



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:40 PM UTC

PDB ID : 8OFQ / pdb_00008ofq
Title : Human adenovirus type 25 fiber-knob protein
Authors : Rizkallah, P.J.; Parker, A.L.; Mundy, R.M.; Baker, A.T.
Deposited on : 2023-03-16
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

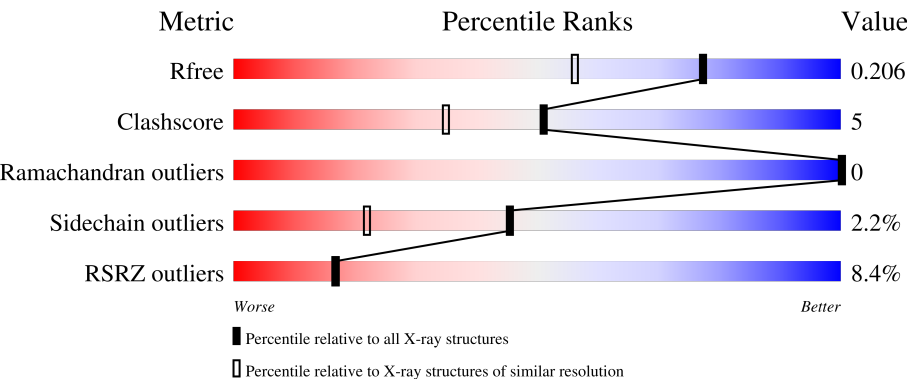
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 $\leq 5\%$. 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	187	 5% 84% 9% . .
1	B	187	 8% 88% 7% . .
1	C	187	 9% 84% 11% . .
1	D	187	 7% 86% 9% . .
1	E	187	 10% 87% 8% . .

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Mol	Chain	Length	Quality of chain
1	F	187	8% 87% 7%
1	G	187	8% 83% 9%
1	H	187	9% 82% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13123 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	179	Total	C	N	O	S	0	4	0
			1481	949	244	284	4			
1	B	179	Total	C	N	O	S	0	5	0
			1489	953	246	286	4			
1	C	179	Total	C	N	O	S	0	4	0
			1479	949	242	284	4			
1	D	179	Total	C	N	O	S	0	3	0
			1470	943	240	283	4			
1	E	179	Total	C	N	O	S	0	3	0
			1470	942	240	284	4			
1	F	179	Total	C	N	O	S	0	6	0
			1492	954	244	290	4			
1	G	179	Total	C	N	O	S	0	8	0
			1508	963	247	294	4			
1	H	179	Total	C	N	O	S	0	4	0
			1478	947	242	285	4			

There are 24 discrepancies between the modelled and reference sequences:

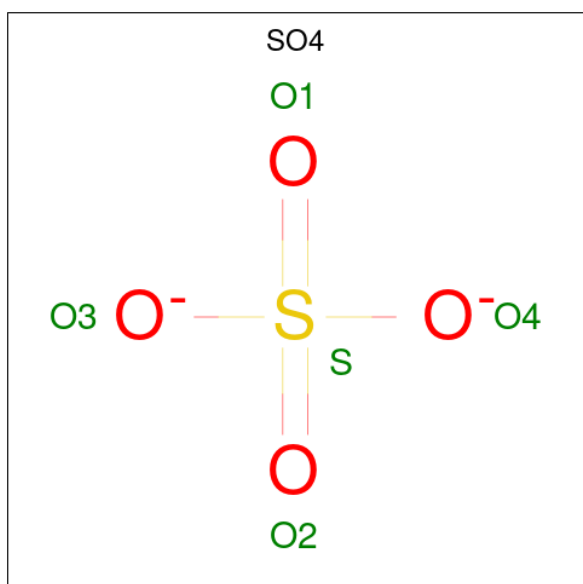
Chain	Residue	Modelled	Actual	Comment	Reference
A	185	ASP	-	expression tag	UNP M0QUM1
A	186	LYS	-	expression tag	UNP M0QUM1
A	187	LEU	-	expression tag	UNP M0QUM1
B	185	ASP	-	expression tag	UNP M0QUM1
B	186	LYS	-	expression tag	UNP M0QUM1
B	187	LEU	-	expression tag	UNP M0QUM1
C	185	ASP	-	expression tag	UNP M0QUM1
C	186	LYS	-	expression tag	UNP M0QUM1
C	187	LEU	-	expression tag	UNP M0QUM1
D	185	ASP	-	expression tag	UNP M0QUM1
D	186	LYS	-	expression tag	UNP M0QUM1
D	187	LEU	-	expression tag	UNP M0QUM1
E	185	ASP	-	expression tag	UNP M0QUM1

