



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:43 PM UTC

PDB ID : 6ITX / pdb_00006itx
Title : Structure of the C-terminal head domain of the avian adenovirus EDSV fiber
Authors : Wei, Q.; Song, Y.
Deposited on : 2018-11-26
Resolution : 2.75 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

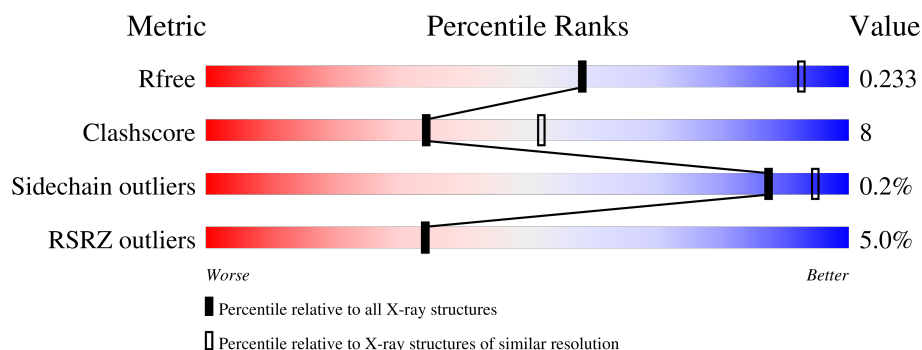
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	301	3% 61%11%27%
1	B	301	2% 62%10%28%
1	C	301	2% 61%11%28%
1	D	301	7% 61%13%26%
1	E	301	3% 54%18%28%
1	F	301	5% 63%10%27%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10245 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	219	Total	C	N	O	S	0	0	0
			1656	1068	269	311	8			
1	B	216	Total	C	N	O	S	0	0	0
			1632	1050	265	309	8			
1	D	223	Total	C	N	O	S	0	0	0
			1684	1083	274	319	8			
1	C	217	Total	C	N	O	S	0	0	0
			1641	1056	267	310	8			
1	E	217	Total	C	N	O	S	0	0	0
			1641	1056	267	310	8			
1	F	221	Total	C	N	O	S	0	0	0
			1666	1073	271	314	8			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP S4TZM6
A	2	GLY	-	expression tag	UNP S4TZM6
A	3	SER	-	expression tag	UNP S4TZM6
A	4	SER	-	expression tag	UNP S4TZM6
A	5	HIS	-	expression tag	UNP S4TZM6
A	6	HIS	-	expression tag	UNP S4TZM6
A	7	HIS	-	expression tag	UNP S4TZM6
A	8	HIS	-	expression tag	UNP S4TZM6
A	9	HIS	-	expression tag	UNP S4TZM6
A	10	HIS	-	expression tag	UNP S4TZM6
A	11	SER	-	expression tag	UNP S4TZM6
A	12	SER	-	expression tag	UNP S4TZM6
A	13	GLY	-	expression tag	UNP S4TZM6
A	14	LEU	-	expression tag	UNP S4TZM6
A	15	VAL	-	expression tag	UNP S4TZM6
A	16	PRO	-	expression tag	UNP S4TZM6
A	17	ARG	-	expression tag	UNP S4TZM6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP S4TZM6
A	19	SER	-	expression tag	UNP S4TZM6
A	20	HIS	-	expression tag	UNP S4TZM6
A	21	MET	-	expression tag	UNP S4TZM6
A	22	ALA	-	expression tag	UNP S4TZM6
A	23	SER	-	expression tag	UNP S4TZM6
A	24	MET	-	expression tag	UNP S4TZM6
A	25	THR	-	expression tag	UNP S4TZM6
A	26	GLY	-	expression tag	UNP S4TZM6
A	27	GLY	-	expression tag	UNP S4TZM6
A	28	GLN	-	expression tag	UNP S4TZM6
A	29	GLN	-	expression tag	UNP S4TZM6
A	30	MET	-	expression tag	UNP S4TZM6
A	31	GLY	-	expression tag	UNP S4TZM6
A	32	ARG	-	expression tag	UNP S4TZM6
A	33	GLY	-	expression tag	UNP S4TZM6
A	34	SER	-	expression tag	UNP S4TZM6
B	1	MET	-	expression tag	UNP S4TZM6
B	2	GLY	-	expression tag	UNP S4TZM6
