



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:41 PM UTC

PDB ID : 3F0Y / pdb_00003f0y
Title : Crystal structure of the human Adenovirus type 14 fiber knob
Authors : Persson, B.D.; Reiter, D.M.; Arnberg, N.; Stehle, T.
Deposited on : 2008-10-27
Resolution : 1.80 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

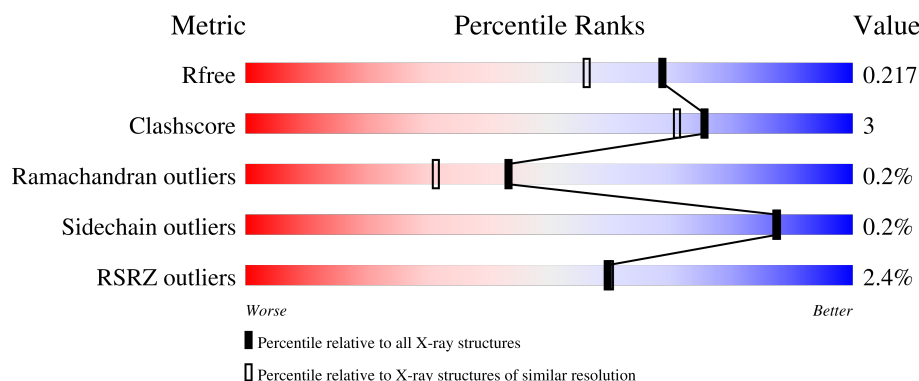
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	208	 2% 90% 5% 5%
1	B	208	 2% 90% 5% 5%
1	C	208	 2% 93% 5% 5%
1	D	208	 3% 87% 8% 5%
1	E	208	 3% 88% 6% 5%

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Mol	Chain	Length	Quality of chain
1	F	208	% 89% 6%5%
1	G	208	3% 90% 6%
1	H	208	% 82% 13%5%
1	I	208	2% 89% 5%5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15886 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	198	Total	C	N	O	S	0	4	0
			1570	986	259	315	10			
1	B	198	Total	C	N	O	S	0	1	0
			1547	969	255	313	10			
1	C	198	Total	C	N	O	S	0	2	0
			1552	974	255	313	10			
1	D	198	Total	C	N	O	S	0	5	0
			1572	989	257	315	11			
1	E	198	Total	C	N	O	S	0	3	0
			1561	982	255	314	10			
1	F	198	Total	C	N	O	S	0	4	0
			1565	985	255	315	10			
1	G	199	Total	C	N	O	S	0	3	0
			1569	988	256	315	10			
1	H	198	Total	C	N	O	S	0	3	0
			1559	978	256	315	10			
1	I	198	Total	C	N	O	S	0	1	0
			1549	970	256	313	10			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	GLY	-	expression tag	UNP Q8V791
A	119	SER	-	expression tag	UNP Q8V791
A	120	HIS	-	expression tag	UNP Q8V791
A	121	MET	-	expression tag	UNP Q8V791
A	122	GLY	-	expression tag	UNP Q8V791
B	118	GLY	-	expression tag	UNP Q8V791
B	119	SER	-	expression tag	UNP Q8V791
B	120	HIS	-	expression tag	UNP Q8V791
B	121	MET	-	expression tag	UNP Q8V791
B	122	GLY	-	expression tag	UNP Q8V791
C	118	GLY	-	expression tag	UNP Q8V791

