5.76	95.45	111.00
1	J	212	VAL	CB-CA-C	-5.64	100.68	111.40
1	C	214	VAL	CB-CA-C	-5.64	100.68	111.40
1	A	212	VAL	CB-CA-C	-5.63	100.70	111.40
1	I	212	VAL	CB-CA-C	-5.62	100.73	111.40

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	2150	0	2045	36	0
1	B	2386	0	2272	29	0
1	C	2160	0	2056	30	0
1	D	2442	0	2337	39	0
1	E	2386	0	2272	35	0
1	F	2442	0	2337	42	0
1	G	2442	0	2337	38	0
1	H	2360	0	2245	36	0
1	I	2442	0	2337	34	0
1	J	2386	0	2271	34	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
2	E	48	0	25	1	0
2	F	48	0	25	1	0
2	G	48	0	25	1	0
2	H	48	0	25	1	0
2	I	48	0	25	1	0
2	J	48	0	25	0	0
3	A	27	0	12	3	0
3	B	38	0	23	2	0
3	C	27	0	12	2	0
3	D	38	0	23	0	0
3	E	27	0	12	3	0
3	F	38	0	23	3	0
3	G	27	0	12	0	0
3	H	27	0	12	1	0
3	I	27	0	12	3	0
3	J	27	0	12	0	0
4	A	70	0	0	4	0
4	B	119	0	0	5	0
4	C	82	0	0	5	0
4	D	118	0	0	4	0
4	E	105	0	0	2	0
4	F	106	0	0	6	0
4	G	118	0	0	3	0
4	H	114	0	0	4	0
4	I	123	0	0	6	0
4	J	101	0	0	7	0
All	All	25435	0	22912	368	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 8.

The worst 5 of 368 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)
3:A:2500:ADQ:H8	3:A:2500:ADQ:H5'1	1.30	1.13
3:F:2505:ADQ:H5'1	3:F:2505:ADQ:H8	1.39	1.04
3:I:2508:ADQ:H5'1	3:I:2508:ADQ:H8	1.41	1.01
3:C:2502:ADQ:H8	3:C:2502:ADQ:H5'1	1.40	1.00
1:F:296:ALA:O	1:F:300:THR:HG23	1.64	0.95

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	266/310 (86%)	254 (96%)	9 (3%)	3 (1%)	17 9
1	B	295/310 (95%)	284 (96%)	10 (3%)	1 (0%)	46 41
1	C	265/310 (86%)	251 (95%)	13 (5%)	1 (0%)	39 33
1	D	304/310 (98%)	292 (96%)	11 (4%)	1 (0%)	46 41
1	E	295/310 (95%)	284 (96%)	10 (3%)	1 (0%)	46 41
1	F	304/310 (98%)	290 (95%)	13 (4%)	1 (0%)	46 41
1	G	304/310 (98%)	291 (96%)	11 (4%)	2 (1%)	26 19
1	H	292/310 (94%)	282 (97%)	10 (3%)	0	100 100
1	I	304/310 (98%)	290 (95%)	14 (5%)	0	100 100
1	J	295/310 (95%)	280 (95%)	12 (4%)	3 (1%)	19 11
All	All	2924/3100 (94%)	2798 (96%)	113 (4%)	13 (0%)	39 33

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	PHE
1	B	263	PRO
1	F	264	PHE
1	J	263	PRO
1	J	259	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	222/256 (87%)	205 (92%)	17 (8%)	16 10
1	B	248/256 (97%)	226 (91%)	22 (9%)	12 7
1	C	224/256 (88%)	208 (93%)	16 (7%)	18 12
1	D	254/256 (99%)	235 (92%)	19 (8%)	17 11
1	E	248/256 (97%)	230 (93%)	18 (7%)	17 11
1	F	254/256 (99%)	235 (92%)	19 (8%)	17 11
1	G	254/256 (99%)	238 (94%)	16 (6%)	22 16
1	H	245/256 (96%)	227 (93%)	18 (7%)	17 11
1	I	254/256 (99%)	234 (92%)	20 (8%)	15 9
1	J	248/256 (97%)	229 (92%)	19 (8%)	16 10
All	All	2451/2560 (96%)	2267 (92%)	184 (8%)	17 11