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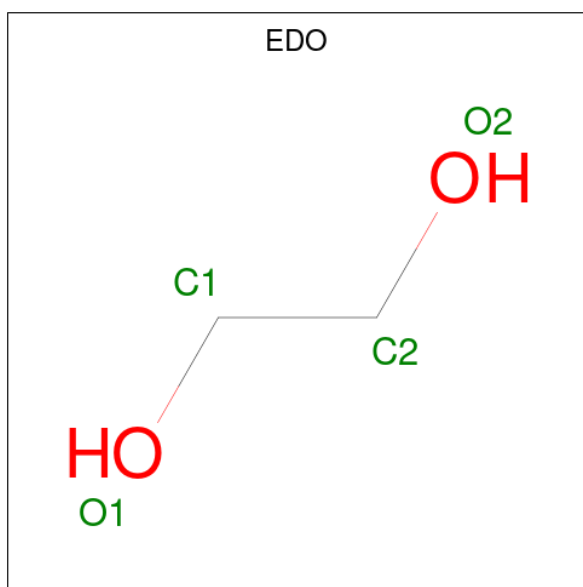
Chain	Residue	Modelled	Actual	Comment	Reference
E	186	LYS	-	expression tag	UNP M0QUM1
E	187	LEU	-	expression tag	UNP M0QUM1
F	185	ASP	-	expression tag	UNP M0QUM1
F	186	LYS	-	expression tag	UNP M0QUM1
F	187	LEU	-	expression tag	UNP M0QUM1
G	185	ASP	-	expression tag	UNP M0QUM1
G	186	LYS	-	expression tag	UNP M0QUM1
G	187	LEU	-	expression tag	UNP M0QUM1
H	185	ASP	-	expression tag	UNP M0QUM1
H	186	LYS	-	expression tag	UNP M0QUM1
H	187	LEU	-	expression tag	UNP M0QUM1

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



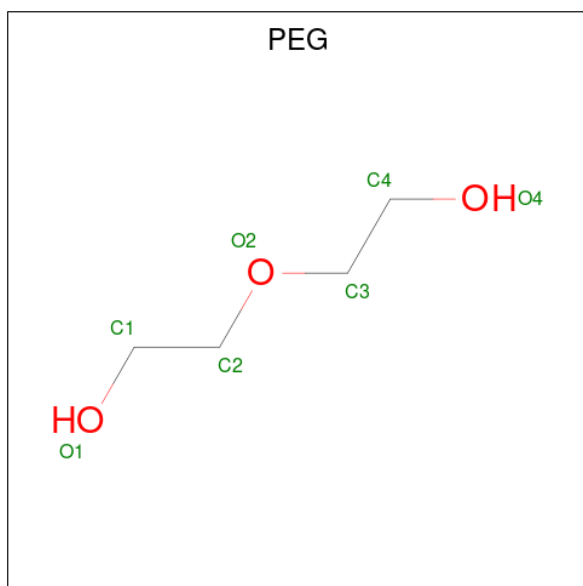
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			7	4	3		

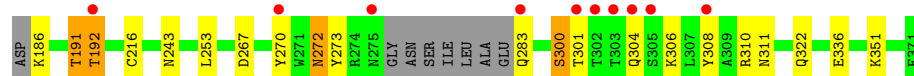
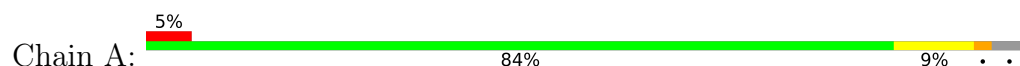
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	183	Total 183	O 183	0	0
5	B	147	Total 147	O 147	0	0
5	C	152	Total 152	O 152	0	0
5	D	159	Total 159	O 159	0	0
5	E	136	Total 136	O 136	0	0
5	F	132	Total 132	O 132	0	0
5	G	174	Total 174	O 174	0	0
5	H	147	Total 147	O 147	0	0

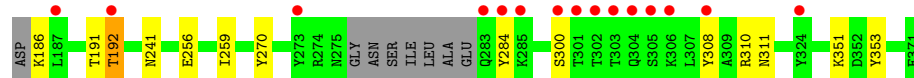
3 Residue-property plots [i](#)

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.

