



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2021 – 07:02 am BST

PDB ID : 6QPN  
Title : Adenovirus species D serotype 49 Fiber-Knob  
Authors : Baker, A.T.; Rizkallah, P.J.  
Deposited on : 2019-02-14  
Resolution : 2.74 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](mailto: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.

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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 : 2.23.1  
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) : 2.23.1

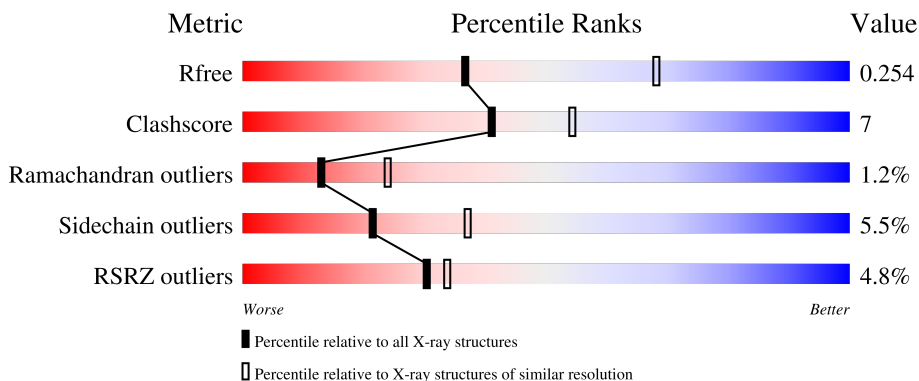
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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.



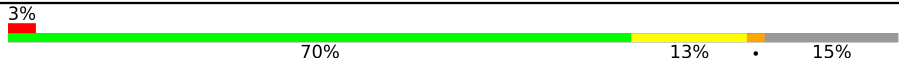
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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  $\geq 3$ , 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	226	 70% 16% 12%
1	B	226	 63% 16% 19%
1	C	226	 69% 17% 13%
1	D	226	 71% 13% 15%
1	E	226	 75% 11% 12%

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Mol	Chain	Length	Quality of chain
1	F	226	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into four segments: a small red segment at the beginning labeled '3%', a large green segment labeled '70%', a yellow segment labeled '13%', and a grey segment at the end labeled '15%'. A small black dot is visible on the grey segment.</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9083 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
			Total	C	N	O	S			
1	A	199	1542	979	252	307	4	0	0	0
1	B	184	1439	919	234	282	4	0	0	0
1	C	196	1523	968	247	304	4	0	0	0
1	D	193	1502	956	244	298	4	0	0	0
1	E	200	1551	984	253	310	4	0	0	0
1	F	193	1502	956	244	298	4	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	373	MET	-	initiating methionine	UNP Q09TX9
A	374	ARG	-	expression tag	UNP Q09TX9
A	375	GLY	-	expression tag	UNP Q09TX9
A	376	SER	-	expression tag	UNP Q09TX9
A	377	HIS	-	expression tag	UNP Q09TX9
A	378	HIS	-	expression tag	UNP Q09TX9
A	379	HIS	-	expression tag	UNP Q09TX9
A	380	HIS	-	expression tag	UNP Q09TX9
A	381	HIS	-	expression tag	UNP Q09TX9
A	382	HIS	-	expression tag	UNP Q09TX9
A	383	GLY	-	expression tag	UNP Q09TX9
A	384	SER	-	expression tag	UNP Q09TX9
B	373	MET	-	initiating methionine	UNP Q09TX9
B	374	ARG	-	expression tag	UNP Q09TX9
B	375	GLY	-	expression tag	UNP Q09TX9
B	376	SER	-	expression tag	UNP Q09TX9
B	377	HIS	-	expression tag	UNP Q09TX9

