wwPDB X-ray Structure Validation Summary Report (i)

Dec 23, 2021 – 06:17 pm GMT

PDB ID	:	7OP2
Title	:	Chadox1/ Chimpanzee adenovirus Y25 fiber knob protein
Authors	:	Rizkallah, P.J.; Baker, A.T.; Parker, A.L.; Teijeira Crespo, A.; Lipka-Lloyd, M.
Deposited on	:	2021-05-28
Resolution	:	1.59 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
https://www.wwpdb.org/validation/2017/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:

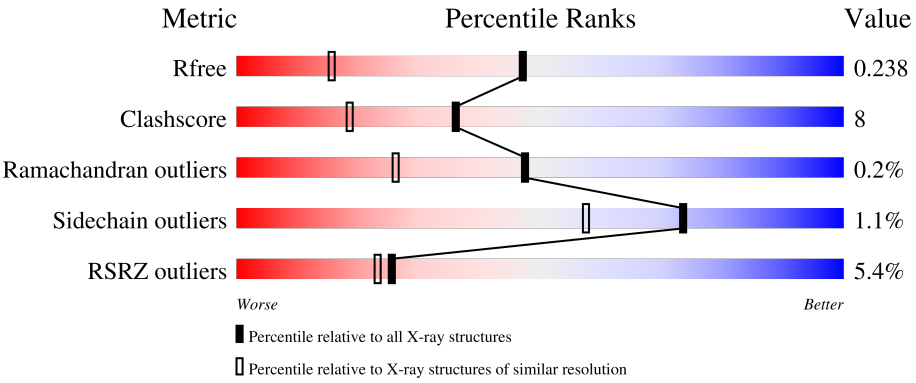
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 1.59 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	187	2% 88% 12%
1	B	187	6% 84% 12%
1	C	187	6% 86% 12%
1	D	187	2% 86% 14%
1	E	187	13% 80% 18%

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Mol	Chain	Length	Quality of chain
1	F	187	6% 86% 13%
1	G	187	% 84% 16%
1	H	187	7% 77% 20%
1	I	187	5% 88% 11%
1	J	187	4% 90% 10%
1	K	187	8% 79% 18%
1	L	187	3% 85% 11%

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	EDO	F	401	-	-	X	-
3	EDO	H	403	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18792 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 Fiber.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	5	0
			1487	939	242	296	10			
1	B	181	Total	C	N	O	S	0	5	0
			1427	903	228	285	11			
1	C	184	Total	C	N	O	S	0	4	0
			1448	916	231	290	11			
1	D	187	Total	C	N	O	S	0	3	0
			1470	932	233	293	12			
1	E	187	Total	C	N	O	S	0	6	0
			1493	942	240	299	12			
1	F	187	Total	C	N	O	S	0	3	0
			1468	927	236	294	11			
1	G	187	Total	C	N	O	S	0	6	0
			1488	941	237	298	12			
1	H	181	Total	C	N	O	S	0	4	0
			1423	902	227	282	12			
1	I	187	Total	C	N	O	S	0	2	0
			1457	921	232	293	11			
1	J	187	Total	C	N	O	S	0	2	0
			1460	922	235	293	10			
1	K	182	Total	C	N	O	S	0	6	0
			1452	921	232	289	10			
1	L	179	Total	C	N	O	S	0	4	0
			1409	892	225	281	11			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	D	2	Total	Ca	0	0
			2	2		

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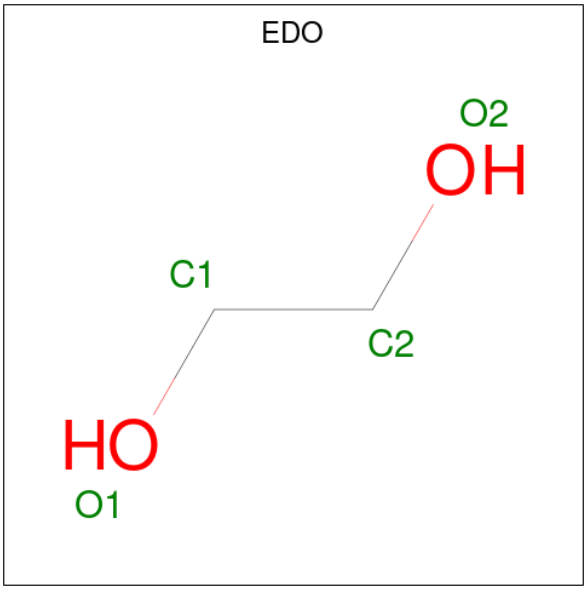
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