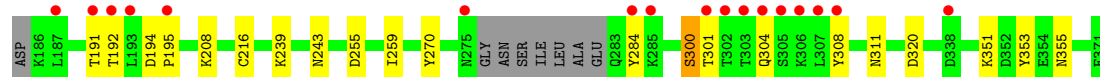
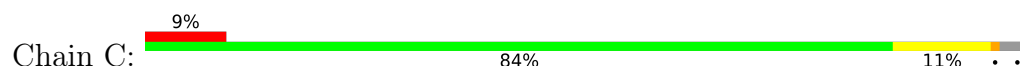
- Molecule 1: Fiber



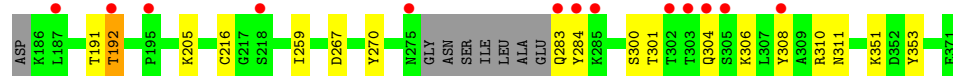
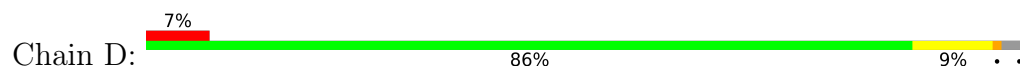
- Molecule 1: Fiber



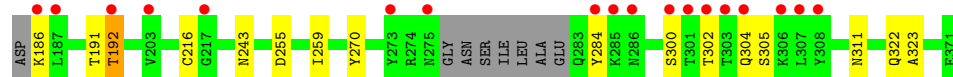
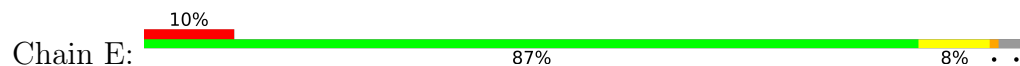
- Molecule 1: Fiber



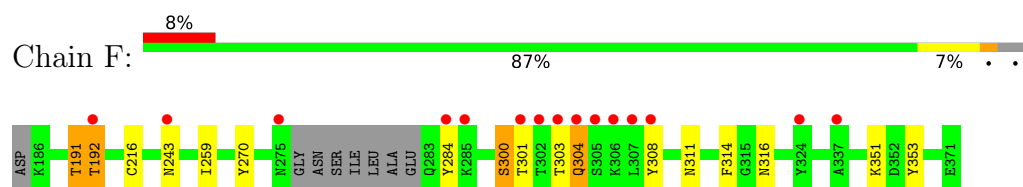
- Molecule 1: Fiber



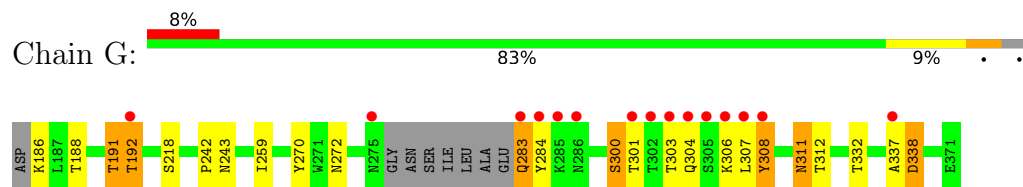
- Molecule 1: Fiber



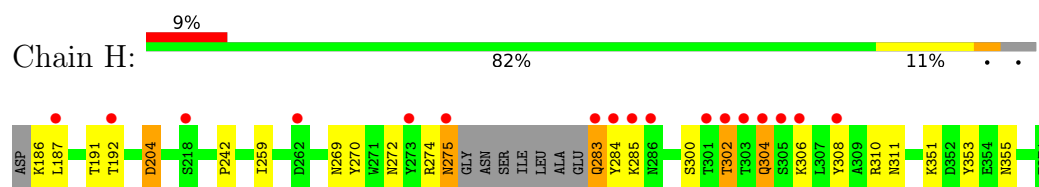
- Molecule 1: Fiber



- Molecule 1: Fiber



- Molecule 1: Fiber



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	126.55Å 126.55Å 251.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.61 – 1.60 82.61 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (82.61-1.60) 100.0 (82.61-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.172 , 0.198 0.183 , 0.206	Depositor DCC
R_{free} test set	9768 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13123	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: SO4, PEG, EDO

