



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:21 AM UTC

PDB ID : 1H7Z / pdb_00001h7z
Title : Adenovirus Ad3 fibre head
Authors : Durmort, C.; Stehlin, C.; Schoehn, G.; Mitraki, A.; Drouet, E.; Cusack, S.;
Burmeister, W.P.
Deposited on : 2001-01-21
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

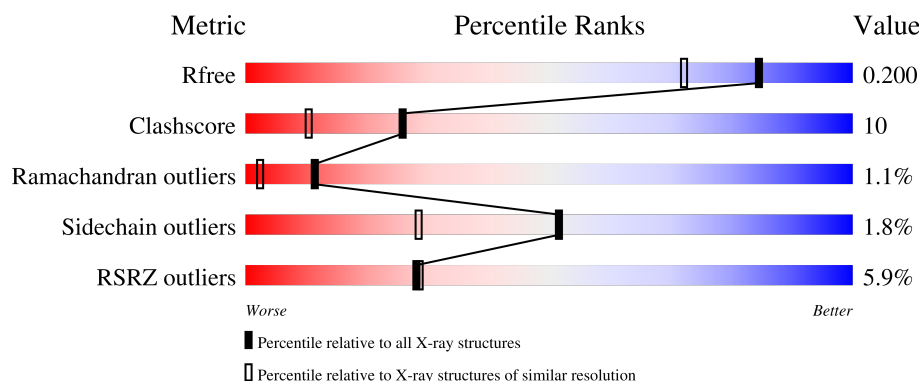
1 Overall quality at a glance

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	194	5% 78% 16% ...
1	B	194	6% 80% 14% ...
1	C	194	7% 76% 19% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5428 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.

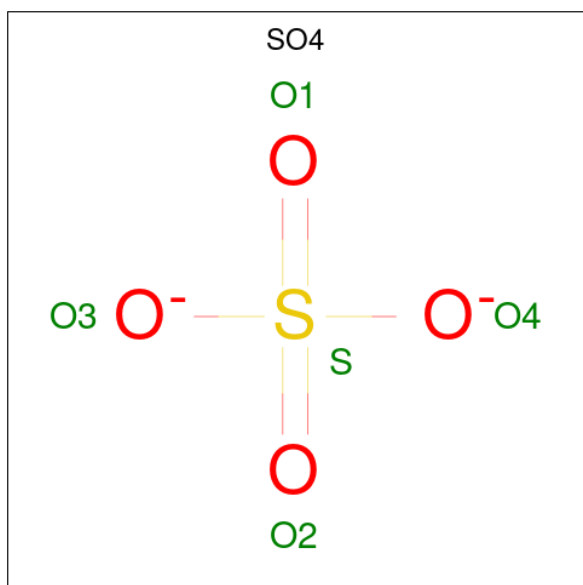
- Molecule 1 is a protein called ADENOVIRUS FIBRE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1499	962	240	291	6			
1	B	191	Total	C	N	O	S	0	0	0
			1499	962	240	291	6			
1	C	191	Total	C	N	O	S	0	0	0
			1499	962	240	291	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	MET	ILE	engineered mutation	UNP P04501
B	126	MET	ILE	engineered mutation	UNP P04501
C	126	MET	ILE	engineered mutation	UNP P04501