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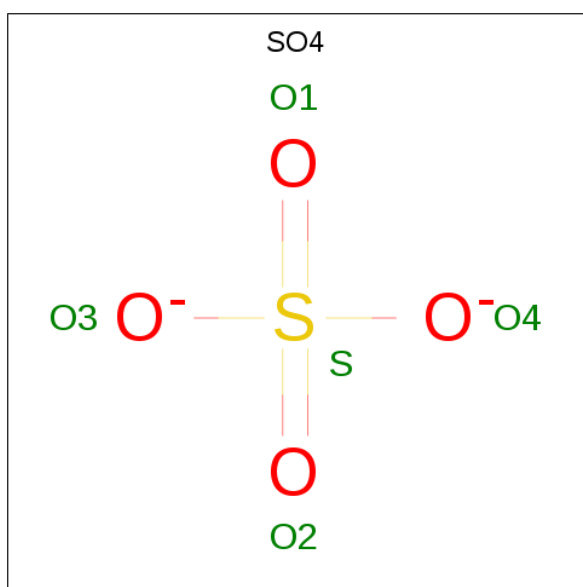
Chain	Residue	Modelled	Actual	Comment	Reference
B	378	HIS	-	expression tag	UNP Q09TX9
B	379	HIS	-	expression tag	UNP Q09TX9
B	380	HIS	-	expression tag	UNP Q09TX9
B	381	HIS	-	expression tag	UNP Q09TX9
B	382	HIS	-	expression tag	UNP Q09TX9
B	383	GLY	-	expression tag	UNP Q09TX9
B	384	SER	-	expression tag	UNP Q09TX9
C	373	MET	-	initiating methionine	UNP Q09TX9
C	374	ARG	-	expression tag	UNP Q09TX9
C	375	GLY	-	expression tag	UNP Q09TX9
C	376	SER	-	expression tag	UNP Q09TX9
C	377	HIS	-	expression tag	UNP Q09TX9
C	378	HIS	-	expression tag	UNP Q09TX9
C	379	HIS	-	expression tag	UNP Q09TX9
C	380	HIS	-	expression tag	UNP Q09TX9
C	381	HIS	-	expression tag	UNP Q09TX9
C	382	HIS	-	expression tag	UNP Q09TX9
C	383	GLY	-	expression tag	UNP Q09TX9
C	384	SER	-	expression tag	UNP Q09TX9
D	373	MET	-	initiating methionine	UNP Q09TX9
D	374	ARG	-	expression tag	UNP Q09TX9
D	375	GLY	-	expression tag	UNP Q09TX9
D	376	SER	-	expression tag	UNP Q09TX9
D	377	HIS	-	expression tag	UNP Q09TX9
D	378	HIS	-	expression tag	UNP Q09TX9
D	379	HIS	-	expression tag	UNP Q09TX9
D	380	HIS	-	expression tag	UNP Q09TX9
D	381	HIS	-	expression tag	UNP Q09TX9
D	382	HIS	-	expression tag	UNP Q09TX9
D	383	GLY	-	expression tag	UNP Q09TX9
D	384	SER	-	expression tag	UNP Q09TX9
E	373	MET	-	initiating methionine	UNP Q09TX9
E	374	ARG	-	expression tag	UNP Q09TX9
E	375	GLY	-	expression tag	UNP Q09TX9
E	376	SER	-	expression tag	UNP Q09TX9
E	377	HIS	-	expression tag	UNP Q09TX9
E	378	HIS	-	expression tag	UNP Q09TX9
E	379	HIS	-	expression tag	UNP Q09TX9
E	380	HIS	-	expression tag	UNP Q09TX9
E	381	HIS	-	expression tag	UNP Q09TX9
E	382	HIS	-	expression tag	UNP Q09TX9
E	383	GLY	-	expression tag	UNP Q09TX9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	384	SER	-	expression tag	UNP Q09TX9
F	373	MET	-	initiating methionine	UNP Q09TX9
F	374	ARG	-	expression tag	UNP Q09TX9
F	375	GLY	-	expression tag	UNP Q09TX9
F	376	SER	-	expression tag	UNP Q09TX9
F	377	HIS	-	expression tag	UNP Q09TX9
F	378	HIS	-	expression tag	UNP Q09TX9
F	379	HIS	-	expression tag	UNP Q09TX9
F	380	HIS	-	expression tag	UNP Q09TX9
F	381	HIS	-	expression tag	UNP Q09TX9
F	382	HIS	-	expression tag	UNP Q09TX9
F	383	GLY	-	expression tag	UNP Q09TX9
F	384	SER	-	expression tag	UNP Q09TX9