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	0.95	0/1514	1.11	3/2056 (0.1%)
1	B	0.96	0/1522	1.10	1/2067 (0.0%)
1	C	0.93	0/1512	1.11	0/2053
1	D	0.96	0/1503	1.12	1/2042 (0.0%)
1	E	0.94	0/1503	1.13	1/2043 (0.0%)
1	F	0.95	0/1525	1.11	2/2072 (0.1%)
1	G	1.01	1/1541 (0.1%)	1.12	2/2094 (0.1%)
1	H	0.98	1/1511 (0.1%)	1.11	2/2053 (0.1%)
All	All	0.96	2/12131 (0.0%)	1.11	12/16480 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	338	ASP	C-O	6.35	1.33	1.23
1	H	302	THR	C-O	5.53	1.30	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	THR	CA-CB-OG1	-5.90	100.75	109.60
1	H	204	ASP	CA-CB-CG	-5.89	106.71	112.60
1	B	192	THR	CA-CB-OG1	-5.56	101.25	109.60
1	H	304	GLN	N-CA-C	-5.46	106.62	113.28
1	F	192	THR	CA-CB-OG1	-5.46	101.41	109.60
1	G	192	THR	CA-CB-OG1	-5.35	101.58	109.60
1	D	192	THR	CA-CB-OG1	-5.33	101.61	109.60
1	E	192	THR	CA-CB-OG1	-5.25	101.72	109.60
1	G	191	THR	N-CA-C	-5.22	102.55	110.28
1	A	267	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	191	THR	N-CA-C	-5.03	102.84	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	191	THR	N-CA-C	-5.01	102.87	110.28

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	1481	0	1463	22	1
1	B	1489	0	1468	7	0
1	C	1479	0	1463	16	0
1	D	1470	0	1451	20	0
1	E	1470	0	1446	12	0
1	F	1492	0	1463	16	0
1	G	1508	0	1477	32	1
1	H	1478	0	1456	16	1
2	C	5	0	0	1	0
2	E	5	0	0	1	0
2	G	5	0	0	0	0
3	E	4	0	6	3	0
4	G	7	0	10	0	0
5	A	183	0	0	5	0
5	B	147	0	0	3	1
5	C	152	0	0	1	0
5	D	159	0	0	6	1
5	E	136	0	0	1	0
5	F	132	0	0	1	0
5	G	174	0	0	4	0
5	H	147	0	0	3	0
All	All	13123	0	11703	124	3

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 5.