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



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

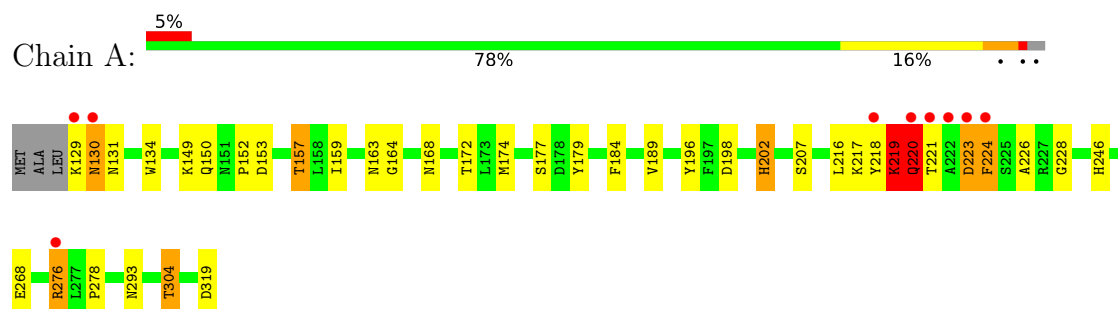
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	275	Total O 275 275	0	0
3	B	290	Total O 290 290	0	0
3	C	326	Total O 326 326	0	0

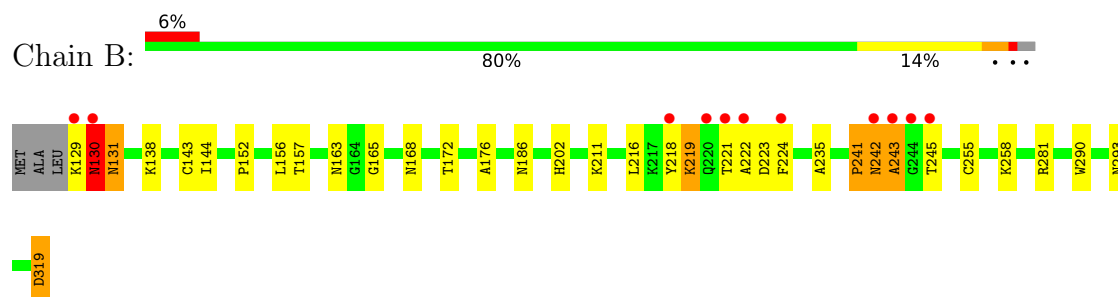
3 Residue-property plots [i](#)

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.

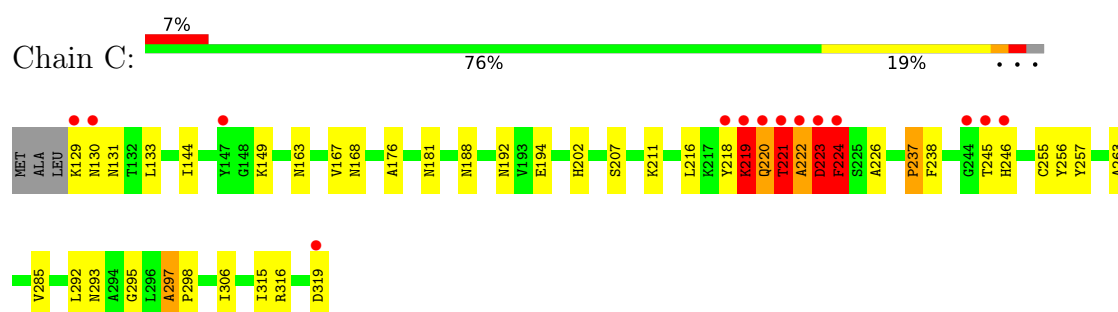
• Molecule 1: ADENOVIRUS FIBRE PROTEIN



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• Molecule 1: ADENOVIRUS FIBRE PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.58Å 96.58Å 154.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 1.60 19.96 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.96-1.60) 95.5 (19.96-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.216 0.169 , 0.200	Depositor DCC
R_{free} test set	5271 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5428	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

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	0.98	3/1536 (0.2%)	2.03	33/2091 (1.6%)
1	B	0.97	1/1536 (0.1%)	1.77	25/2091 (1.2%)
1	C	1.06	0/1536	1.93	33/2091 (1.6%)
All	All	1.00	4/4608 (0.1%)	1.91	91/6273 (1.5%)