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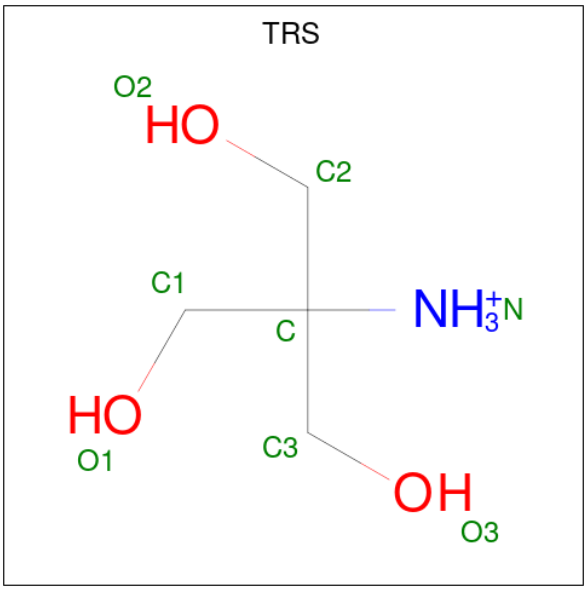
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	K	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C N O 8 4 1 3	0	0
4	D	1	Total C N O 16 8 2 6	0	1

- Molecule 5 is water.

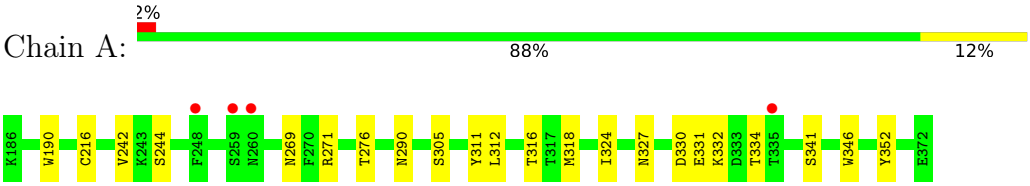
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	116	Total O 116 116	0	0
5	B	86	Total O 86 86	0	0
5	C	106	Total O 106 106	0	0
5	D	115	Total O 115 115	0	0
5	E	75	Total O 75 75	0	0
5	F	110	Total O 110 110	0	0
5	G	109	Total O 109 109	0	0
5	H	78	Total O 78 78	0	0
5	I	109	Total O 109 109	0	0
5	J	108	Total O 108 108	0	0
5	K	97	Total O 97 97	0	0
5	L	97	Total O 97 97	0	0

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.

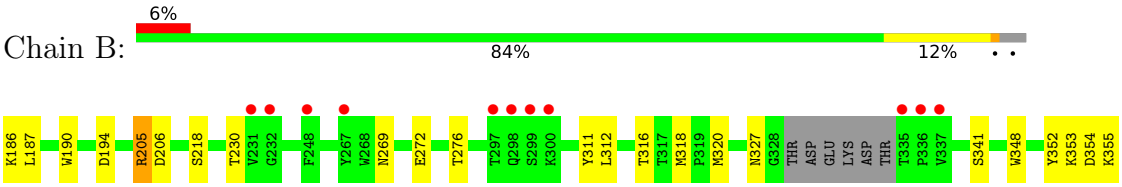
• Molecule 1: Fiber

Chain A:



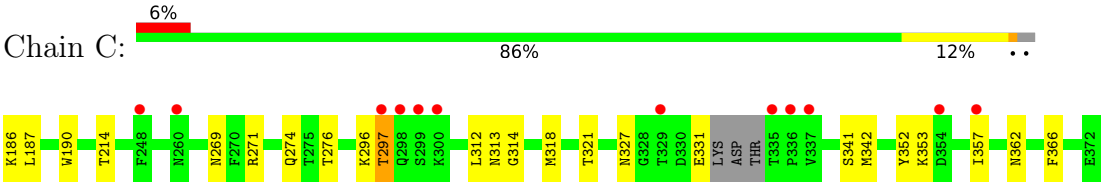
• Molecule 1: Fiber

Chain B:



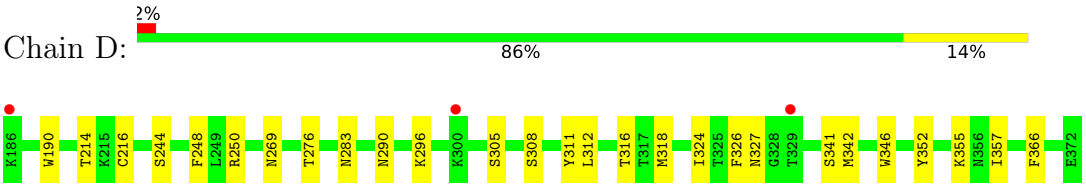
• Molecule 1: Fiber

Chain C:



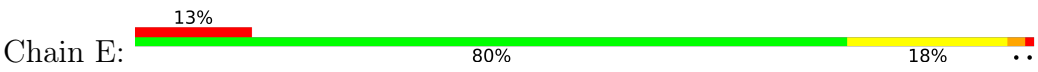
• Molecule 1: Fiber

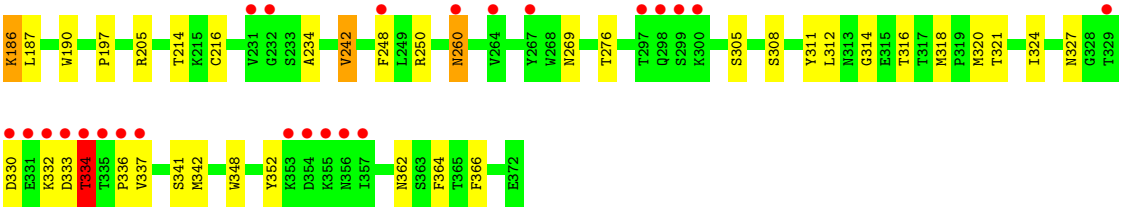
Chain D:



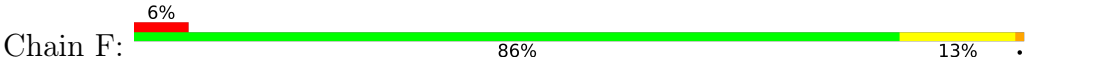
• Molecule 1: Fiber

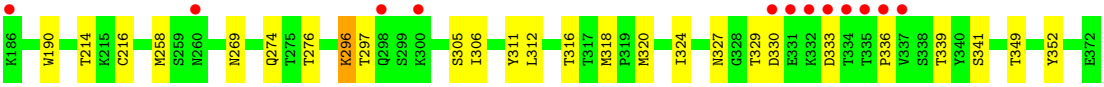
Chain E:



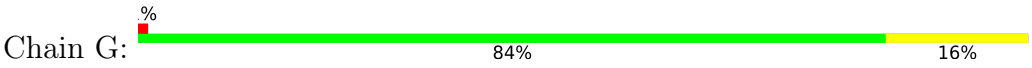


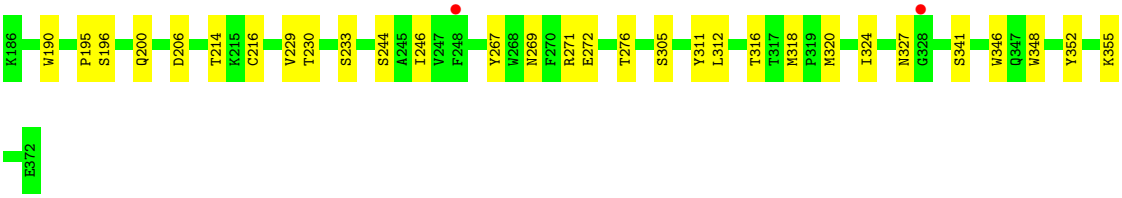
• Molecule 1: Fiber



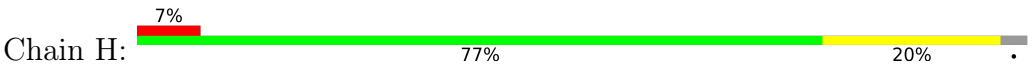


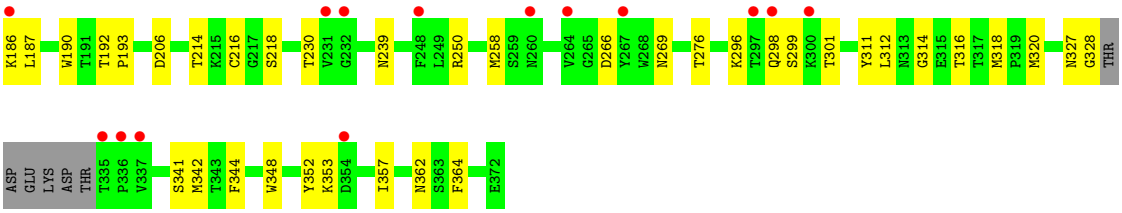
• Molecule 1: Fiber



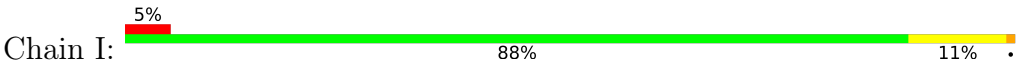


• Molecule 1: Fiber

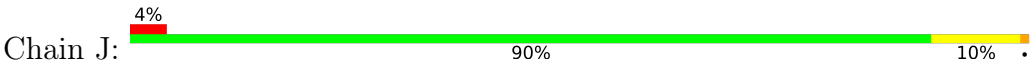




• Molecule 1: Fiber

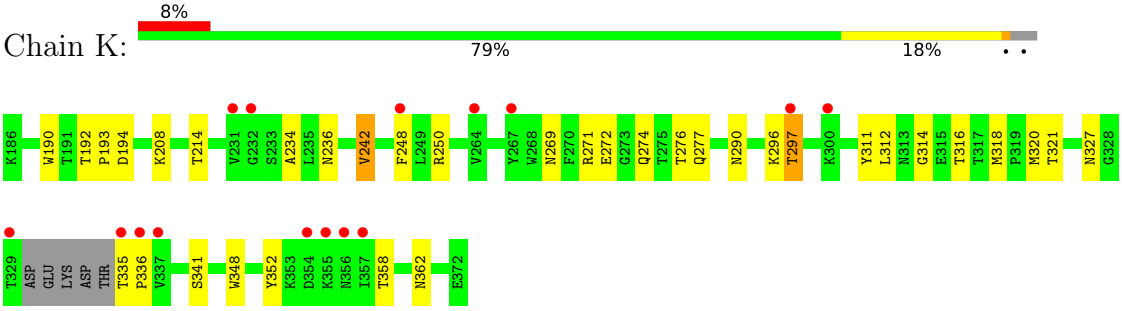


• Molecule 1: Fiber



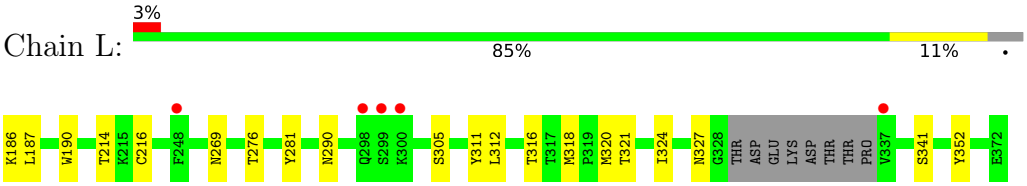
• Molecule 1: Fiber

Chain K:



• Molecule 1: Fiber

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.43Å 112.26Å 98.61Å 90.00° 92.61° 90.00°	Depositor
Resolution (Å)	74.04 – 1.59 74.04 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.7 (74.04-1.59) 99.7 (74.04-1.59)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.224 , 0.244 0.219 , 0.238	Depositor DCC
R_{free} test set	14210 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.094 for h,-k,-l 0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.897 for H, K, L 0.103 for -h,-k,l	Depositor
Outliers	8 of 285749 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18792	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4197e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: EDO, CA, TRS