All (124) 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:G:307:LEU:HB3	1:G:311[B]:ASN:ND2	1.54	1.22
1:G:307:LEU:CB	1:G:311[B]:ASN:HD21	1.55	1.17
1:G:307:LEU:HB3	1:G:311[B]:ASN:HD21	0.99	1.11
1:A:351[B]:LYS:HB3	1:A:351[B]:LYS:HZ3	1.31	0.93
1:E:322[B]:GLN:NE2	5:E:501:HOH:O	2.13	0.82
1:D:304:GLN:HG3	1:G:304:GLN:HG2	1.62	0.82
1:G:307:LEU:HD13	1:G:311[B]:ASN:ND2	1.95	0.81
1:A:351[B]:LYS:HB3	1:A:351[B]:LYS:NZ	1.96	0.79
1:A:351[B]:LYS:NZ	1:A:351[B]:LYS:CB	2.49	0.73
1:C:355:ASN:HB3	5:C:510:HOH:O	1.88	0.73
1:A:351[B]:LYS:HZ3	1:A:351[B]:LYS:CB	2.00	0.72
1:F:351[B]:LYS:HD3	1:F:353:TYR:CE1	2.25	0.72
1:D:306:LYS:CE	1:G:306:LYS:HD3	2.21	0.71
1:G:312:THR:OG1	1:G:332[B]:THR:HG22	1.91	0.70
1:B:351[B]:LYS:HD3	1:B:353:TYR:CE1	2.27	0.69
1:C:351:LYS:HD3	1:C:353:TYR:CE1	2.27	0.69
1:D:306:LYS:HE2	1:G:306:LYS:HD3	1.73	0.69
1:F:316:ASN:ND2	5:F:401:HOH:O	2.25	0.69
1:D:351:LYS:HD3	1:D:353:TYR:CE1	2.29	0.68
1:H:351[B]:LYS:HD3	1:H:353:TYR:CE1	2.30	0.67
1:G:307:LEU:CB	1:G:311[B]:ASN:ND2	2.32	0.66
1:A:283:GLN:N	5:A:401:HOH:O	2.28	0.66
1:G:304:GLN:OE1	1:G:306:LYS:CD	2.44	0.65
1:E:302:THR:HG23	1:E:305:SER:H	1.62	0.65
1:G:304:GLN:OE1	1:G:306:LYS:HD2	1.96	0.65
1:G:307:LEU:CD1	1:G:311[B]:ASN:ND2	2.60	0.65
1:H:272:ASN:HD21	1:H:283:GLN:HG2	1.66	0.61
1:C:194:ASP:O	1:C:208:LYS:CE	2.49	0.60
1:E:216[B]:CYS:HB2	1:F:216[B]:CYS:HG	1.67	0.60
1:A:322:GLN:NE2	5:A:402:HOH:O	2.34	0.59
1:D:205[A]:LYS:HE3	5:D:518:HOH:O	2.01	0.59
1:E:323:ALA:HB3	3:E:402:EDO:H11	1.83	0.59
1:H:269:ASN:ND2	5:H:401:HOH:O	2.21	0.58
1:D:205[A]:LYS:CE	5:D:518:HOH:O	2.52	0.58
1:A:272:ASN:HD22	1:A:273:TYR:H	1.53	0.57
1:H:355[B]:ASN:ND2	5:H:403:HOH:O	2.38	0.57
1:B:191:THR:HA	1:B:270:TYR:O	2.06	0.56
1:D:308:TYR:CE1	1:G:303:THR:O	2.59	0.56
1:G:307:LEU:CG	1:G:311[B]:ASN:HD21	2.18	0.56
1:H:304:GLN:HB3	1:H:306:LYS:HE3	1.87	0.56
1:G:337:ALA:HB3	5:G:567:HOH:O	2.05	0.56
1:D:308:TYR:HE1	1:G:303:THR:O	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:THR:HA	1:C:270:TYR:O	2.06	0.55
1:D:306:LYS:NZ	5:D:401:HOH:O	2.21	0.55
1:A:191:THR:HA	1:A:270:TYR:O	2.07	0.55
1:E:191:THR:HA	1:E:270:TYR:O	2.06	0.55
1:G:191:THR:HA	1:G:270:TYR:O	2.05	0.55
1:A:351[B]:LYS:HG2	5:A:519:HOH:O	2.05	0.55
1:D:191:THR:HA	1:D:270:TYR:O	2.07	0.55
1:B:241[A]:ASN:ND2	5:B:404:HOH:O	2.40	0.55
1:G:283:GLN:N	1:G:283:GLN:OE1	2.40	0.54
1:C:194:ASP:O	1:C:208:LYS:HE3	2.07	0.54
1:F:191:THR:HA	1:F:270:TYR:O	2.08	0.53
1:H:191:THR:HA	1:H:270:TYR:O	2.09	0.53
1:C:243:ASN:HD21	1:F:243:ASN:HD22	1.56	0.53
1:H:274:ARG:O	1:H:275:ASN:HB2	2.11	0.50
5:B:485:HOH:O	1:C:308:TYR:HB3	2.11	0.49
1:C:195:PRO:HA	1:C:208:LYS:HE3	1.95	0.49
1:E:302:THR:HG23	1:E:305:SER:N	2.28	0.49
1:H:275:ASN:C	1:H:275:ASN:HD22	2.21	0.48
1:A:253:LEU:CD2	1:A:336:GLU:HG3	2.44	0.48