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

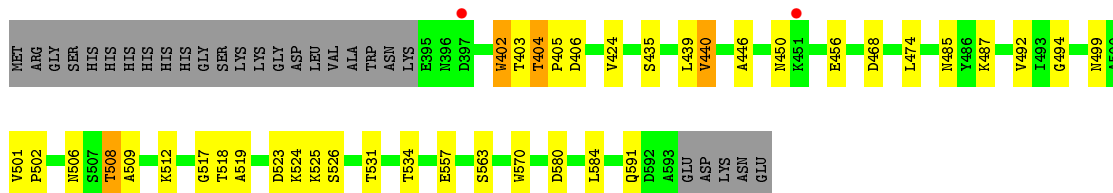
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 3 3	0	0
3	B	2	Total O 2 2	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0
3	F	2	Total O 2 2	0	0

### 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.

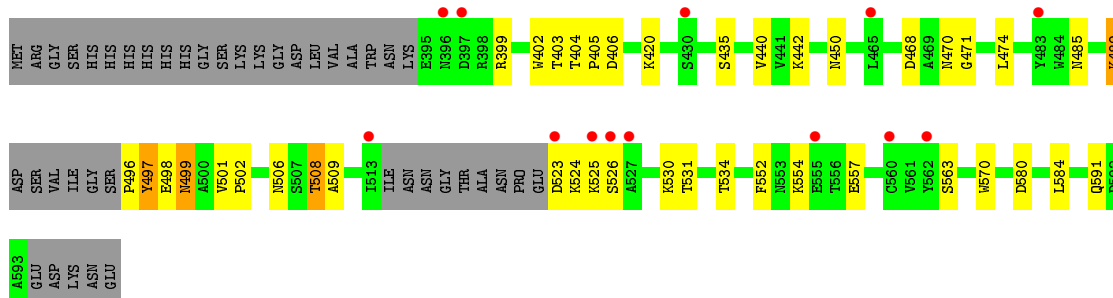
- Molecule 1: Fiber

Chain A: 



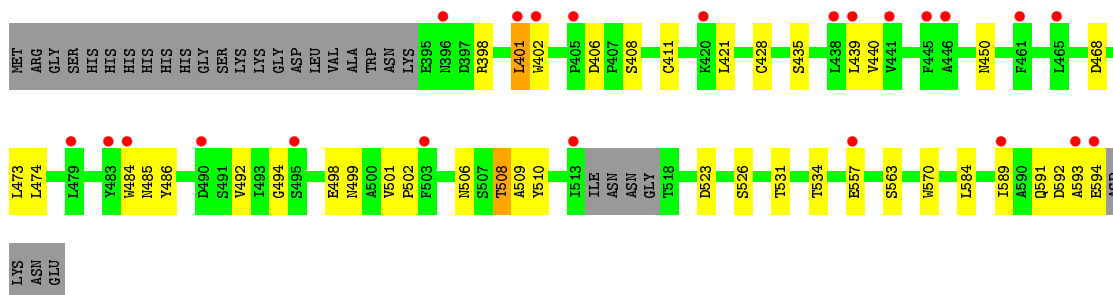
- Molecule 1: Fiber

Chain B: 



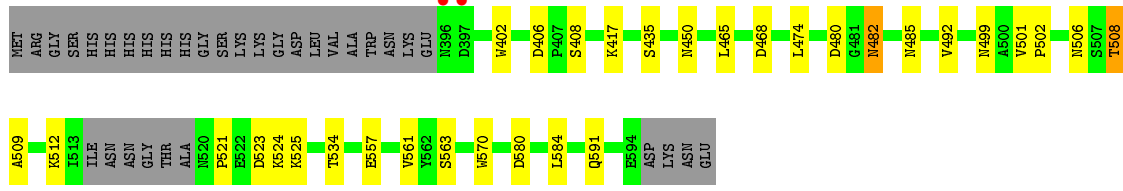
- Molecule 1: Fiber

Chain C: 