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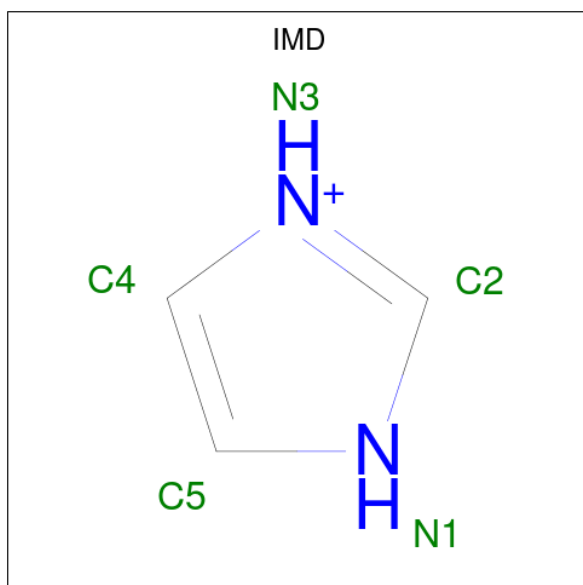
Chain	Residue	Modelled	Actual	Comment	Reference
C	119	SER	-	expression tag	UNP Q8V791
C	120	HIS	-	expression tag	UNP Q8V791
C	121	MET	-	expression tag	UNP Q8V791
C	122	GLY	-	expression tag	UNP Q8V791
D	118	GLY	-	expression tag	UNP Q8V791
D	119	SER	-	expression tag	UNP Q8V791
D	120	HIS	-	expression tag	UNP Q8V791
D	121	MET	-	expression tag	UNP Q8V791
D	122	GLY	-	expression tag	UNP Q8V791
E	118	GLY	-	expression tag	UNP Q8V791
E	119	SER	-	expression tag	UNP Q8V791
E	120	HIS	-	expression tag	UNP Q8V791
E	121	MET	-	expression tag	UNP Q8V791
E	122	GLY	-	expression tag	UNP Q8V791
F	118	GLY	-	expression tag	UNP Q8V791
F	119	SER	-	expression tag	UNP Q8V791
F	120	HIS	-	expression tag	UNP Q8V791
F	121	MET	-	expression tag	UNP Q8V791
F	122	GLY	-	expression tag	UNP Q8V791
G	118	GLY	-	expression tag	UNP Q8V791
G	119	SER	-	expression tag	UNP Q8V791
G	120	HIS	-	expression tag	UNP Q8V791
G	121	MET	-	expression tag	UNP Q8V791
G	122	GLY	-	expression tag	UNP Q8V791
H	118	GLY	-	expression tag	UNP Q8V791
H	119	SER	-	expression tag	UNP Q8V791
H	120	HIS	-	expression tag	UNP Q8V791
H	121	MET	-	expression tag	UNP Q8V791
H	122	GLY	-	expression tag	UNP Q8V791
I	118	GLY	-	expression tag	UNP Q8V791
I	119	SER	-	expression tag	UNP Q8V791
I	120	HIS	-	expression tag	UNP Q8V791
I	121	MET	-	expression tag	UNP Q8V791
I	122	GLY	-	expression tag	UNP Q8V791

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 5 3 2	0	0
3	A	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	183	Total O 183 183	0	0
4	B	225	Total O 225 225	0	0
4	C	185	Total O 185 185	0	0
4	D	216	Total O 216 216	0	0
4	E	199	Total O 199 199	0	0
4	F	223	Total O 223 223	0	0
4	G	218	Total O 218 218	0	0
4	H	183	Total O 183 183	0	0
4	I	171	Total O 171 171	0	0

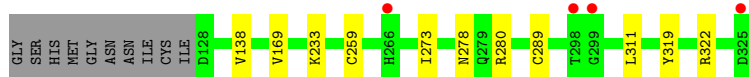
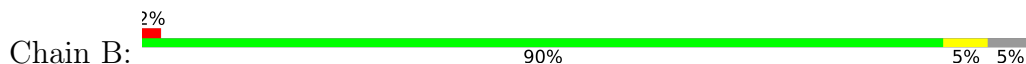
3 Residue-property plots [i](#)

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.

