



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 03:08 AM UTC

PDB ID : 28NU / pdb\_000028nu  
Title : Human Adenovirus type C5 knob protein with the KO1 mutation  
Authors : Rizkallah, P.J.; Swift, E.A.; Parker, A.L.  
Deposited on : 2026-02-10  
Resolution : 2.60 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](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.

The types of validation reports are described at

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

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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

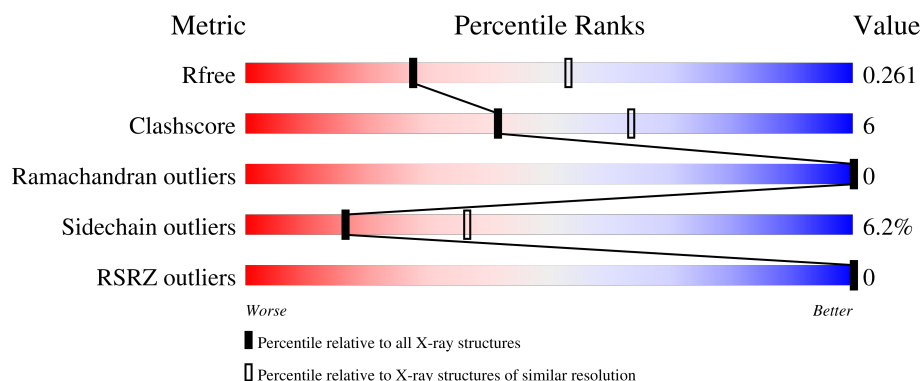
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*






The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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  $\geq 3$ , 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	186	 83% 15% ..
1	B	186	 83% 15% ..
1	C	186	 81% 16% ..
1	D	186	 82% 16% ..
1	E	186	 82% 16% ..

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Mol	Chain	Length	Quality of chain
1	F	186	 83%15%

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	PEG	E	602	-	-	X	-
3	PEG	F	602	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9140 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 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	2	0
			1446	915	235	292	4			
1	B	186	Total	C	N	O	S	0	2	0
			1446	915	235	292	4			
1	C	186	Total	C	N	O	S	0	2	0
			1446	915	235	292	4			
1	D	186	Total	C	N	O	S	0	2	0
			1446	915	235	292	4			
1	E	186	Total	C	N	O	S	0	2	0
			1446	915	235	292	4			
1	F	186	Total	C	N	O	S	0	2	0
			1446	915	235	292	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	ASP	-	expression tag	UNP P11818
A	408	GLU	SER	conflict	UNP P11818
A	409	ALA	PRO	conflict	UNP P11818
A	437	THR	SER	conflict	UNP P11818
A	464	ASP	ASN	conflict	UNP P11818
B	396	ASP	-	expression tag	UNP P11818
B	408	GLU	SER	conflict	UNP P11818
B	409	ALA	PRO	conflict	UNP P11818
B	437	THR	SER	conflict	UNP P11818
B	464	ASP	ASN	conflict	UNP P11818
C	396	ASP	-	expression tag	UNP P11818
C	408	GLU	SER	conflict	UNP P11818
C	409	ALA	PRO	conflict	UNP P11818
C	437	THR	SER	conflict	UNP P11818
C	464	ASP	ASN	conflict	UNP P11818
D	396	ASP	-	expression tag	UNP P11818
D	408	GLU	SER	conflict	UNP P11818