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	0.79	0/1520	0.82	0/2070
1	B	0.76	1/1459 (0.1%)	0.80	1/1988 (0.1%)
1	C	0.74	0/1480	0.78	0/2015
1	D	0.76	0/1504	0.78	0/2050
1	E	0.76	0/1526	0.82	0/2078
1	F	0.74	0/1501	0.80	0/2045
1	G	0.83	1/1521 (0.1%)	0.81	0/2073
1	H	0.77	0/1455	0.81	0/1981
1	I	0.75	0/1490	0.80	0/2031
1	J	0.78	0/1493	0.82	1/2035 (0.0%)
1	K	0.76	0/1485	0.82	0/2024
1	L	0.73	0/1440	0.77	0/1960
All	All	0.77	2/17874 (0.0%)	0.80	2/24350 (0.0%)

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	E	0	3
1	F	0	1
1	G	0	1
1	I	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	233	SER	CB-OG	5.94	1.50	1.42
1	B	272	GLU	CD-OE1	-5.10	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	250	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	B	205	ARG	NE-CZ-NH2	-5.34	117.63	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	260	ASN	Mainchain
1	E	334	THR	Peptide
1	E	336	PRO	Peptide
1	F	296	LYS	Mainchain
1	G	355	LYS	Mainchain

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	1487	0	1449	21	0
1	B	1427	0	1384	28	0
1	C	1448	0	1404	24	0
1	D	1470	0	1426	34	0
1	E	1493	0	1449	39	0
1	F	1468	0	1425	28	0
1	G	1488	0	1449	29	0
1	H	1423	0	1383	32	0
1	I	1457	0	1413	17	0
1	J	1460	0	1417	13	0
1	K	1452	0	1406	27	0
1	L	1409	0	1364	20	0
2	A	1	0	0	0	0
2	D	2	0	0	0	0
2	G	1	0	0	0	0
3	A	4	0	6	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
3	E	4	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	4	0	6	8	0
3	G	16	0	24	4	0
3	H	12	0	17	4	0
3	I	8	0	12	1	0
3	J	8	0	12	0	0
3	K	4	0	6	0	0
3	L	8	0	12	1	0
4	D	24	0	36	3	0
5	A	116	0	0	1	0
5	B	86	0	0	1	0
5	C	106	0	0	1	0
5	D	115	0	0	3	0
5	E	75	0	0	0	0
5	F	110	0	0	0	0
5	G	109	0	0	4	0
5	H	78	0	0	0	0
5	I	109	0	0	2	0
5	J	108	0	0	0	0
5	K	97	0	0	4	0
5	L	97	0	0	0	0
All	All	18792	0	17118	279	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 279 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:271[B]:ARG:NH1	1:B:218[B]:SER:OG	1.85	1.09
1:E:334:THR:HG23	1:E:337:VAL:HA	1.31	1.09
1:A:331:GLU:O	1:A:334:THR:HG22	1.58	1.03
1:D:318[A]:MET:CE	1:D:357:ILE:HD13	1.93	0.98
1:L:312:LEU:HB2	1:L:320[A]:MET:HE3	1.50	0.94

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	190/187 (102%)	183 (96%)	7 (4%)	0	100 100
1	B	182/187 (97%)	177 (97%)	5 (3%)	0	100 100
1	C	184/187 (98%)	175 (95%)	8 (4%)	1 (0%)	29 11
1	D	188/187 (100%)	181 (96%)	7 (4%)	0	100 100
1	E	191/187 (102%)	181 (95%)	8 (4%)	2 (1%)	15 3
1	F	188/187 (100%)	181 (96%)	7 (4%)	0	100 100
1	G	191/187 (102%)	185 (97%)	6 (3%)	0	100 100
1	H	181/187 (97%)	175 (97%)	6 (3%)	0	100 100
1	I	187/187 (100%)	180 (96%)	7 (4%)	0	100 100
1	J	187/187 (100%)	179 (96%)	8 (4%)	0	100 100
1	K	183/187 (98%)	173 (94%)	9 (5%)	1 (0%)	29 11
1	L	179/187 (96%)	173 (97%)	6 (3%)	0	100 100
All	All	2231/2244 (99%)	2143 (96%)	84 (4%)	4 (0%)	47 26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	334	THR
1	K	297	THR
1	C	297	THR
1	E	332	LYS