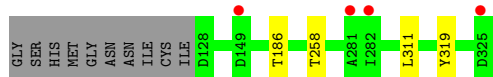
- Molecule 1: Fiber protein



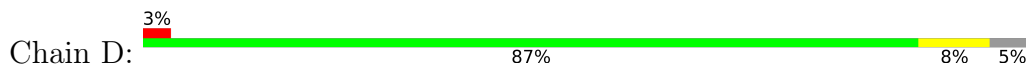
- Molecule 1: Fiber protein



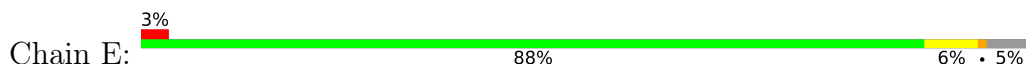
- Molecule 1: Fiber protein



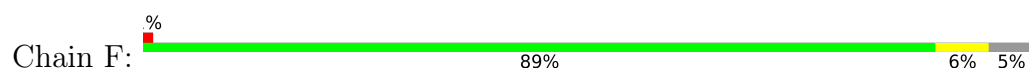
- Molecule 1: Fiber protein



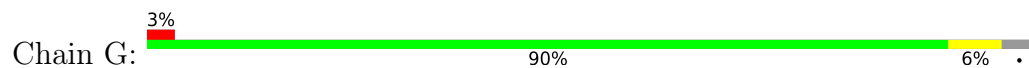
- Molecule 1: Fiber protein



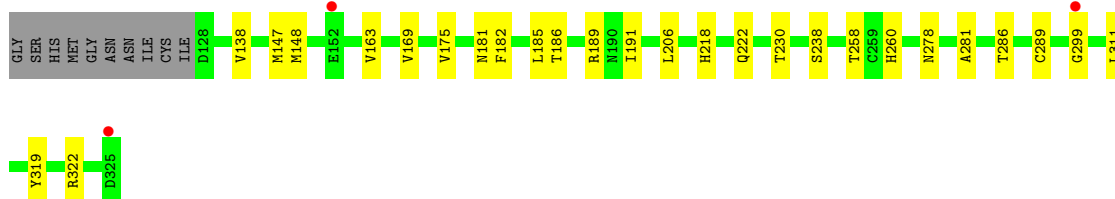
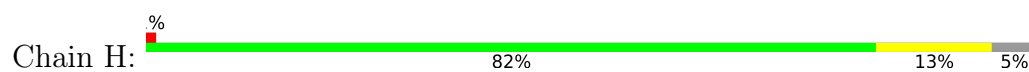
- Molecule 1: Fiber protein



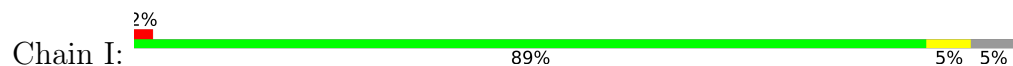
- Molecule 1: Fiber protein



- Molecule 1: Fiber protein



- Molecule 1: Fiber protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	106.47Å 106.47Å 311.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.40 – 1.80 47.40 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.40-1.80) 99.3 (47.40-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.188 , 0.215 0.192 , 0.217	Depositor DCC
R_{free} test set	9272 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15886	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: IMD, GOL

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	0.34	0/1617	0.58	0/2205
1	B	0.35	0/1584	0.58	0/2160
1	C	0.35	0/1592	0.57	0/2172
1	D	0.36	0/1622	0.61	1/2212 (0.0%)
1	E	0.36	0/1605	0.61	2/2190 (0.1%)
1	F	0.35	0/1612	0.58	0/2200
1	G	0.35	0/1613	0.60	0/2201
1	H	0.35	0/1599	0.58	0/2182
1	I	0.35	0/1586	0.62	2/2163 (0.1%)
All	All	0.35	0/14430	0.59	5/19685 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	I	281	ALA	CA-C-N	5.92	132.36	121.70
1	I	281	ALA	C-N-CA	5.92	132.36	121.70
1	D	299	GLY	N-CA-C	-5.65	105.65	112.48
1	E	151	SER	CA-C-N	5.39	131.40	121.70
1	E	151	SER	C-N-CA	5.39	131.40	121.70