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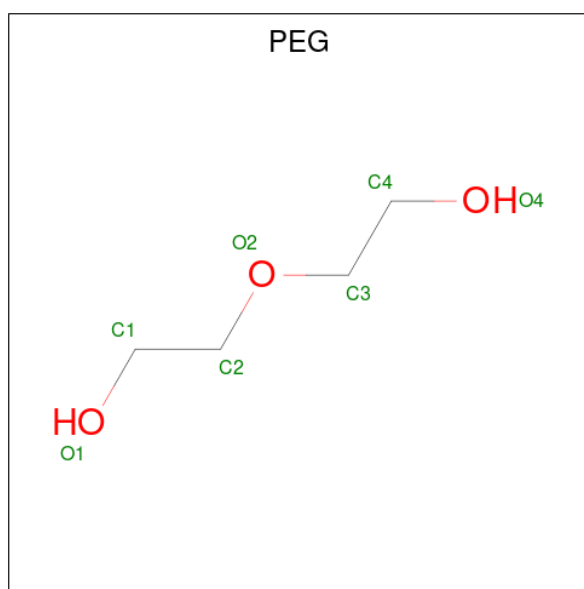
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Chain	Residue	Modelled	Actual	Comment	Reference
D	409	ALA	PRO	conflict	UNP P11818
D	437	THR	SER	conflict	UNP P11818
D	464	ASP	ASN	conflict	UNP P11818
E	396	ASP	-	expression tag	UNP P11818
E	408	GLU	SER	conflict	UNP P11818
E	409	ALA	PRO	conflict	UNP P11818
E	437	THR	SER	conflict	UNP P11818
E	464	ASP	ASN	conflict	UNP P11818
F	396	ASP	-	expression tag	UNP P11818
F	408	GLU	SER	conflict	UNP P11818
F	409	ALA	PRO	conflict	UNP P11818
F	437	THR	SER	conflict	UNP P11818
F	464	ASP	ASN	conflict	UNP P11818

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

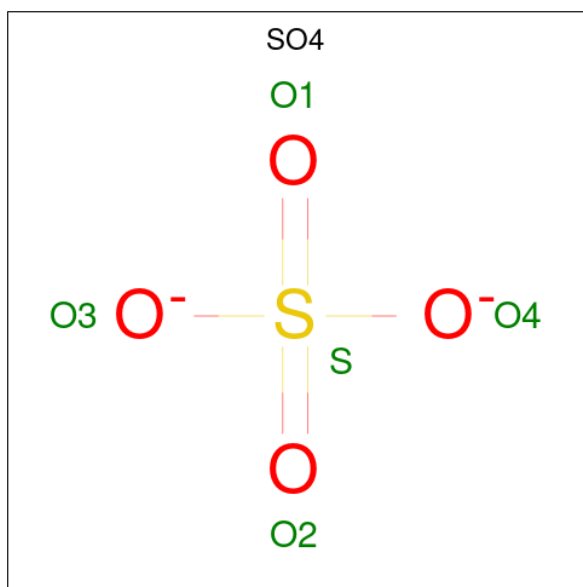
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

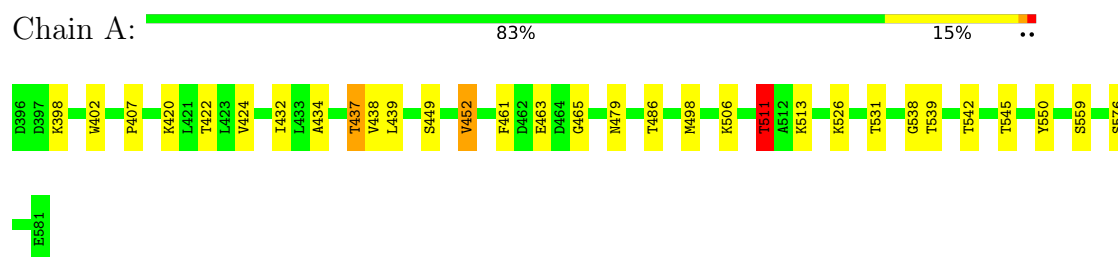
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total 70	O 70	0	0
5	B	62	Total 62	O 62	0	0
5	C	62	Total 62	O 62	0	0
5	D	67	Total 67	O 67	0	0
5	E	63	Total 63	O 63	0	0
5	F	65	Total 65	O 65	0	0