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	3
1	B	0	1
1	C	0	2
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	LYS	C-N	-10.48	1.20	1.33
1	B	319	ASP	C-O	7.82	1.39	1.23
1	A	219	LYS	C-O	5.90	1.31	1.24
1	A	221	THR	N-CA	-5.84	1.39	1.46

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	LYS	O-C-N	-30.62	81.86	122.59
1	A	219	LYS	CA-C-O	-19.41	92.75	120.51
1	C	319	ASP	CA-CB-CG	19.38	131.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	GLN	O-C-N	-17.25	101.86	123.26
1	C	224	PHE	CA-CB-CG	13.86	127.66	113.80
1	C	221	THR	N-CA-C	13.83	140.26	110.80
1	C	319	ASP	CA-C-O	-13.34	80.99	121.00
1	A	221	THR	N-CA-CB	13.20	132.15	110.37
1	A	219	LYS	CA-C-N	12.99	142.62	121.58
1	A	219	LYS	C-N-CA	12.99	142.62	121.58
1	A	219	LYS	N-CA-C	12.55	137.53	110.80
1	A	217	LYS	CA-C-N	9.81	136.60	122.77
1	A	217	LYS	C-N-CA	9.81	136.60	122.77
1	B	319	ASP	CA-CB-CG	9.75	122.35	112.60
1	B	130	ASN	CA-CB-CG	-9.63	102.97	112.60
1	B	245	THR	O-C-N	-9.10	112.12	122.86
1	C	223	ASP	N-CA-C	-9.02	101.82	112.92
1	C	224	PHE	CA-C-O	8.96	130.04	120.36
1	B	242	ASN	O-C-N	8.65	134.09	122.59
1	A	220	GLN	CA-C-O	-8.45	109.67	119.98
1	C	263	ALA	O-C-N	8.21	132.54	122.86
1	A	218	TYR	CA-C-N	8.00	136.81	121.54
1	A	218	TYR	C-N-CA	8.00	136.81	121.54
1	A	223	ASP	N-CA-C	-7.81	94.89	108.08
1	A	223	ASP	CB-CA-C	7.73	125.59	116.63
1	B	319	ASP	CA-C-O	-7.58	98.25	121.00
1	C	285	VAL	O-C-N	7.49	131.11	123.10
1	C	181	ASN	OD1-CG-ND2	7.34	129.94	122.60
1	B	222	ALA	N-CA-C	-7.07	103.82	113.30
1	A	246	HIS	CA-CB-CG	-7.00	106.80	113.80
1	A	218	TYR	O-C-N	-6.80	115.31	123.27
1	A	293	ASN	CA-CB-CG	-6.77	105.83	112.60
1	C	221	THR	CB-CA-C	-6.75	96.99	110.42
1	A	220	GLN	CA-C-N	6.71	131.56	122.84
1	A	220	GLN	C-N-CA	6.71	131.56	122.84
1	C	224	PHE	O-C-N	-6.63	115.41	123.30
1	C	263	ALA	CA-C-O	-6.60	114.37	121.56
1	B	319	ASP	CB-CA-C	-6.50	97.75	110.10
1	B	202	HIS	CA-CB-CG	-6.36	107.44	113.80
1	B	245	THR	CA-C-O	6.33	128.46	121.56
1	A	217	LYS	O-C-N	-6.32	114.03	122.43
1	C	207	SER	O-C-N	6.12	131.06	122.36