1:E:323:ALA:CB	3:E:402:EDO:H11	2.44	0.48
1:G:242:PRO:HA	5:G:588:HOH:O	2.14	0.48
1:G:307:LEU:CD1	1:G:311[B]:ASN:HD21	2.24	0.48
1:D:283:GLN:OE1	1:D:283:GLN:HA	2.14	0.47
1:A:301:THR:O	1:A:304:GLN:O	2.31	0.47
1:H:187:LEU:HD12	1:H:187:LEU:N	2.30	0.47
1:C:255:ASP:HA	2:C:401:SO4:O2	2.15	0.47
1:D:259:ILE:HD13	1:D:284:TYR:CE1	2.50	0.46
1:D:306:LYS:HE3	1:G:306:LYS:HD3	1.97	0.46
1:G:272:ASN:HD21	1:G:283:GLN:HB2	1.80	0.46
1:A:306:LYS:HE2	1:C:320:ASP:OD1	2.14	0.46
1:B:308:TYR:CD2	1:B:310[B]:ARG:NH2	2.84	0.46
1:C:301:THR:O	1:C:304:GLN:O	2.34	0.46
1:E:255:ASP:HA	2:E:401:SO4:O3	2.15	0.46
1:F:301:THR:O	1:F:304:GLN:O	2.35	0.46
1:A:351[A]:LYS:NZ	5:A:408:HOH:O	2.46	0.45
1:H:242:PRO:HA	5:H:501:HOH:O	2.17	0.45
5:D:536:HOH:O	1:G:308:TYR:HB2	2.16	0.45
1:B:259:ILE:HD13	1:B:284:TYR:CE1	2.52	0.45
1:G:301:THR:O	1:G:304:GLN:O	2.35	0.45
1:F:259:ILE:HD13	1:F:284:TYR:CE1	2.52	0.45
1:G:307:LEU:CG	1:G:311[B]:ASN:ND2	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:THR:C	1:E:192:THR:O	2.59	0.44
1:A:191:THR:C	1:A:192:THR:O	2.60	0.44
1:A:243:ASN:HD22	1:E:243:ASN:HD21	1.64	0.44
1:D:191:THR:C	1:D:192:THR:O	2.60	0.44
1:A:308:TYR:CD2	1:A:310[B]:ARG:NH2	2.86	0.44
1:H:259:ILE:HD13	1:H:284:TYR:CE1	2.52	0.43
1:A:304:GLN:HB3	1:F:304:GLN:OE1	2.18	0.43
1:H:304:GLN:O	1:H:304:GLN:NE2	2.50	0.43
1:D:205[A]:LYS:NZ	1:D:267:ASP:OD2	2.51	0.43
1:D:216[B]:CYS:HG	1:F:216[B]:CYS:HB2	1.84	0.43
1:C:191:THR:C	1:C:192:THR:O	2.60	0.43
1:G:191:THR:C	1:G:192:THR:O	2.60	0.43
1:D:216[B]:CYS:HB2	1:E:216[B]:CYS:HG	1.83	0.43
1:A:308:TYR:CZ	1:F:303:THR:O	2.72	0.43
1:H:308:TYR:CD2	1:H:310:ARG:NH2	2.87	0.43
1:C:239[A]:LYS:HA	1:C:239[A]:LYS:HD3	1.83	0.43
1:C:259:ILE:HD13	1:C:284:TYR:CE2	2.54	0.43
3:E:402:EDO:H22	1:F:314:PHE:CE1	2.54	0.43
1:E:259:ILE:HD13	1:E:284:TYR:CE2	2.54	0.43
1:H:283:GLN:HE21	1:H:283:GLN:HB3	1.65	0.43
1:A:272:ASN:ND2	1:A:273:TYR:H	2.15	0.42
1:B:256:GLU:HG2	5:B:496:HOH:O	2.20	0.42
1:D:310:ARG:HD2	5:D:530:HOH:O	2.19	0.42
1:A:300:SER:HB2	1:A:304:GLN:O	2.19	0.42
5:A:439:HOH:O	1:F:308:TYR:HB2	2.18	0.42
1:G:259:ILE:HD13	1:G:284:TYR:CE1	2.54	0.42
1:F:191:THR:C	1:F:192:THR:O	2.60	0.42
1:D:301:THR:OG1	1:D:304:GLN:HB2	2.20	0.41
1:G:304:GLN:OE1	1:G:306:LYS:CG	2.68	0.41
1:D:205[A]:LYS:HE2	5:D:518:HOH:O	2.19	0.41
1:G:186:LYS:N	5:G:507:HOH:O	2.53	0.41
1:B:191:THR:C	1:B:192:THR:O	2.60	0.41
1:G:300:SER:HB2	1:G:304:GLN:O	2.21	0.41
1:A:216[B]:CYS:HG	1:C:216[B]:CYS:HB2	1.86	0.41
1:F:243:ASN:HD21	1:G:243:ASN:HD22	1.68	0.41
1:H:191:THR:C	1:H:192:THR:O	2.60	0.41
1:H:302:THR:HG22	1:H:304:GLN:H	1.86	0.41
1:A:308:TYR:CE2	1:F:303:THR:O	2.73	0.40
1:C:300:SER:HB2	1:C:304:GLN:O	2.21	0.40
1:F:300:SER:HB2	1:F:304:GLN:O	2.22	0.40
1:G:338:ASP:HB2	5:G:502:HOH:O	2.21	0.40