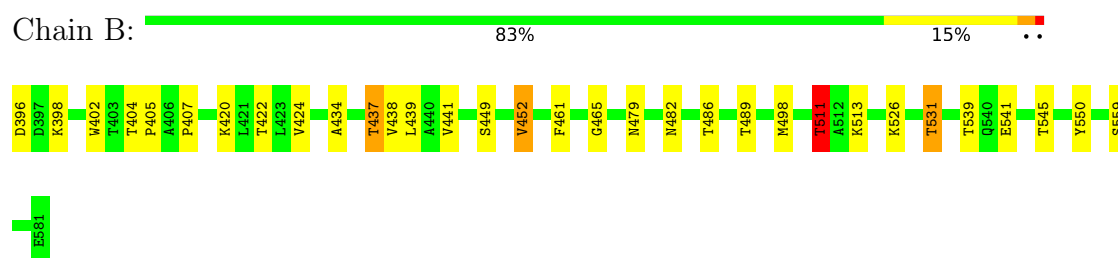
### 3 Residue-property plots [i](#)

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.

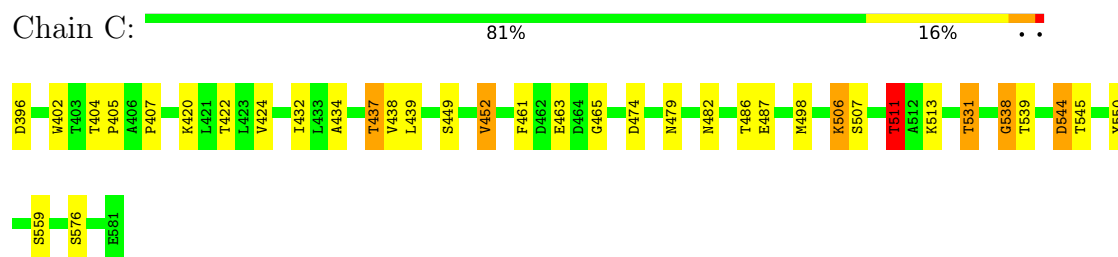
- Molecule 1: Fiber protein



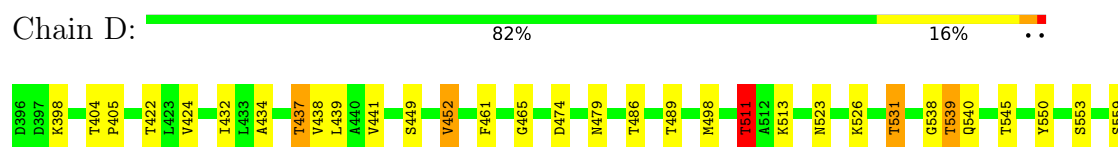
- Molecule 1: Fiber protein



- Molecule 1: Fiber protein



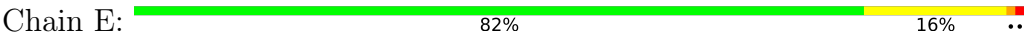
- Molecule 1: Fiber protein



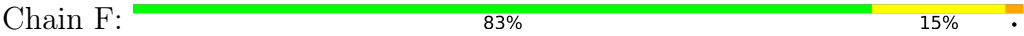




• Molecule 1: Fiber protein



• Molecule 1: Fiber protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.98Å 139.98Å 139.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.20 – 2.60 57.20 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (57.20-2.60) 99.6 (57.20-2.60)	Depositor EDS
$R_{merge}$	0.39	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.214 , 0.257 0.218 , 0.261	Depositor DCC
$R_{free}$ test set	4317 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.459 for -h,-l,-k 0.458 for -h,l,k 0.458 for l,-k,h 0.459 for -l,-k,-h 0.460 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9140	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, MG, 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	1.09	2/1479 (0.1%)	1.30	1/2019 (0.0%)
1	B	1.10	1/1479 (0.1%)	1.28	1/2019 (0.0%)
1	C	1.08	2/1479 (0.1%)	1.29	2/2019 (0.1%)
1	D	1.08	2/1479 (0.1%)	1.29	1/2019 (0.0%)
1	E	1.08	1/1479 (0.1%)	1.27	1/2019 (0.0%)
1	F	1.11	3/1479 (0.2%)	1.27	1/2019 (0.0%)
All	All	1.09	11/8874 (0.1%)	1.28	7/12114 (0.1%)