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	1570	0	1505	6	0
1	B	1547	0	1475	7	0
1	C	1552	0	1486	4	0
1	D	1572	0	1508	13	0
1	E	1561	0	1494	15	0
1	F	1565	0	1502	11	0
1	G	1569	0	1506	10	0
1	H	1559	0	1492	21	0
1	I	1549	0	1476	11	0
2	A	12	0	16	0	0
2	C	6	0	8	0	0
2	H	6	0	8	0	0
3	A	10	0	10	0	0
3	C	5	0	5	0	0
4	A	183	0	0	0	0
4	B	225	0	0	2	0
4	C	185	0	0	2	0
4	D	216	0	0	0	0
4	E	199	0	0	0	0
4	F	223	0	0	1	0
4	G	218	0	0	1	0
4	H	183	0	0	1	0
4	I	171	0	0	0	0
All	All	15886	0	13491	83	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 3.

All (83) 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:I:281:ALA:HA	1:I:282:ILE:HG23	1.47	0.94
1:D:151:SER:HA	1:D:152:GLU:HB2	1.53	0.89
1:G:319[B]:TYR:OH	1:H:319:TYR:OH	1.88	0.88
1:E:319[A]:TYR:OH	1:F:319[A]:TYR:OH	1.93	0.85
1:E:319[B]:TYR:OH	1:F:319[B]:TYR:OH	1.99	0.81
1:I:281:ALA:HA	1:I:282:ILE:CG2	2.10	0.81
1:D:151:SER:HA	1:D:152:GLU:CB	2.12	0.80
1:E:151:SER:HA	1:E:152:GLU:HB2	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:281:ALA:CA	1:I:282:ILE:HG23	2.13	0.78
1:E:151:SER:HA	1:E:152:GLU:CB	2.25	0.66
1:C:258[B]:THR:HG22	4:C:1406:HOH:O	1.95	0.66
1:E:151:SER:CA	1:E:152:GLU:HB2	2.29	0.61
1:D:218:HIS:HE1	1:D:230:THR:H	1.47	0.60
1:I:281:ALA:HA	1:I:282:ILE:CB	2.31	0.60
1:D:151:SER:CA	1:D:152:GLU:CB	2.81	0.59
1:I:281:ALA:HA	1:I:282:ILE:CG1	2.33	0.58
1:G:218:HIS:HE1	1:G:230:THR:H	1.53	0.57
1:B:319:TYR:OH	1:C:319:TYR:OH	2.02	0.57
1:A:169:VAL:HG23	1:A:322:ARG:HB3	1.88	0.56
1:D:186:THR:CG2	1:D:311:LEU:HD13	2.35	0.56
1:D:184[A]:MET:HE3	1:D:187:THR:HG21	1.87	0.54
1:E:218:HIS:HE1	1:E:230:THR:H	1.54	0.54
1:F:281:ALA:HB1	1:F:286[A]:THR:OG1	2.07	0.53
1:H:186:THR:CG2	1:H:311:LEU:HD13	2.38	0.52
1:H:169:VAL:HG23	1:H:322:ARG:HB3	1.92	0.52
1:G:165[A]:THR:HG22	1:H:163:VAL:HG11	1.92	0.52
1:I:185:LEU:HD22	1:I:191:ILE:HD12	1.91	0.52
1:H:186:THR:HG22	1:H:311:LEU:HD13	1.92	0.51
1:D:169:VAL:HG23	1:D:322:ARG:HB3	1.93	0.50
1:B:278:ASN:HD22	1:B:289:CYS:H	1.58	0.50
1:A:321:ILE:HD13	1:B:138:VAL:HG22	1.94	0.49
1:H:278:ASN:HD22	1:H:289:CYS:H	1.61	0.49
1:G:186:THR:CG2	1:G:311:LEU:HD13	2.43	0.49
1:D:238:SER:OG	1:E:222:GLN:NE2	2.45	0.49
1:G:147:MET:O	4:G:1644:HOH:O	2.19	0.49
1:D:218:HIS:CE1	1:D:230:THR:H	2.29	0.48
1:E:319[B]:TYR:CZ	1:F:319[B]:TYR:OH	2.67	0.48
1:H:185:LEU:HD22	1:H:191:ILE:HD12	1.95	0.48
1:I:169:VAL:HG23	1:I:322:ARG:HB3	1.95	0.48
1:F:169:VAL:HG23	1:F:322:ARG:HB3	1.95	0.48
1:I:186:THR:CG2	1:I:311:LEU:HD13	2.44	0.47