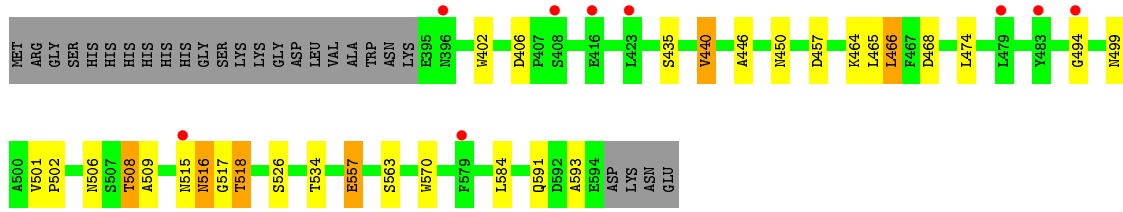
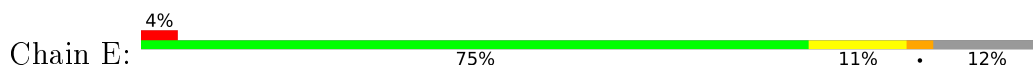


- Molecule 1: Fiber

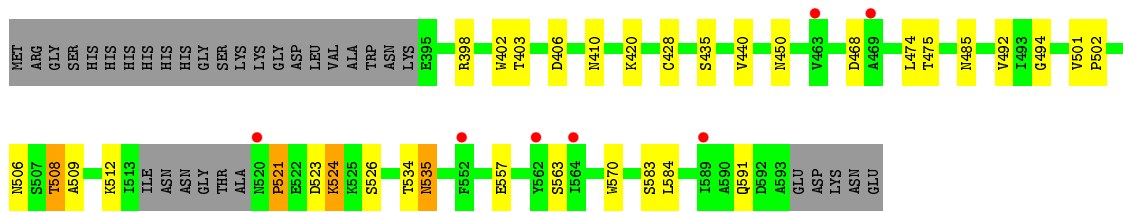




• Molecule 1: Fiber



• Molecule 1: Fiber



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.83Å 56.28Å 115.70Å 90.00° 112.95° 90.00°	Depositor
Resolution (Å)	106.54 – 2.74 106.54 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.7 (106.54-2.74) 98.7 (106.54-2.74)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.73Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.211 , 0.259 0.212 , 0.254	Depositor DCC
$R_{free}$ test set	1609 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.7	Xtrriage
Anisotropy	0.324	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 57.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.69	0/1576	0.94	2/2141 (0.1%)
1	B	0.69	0/1470	0.91	0/1991
1	C	0.67	0/1556	0.89	0/2112
1	D	0.69	0/1535	0.90	0/2083
1	E	0.66	0/1585	0.86	0/2153
1	F	0.66	0/1535	0.87	0/2083
All	All	0.68	0/9257	0.89	2/12563 (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	B	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	THR	CA-CB-OG1	-8.84	90.43	109.00
1	A	456	GLU	CB-CA-C	5.16	120.71	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	497	TYR	Peptide
1	B	499	ASN	Peptide

## 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	1542	0	1524	32	0
1	B	1439	0	1429	27	0
1	C	1523	0	1503	35	1
1	D	1502	0	1485	16	1
1	E	1551	0	1530	25	0
1	F	1502	0	1485	18	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	D	5	0	0	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	F	2	0	0	0	0
All	All	9083	0	8956	128	2

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 7.