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	A	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	538	GLY	C-O	6.99	1.30	1.23
1	C	438	VAL	C-O	6.47	1.30	1.24
1	A	538	GLY	C-O	6.42	1.30	1.23
1	F	438	VAL	C-O	6.31	1.30	1.24
1	D	438	VAL	C-O	6.26	1.30	1.24
1	D	538	GLY	C-O	6.16	1.30	1.23
1	E	438	VAL	C-O	6.03	1.30	1.24
1	B	438	VAL	C-O	5.76	1.29	1.24
1	A	438	VAL	C-O	5.50	1.29	1.24
1	F	538	GLY	C-O	5.16	1.29	1.23
1	F	475	PRO	C-O	-5.07	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	511	THR	CB-CA-C	5.57	118.72	109.53
1	E	511	THR	CB-CA-C	5.48	118.57	109.53
1	C	544	ASP	CA-CB-CG	5.46	118.06	112.60
1	C	511	THR	CB-CA-C	5.36	118.38	109.53
1	F	511	THR	CB-CA-C	5.34	118.34	109.53
1	B	511	THR	CB-CA-C	5.32	118.31	109.53
1	A	511	THR	CB-CA-C	5.30	118.27	109.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	542	THR	Peptide

## 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	1446	0	1401	16	0
1	B	1446	0	1401	23	0
1	C	1446	0	1401	22	0
1	D	1446	0	1401	22	0
1	E	1446	0	1401	25	0
1	F	1446	0	1401	21	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	7	0	10	3	0
3	B	14	0	20	3	0
3	C	7	0	10	3	0
3	D	14	0	20	2	0
3	E	14	0	20	7	0
3	F	7	0	10	7	0
4	C	5	0	0	0	0
4	F	5	0	0	0	0
5	A	70	0	0	0	0
5	B	62	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	62	0	0	1	0
5	D	67	0	0	1	0
5	E	63	0	0	1	0
5	F	65	0	0	0	0
All	All	9140	0	8496	110	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 6.