1:A:190:ASN:ND2	1:A:297[A]:ASN:OD1	2.48	0.47
1:H:218:HIS:CE1	1:H:230:THR:H	2.33	0.46
1:B:169:VAL:HG23	1:B:322:ARG:HB3	1.97	0.46
1:F:218:HIS:HE1	1:F:230:THR:H	1.62	0.46
1:D:186:THR:O	1:D:301:ALA:HB1	2.16	0.46
1:D:222:GLN:NE2	1:F:238:SER:OG	2.49	0.46
1:E:278:ASN:HD22	1:E:289:CYS:H	1.63	0.46
1:C:258[B]:THR:HG23	4:C:958:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:VAL:HG23	1:E:322:ARG:HB3	1.99	0.45
1:F:147:MET:O	4:F:1642:HOH:O	2.21	0.45
1:E:165:THR:HG22	1:F:163:VAL:HG11	1.99	0.44
1:F:147:MET:HE3	1:F:175[A]:VAL:HG11	1.99	0.44
1:E:171:ALA:O	1:E:317:THR:HA	2.17	0.44
1:H:147:MET:HE3	1:H:175[A]:VAL:HG11	1.99	0.44
1:A:255:ILE:HG23	4:B:85:HOH:O	2.17	0.43
1:A:185:LEU:HD22	1:A:191:ILE:HD12	2.00	0.43
1:H:281:ALA:HB1	1:H:286[A]:THR:OG1	2.19	0.43
1:B:311:LEU:C	1:B:311:LEU:HD23	2.43	0.43
1:I:209:LEU:HD21	1:I:283:ARG:NH1	2.34	0.43
1:A:138:VAL:HG21	1:A:222:GLN:NE2	2.33	0.43
1:F:171:ALA:O	1:F:317:THR:HA	2.19	0.43
1:B:233:LYS:NZ	4:B:1024:HOH:O	2.52	0.42
1:D:147:MET:HE3	1:D:175[A]:VAL:HG11	2.00	0.42
1:G:319[B]:TYR:CZ	1:H:319:TYR:OH	2.70	0.42
1:H:206:LEU:HD12	1:H:286[A]:THR:HG22	2.01	0.42
1:H:258[A]:THR:HG23	4:H:692:HOH:O	2.18	0.42
1:B:259:CYS:SG	1:B:273:ILE:HD11	2.59	0.42
1:G:238:SER:OG	1:H:222:GLN:NE2	2.52	0.42
1:H:238:SER:OG	1:I:222:GLN:NE2	2.53	0.42
1:G:169:VAL:HG23	1:G:322:ARG:HB3	2.01	0.42
1:H:206:LEU:CD1	1:H:286[A]:THR:HG22	2.50	0.42
1:E:151:SER:HA	1:E:152:GLU:CG	2.50	0.42
1:H:148:MET:HE1	1:H:181:ASN:HB2	2.02	0.41
1:E:151:SER:CA	1:E:152:GLU:CB	2.95	0.41
1:H:189:ARG:NH1	1:H:299:GLY:O	2.54	0.41
1:E:146:GLN:NE2	1:E:151:SER:O	2.54	0.41
1:G:321:ILE:HD13	1:H:138:VAL:HG22	2.02	0.41
1:G:256:TYR:CD1	1:H:260:HIS:HB2	2.56	0.41
1:H:148:MET:HE2	1:H:182:PHE:HB2	2.03	0.41
1:I:236:MET:HA	1:I:236:MET:HE2	2.03	0.40
1:C:186:THR:CG2	1:C:311:LEU:HD13	2.51	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	200/208 (96%)	195 (98%)	5 (2%)	0	100	100
1	B	197/208 (95%)	192 (98%)	5 (2%)	0	100	100
1	C	198/208 (95%)	194 (98%)	4 (2%)	0	100	100
1	D	201/208 (97%)	192 (96%)	7 (4%)	2 (1%)	12	4
1	E	199/208 (96%)	194 (98%)	4 (2%)	1 (0%)	24	14
1	F	200/208 (96%)	196 (98%)	4 (2%)	0	100	100
1	G	200/208 (96%)	198 (99%)	2 (1%)	0	100	100
1	H	199/208 (96%)	192 (96%)	7 (4%)	0	100	100
1	I	197/208 (95%)	191 (97%)	5 (2%)	1 (0%)	24	14
All	All	1791/1872 (96%)	1744 (97%)	43 (2%)	4 (0%)	43	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	152	GLU
1	E	152	GLU
1	I	282	ILE
1	D	300	ASP