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	139	VAL
1	F	157	GLU
1	J	124	THR
1	E	181	MET
1	F	79	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	95	GLN
1	G	138	ASN
1	J	169	ASN
1	F	102	HIS
1	F	254	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	A	78	1	3,6,7	0.52	0	1,6,8	2.01	1 (100%)
1	CSO	B	78	1	3,6,7	0.48	0	1,6,8	1.97	0
1	CSO	C	78	1	3,6,7	0.67	0	1,6,8	2.00	0
1	CSO	D	78	1	3,6,7	0.67	0	1,6,8	1.91	0
1	CSO	E	78	1	3,6,7	0.73	0	1,6,8	1.92	0
1	CSO	F	78	1	3,6,7	0.54	0	1,6,8	2.07	1 (100%)
1	CSO	G	78	1	3,6,7	0.67	0	1,6,8	1.79	0
1	CSO	H	78	1	3,6,7	0.59	0	1,6,8	2.25	1 (100%)
1	CSO	I	78	1	3,6,7	0.61	0	1,6,8	1.71	0
1	CSO	J	78	1	3,6,7	0.60	0	1,6,8	1.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	A	78	1	-	0/1/5/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	B	78	1	-	0/1/5/7	0/0/0/0
1	CSO	C	78	1	-	0/1/5/7	0/0/0/0
1	CSO	D	78	1	-	0/1/5/7	0/0/0/0
1	CSO	E	78	1	-	0/1/5/7	0/0/0/0
1	CSO	F	78	1	-	0/1/5/7	0/0/0/0
1	CSO	G	78	1	-	0/1/5/7	0/0/0/0
1	CSO	H	78	1	-	0/1/5/7	0/0/0/0
1	CSO	I	78	1	-	0/1/5/7	0/0/0/0
1	CSO	J	78	1	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	78	CSO	O-C-CA	-2.25	119.63	125.49
1	F	78	CSO	O-C-CA	-2.07	120.10	125.49
1	A	78	CSO	O-C-CA	-2.01	120.25	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	78	CSO	1	0
1	B	78	CSO	1	0
1	C	78	CSO	1	0
1	D	78	CSO	1	0
1	E	78	CSO	1	0
1	F	78	CSO	1	0
1	G	78	CSO	1	0
1	H	78	CSO	1	0
1	I	78	CSO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

20 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	$\#\|Z\| > 2$
2	NAP	A	2400	-	42,52,52	1.90	11 (26%)	54,80,80	2.00	10 (18%)
3	ADQ	A	2500	-	22,29,41	1.33	3 (13%)	27,45,63	2.55	3 (11%)
2	NAP	B	2401	-	42,52,52	1.72	9 (21%)	54,80,80	2.00	10 (18%)
3	ADQ	B	2501	-	33,41,41	1.40	5 (15%)	44,63,63	2.27	8 (18%)
2	NAP	C	2402	-	42,52,52	1.73	8 (19%)	54,80,80	2.04	10 (18%)
3	ADQ	C	2502	-	22,29,41	1.09	2 (9%)	27,45,63	2.53	2 (7%)
2	NAP	D	2403	-	42,52,52	1.82	10 (23%)	54,80,80	1.93	10 (18%)
3	ADQ	D	2503	-	33,41,41	1.52	4 (12%)	44,63,63	2.49	7 (15%)
2	NAP	E	2404	-	42,52,52	1.91	9 (21%)	54,80,80	1.97	12 (22%)
3	ADQ	E	2504	-	22,29,41	1.16	4 (18%)	27,45,63	2.58	3 (11%)
2	NAP	F	2405	-	42,52,52	1.80	10 (23%)	54,80,80	2.06	11 (20%)
3	ADQ	F	2505	-	33,41,41	1.50	6 (18%)	44,63,63	2.31	8 (18%)
2	NAP	G	2406	-	42,52,52	1.93	10 (23%)	54,80,80	1.97	13 (24%)
3	ADQ	G	2506	-	22,29,41	1.41	2 (9%)	27,45,63	2.48	2 (7%)
2	NAP	H	2407	-	42,52,52	1.78	9 (21%)	54,80,80	1.97	10 (18%)
3	ADQ	H	2507	-	22,29,41	1.41	3 (13%)	27,45,63	2.51	2 (7%)
2	NAP	I	2408	-	42,52,52	1.78	10 (23%)	54,80,80	1.97	10 (18%)
3	ADQ	I	2508	-	22,29,41	1.00	2 (9%)	27,45,63	2.49	2 (7%)
2	NAP	J	2409	-	42,52,52	1.94	10 (23%)	54,80,80	2.01	9 (16%)
3	ADQ	J	2509	-	22,29,41	1.27	3 (13%)	27,45,63	2.63	3 (11%)