All (110) 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:441:VAL:HB	3:E:602:PEG:H22	1.47	0.96
1:F:439:LEU:HD22	3:F:602:PEG:H32	1.62	0.82
1:E:561:HIS:HD2	5:E:760:HOH:O	1.73	0.70
1:C:439:LEU:HD22	3:C:602:PEG:H32	1.76	0.68
1:E:511:THR:HB	3:F:602:PEG:H42	1.76	0.68
1:B:439:LEU:HD22	3:B:601:PEG:H32	1.75	0.68
1:A:526:LYS:HB2	1:B:531[B]:THR:HG21	1.76	0.66
1:D:561:HIS:HD2	5:D:766:HOH:O	1.80	0.65
1:E:441:VAL:HA	3:E:602:PEG:H12	1.77	0.64
1:B:479:ASN:HB3	1:B:486:THR:HB	1.80	0.64
1:A:479:ASN:HB3	1:A:486:THR:HB	1.80	0.64
1:D:479:ASN:HB3	1:D:486:THR:HB	1.80	0.63
1:C:479:ASN:HB3	1:C:486:THR:HB	1.80	0.63
1:F:479:ASN:HB3	1:F:486:THR:HB	1.80	0.63
1:E:479:ASN:HB3	1:E:486:THR:HB	1.81	0.62
1:D:526:LYS:HB2	1:F:531[B]:THR:HG21	1.81	0.62
3:B:601:PEG:H42	1:C:511:THR:HB	1.81	0.61
1:E:531[B]:THR:HG21	1:F:526:LYS:HB2	1.82	0.61
1:A:439:LEU:HD13	3:A:602:PEG:H31	1.82	0.61
1:D:439:LEU:HD22	3:D:602:PEG:H31	1.83	0.61
3:A:602:PEG:H42	1:B:511:THR:HB	1.84	0.59
1:A:439:LEU:HD22	3:A:602:PEG:H32	1.83	0.59
1:E:441:VAL:HA	3:E:602:PEG:C1	2.33	0.58
1:E:531[B]:THR:HG21	1:F:526:LYS:CB	2.35	0.57
1:D:531[B]:THR:HG21	1:E:526:LYS:HB2	1.87	0.56
1:A:526:LYS:CB	1:B:531[B]:THR:HG21	2.36	0.56
1:B:526:LYS:HB2	1:C:531[B]:THR:HG21	1.86	0.56
1:D:531[B]:THR:HG21	1:E:526:LYS:CB	2.35	0.56
1:E:439:LEU:HD22	3:E:601:PEG:H22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:526:LYS:CB	1:F:531[B]:THR:HG21	2.36	0.54
1:B:437:THR:HG21	1:C:513:LYS:HG3	1.90	0.53
1:A:437:THR:HG21	1:B:513:LYS:HG3	1.91	0.53
1:E:513:LYS:HB2	3:F:602:PEG:H12	1.91	0.53
1:E:513:LYS:HG3	1:F:437:THR:HG21	1.91	0.53
1:A:511:THR:HB	3:C:602:PEG:H42	1.91	0.53
1:C:439:LEU:HD13	3:C:602:PEG:H31	1.89	0.53
1:D:437:THR:HG21	1:F:513:LYS:HG3	1.91	0.52
1:B:526:LYS:CB	1:C:531[B]:THR:HG21	2.39	0.52
1:D:513:LYS:HG3	1:E:437:THR:HG21	1.91	0.52
1:A:422:THR:HB	1:A:437:THR:HG23	1.92	0.52
1:A:513:LYS:HG3	1:C:437:THR:HG21	1.92	0.52
1:C:487:GLU:HB3	5:C:745:HOH:O	2.10	0.52
1:E:422:THR:HB	1:E:437:THR:HG23	1.92	0.51
1:D:422:THR:HB	1:D:437:THR:HG23	1.92	0.50
1:F:422:THR:HB	1:F:437:THR:HG23	1.92	0.50
1:B:422:THR:HB	1:B:437:THR:HG23	1.93	0.50
1:C:538:GLY:HA2	1:C:544:ASP:OD2	2.12	0.50
1:D:449:SER:O	1:D:452:VAL:HG13	2.12	0.50
1:C:422:THR:HB	1:C:437:THR:HG23	1.94	0.49
1:F:489:THR:O	1:F:489:THR:HG23	2.12	0.49
1:D:489:THR:HG23	1:D:489:THR:O	2.13	0.49
1:B:449:SER:O	1:B:452:VAL:HG13	2.12	0.49
1:F:449:SER:O	1:F:452:VAL:HG13	2.13	0.48