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	178/182 (98%)	177 (99%)	1 (1%)	78	77
1	B	175/182 (96%)	174 (99%)	1 (1%)	78	77
1	C	176/182 (97%)	176 (100%)	0	100	100
1	D	179/182 (98%)	179 (100%)	0	100	100
1	E	177/182 (97%)	177 (100%)	0	100	100
1	F	178/182 (98%)	178 (100%)	0	100	100
1	G	178/182 (98%)	178 (100%)	0	100	100
1	H	177/182 (97%)	177 (100%)	0	100	100
1	I	175/182 (96%)	174 (99%)	1 (1%)	78	77
All	All	1593/1638 (97%)	1590 (100%)	3 (0%)	87	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	ARG
1	B	280	ARG
1	I	282	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	190	ASN
1	A	222	GLN
1	A	223	ASN
1	A	305	GLN
1	B	130	ASN
1	B	192	ASN
1	B	222	GLN
1	B	231	ASN
1	B	253	ASN
1	B	278	ASN
1	C	247	ASN
1	C	253	ASN
1	C	305	GLN
1	D	218	HIS
1	D	222	GLN
1	D	231	ASN
1	D	247	ASN

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Mol	Chain	Res	Type
1	D	266	HIS
1	E	130	ASN
1	E	218	HIS
1	E	222	GLN
1	E	278	ASN
1	F	218	HIS
1	F	253	ASN
1	G	130	ASN
1	G	132	ASN
1	G	180	ASN
1	G	218	HIS
1	G	222	GLN
1	G	231	ASN
1	H	130	ASN
1	H	180	ASN
1	H	222	GLN
1	H	231	ASN
1	H	278	ASN
1	H	279	GLN
1	H	297	ASN
1	I	218	HIS
1	I	222	GLN
1	I	247	ASN
1	I	253	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 ⓘ

7 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	GOL	H	1	-	5,5,5	0.41	0	5,5,5	0.21	0
2	GOL	A	2	-	5,5,5	0.35	0	5,5,5	0.30	0
2	GOL	A	3	-	5,5,5	0.37	0	5,5,5	0.23	0
2	GOL	C	4	-	5,5,5	0.38	0	5,5,5	0.25	0
3	IMD	A	326	-	5,5,5	0.62	0	5,5,5	0.43	0
3	IMD	C	2	-	5,5,5	0.64	0	5,5,5	0.44	0
3	IMD	A	1	-	5,5,5	0.63	0	5,5,5	0.45	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
2	GOL	H	1	-	-	0/4/4/4	-
2	GOL	A	2	-	-	4/4/4/4	-
2	GOL	A	3	-	-	2/4/4/4	-
2	GOL	C	4	-	-	4/4/4/4	-
3	IMD	A	326	-	-	-	0/1/1/1
3	IMD	C	2	-	-	-	0/1/1/1
3	IMD	A	1	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2	GOL	O1-C1-C2-C3
2	A	2	GOL	C1-C2-C3-O3
2	A	3	GOL	C1-C2-C3-O3
2	C	4	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	C	4	GOL	C1-C2-C3-O3
2	A	2	GOL	O2-C2-C3-O3
2	A	3	GOL	O2-C2-C3-O3
2	A	2	GOL	O1-C1-C2-O2
2	C	4	GOL	O2-C2-C3-O3
2	C	4	GOL	O1-C1-C2-O2