All (128) 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:B:403:THR:O	1:B:404:THR:HG22	1.59	1.03
1:A:424:VAL:HG21	1:C:589:ILE:HD12	1.56	0.85
1:E:502:PRO:HG3	1:E:593:ALA:HB2	1.57	0.85
1:E:518:THR:CG2	1:E:518:THR:O	2.27	0.82
1:C:401:LEU:HD11	1:C:486:TYR:CE1	2.16	0.80
1:C:411:CYS:SG	1:C:421:LEU:HB3	2.24	0.77
1:A:508:THR:HG22	1:B:406:ASP:CB	2.14	0.77
1:D:580:ASP:OD1	1:E:526:SER:OG	2.01	0.77
1:A:402:TRP:CZ3	1:C:589:ILE:HD11	2.20	0.76
1:F:403:THR:HG21	1:F:410:ASN:HD21	1.51	0.75
1:B:403:THR:O	1:B:404:THR:CG2	2.36	0.74
1:B:404:THR:OG1	1:B:405:PRO:HD2	1.89	0.72
1:F:403:THR:CG2	1:F:410:ASN:ND2	2.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:THR:HG22	1:B:406:ASP:HB2	1.70	0.72
1:F:403:THR:HG21	1:F:410:ASN:ND2	2.04	0.72
1:E:518:THR:O	1:E:518:THR:HG23	1.90	0.71
1:A:526:SER:OG	1:B:580:ASP:OD1	2.06	0.71
1:A:524:LYS:O	1:B:420:LYS:NZ	2.25	0.69
1:A:402:TRP:HZ3	1:C:589:ILE:HD11	1.58	0.68
1:A:404:THR:CG2	1:A:405:PRO:HD2	2.25	0.67
1:E:502:PRO:HG3	1:E:593:ALA:CB	2.25	0.66
1:B:501:VAL:N	1:B:502:PRO:HD2	2.11	0.66
1:E:464:LYS:HB3	1:E:466:LEU:HD11	1.78	0.65
1:C:473:LEU:HD21	1:C:484:TRP:HE1	1.61	0.64
1:A:517:GLY:C	1:A:519:ALA:H	2.00	0.62
1:A:508:THR:HG22	1:B:406:ASP:HB3	1.81	0.62
1:E:465:LEU:C	1:E:466:LEU:HD12	2.20	0.62
1:C:510:TYR:OH	1:C:589:ILE:HG22	1.99	0.61
1:A:580:ASP:OD1	1:C:526:SER:OG	2.17	0.60
1:E:466:LEU:CD1	1:E:466:LEU:N	2.65	0.60
1:B:508:THR:HG22	1:C:406:ASP:HB2	1.85	0.59
1:D:417:LYS:HE3	1:D:480:ASP:OD2	2.03	0.59
1:B:471:GLY:O	1:B:498:GLU:OE2	2.21	0.58
1:C:411:CYS:SG	1:C:421:LEU:CB	2.91	0.58
1:B:530:LYS:HE2	1:B:552:PHE:O	2.03	0.58
1:C:473:LEU:HD21	1:C:484:TRP:NE1	2.18	0.58
1:B:485:ASN:ND2	1:B:496:PRO:HB3	2.19	0.57
1:E:450:ASN:HD21	1:E:570:TRP:HE1	1.53	0.57
1:A:450:ASN:HD21	1:A:570:TRP:HE1	1.54	0.56
1:C:510:TYR:CZ	1:C:589:ILE:HG22	2.40	0.56
1:F:450:ASN:HD21	1:F:570:TRP:HE1	1.53	0.56
1:E:516:ASN:O	1:E:518:THR:N	2.39	0.56
1:D:450:ASN:HD21	1:D:570:TRP:HE1	1.53	0.55
1:D:508:THR:HG22	1:F:406:ASP:HB2	1.88	0.55
1:F:506:ASN:HD22	1:F:509:ALA:H	1.55	0.55
1:D:512:LYS:NZ	1:D:561:VAL:O	2.39	0.55
1:A:403:THR:O	1:A:404:THR:C	2.43	0.54
1:C:468:ASP:HB3	1:C:474:LEU:HD11	1.88	0.54
1:A:404:THR:HG23	1:A:405:PRO:HD2	1.89	0.54
1:C:450:ASN:HD21	1:C:570:TRP:HE1	1.54	0.54
1:C:506:ASN:HD22	1:C:509:ALA:H	1.55	0.54
1:B:506:ASN:HD22	1:B:509:ALA:H	1.56	0.54
1:D:524:LYS:O	1:F:420:LYS:NZ	2.41	0.53
1:E:466:LEU:HD12	1:E:466:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:ASN:HD22	1:D:509:ALA:H	1.55	0.53
1:B:450:ASN:HD21	1:B:570:TRP:HE1	1.55	0.53
1:C:593:ALA:O	1:C:594:GLU:C	2.47	0.53
1:B:468:ASP:HB3	1:B:474:LEU:HD21	1.91	0.52
1:A:506:ASN:HD22	1:A:509:ALA:H	1.57	0.52
1:F:506:ASN:HA	1:F:591:GLN:OE1	2.10	0.52
1:B:508:THR:HG22	1:C:406:ASP:CB	2.39	0.52
1:D:534:THR:HG21	1:D:584:LEU:HD11	1.92	0.51
1:A:506:ASN:HA	1:A:591:GLN:OE1	2.11	0.51