1:C:449:SER:O	1:C:452:VAL:HG13	2.14	0.48
1:A:449:SER:O	1:A:452:VAL:HG13	2.13	0.48
1:B:489:THR:O	1:B:489:THR:HG23	2.13	0.47
1:E:489:THR:O	1:E:489:THR:HG23	2.14	0.47
3:B:602:PEG:H41	1:D:511:THR:HG22	1.96	0.46
1:F:439:LEU:HD13	3:F:602:PEG:H31	1.97	0.45
1:D:424:VAL:O	1:D:434:ALA:HA	2.17	0.45
1:F:439:LEU:HB2	3:F:602:PEG:H11	1.99	0.44
1:E:461:PHE:HB3	1:E:465:GLY:HA2	2.00	0.44
1:C:424:VAL:O	1:C:434:ALA:HA	2.17	0.44
1:A:424:VAL:O	1:A:434:ALA:HA	2.17	0.44
1:E:513:LYS:H	3:F:602:PEG:H21	1.83	0.44
1:B:424:VAL:O	1:B:434:ALA:HA	2.18	0.44
1:B:461:PHE:HB3	1:B:465:GLY:HA2	2.00	0.44
1:E:424:VAL:O	1:E:434:ALA:HA	2.18	0.43
1:E:513:LYS:N	3:F:602:PEG:H21	2.33	0.43
1:B:498:MET:HB3	1:B:550:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:539:THR:HG23	1:D:553:SER:OG	2.19	0.43
1:E:512:ALA:HB2	1:F:523:ASN:HA	1.99	0.43
1:D:461:PHE:HB3	1:D:465:GLY:HA2	2.00	0.43
1:F:424:VAL:O	1:F:434:ALA:HA	2.17	0.43
1:F:461:PHE:HB3	1:F:465:GLY:HA2	2.00	0.43
1:A:498:MET:HB3	1:A:550:TYR:CD1	2.54	0.43
1:C:461:PHE:HB3	1:C:465:GLY:HA2	2.00	0.43
1:B:404:THR:HB	1:B:405:PRO:HD2	2.01	0.43
1:E:498:MET:HB3	1:E:550:TYR:CD1	2.54	0.43
1:D:498:MET:HB3	1:D:550:TYR:CD1	2.54	0.43
1:F:498:MET:HB3	1:F:550:TYR:CD1	2.54	0.42
3:E:601:PEG:H11	3:E:602:PEG:H41	2.00	0.42
1:F:432:ILE:O	1:F:576:SER:HA	2.19	0.42
1:D:531[B]:THR:HG21	1:E:526:LYS:HB3	2.01	0.42
1:B:441:VAL:HB	3:E:602:PEG:C2	2.35	0.42
1:C:498:MET:HB3	1:C:550:TYR:CD1	2.54	0.42
1:D:432:ILE:O	1:D:576:SER:HA	2.19	0.42
1:A:461:PHE:HB3	1:A:465:GLY:HA2	2.00	0.42
1:D:441:VAL:HB	3:D:603:PEG:H21	2.02	0.42
1:E:432:ILE:O	1:E:576:SER:HA	2.20	0.41
1:A:407:PRO:O	1:A:420:LYS:HE2	2.21	0.41
1:C:404:THR:HB	1:C:405:PRO:HD2	2.03	0.41
1:D:523:ASN:HA	1:F:512:ALA:HB2	2.02	0.41
1:B:441:VAL:HB	3:E:602:PEG:H31	2.02	0.41
1:E:396:ASP:HB2	1:E:482:ASN:HA	2.03	0.41
1:A:402:TRP:CD1	1:A:402:TRP:C	2.99	0.41
1:C:506:LYS:O	1:C:507:SER:HB2	2.21	0.41
1:A:432:ILE:O	1:A:576:SER:HA	2.20	0.41
1:B:396:ASP:HB2	1:B:482:ASN:HA	2.02	0.41
1:B:437:THR:HG21	1:C:513:LYS:CG	2.51	0.41
1:E:404:THR:HB	1:E:405:PRO:HD2	2.03	0.41
1:C:407:PRO:O	1:C:420:LYS:HE2	2.20	0.41
1:D:404:THR:HB	1:D:405:PRO:HD2	2.03	0.41
1:F:402:TRP:C	1:F:402:TRP:CD1	2.99	0.41
1:B:407:PRO:O	1:B:420:LYS:HE2	2.21	0.40
1:B:402:TRP:C	1:B:402:TRP:CD1	2.99	0.40
1:C:402:TRP:CD1	1:C:402:TRP:C	2.99	0.40
1:C:396:ASP:HB2	1:C:482:ASN:HA	2.04	0.40
1:C:432:ILE:O	1:C:576:SER:HA	2.20	0.40
1:F:489:THR:O	1:F:489:THR:CG2	2.69	0.40