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, 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	198/208 (95%)	0.26	5 (2%) 58 58	10, 22, 26, 30	4 (2%)
1	B	198/208 (95%)	-0.10	4 (2%) 65 65	10, 16, 23, 26	1 (0%)
1	C	198/208 (95%)	0.20	4 (2%) 65 65	10, 21, 27, 30	2 (1%)
1	D	198/208 (95%)	0.01	7 (3%) 47 47	8, 17, 24, 26	5 (2%)
1	E	198/208 (95%)	0.08	6 (3%) 52 52	8, 18, 25, 28	3 (1%)
1	F	198/208 (95%)	-0.19	3 (1%) 72 72	7, 16, 23, 25	4 (2%)
1	G	199/208 (95%)	-0.02	6 (3%) 52 52	9, 17, 25, 29	3 (1%)
1	H	198/208 (95%)	0.09	3 (1%) 72 72	8, 19, 25, 29	3 (1%)
1	I	198/208 (95%)	0.23	4 (2%) 65 65	13, 21, 27, 31	1 (0%)
All	All	1783/1872 (95%)	0.06	42 (2%) 59 60	7, 18, 26, 31	26 (1%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	282	ILE	5.2
1	F	282	ILE	4.9
1	G	127	ILE	4.9
1	A	282	ILE	4.5
1	C	282	ILE	4.3
1	D	298	THR	3.8
1	G	305	GLN	3.8
1	G	308	ALA	3.7
1	D	152	GLU	3.7
1	A	149	ASP	3.6
1	E	152	GLU	3.2
1	D	300	ASP	3.1
1	G	306	THR	3.1
1	D	266	HIS	3.0
1	I	281	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	149	ASP	2.9
1	E	305	GLN	2.9
1	G	307	SER	2.8
1	B	298	THR	2.7
1	G	304	GLY	2.7
1	D	247	ASN	2.5
1	A	325	ASP	2.4
1	D	189	ARG	2.4
1	H	152	GLU	2.4
1	E	266	HIS	2.4
1	B	325	ASP	2.3
1	D	325	ASP	2.3
1	B	299	GLY	2.3
1	C	325	ASP	2.3
1	H	325	ASP	2.3
1	I	325	ASP	2.3
1	A	281	ALA	2.2
1	F	325	ASP	2.2
1	E	151	SER	2.2
1	F	189	ARG	2.2
1	C	149	ASP	2.1
1	I	300	ASP	2.1
1	A	266	HIS	2.1
1	H	299	GLY	2.0
1	C	281	ALA	2.0
1	B	266	HIS	2.0
1	E	306	THR	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($\text{\AA}^2$)	Q<0.9
2	GOL	A	2	6/6	0.58	0.26	42,42,42,42	0
2	GOL	C	4	6/6	0.66	0.26	63,63,63,63	0
2	GOL	A	3	6/6	0.69	0.23	47,47,47,48	0
3	IMD	A	1	5/5	0.70	0.21	55,55,55,55	0
2	GOL	H	1	6/6	0.74	0.24	32,32,32,32	6
3	IMD	C	2	5/5	0.80	0.17	47,47,47,47	0
3	IMD	A	326	5/5	0.82	0.23	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.