All (3) 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)
5:B:528:HOH:O	5:D:502:HOH:O[2_665]	1.98	0.22
1:G:188:THR:OG1	1:G:218[A]:SER:OG[2_665]	2.17	0.03
1:A:322:GLN:OE1	1:H:355[B]:ASN:ND2[9_554]	2.18	0.02

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	179/187 (96%)	174 (97%)	5 (3%)	0	100	100
1	B	180/187 (96%)	174 (97%)	6 (3%)	0	100	100
1	C	179/187 (96%)	174 (97%)	5 (3%)	0	100	100
1	D	178/187 (95%)	173 (97%)	5 (3%)	0	100	100
1	E	178/187 (95%)	172 (97%)	6 (3%)	0	100	100
1	F	181/187 (97%)	176 (97%)	5 (3%)	0	100	100
1	G	183/187 (98%)	177 (97%)	6 (3%)	0	100	100
1	H	179/187 (96%)	173 (97%)	6 (3%)	0	100	100
All	All	1437/1496 (96%)	1393 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	168/170 (99%)	164 (98%)	4 (2%)	43	19
1	B	169/170 (99%)	166 (98%)	3 (2%)	51	28
1	C	168/170 (99%)	166 (99%)	2 (1%)	63	43
1	D	167/170 (98%)	165 (99%)	2 (1%)	63	43
1	E	167/170 (98%)	163 (98%)	4 (2%)	43	19
1	F	170/170 (100%)	167 (98%)	3 (2%)	51	28
1	G	172/170 (101%)	167 (97%)	5 (3%)	37	14
1	H	168/170 (99%)	161 (96%)	7 (4%)	26	7
All	All	1349/1360 (99%)	1319 (98%)	30 (2%)	45	22

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	LYS
1	A	272	ASN
1	A	300	SER
1	A	311	ASN
1	B	186	LYS
1	B	300	SER
1	B	311	ASN
1	C	300	SER
1	C	311	ASN
1	D	300	SER
1	D	311	ASN
1	E	186	LYS
1	E	300	SER
1	E	304	GLN
1	E	311	ASN
1	F	300	SER
1	F	304	GLN
1	F	311	ASN
1	G	283	GLN
1	G	300	SER
1	G	308	TYR
1	G	311[A]	ASN
1	G	311[B]	ASN
1	H	186	LYS
1	H	204	ASP
1	H	275	ASN
1	H	283	GLN