There are no symmetry-related clashes.

## 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	186/186 (100%)	170 (91%)	16 (9%)	0	100	100
1	B	186/186 (100%)	174 (94%)	12 (6%)	0	100	100
1	C	186/186 (100%)	172 (92%)	14 (8%)	0	100	100
1	D	186/186 (100%)	171 (92%)	15 (8%)	0	100	100
1	E	186/186 (100%)	173 (93%)	13 (7%)	0	100	100
1	F	186/186 (100%)	174 (94%)	12 (6%)	0	100	100
All	All	1116/1116 (100%)	1034 (93%)	82 (7%)	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	161/159 (101%)	150 (93%)	11 (7%)	14	32
1	B	161/159 (101%)	151 (94%)	10 (6%)	16	36
1	C	161/159 (101%)	150 (93%)	11 (7%)	14	32
1	D	161/159 (101%)	150 (93%)	11 (7%)	14	32
1	E	161/159 (101%)	150 (93%)	11 (7%)	14	32
1	F	161/159 (101%)	150 (93%)	11 (7%)	14	32
All	All	966/954 (101%)	901 (93%)	65 (7%)	16	33



All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	398	LYS
1	A	437	THR
1	A	452	VAL
1	A	463	GLU
1	A	506	LYS
1	A	511	THR
1	A	531[A]	THR
1	A	531[B]	THR
1	A	539	THR
1	A	545	THR
1	A	559	SER
1	B	398	LYS
1	B	437	THR
1	B	452	VAL
1	B	511	THR
1	B	531[A]	THR
1	B	531[B]	THR
1	B	539	THR
1	B	541	GLU
1	B	545	THR
1	B	559	SER
1	C	437	THR
1	C	452	VAL
1	C	463	GLU
1	C	474	ASP
1	C	506	LYS
1	C	511	THR
1	C	531[A]	THR
1	C	531[B]	THR
1	C	539	THR
1	C	545	THR
1	C	559	SER
1	D	398	LYS
1	D	437	THR
1	D	452	VAL
1	D	474	ASP
1	D	511	THR
1	D	531[A]	THR
1	D	531[B]	THR
1	D	539	THR
1	D	540	GLN
1	D	545	THR