1:E:506:ASN:HA	1:E:591:GLN:OE1	2.10	0.51
1:A:525:LYS:HE2	1:B:406:ASP:OD2	2.10	0.51
1:B:506:ASN:HA	1:B:591:GLN:OE1	2.10	0.51
1:B:534:THR:HG21	1:B:584:LEU:HD11	1.93	0.51
1:B:485:ASN:OD1	1:B:497:TYR:O	2.29	0.51
1:E:468:ASP:HB3	1:E:474:LEU:HD21	1.92	0.51
1:C:401:LEU:HD11	1:C:486:TYR:CD1	2.46	0.51
1:C:506:ASN:HA	1:C:591:GLN:OE1	2.10	0.51
1:D:506:ASN:HA	1:D:591:GLN:OE1	2.11	0.51
1:E:506:ASN:HD22	1:E:509:ALA:H	1.57	0.51
1:E:515:ASN:C	1:E:516:ASN:HD22	2.15	0.51
1:A:468:ASP:HB3	1:A:474:LEU:HD21	1.93	0.50
1:E:518:THR:O	1:E:518:THR:HG22	2.10	0.50
1:D:501:VAL:N	1:D:502:PRO:CD	2.75	0.50
1:E:534:THR:HG21	1:E:584:LEU:HD11	1.94	0.50
1:D:468:ASP:HB3	1:D:474:LEU:HD21	1.93	0.50
1:C:501:VAL:N	1:C:502:PRO:CD	2.75	0.49
1:F:403:THR:CG2	1:F:410:ASN:HD22	2.23	0.49
1:F:501:VAL:N	1:F:502:PRO:CD	2.76	0.49
1:C:473:LEU:N	1:C:473:LEU:CD2	2.75	0.49
1:F:468:ASP:HB3	1:F:474:LEU:HD21	1.94	0.49
1:A:501:VAL:N	1:A:502:PRO:CD	2.75	0.49
1:E:501:VAL:N	1:E:502:PRO:CD	2.76	0.48
1:A:403:THR:O	1:A:404:THR:O	2.31	0.48
1:A:439:LEU:HD22	1:C:526:SER:HB2	1.94	0.48
1:A:534:THR:HG21	1:A:584:LEU:HD11	1.96	0.47
1:F:534:THR:C	1:F:535:ASN:HD22	2.17	0.47
1:D:485:ASN:HB3	1:D:492:VAL:HB	1.97	0.46
1:D:508:THR:HG22	1:F:406:ASP:CB	2.46	0.46
1:C:474:LEU:CD1	1:C:474:LEU:N	2.79	0.46
1:C:534:THR:HG21	1:C:584:LEU:HD11	1.98	0.46
1:B:524:LYS:N	1:B:524:LYS:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:SER:HB3	1:C:439:LEU:HD22	1.98	0.45
1:A:404:THR:HG22	1:A:405:PRO:HD2	1.98	0.45
1:A:402:TRP:CE3	1:C:589:ILE:HD11	2.52	0.45
1:B:501:VAL:N	1:B:502:PRO:CD	2.78	0.45
1:D:406:ASP:CB	1:E:508:THR:HG22	2.48	0.44
1:C:398:ARG:O	1:C:398:ARG:HG3	2.18	0.44
1:A:512:LYS:HB3	1:A:512:LYS:HE2	1.61	0.44
1:B:470:ASN:HB3	1:B:499:ASN:HD22	1.82	0.44
1:E:499:ASN:ND2	1:E:501:VAL:HG23	2.33	0.44
1:F:523:ASP:O	1:F:524:LYS:HG2	2.18	0.44
1:A:440:VAL:HG23	1:A:446:ALA:HA	2.00	0.43
1:B:525:LYS:HE2	1:F:398:ARG:HH12	1.83	0.43
1:C:474:LEU:N	1:C:474:LEU:HD12	2.33	0.43
1:C:468:ASP:N	1:C:474:LEU:HD11	2.34	0.43
1:D:499:ASN:ND2	1:D:501:VAL:HG23	2.34	0.43
1:A:403:THR:O	1:A:403:THR:OG1	2.37	0.43
1:C:499:ASN:ND2	1:C:501:VAL:HG23	2.34	0.43
1:E:502:PRO:CG	1:E:593:ALA:HB2	2.39	0.43
1:B:489:LYS:N	1:B:489:LYS:HD2	2.34	0.43
1:E:464:LYS:HE3	1:E:557:GLU:OE1	2.19	0.42
1:A:406:ASP:HB2	1:C:508:THR:HG22	2.01	0.42
1:A:406:ASP:CB	1:C:508:THR:HG22	2.49	0.42
1:F:485:ASN:HB3	1:F:492:VAL:HB	2.02	0.41
1:C:473:LEU:N	1:C:473:LEU:HD22	2.34	0.41
1:D:465:LEU:HD12	1:D:465:LEU:N	2.35	0.41
1:F:534:THR:HG21	1:F:584:LEU:HD11	2.03	0.41
1:A:485:ASN:HB3	1:A:492:VAL:HB	2.02	0.41
1:A:487:LYS:NZ	1:C:592:ASP:OD2	2.54	0.41
1:E:406:ASP:HB2	1:F:508:THR:HG22	2.03	0.41
1:C:485:ASN:HB3	1:C:492:VAL:HB	2.02	0.40
1:E:465:LEU:HD12	1:E:465:LEU:N	2.36	0.40
1:A:499:ASN:ND2	1:A:501:VAL:HG23	2.36	0.40
1:E:440:VAL:HG23	1:E:446:ALA:HA	2.04	0.40

