



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 04:50 pm BST

PDB ID : 8OFQ
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

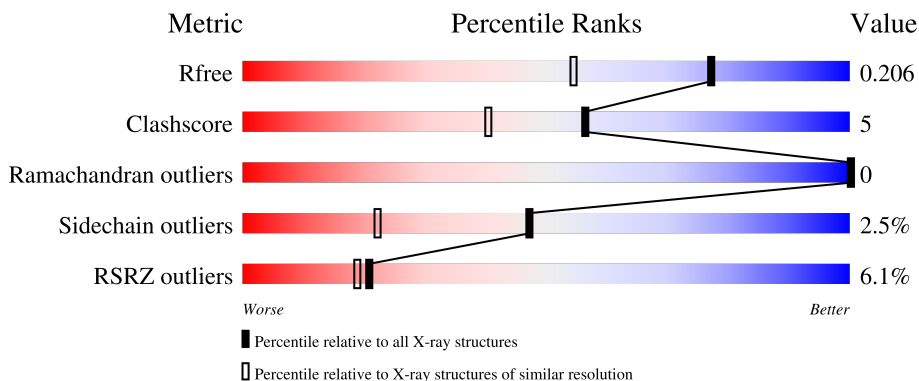
1 Overall quality at a glance i

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.



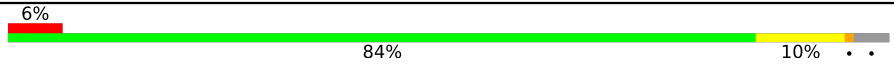
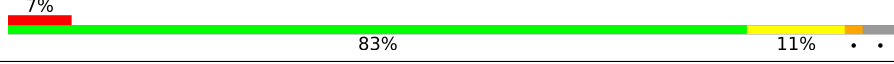
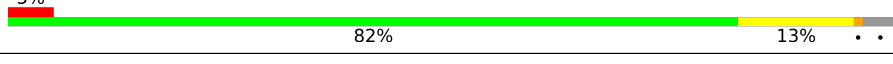
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 $\leq 5\%$. 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	
1	B	187	
1	C	187	
1	D	187	
1	E	187	

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Mol	Chain	Length	Quality of chain
1	F	187	 6% 84% 10% . .
1	G	187	 7% 83% 11% . .
1	H	187	 5% 82% 13% . .

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
			Total	C	N	O	S			
1	A	179	1481	949	244	284	4	0	4	0
1	B	179	1489	953	246	286	4	0	5	0
1	C	179	1479	949	242	284	4	0	4	0
1	D	179	1470	943	240	283	4	0	3	0
1	E	179	1470	942	240	284	4	0	3	0
1	F	179	1492	954	244	290	4	0	6	0
1	G	179	1508	963	247	294	4	0	8	0
1	H	179	1478	947	242	285	4	0	4	0

There are 24 discrepancies between the modelled and reference sequences:

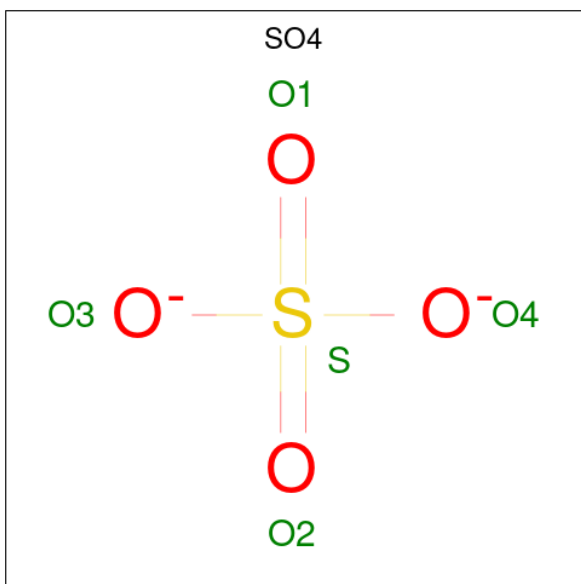
Chain	Residue	Modelled	Actual	Comment	Reference
A	185	ASP	-	expression tag	UNP M0QUM1
A	186	LYS	-	expression tag	UNP M0QUM1
A	187	LEU	-	expression tag	UNP M0QUM1
B	185	ASP	-	expression tag	UNP M0QUM1
B	186	LYS	-	expression tag	UNP M0QUM1
B	187	LEU	-	expression tag	UNP M0QUM1
C	185	ASP	-	expression tag	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 (three-letter code: SO4) (formula: O₄S).