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	170/165 (103%)	167 (98%)	3 (2%)	59 36
1	B	164/165 (99%)	163 (99%)	1 (1%)	86 77
1	C	166/165 (101%)	164 (99%)	2 (1%)	71 54
1	D	168/165 (102%)	167 (99%)	1 (1%)	86 77
1	E	171/165 (104%)	168 (98%)	3 (2%)	59 36
1	F	168/165 (102%)	165 (98%)	3 (2%)	59 36
1	G	171/165 (104%)	170 (99%)	1 (1%)	86 77
1	H	163/165 (99%)	161 (99%)	2 (1%)	71 54
1	I	167/165 (101%)	165 (99%)	2 (1%)	71 54
1	J	167/165 (101%)	165 (99%)	2 (1%)	71 54
1	K	166/165 (101%)	164 (99%)	2 (1%)	71 54
1	L	161/165 (98%)	160 (99%)	1 (1%)	86 77
All	All	2002/1980 (101%)	1979 (99%)	23 (1%)	73 57

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	190	TRP
1	I	300	LYS
1	I	190	TRP
1	J	190	TRP
1	D	190	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	327	ASN
1	K	274	GLN
1	J	219	GLN
1	J	304	ASN
1	K	304	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 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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	EDO	H	402	-	3,3,3	0.21	0	2,2,2	0.38	0
3	EDO	J	402	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	I	401	-	3,3,3	0.06	0	2,2,2	0.19	0
3	EDO	A	402	-	3,3,3	0.24	0	2,2,2	0.21	0
3	EDO	C	401	-	3,3,3	0.44	0	2,2,2	0.35	0
3	EDO	G	405	-	3,3,3	0.04	0	2,2,2	0.38	0
4	TRS	D	405[B]	-	7,7,7	0.30	0	9,9,9	0.30	0
3	EDO	E	401	-	3,3,3	0.02	0	2,2,2	0.21	0
3	EDO	I	402	-	3,3,3	0.04	0	2,2,2	0.11	0
3	EDO	D	403	-	3,3,3	0.24	0	2,2,2	0.36	0
3	EDO	J	401	-	3,3,3	0.27	0	2,2,2	0.37	0
3	EDO	K	401	-	3,3,3	0.45	0	2,2,2	0.26	0
3	EDO	L	401	-	3,3,3	0.30	0	2,2,2	0.29	0
3	EDO	G	404	-	3,3,3	0.36	0	2,2,2	0.44	0
3	EDO	G	403	-	3,3,3	0.26	0	2,2,2	0.26	0
3	EDO	H	401	-	3,3,3	0.30	0	2,2,2	0.10	0
3	EDO	F	401	-	3,3,3	0.80	0	2,2,2	0.29	0
4	TRS	D	405[A]	-	7,7,7	0.33	0	9,9,9	0.39	0
4	TRS	D	404	-	7,7,7	0.21	0	9,9,9	0.42	0
3	EDO	H	403	-	3,3,3	0.71	0	2,2,2	0.30	0
3	EDO	G	402	-	3,3,3	0.23	0	2,2,2	0.40	0
3	EDO	L	402	-	3,3,3	0.28	0	2,2,2	0.06	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
3	EDO	H	402	-	-	1/1/1/1	-
3	EDO	J	402	-	-	0/1/1/1	-
3	EDO	I	401	-	-	0/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	C	401	-	-	0/1/1/1	-
3	EDO	G	405	-	-	1/1/1/1	-
4	TRS	D	405[B]	-	-	3/9/9/9	-
3	EDO	E	401	-	-	1/1/1/1	-
3	EDO	I	402	-	-	1/1/1/1	-
3	EDO	D	403	-	-	0/1/1/1	-
3	EDO	J	401	-	-	0/1/1/1	-
3	EDO	K	401	-	-	0/1/1/1	-
3	EDO	L	401	-	-	0/1/1/1	-
3	EDO	G	404	-	-	1/1/1/1	-
3	EDO	G	403	-	-	0/1/1/1	-
3	EDO	H	401	-	-	0/1/1/1	-
3	EDO	F	401	-	-	0/1/1/1	-
4	TRS	D	405[A]	-	-	6/9/9/9	-
4	TRS	D	404	-	-	6/9/9/9	-
3	EDO	H	403	-	-	1/1/1/1	-
3	EDO	G	402	-	-	0/1/1/1	-
3	EDO	L	402	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	404	TRS	C1-C-C2-O2
4	D	404	TRS	C3-C-C2-O2
4	D	404	TRS	N-C-C2-O2
4	D	405[A]	TRS	C2-C-C1-O1
4	D	405[A]	TRS	C1-C-C2-O2