All (2) 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:D:482:ASN:ND2	1:D:482:ASN:ND2 2_655	1.99	0.21
1:C:498:GLU:OE1	1:F:475:THR:OG1 2_656	2.08	0.12

## 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	197/226 (87%)	179 (91%)	15 (8%)	3 (2%)	10	18
1	B	178/226 (79%)	168 (94%)	9 (5%)	1 (1%)	25	44
1	C	192/226 (85%)	179 (93%)	11 (6%)	2 (1%)	15	28
1	D	189/226 (84%)	174 (92%)	13 (7%)	2 (1%)	14	26
1	E	198/226 (88%)	181 (91%)	14 (7%)	3 (2%)	10	18
1	F	189/226 (84%)	171 (90%)	15 (8%)	3 (2%)	9	17
All	All	1143/1356 (84%)	1052 (92%)	77 (7%)	14 (1%)	13	24

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	THR
1	A	557	GLU
1	C	557	GLU
1	D	521	PRO
1	F	521	PRO
1	D	557	GLU
1	E	517	GLY
1	E	557	GLU
1	B	557	GLU
1	F	557	GLU
1	E	494	GLY
1	C	494	GLY
1	F	494	GLY
1	A	494	GLY

### 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	175/198 (88%)	168 (96%)	7 (4%)	31	52
1	B	163/198 (82%)	152 (93%)	11 (7%)	16	29
1	C	173/198 (87%)	163 (94%)	10 (6%)	20	35
1	D	171/198 (86%)	163 (95%)	8 (5%)	26	45
1	E	176/198 (89%)	167 (95%)	9 (5%)	24	41
1	F	171/198 (86%)	159 (93%)	12 (7%)	15	27
All	All	1029/1188 (87%)	972 (94%)	57 (6%)	21	37

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402	TRP
1	A	435	SER
1	A	440	VAL
1	A	508	THR
1	A	523	ASP
1	A	531	THR
1	A	563	SER
1	B	399	ARG
1	B	402	TRP
1	B	435	SER
1	B	440	VAL
1	B	442	LYS
1	B	489	LYS
1	B	508	THR
1	B	523	ASP
1	B	531	THR
1	B	554	LYS
1	B	563	SER
1	C	401	LEU
1	C	402	TRP
1	C	408	SER
1	C	428	CYS
1	C	435	SER
1	C	440	VAL
1	C	508	THR
1	C	523	ASP
1	C	531	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	563	SER
1	D	402	TRP
1	D	408	SER
1	D	435	SER
1	D	482	ASN
1	D	508	THR
1	D	523	ASP
1	D	525	LYS
1	D	563	SER
1	E	402	TRP
1	E	435	SER
1	E	440	VAL
1	E	457	ASP
1	E	466	LEU
1	E	508	THR
1	E	516	ASN
1	E	518	THR
1	E	563	SER
1	F	402	TRP
1	F	428	CYS
1	F	435	SER
1	F	440	VAL
1	F	508	THR
1	F	512	LYS
1	F	521	PRO
1	F	524	LYS
1	F	526	SER
1	F	535	ASN
1	F	563	SER
1	F	583	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	450	ASN
1	A	482	ASN
1	A	506	ASN
1	A	516	ASN
1	A	535	ASN
1	A	576	ASN
1	B	450	ASN
1	B	485	ASN