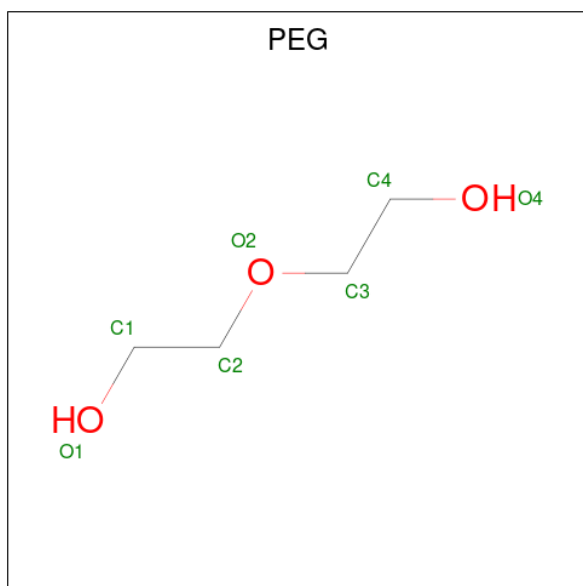
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

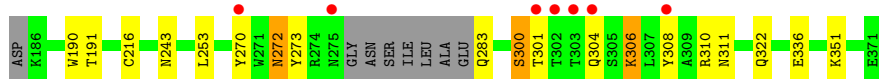
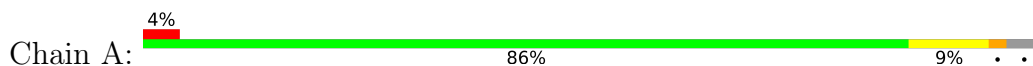
- Molecule 5 is water.

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

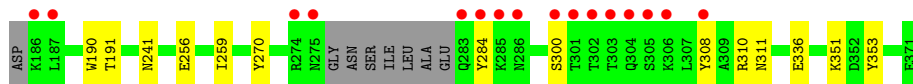
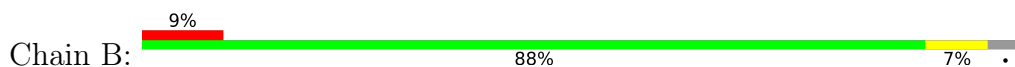
3 Residue-property plots [i](#)

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.

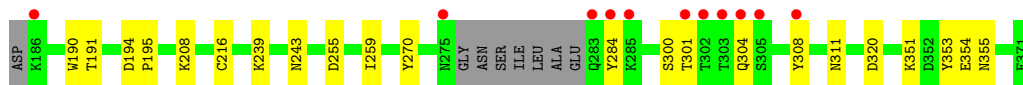
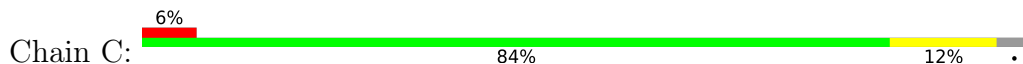
- Molecule 1: Fiber



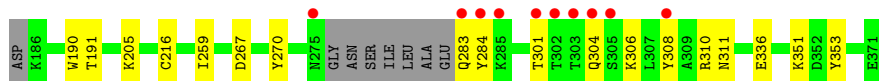
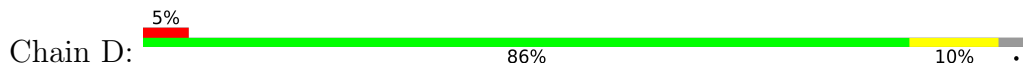
- Molecule 1: Fiber



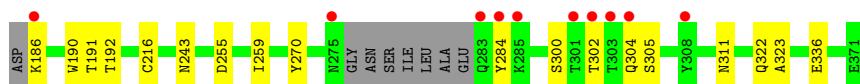
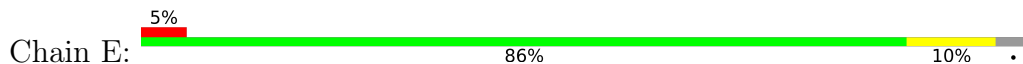
- Molecule 1: Fiber



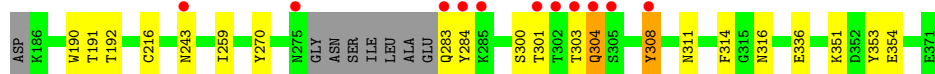
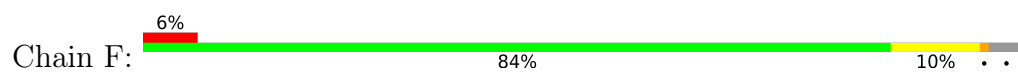
- Molecule 1: Fiber