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Mol	Chain	Res	Type
1	D	559	SER
1	E	437	THR
1	E	463	GLU
1	E	474	ASP
1	E	506	LYS
1	E	511	THR
1	E	531[A]	THR
1	E	531[B]	THR
1	E	539	THR
1	E	541	GLU
1	E	545	THR
1	E	559	SER
1	F	437	THR
1	F	452	VAL
1	F	463	GLU
1	F	506	LYS
1	F	511	THR
1	F	531[A]	THR
1	F	531[B]	THR
1	F	539	THR
1	F	541	GLU
1	F	545	THR
1	F	559	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	519	GLN
1	A	565	ASN
1	B	519	GLN
1	B	565	ASN
1	C	519	GLN
1	C	565	ASN
1	D	519	GLN
1	D	540	GLN
1	D	565	ASN
1	E	519	GLN
1	E	565	ASN
1	F	565	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	PEG	D	603	-	6,6,6	0.40	0	5,5,5	0.13	0
3	PEG	E	601	-	6,6,6	0.44	0	5,5,5	0.25	0
4	SO4	C	601	-	4,4,4	0.28	0	6,6,6	0.08	0
3	PEG	D	602	-	6,6,6	0.47	0	5,5,5	0.23	0
3	PEG	B	601	-	6,6,6	0.50	0	5,5,5	0.21	0
3	PEG	E	602	-	6,6,6	0.71	0	5,5,5	0.40	0
3	PEG	A	602	-	6,6,6	0.48	0	5,5,5	0.23	0
3	PEG	C	602	-	6,6,6	0.44	0	5,5,5	0.20	0
3	PEG	B	602	-	6,6,6	0.35	0	5,5,5	0.14	0
4	SO4	F	601	-	4,4,4	0.32	0	6,6,6	0.09	0
3	PEG	F	602	-	6,6,6	0.44	0	5,5,5	0.25	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	PEG	D	603	-	-	3/4/4/4	-
3	PEG	E	601	-	-	2/4/4/4	-
3	PEG	D	602	-	-	3/4/4/4	-
3	PEG	B	601	-	-	0/4/4/4	-
3	PEG	E	602	-	-	2/4/4/4	-
3	PEG	A	602	-	-	2/4/4/4	-
3	PEG	C	602	-	-	0/4/4/4	-
3	PEG	B	602	-	-	3/4/4/4	-
3	PEG	F	602	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	603	PEG	O2-C3-C4-O4
3	B	602	PEG	C4-C3-O2-C2
3	B	602	PEG	C1-C2-O2-C3
3	B	602	PEG	O2-C3-C4-O4
3	E	602	PEG	O2-C3-C4-O4
3	D	603	PEG	C4-C3-O2-C2
3	D	602	PEG	C1-C2-O2-C3
3	E	601	PEG	C4-C3-O2-C2
3	E	602	PEG	C1-C2-O2-C3
3	E	601	PEG	O2-C3-C4-O4
3	D	602	PEG	O2-C3-C4-O4
3	D	603	PEG	O1-C1-C2-O2
3	A	602	PEG	O1-C1-C2-O2
3	D	602	PEG	O1-C1-C2-O2
3	A	602	PEG	C1-C2-O2-C3

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	603	PEG	1	0
3	E	601	PEG	2	0
3	D	602	PEG	1	0
3	B	601	PEG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	602	PEG	6	0
3	A	602	PEG	3	0
3	C	602	PEG	3	0
3	B	602	PEG	1	0
3	F	602	PEG	7	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	186/186 (100%)	-1.46	0 100 100	18, 42, 93, 155	2 (1%)
1	B	186/186 (100%)	-1.43	0 100 100	18, 42, 95, 147	2 (1%)
1	C	186/186 (100%)	-1.44	0 100 100	19, 42, 91, 145	2 (1%)
1	D	186/186 (100%)	-1.45	0 100 100	18, 42, 91, 152	2 (1%)
1	E	186/186 (100%)	-1.44	0 100 100	17, 42, 94, 141	2 (1%)
1	F	186/186 (100%)	-1.43	0 100 100	19, 42, 92, 145	2 (1%)
All	All	1116/1116 (100%)	-1.44	0 100 100	17, 42, 95, 155	12 (1%)

There are no RSRZ outliers to report.

### 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, 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
3	PEG	C	602	7/7	0.98	0.08	66,71,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	B	601	7/7	0.99	0.09	53,62,68,70	0
3	PEG	B	602	7/7	0.99	0.06	56,71,82,88	0
3	PEG	A	602	7/7	0.99	0.11	58,62,69,69	0
3	PEG	D	602	7/7	0.99	0.07	62,67,69,73	0
3	PEG	D	603	7/7	0.99	0.10	56,67,72,75	0
3	PEG	E	601	7/7	0.99	0.05	61,71,76,76	0
3	PEG	E	602	7/7	0.99	0.13	47,63,67,69	0
3	PEG	F	602	7/7	0.99	0.10	61,65,71,71	0
4	SO4	C	601	5/5	0.99	0.04	78,80,94,101	0
4	SO4	F	601	5/5	0.99	0.04	83,84,89,102	0
2	MG	D	601	1/1	1.00	0.04	50,50,50,50	0
2	MG	A	601	1/1	1.00	0.02	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.