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Mol	Chain	Res	Type
1	H	285	LYS
1	H	300	SER
1	H	311	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	A	311	ASN
1	B	269	ASN
1	B	304	GLN
1	B	311	ASN
1	C	243	ASN
1	C	269	ASN
1	C	311	ASN
1	C	322	GLN
1	D	269	ASN
1	D	304	GLN
1	D	311	ASN
1	E	243	ASN
1	E	269	ASN
1	E	304	GLN
1	E	311	ASN
1	F	243	ASN
1	F	269	ASN
1	F	311	ASN
1	F	346	ASN
1	G	223	ASN
1	G	269	ASN
1	G	283	GLN
1	G	286	ASN
1	G	346	ASN
1	H	269	ASN
1	H	275	ASN
1	H	283	GLN
1	H	311	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	E	401	-	4,4,4	0.33	0	6,6,6	0.11	0
4	PEG	G	402	-	6,6,6	0.21	0	5,5,5	0.07	0
3	EDO	E	402	-	3,3,3	0.20	0	2,2,2	0.28	0
2	SO4	C	401	-	4,4,4	0.30	0	6,6,6	0.07	0
2	SO4	G	401	-	4,4,4	0.21	0	6,6,6	0.09	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	E	402	-	-	1/1/1/1	-
4	PEG	G	402	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	402	PEG	O1-C1-C2-O2
3	E	402	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	SO4	1	0
3	E	402	EDO	3	0
2	C	401	SO4	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, 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	179/187 (95%)	0.14	10 (5%)	30 31	12, 23, 57, 95	4 (2%)
1	B	179/187 (95%)	0.37	15 (8%)	17 17	13, 28, 71, 114	5 (2%)
1	C	179/187 (95%)	0.36	17 (9%)	14 14	13, 27, 65, 126	4 (2%)
1	D	179/187 (95%)	0.24	13 (7%)	21 21	13, 25, 60, 91	3 (1%)
1	E	179/187 (95%)	0.42	18 (10%)	12 12	12, 28, 68, 114	3 (1%)
1	F	179/187 (95%)	0.38	15 (8%)	17 17	12, 28, 65, 127	6 (3%)
1	G	179/187 (95%)	0.21	15 (8%)	17 17	8, 22, 61, 126	8 (4%)
1	H	179/187 (95%)	0.41	17 (9%)	14 14	12, 27, 68, 112	4 (2%)
All	All	1432/1496 (95%)	0.32	120 (8%)	17 17	8, 26, 65, 127	37 (2%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	303	THR	7.2
1	G	284	TYR	7.1
1	H	303	THR	6.9
1	H	284	TYR	6.8
1	H	304	GLN	6.8
1	G	303	THR	6.7
1	E	303	THR	5.9
1	B	303	THR	5.8
1	C	303	THR	5.8
1	E	302	THR	5.8
1	B	284	TYR	5.3
1	G	302	THR	5.2
1	A	303	THR	5.0
1	C	284	TYR	5.0
1	F	302	THR	4.9
1	B	308	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	H	308	TYR	4.3
1	D	303	THR	4.3
1	B	302	THR	4.3
1	G	301	THR	4.2
1	C	302	THR	4.1
1	F	305	SER	4.1
1	E	304	GLN	4.1
1	E	284	TYR	4.1
1	E	308	TYR	4.0
1	D	284	TYR	4.0
1	F	284	TYR	4.0
1	B	305	SER	4.0
1	G	285	LYS	4.0
1	A	308	TYR	3.8
1	F	308	TYR	3.8
1	A	302	THR	3.8
1	G	308	TYR	3.8
1	C	285	LYS	3.7
1	D	308	TYR	3.7
1	H	302	THR	3.6
1	A	270	TYR	3.6
1	F	307	LEU	3.5
1	H	283	GLN	3.5
1	C	308	TYR	3.5
1	H	285	LYS	3.5
1	A	304	GLN	3.4
1	D	305	SER	3.4
1	G	307	LEU	3.4
1	G	283	GLN	3.2
1	A	275	ASN	3.2
1	E	301	THR	3.2
1	E	275	ASN	3.1
1	C	193	LEU	3.1
1	D	275	ASN	3.1
1	G	286	ASN	3.1
1	D	302	THR	3.0
1	F	301	THR	3.0
1	B	306	LYS	3.0
1	A	301	THR	2.9
1	B	301	THR	2.9
1	H	273	TYR	2.9
1	H	301	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	304	GLN	2.9
1	C	305	SER	2.9
1	H	305	SER	2.9
1	C	301	THR	2.9
1	H	275	ASN	2.9
1	D	192	THR	2.8
1	E	186	LYS	2.8
1	B	283	GLN	2.8
1	C	304	GLN	2.8
1	D	285	LYS	2.8
1	A	192	THR	2.8
1	G	305	SER	2.7
1	B	300	SER	2.7
1	F	304	GLN	2.7
1	G	304	GLN	2.6
1	B	285	LYS	2.6
1	F	337	ALA	2.6
1	D	283	GLN	2.5
1	E	306	LYS	2.5
1	E	273	TYR	2.5
1	C	338	ASP	2.5
1	D	304	GLN	2.5
1	E	217	GLY	2.5
1	G	306	LYS	2.4
1	G	192	THR	2.4
1	B	187	LEU	2.4
1	G	275	ASN	2.4
1	D	187	LEU	2.3
1	G	337	ALA	2.3
1	E	192	THR	2.3
1	B	324	TYR	2.3
1	H	218	SER	2.3
1	B	192	THR	2.3
1	C	192	THR	2.3
1	F	275	ASN	2.3
1	E	285	LYS	2.3
1	C	195	PRO	2.2
1	F	243	ASN	2.2
1	C	187	LEU	2.2
1	A	305	SER	2.2
1	B	273	TYR	2.2
1	C	191	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	192	THR	2.2
1	F	285	LYS	2.2
1	C	275	ASN	2.2
1	F	192	THR	2.2
1	F	306	LYS	2.2
1	H	187	LEU	2.2
1	C	306	LYS	2.2
1	F	324	TYR	2.2
1	E	300	SER	2.2
1	E	203	VAL	2.1
1	A	283	GLN	2.1
1	E	307	LEU	2.1
1	H	286	ASN	2.1
1	C	307	LEU	2.1
1	H	262	ASP	2.1
1	D	218	SER	2.1
1	E	187	LEU	2.1
1	H	306	LYS	2.1
1	E	286	ASN	2.0
1	D	195	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	E	401	5/5	0.52	0.18	79,88,97,100	0
2	SO4	C	401	5/5	0.54	0.19	66,83,93,96	0
4	PEG	G	402	7/7	0.77	0.17	51,53,57,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	E	402	4/4	0.83	0.15	31,34,36,40	0
2	SO4	G	401	5/5	0.89	0.20	21,25,25,27	5

6.5 Other polymers [i](#)

There are no such residues in this entry.