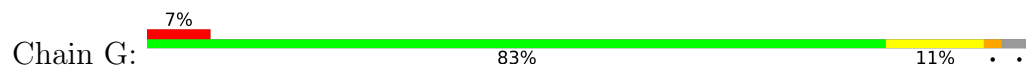
- Molecule 1: Fiber



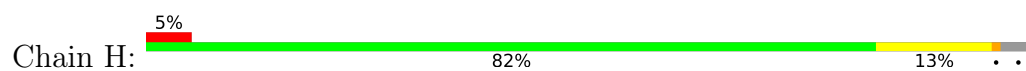
- Molecule 1: Fiber



- 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) 99.9 (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)	Xtrriage
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	Xtrriage
Anisotropy	0.020	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtrriage
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

Xtrriage'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	0.70	0/1514	0.80	0/2056
1	B	0.72	1/1522 (0.1%)	0.78	0/2067
1	C	0.69	1/1512 (0.1%)	0.78	0/2053
1	D	0.73	1/1503 (0.1%)	0.79	0/2042
1	E	0.68	1/1503 (0.1%)	0.80	0/2043
1	F	0.71	2/1525 (0.1%)	0.78	0/2072
1	G	0.76	1/1541 (0.1%)	0.81	0/2094
1	H	0.73	1/1511 (0.1%)	0.77	0/2053
All	All	0.71	8/12131 (0.1%)	0.79	0/16480

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	336	GLU	CD-OE2	8.12	1.34	1.25
1	B	336	GLU	CD-OE2	7.86	1.34	1.25
1	H	336	GLU	CD-OE2	7.09	1.33	1.25
1	F	354	GLU	CD-OE2	-6.84	1.18	1.25
1	F	336	GLU	CD-OE2	5.68	1.31	1.25
1	E	336	GLU	CD-OE2	5.47	1.31	1.25
1	G	338	ASP	C-O	5.46	1.33	1.23
1	C	354	GLU	CD-OE2	-5.44	1.19	1.25

There are no bond angle outliers.

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	21	1
1	B	1489	0	1468	6	0
1	C	1479	0	1463	15	0
1	D	1470	0	1451	19	0
1	E	1470	0	1446	12	0
1	F	1492	0	1463	16	0
1	G	1508	0	1477	31	1
1	H	1478	0	1456	15	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	118	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 (118) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:306:LYS:NZ	5:D:401:HOH:O	2.21	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
1:C:191:THR:HA	1:C:270:TYR:O	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:351[A]:LYS:NZ	5:A:408:HOH:O	2.46	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: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
1:A:243:ASN:HD22	1:E:243:ASN:HD21	1.64	0.44
1:H:275:ASN:C	1:H:275:ASN:HD22	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:F:191:THR:C	1:F: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:E:191:THR:C	1:E:192:THR:O	2.59	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 [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	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 [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	168/170 (99%)	163 (97%)	5 (3%)	41	16
1	B	169/170 (99%)	166 (98%)	3 (2%)	59	36
1	C	168/170 (99%)	166 (99%)	2 (1%)	71	54
1	D	167/170 (98%)	165 (99%)	2 (1%)	71	54
1	E	167/170 (98%)	162 (97%)	5 (3%)	41	16
1	F	170/170 (100%)	165 (97%)	5 (3%)	42	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	172/170 (101%)	168 (98%)	4 (2%)	50	25
1	H	168/170 (99%)	160 (95%)	8 (5%)	25	7
All	All	1349/1360 (99%)	1315 (98%)	34 (2%)	47	22

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	TRP
1	A	272	ASN
1	A	300	SER
1	A	306	LYS
1	A	311	ASN
1	B	190	TRP
1	B	300	SER
1	B	311	ASN
1	C	190	TRP
1	C	311	ASN
1	D	190	TRP
1	D	311	ASN
1	E	186	LYS
1	E	190	TRP
1	E	300	SER
1	E	304	GLN
1	E	311	ASN
1	F	190	TRP
1	F	283	GLN
1	F	304	GLN
1	F	308	TYR
1	F	311	ASN
1	G	190	TRP
1	G	308	TYR
1	G	311[A]	ASN
1	G	311[B]	ASN
1	H	186	LYS
1	H	190	TRP
1	H	204	ASP
1	H	275	ASN
1	H	283	GLN
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 (25) 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	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	269	ASN
1	F	311	ASN
1	G	243	ASN
1	G	269	ASN
1	G	283	GLN
1	G	286	ASN
1	H	269	ASN
1	H	275	ASN
1	H	283	GLN
1	H	311	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

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	0.36	0	6,6,6	0.07	0
4	PEG	G	402	-	6,6,6	0.20	0	5,5,5	0.07	0
2	SO4	C	401	-	4,4,4	0.33	0	6,6,6	0.05	0
3	EDO	E	402	-	3,3,3	0.20	0	2,2,2	0.36	0
2	SO4	G	401	-	4,4,4	0.15	0	6,6,6	0.07	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	G	402	-	-	1/4/4/4	-
3	EDO	E	402	-	-	1/1/1/1	-