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	NAP	A	2400	-	-	0/27/67/67	0/5/5/5
3	ADQ	A	2500	-	-	0/12/32/59	0/3/3/4
2	NAP	B	2401	-	-	0/27/67/67	0/5/5/5
3	ADQ	B	2501	-	-	0/19/59/59	0/4/4/4
2	NAP	C	2402	-	-	0/27/67/67	0/5/5/5
3	ADQ	C	2502	-	-	0/12/32/59	0/3/3/4
2	NAP	D	2403	-	-	0/27/67/67	0/5/5/5
3	ADQ	D	2503	-	-	0/19/59/59	0/4/4/4
2	NAP	E	2404	-	-	0/27/67/67	0/5/5/5
3	ADQ	E	2504	-	-	0/12/32/59	0/3/3/4
2	NAP	F	2405	-	-	0/27/67/67	0/5/5/5
3	ADQ	F	2505	-	-	0/19/59/59	0/4/4/4
2	NAP	G	2406	-	1/1/12/12	0/27/67/67	0/5/5/5
3	ADQ	G	2506	-	-	0/12/32/59	0/3/3/4
2	NAP	H	2407	-	-	0/27/67/67	0/5/5/5
3	ADQ	H	2507	-	-	0/12/32/59	0/3/3/4
2	NAP	I	2408	-	-	0/27/67/67	0/5/5/5
3	ADQ	I	2508	-	-	0/12/32/59	0/3/3/4
2	NAP	J	2409	-	-	0/27/67/67	0/5/5/5
3	ADQ	J	2509	-	-	0/12/32/59	0/3/3/4

The worst 5 of 130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2503	ADQ	PB-O3B	-4.94	1.47	1.60
3	F	2505	ADQ	PB-O3B	-4.03	1.49	1.60
3	B	2501	ADQ	PB-O3B	-3.58	1.50	1.60
2	D	2403	NAP	P2B-O3X	-2.77	1.44	1.54
2	I	2408	NAP	P2B-O3X	-2.62	1.45	1.54

The worst 5 of 145 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	2509	ADQ	N3-C2-N1	-12.66	119.20	128.89
3	F	2505	ADQ	N3-C2-N1	-12.57	119.27	128.89
3	E	2504	ADQ	N3-C2-N1	-12.43	119.38	128.89
3	B	2501	ADQ	N3-C2-N1	-12.30	119.47	128.89
3	D	2503	ADQ	N3-C2-N1	-12.30	119.48	128.89

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	2406	NAP	C4B

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2400	NAP	1	0
3	A	2500	ADQ	3	0
2	B	2401	NAP	1	0
3	B	2501	ADQ	2	0
3	C	2502	ADQ	2	0
2	E	2404	NAP	1	0
3	E	2504	ADQ	3	0
2	F	2405	NAP	1	0
3	F	2505	ADQ	3	0
2	G	2406	NAP	1	0
2	H	2407	NAP	1	0
3	H	2507	ADQ	1	0
2	I	2408	NAP	1	0
3	I	2508	ADQ	3	0

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.