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	401	EDO	1	0
3	G	405	EDO	1	0
3	E	401	EDO	1	0
3	G	404	EDO	3	0
3	F	401	EDO	8	0
4	D	405[A]	TRS	1	0
4	D	404	TRS	2	0
3	H	403	EDO	4	0
3	L	402	EDO	1	0

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

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	187/187 (100%)	-0.06	4 (2%) 63 62	15, 22, 36, 48	0
1	B	181/187 (96%)	0.41	12 (6%) 18 17	15, 27, 50, 84	0
1	C	184/187 (98%)	0.17	12 (6%) 18 17	15, 25, 48, 78	0
1	D	187/187 (100%)	-0.02	3 (1%) 72 71	15, 22, 38, 55	0
1	E	187/187 (100%)	0.54	24 (12%) 3 3	15, 28, 61, 91	0
1	F	187/187 (100%)	0.05	12 (6%) 19 17	14, 22, 47, 85	0
1	G	187/187 (100%)	-0.14	2 (1%) 80 80	15, 20, 36, 44	0
1	H	181/187 (96%)	0.44	14 (7%) 13 11	15, 28, 52, 82	0
1	I	187/187 (100%)	0.17	10 (5%) 26 24	15, 23, 47, 69	0
1	J	187/187 (100%)	-0.01	7 (3%) 41 39	15, 23, 41, 59	0
1	K	182/187 (97%)	0.33	15 (8%) 11 10	13, 24, 44, 69	0
1	L	179/187 (95%)	-0.00	5 (2%) 53 50	15, 24, 41, 58	0
All	All	2216/2244 (98%)	0.16	120 (5%) 25 23	13, 24, 46, 91	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	THR	8.5
1	L	300	LYS	7.8
1	H	335	THR	7.4
1	K	231	VAL	7.0
1	K	267	TYR	6.9

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

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

6.3 Carbohydrates (i)

There are no 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
4	TRS	D	404	8/8	0.70	0.21	39,47,49,55	0
3	EDO	I	402	4/4	0.83	0.14	40,45,47,54	0
3	EDO	G	404	4/4	0.83	0.15	35,39,40,43	0
3	EDO	L	402	4/4	0.84	0.12	30,35,35,40	0
4	TRS	D	405[A]	8/8	0.86	0.19	15,19,22,22	8
4	TRS	D	405[B]	8/8	0.86	0.19	20,21,22,24	8
3	EDO	K	401	4/4	0.87	0.13	18,20,21,22	0
3	EDO	E	401	4/4	0.89	0.14	47,47,49,49	0
3	EDO	G	405	4/4	0.89	0.11	38,38,39,40	0
3	EDO	I	401	4/4	0.89	0.09	40,42,43,44	0
3	EDO	H	402	4/4	0.91	0.11	29,30,31,32	0
3	EDO	H	401	4/4	0.91	0.12	20,21,22,23	0
3	EDO	J	402	4/4	0.93	0.08	19,21,22,23	0
3	EDO	G	402	4/4	0.94	0.10	20,24,25,26	0
3	EDO	H	403	4/4	0.95	0.10	18,22,23,23	0
3	EDO	L	401	4/4	0.95	0.09	20,21,23,24	0
3	EDO	F	401	4/4	0.95	0.10	19,20,20,20	0
3	EDO	C	401	4/4	0.96	0.08	17,19,20,20	0
3	EDO	J	401	4/4	0.96	0.08	19,24,25,26	0
3	EDO	A	402	4/4	0.96	0.07	23,25,27,27	0
3	EDO	D	403	4/4	0.97	0.08	17,21,21,22	0
2	CA	D	402	1/1	0.98	0.04	28,28,28,28	0
2	CA	G	401	1/1	0.98	0.04	32,32,32,32	0
3	EDO	G	403	4/4	0.98	0.05	20,22,22,24	0
2	CA	A	401	1/1	0.99	0.04	18,18,18,18	0
2	CA	D	401	1/1	0.99	0.04	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.