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	SO4	1	0
3	E	402	EDO	3	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%)	-0.17	7 (3%) 39 36	16, 24, 57, 95	0
1	B	179/187 (95%)	0.06	16 (8%) 9 8	17, 28, 71, 114	0
1	C	179/187 (95%)	0.08	11 (6%) 21 19	16, 28, 65, 126	0
1	D	179/187 (95%)	-0.16	10 (5%) 24 22	16, 26, 60, 91	0
1	E	179/187 (95%)	-0.02	10 (5%) 24 22	17, 28, 68, 114	0
1	F	179/187 (95%)	-0.01	11 (6%) 21 19	17, 29, 65, 127	0
1	G	179/187 (95%)	0.11	13 (7%) 15 13	15, 23, 61, 126	0
1	H	179/187 (95%)	0.04	10 (5%) 24 22	17, 27, 68, 112	0
All	All	1432/1496 (95%)	-0.01	88 (6%) 21 19	15, 26, 65, 127	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	303	THR	20.2
1	G	302	THR	20.0
1	C	303	THR	14.1
1	F	303	THR	12.2
1	F	302	THR	11.9
1	H	284	TYR	11.8
1	C	302	THR	10.8
1	B	303	THR	10.4
1	B	302	THR	10.4
1	G	284	TYR	9.4
1	H	303	THR	9.2
1	H	304	GLN	9.2
1	B	284	TYR	9.2
1	C	283	GLN	9.1
1	G	283	GLN	8.9
1	B	283	GLN	8.9

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Mol	Chain	Res	Type	RSRZ
1	A	303	THR	8.7
1	H	283	GLN	8.1
1	C	284	TYR	7.6
1	E	275	ASN	7.3
1	E	284	TYR	7.0
1	G	301	THR	6.5
1	C	285	LYS	6.4
1	F	283	GLN	6.3
1	A	275	ASN	6.2
1	H	275	ASN	6.0
1	B	305	SER	5.9
1	A	304	GLN	5.7
1	E	283	GLN	5.7
1	E	303	THR	5.7
1	D	303	THR	5.3
1	B	308	TYR	5.2
1	B	275	ASN	5.2
1	H	305	SER	5.0
1	D	308	TYR	4.8
1	D	302	THR	4.6
1	G	304	GLN	4.6
1	A	302	THR	4.6
1	F	275	ASN	4.4
1	F	284	TYR	4.4
1	B	304	GLN	4.3
1	C	275	ASN	4.3
1	H	301	THR	4.3
1	C	301	THR	4.3
1	G	275	ASN	4.3
1	F	301	THR	4.2
1	D	275	ASN	4.2
1	G	286	ASN	4.2
1	E	304	GLN	4.2
1	H	308	TYR	4.2
1	D	305	SER	4.1
1	E	285	LYS	3.9
1	E	186	LYS	3.8
1	D	284	TYR	3.8
1	F	308	TYR	3.7
1	E	302	THR	3.7
1	B	300	SER	3.6
1	B	285	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	283	GLN	3.4
1	A	301	THR	3.4
1	E	308	TYR	3.2
1	A	308	TYR	3.2
1	C	308	TYR	3.1
1	B	186	LYS	3.0
1	D	301	THR	3.0
1	G	308	TYR	2.9
1	A	270	TYR	2.9
1	F	285	LYS	2.9
1	B	306	LYS	2.8
1	H	273	TYR	2.7
1	F	304	GLN	2.7
1	G	300	SER	2.6
1	H	285	LYS	2.6
1	F	305	SER	2.6
1	D	304	GLN	2.5
1	E	301	THR	2.3
1	D	285	LYS	2.3
1	G	285	LYS	2.3
1	B	286	ASN	2.3
1	G	306	LYS	2.2
1	C	304	GLN	2.2
1	C	186	LYS	2.2
1	B	187	LEU	2.1
1	B	301	THR	2.1
1	C	305	SER	2.1
1	G	307	LEU	2.1
1	F	243	ASN	2.1
1	B	274	ARG	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PEG	G	402	7/7	0.70	0.12	51,53,57,61	0
3	EDO	E	402	4/4	0.81	0.27	31,34,36,40	0
2	SO4	C	401	5/5	0.84	0.52	66,83,93,96	0
2	SO4	E	401	5/5	0.89	0.33	79,88,97,100	0
2	SO4	G	401	5/5	0.89	0.16	21,25,25,27	5

6.5 Other polymers [i](#)

There are no such residues in this entry.