1	B	242	ASN	CA-C-O	-6.09	111.80	120.51
1	A	179	TYR	O-C-N	6.09	128.34	122.07
1	B	138	LYS	O-C-N	-6.08	116.75	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	PRO	N-CA-C	-6.00	101.78	111.14
1	B	224	PHE	N-CA-C	5.90	119.25	110.52
1	B	235	ALA	CA-C-N	-5.85	115.96	123.16
1	B	235	ALA	C-N-CA	-5.85	115.96	123.16
1	A	134	TRP	N-CA-C	5.85	116.81	108.74
1	A	223	ASP	CA-C-O	-5.84	109.50	119.13
1	C	167	VAL	O-C-N	5.84	129.10	123.14
1	C	297	ALA	N-CA-C	5.67	116.84	109.64
1	A	157	THR	CA-C-O	-5.58	114.38	120.36
1	C	257	TYR	CA-C-O	-5.58	114.33	120.30
1	C	202	HIS	CA-CB-CG	-5.56	108.24	113.80
1	C	257	TYR	O-C-N	5.53	129.68	123.27
1	A	304	THR	CA-C-N	-5.52	113.22	120.95
1	A	304	THR	C-N-CA	-5.52	113.22	120.95
1	B	255	CYS	N-CA-CB	5.51	120.80	110.87
1	A	207	SER	N-CA-CB	-5.46	102.50	110.53
1	C	255	CYS	CA-C-O	-5.42	114.93	121.32
1	C	238	PHE	CA-CB-CG	-5.41	108.39	113.80
1	C	220	GLN	CA-C-O	-5.41	112.78	120.51
1	C	176	ALA	O-C-N	5.38	128.89	122.21
1	A	130	ASN	N-CA-C	-5.34	99.43	110.80
1	B	186	ASN	CA-C-O	-5.33	115.14	121.16
1	B	290	TRP	O-C-N	5.33	129.58	123.29
1	B	241	PRO	CB-CA-C	-5.30	104.62	111.46
1	A	202	HIS	CA-CB-CG	-5.24	108.56	113.80
1	A	276	ARG	CD-NE-CZ	5.18	131.66	124.40
1	B	176	ALA	O-C-N	5.18	127.31	122.18
1	C	263	ALA	CA-C-N	-5.18	115.57	122.72
1	C	263	ALA	C-N-CA	-5.18	115.57	122.72
1	B	290	TRP	CA-C-O	-5.16	114.75	120.38
1	A	218	TYR	N-CA-C	5.14	116.78	108.34
1	B	165	GLY	O-C-N	5.14	129.91	122.26
1	C	219	LYS	N-CA-C	5.12	121.70	110.80
1	C	316	ARG	O-C-N	5.11	128.80	123.03
1	A	198	ASP	CA-CB-CG	5.08	117.69	112.60
1	C	306	ILE	O-C-N	-5.08	117.58	123.07
1	B	143	CYS	N-CA-CB	-5.07	102.09	111.53
1	C	295	GLY	CA-C-O	5.07	125.88	120.30
1	C	237	PRO	CA-C-O	5.07	128.57	122.08
1	C	133	LEU	CA-C-N	-5.06	113.70	122.10
1	C	133	LEU	C-N-CA	-5.06	113.70	122.10
1	C	246	HIS	CB-CG-CD2	5.03	137.74	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	256	TYR	CA-C-O	5.02	127.07	121.40
1	A	224	PHE	CA-C-O	-5.00	115.93	121.28
1	B	156	LEU	CA-C-N	-5.00	116.12	122.77
1	B	156	LEU	C-N-CA	-5.00	116.12	122.77