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Mol	Chain	Res	Type
1	B	499	ASN
1	B	506	ASN
1	B	535	ASN
1	B	576	ASN
1	C	396	ASN
1	C	450	ASN
1	C	482	ASN
1	C	506	ASN
1	C	535	ASN
1	C	576	ASN
1	D	450	ASN
1	D	482	ASN
1	D	488	ASN
1	D	506	ASN
1	D	535	ASN
1	D	576	ASN
1	E	450	ASN
1	E	482	ASN
1	E	506	ASN
1	E	516	ASN
1	E	535	ASN
1	E	576	ASN
1	F	450	ASN
1	F	482	ASN
1	F	506	ASN
1	F	535	ASN
1	F	576	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](#)

3 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	SO4	D	601	-	4,4,4	0.39	0	6,6,6	0.06	0
2	SO4	A	601	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SO4	B	601	-	4,4,4	0.38	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	199/226 (88%)	0.10	2 (1%) 82 86	51, 81, 131, 143	0
1	B	184/226 (81%)	0.46	13 (7%) 16 17	51, 90, 164, 194	0
1	C	196/226 (86%)	0.77	23 (11%) 4 4	75, 127, 173, 211	0
1	D	193/226 (85%)	0.12	2 (1%) 82 86	48, 75, 128, 190	0
1	E	200/226 (88%)	0.38	9 (4%) 33 36	65, 106, 152, 180	0
1	F	193/226 (85%)	0.29	7 (3%) 42 47	67, 99, 150, 205	0
All	All	1165/1356 (85%)	0.35	56 (4%) 30 34	48, 95, 160, 211	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	445	PHE	6.8
1	C	490	ASP	5.5
1	E	396	ASN	5.1
1	B	555	GLU	4.9
1	E	579	PHE	4.5
1	C	465	LEU	4.4
1	C	441	VAL	4.4
1	C	405	PRO	4.2
1	C	401	LEU	4.0
1	E	494	GLY	3.9
1	C	446	ALA	3.9
1	C	484	TRP	3.7
1	B	525	LYS	3.5
1	B	562	TYR	3.4
1	B	465	LEU	3.3
1	D	396	ASN	3.2
1	C	557	GLU	3.2
1	A	397	ASP	3.1
1	F	552	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	593	ALA	3.0
1	C	439	LEU	2.9
1	E	483	TYR	2.8
1	B	560	CYS	2.7
1	C	461	PHE	2.7
1	E	408	SER	2.7
1	B	523	ASP	2.6
1	B	397	ASP	2.5
1	B	483	TYR	2.4
1	B	527	ALA	2.4
1	C	396	ASN	2.4
1	C	589	ILE	2.3
1	B	526	SER	2.3
1	F	562	TYR	2.3
1	C	594	GLU	2.3
1	C	420	LYS	2.3
1	C	438	LEU	2.3
1	B	430	SER	2.2
1	C	495	SER	2.2
1	F	589	ILE	2.2
1	F	520	ASN	2.2
1	C	483	TYR	2.2
1	B	513	ILE	2.2
1	C	479	LEU	2.2
1	E	416	GLU	2.2
1	C	402	TRP	2.1
1	D	397	ASP	2.1
1	F	463	VAL	2.1
1	A	451	LYS	2.1
1	E	479	LEU	2.1
1	C	503	PHE	2.1
1	F	564	ILE	2.1
1	F	469	ALA	2.1
1	B	396	ASN	2.1
1	E	515	ASN	2.0
1	C	513	ILE	2.0
1	E	423	LEU	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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	B	601	5/5	0.86	0.37	154,154,166,174	0
2	SO4	D	601	5/5	0.91	0.58	112,119,122,124	5
2	SO4	A	601	5/5	0.94	0.61	144,145,148,161	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.