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	LYS	Mainchain
1	A	220	GLN	Peptide,Mainchain
1	B	293	ASN	Mainchain
1	C	219	LYS	Mainchain
1	C	221	THR	Mainchain

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	1499	0	1470	39	0
1	B	1499	0	1471	24	0
1	C	1499	0	1471	31	0
2	A	10	0	0	1	0
2	B	15	0	0	0	0
2	C	15	0	0	1	0
3	A	275	0	0	5	0
3	B	290	0	0	8	1
3	C	326	0	0	6	1
All	All	5428	0	4412	85	1

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 10.

All (85) 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:A:220:GLN:HG3	1:A:223:ASP:OD1	1.44	1.15
1:A:129:LYS:O	1:A:130:ASN:HB2	1.53	1.04
1:A:220:GLN:CG	1:A:223:ASP:OD1	2.11	0.96
1:A:219:LYS:O	1:A:220:GLN:HG2	1.75	0.87
1:C:131:ASN:HB3	3:C:2076:HOH:O	1.75	0.85
1:A:129:LYS:O	1:A:130:ASN:CB	2.32	0.73
1:C:216:LEU:HD12	1:C:219:LYS:HG3	1.70	0.73
1:C:224:PHE:CE1	1:C:226:ALA:HB2	2.25	0.72
1:B:281:ARG:NH1	3:B:2232:HOH:O	2.23	0.71
1:A:220:GLN:CB	1:A:223:ASP:OD1	2.38	0.71
1:B:218:TYR:O	1:B:219:LYS:HB2	1.91	0.69
1:B:130:ASN:OD1	1:B:218:TYR:O	2.11	0.68
1:A:149:LYS:HG3	2:A:1321:SO4:O4	1.94	0.68
1:C:129:LYS:HG2	1:C:129:LYS:O	1.96	0.65
1:A:168:ASN:HD22	1:C:163:ASN:ND2	1.95	0.64
1:C:224:PHE:HE1	1:C:226:ALA:HB2	1.60	0.64
1:A:219:LYS:O	1:A:219:LYS:HD3	1.96	0.64
1:B:129:LYS:O	1:B:130:ASN:ND2	2.31	0.63
1:A:168:ASN:HD22	1:C:163:ASN:HD21	1.47	0.61
1:C:219:LYS:HG2	3:C:2001:HOH:O	1.99	0.61
1:B:281:ARG:HG3	3:B:2232:HOH:O	2.00	0.60
1:A:219:LYS:O	1:A:220:GLN:CG	2.49	0.59
1:A:202:HIS:CE1	1:A:224:PHE:O	2.55	0.59
1:A:163:ASN:HD21	1:B:168:ASN:HD22	1.52	0.58
1:A:159:ILE:CD1	1:C:315:ILE:HG12	2.35	0.56
1:C:221:THR:HG22	3:C:2178:HOH:O	2.05	0.56
1:B:258:LYS:HE3	3:B:2217:HOH:O	2.05	0.56
1:A:163:ASN:ND2	1:B:168:ASN:HD22	2.04	0.55
1:B:243:ALA:HB2	3:B:2190:HOH:O	2.06	0.55
1:B:144:ILE:HD12	1:B:211:LYS:HE3	1.89	0.55
1:A:131:ASN:HB3	3:A:2066:HOH:O	2.06	0.55
1:B:218:TYR:O	1:B:219:LYS:CB	2.51	0.54
1:C:216:LEU:CD1	1:C:219:LYS:HG3	2.37	0.54
1:C:221:THR:OG1	1:C:223:ASP:HB2	2.07	0.54
1:A:220:GLN:HB3	1:A:223:ASP:OD1	2.06	0.54
1:A:224:PHE:CE1	1:A:226:ALA:HB2	2.43	0.54
1:A:220:GLN:NE2	3:A:2136:HOH:O	2.41	0.53
1:A:228:GLY:HA3	1:A:319:ASP:OD1	2.09	0.53
1:A:219:LYS:O	1:A:219:LYS:CD	2.57	0.52
1:A:268:GLU:HG3	3:A:2181:HOH:O	2.08	0.52
1:C:221:THR:CB	1:C:223:ASP:HB2	2.39	0.52
1:B:163:ASN:ND2	1:C:168:ASN:HD22	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASN:HA	3:B:2002:HOH:O	2.11	0.50
1:A:150:GLN:HG3	3:A:2026:HOH:O	2.11	0.50
1:A:202:HIS:HE1	1:A:224:PHE:O	1.94	0.50
1:A:220:GLN:HB3	1:A:223:ASP:HA	1.94	0.50
1:C:237:PRO:HG2	3:C:2233:HOH:O	2.12	0.50
1:A:219:LYS:O	1:A:220:GLN:CB	2.58	0.50
1:B:223:ASP:HA	3:B:2158:HOH:O	2.11	0.49
1:B:242:ASN:O	1:B:243:ALA:O	2.30	0.49
1:C:144:ILE:HD12	1:C:211:LYS:HE3	1.93	0.49
1:C:131:ASN:CB	3:C:2076:HOH:O	2.48	0.49
1:A:224:PHE:HE1	1:A:226:ALA:HB2	1.78	0.48
1:C:221:THR:HB	1:C:223:ASP:HB2	1.96	0.47
1:B:163:ASN:HD21	1:C:168:ASN:HD22	1.62	0.47
1:C:216:LEU:HD11	1:C:224:PHE:HB2	1.96	0.47
1:C:221:THR:O	1:C:222:ALA:HB3	2.14	0.47
1:A:157:THR:HB	1:A:172:THR:HG22	1.97	0.46
1:A:174:MET:HE3	1:A:304:THR:HG21	1.98	0.46
1:A:220:GLN:NE2	1:A:224:PHE:CE2	2.83	0.46
1:A:276:ARG:NH2	3:A:2211:HOH:O	2.47	0.46
1:C:129:LYS:O	1:C:130:ASN:OD1	2.34	0.46
1:C:216:LEU:HD12	1:C:219:LYS:CG	2.43	0.45
1:B:130:ASN:HB3	1:B:216:LEU:HD13	1.99	0.44
1:B:221:THR:HB	1:B:223:ASP:OD1	2.18	0.44
1:C:129:LYS:O	1:C:129:LYS:CG	2.65	0.44
1:C:218:TYR:HE1	3:C:2003:HOH:O	2.00	0.43
1:A:153:ASP:HB2	1:A:177:SER:HB3	2.00	0.43
1:A:164:GLY:HA2	1:B:131:ASN:HD21	1.84	0.43
1:C:149:LYS:HG3	2:C:1320:SO4:O1	2.18	0.43
1:C:130:ASN:HD22	1:C:216:LEU:HD13	1.83	0.43
1:A:130:ASN:OD1	1:A:216:LEU:HD13	2.19	0.42
1:C:192:ASN:HB3	1:C:194:GLU:OE2	2.17	0.42
1:B:218:TYR:CD1	1:B:218:TYR:N	2.87	0.42
1:A:184:PHE:HD1	1:A:189:VAL:HG21	1.84	0.42
1:B:131:ASN:C	1:B:131:ASN:ND2	2.78	0.42
1:A:224:PHE:N	1:A:224:PHE:CD2	2.87	0.41
1:A:159:ILE:HD11	1:C:315:ILE:CD1	2.51	0.41
1:B:243:ALA:CA	3:B:2190:HOH:O	2.68	0.41
1:C:188:ASN:OD1	1:C:293:ASN:OD1	2.38	0.41
1:A:220:GLN:NE2	1:A:224:PHE:CD2	2.88	0.41
1:C:297:ALA:HA	1:C:298:PRO:HD3	1.96	0.41
1:B:157:THR:HB	1:B:172:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:TYR:CD1	1:A:278:PRO:HG3	2.56	0.41
1:B:241:PRO:O	3:B:2186:HOH:O	2.22	0.41

All (1) 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)
3:B:2228:HOH:O	3:C:2211:HOH:O[5_665]	2.14	0.06

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	189/194 (97%)	180 (95%)	8 (4%)	1 (0%)	24	10
1	B	189/194 (97%)	180 (95%)	6 (3%)	3 (2%)	7	1
1	C	189/194 (97%)	179 (95%)	8 (4%)	2 (1%)	11	2
All	All	567/582 (97%)	539 (95%)	22 (4%)	6 (1%)	11	2

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	LYS
1	B	130	ASN
1	B	219	LYS
1	B	243	ALA
1	C	220	GLN
1	C	222	ALA

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	167/169 (99%)	166 (99%)	1 (1%)	78	66
1	B	167/169 (99%)	164 (98%)	3 (2%)	51	28
1	C	167/169 (99%)	162 (97%)	5 (3%)	36	13
All	All	501/507 (99%)	492 (98%)	9 (2%)	51	28

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	PRO
1	B	131	ASN
1	B	152	PRO
1	B	319	ASP
1	C	221	THR
1	C	223	ASP
1	C	224	PHE
1	C	245	THR
1	C	292	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	202	HIS
1	A	242	ASN
1	A	293	ASN
1	B	131	ASN
1	B	163	ASN
1	B	249	ASN
1	B	293	ASN
1	C	163	ASN
1	C	192	ASN
1	C	202	HIS
1	C	247	ASN

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Mol	Chain	Res	Type
1	C	249	ASN
1	C	254	GLN
1	C	293	ASN
1	C	302	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	C	1320	-	4,4,4	0.67	0	6,6,6	0.34	0
2	SO4	B	1320	-	4,4,4	0.69	0	6,6,6	0.48	0
2	SO4	A	1321	-	4,4,4	0.66	0	6,6,6	0.10	0
2	SO4	C	1322	-	4,4,4	0.68	0	6,6,6	0.70	0
2	SO4	A	1320	-	4,4,4	0.68	0	6,6,6	0.29	0
2	SO4	C	1321	-	4,4,4	0.69	0	6,6,6	0.18	0
2	SO4	B	1322	-	4,4,4	0.71	0	6,6,6	0.75	0
2	SO4	B	1321	-	4,4,4	0.75	0	6,6,6	0.36	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1320	SO4	1	0
2	A	1321	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	191/194 (98%)	0.17	9 (4%) 36 38	22, 32, 54, 77	0
1	B	191/194 (98%)	-0.01	11 (5%) 29 29	20, 28, 61, 76	0
1	C	191/194 (98%)	0.04	14 (7%) 21 21	21, 29, 60, 77	0
All	All	573/582 (98%)	0.07	34 (5%) 28 29	20, 30, 60, 77	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	GLN	7.9
1	A	221	THR	7.8
1	B	243	ALA	6.1
1	A	220	GLN	6.0
1	C	221	THR	6.0
1	C	218	TYR	5.8
1	C	224	PHE	5.3
1	B	218	TYR	5.2
1	A	222	ALA	5.1
1	C	222	ALA	4.9
1	B	130	ASN	4.8
1	A	218	TYR	4.4
1	B	129	LYS	4.4
1	B	221	THR	4.3
1	B	244	GLY	4.3
1	B	222	ALA	4.2
1	A	224	PHE	4.2
1	A	130	ASN	4.2
1	C	219	LYS	3.9
1	B	224	PHE	3.5
1	A	223	ASP	3.4
1	C	129	LYS	3.2
1	C	147	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	245	THR	3.2
1	B	242	ASN	3.0
1	C	220	GLN	2.7
1	C	130	ASN	2.6
1	A	276	ARG	2.5
1	C	223	ASP	2.4
1	A	129	LYS	2.3
1	C	246	HIS	2.3
1	B	245	THR	2.1
1	C	244	GLY	2.0
1	C	319	ASP	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	B	1320	5/5	0.76	0.14	52,60,63,69	0
2	SO4	B	1322	5/5	0.81	0.13	40,44,68,80	5
2	SO4	A	1321	5/5	0.82	0.16	60,71,77,80	5
2	SO4	C	1320	5/5	0.83	0.14	57,63,80,80	0
2	SO4	C	1321	5/5	0.87	0.12	49,57,69,77	5
2	SO4	B	1321	5/5	0.88	0.11	48,48,55,64	5
2	SO4	A	1320	5/5	0.90	0.10	53,54,67,79	0
2	SO4	C	1322	5/5	0.94	0.09	36,41,52,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.