B	3	SER	-	expression tag	UNP S4TZM6
B	4	SER	-	expression tag	UNP S4TZM6
B	5	HIS	-	expression tag	UNP S4TZM6
B	6	HIS	-	expression tag	UNP S4TZM6
B	7	HIS	-	expression tag	UNP S4TZM6
B	8	HIS	-	expression tag	UNP S4TZM6
B	9	HIS	-	expression tag	UNP S4TZM6
B	10	HIS	-	expression tag	UNP S4TZM6
B	11	SER	-	expression tag	UNP S4TZM6
B	12	SER	-	expression tag	UNP S4TZM6
B	13	GLY	-	expression tag	UNP S4TZM6
B	14	LEU	-	expression tag	UNP S4TZM6
B	15	VAL	-	expression tag	UNP S4TZM6
B	16	PRO	-	expression tag	UNP S4TZM6
B	17	ARG	-	expression tag	UNP S4TZM6
B	18	GLY	-	expression tag	UNP S4TZM6
B	19	SER	-	expression tag	UNP S4TZM6
B	20	HIS	-	expression tag	UNP S4TZM6
B	21	MET	-	expression tag	UNP S4TZM6
B	22	ALA	-	expression tag	UNP S4TZM6
B	23	SER	-	expression tag	UNP S4TZM6
B	24	MET	-	expression tag	UNP S4TZM6
B	25	THR	-	expression tag	UNP S4TZM6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	GLY	-	expression tag	UNP S4TZM6
B	27	GLY	-	expression tag	UNP S4TZM6
B	28	GLN	-	expression tag	UNP S4TZM6
B	29	GLN	-	expression tag	UNP S4TZM6
B	30	MET	-	expression tag	UNP S4TZM6
B	31	GLY	-	expression tag	UNP S4TZM6
B	32	ARG	-	expression tag	UNP S4TZM6
B	33	GLY	-	expression tag	UNP S4TZM6
B	34	SER	-	expression tag	UNP S4TZM6
D	1	MET	-	expression tag	UNP S4TZM6
D	2	GLY	-	expression tag	UNP S4TZM6
D	3	SER	-	expression tag	UNP S4TZM6
D	4	SER	-	expression tag	UNP S4TZM6
D	5	HIS	-	expression tag	UNP S4TZM6
D	6	HIS	-	expression tag	UNP S4TZM6
D	7	HIS	-	expression tag	UNP S4TZM6
D	8	HIS	-	expression tag	UNP S4TZM6
D	9	HIS	-	expression tag	UNP S4TZM6
D	10	HIS	-	expression tag	UNP S4TZM6
D	11	SER	-	expression tag	UNP S4TZM6
D	12	SER	-	expression tag	UNP S4TZM6
D	13	GLY	-	expression tag	UNP S4TZM6
D	14	LEU	-	expression tag	UNP S4TZM6
D	15	VAL	-	expression tag	UNP S4TZM6
D	16	PRO	-	expression tag	UNP S4TZM6
D	17	ARG	-	expression tag	UNP S4TZM6
D	18	GLY	-	expression tag	UNP S4TZM6
D	19	SER	-	expression tag	UNP S4TZM6
D	20	HIS	-	expression tag	UNP S4TZM6
D	21	MET	-	expression tag	UNP S4TZM6
D	22	ALA	-	expression tag	UNP S4TZM6
D	23	SER	-	expression tag	UNP S4TZM6
D	24	MET	-	expression tag	UNP S4TZM6
D	25	THR	-	expression tag	UNP S4TZM6
D	26	GLY	-	expression tag	UNP S4TZM6
D	27	GLY	-	expression tag	UNP S4TZM6
D	28	GLN	-	expression tag	UNP S4TZM6
D	29	GLN	-	expression tag	UNP S4TZM6
D	30	MET	-	expression tag	UNP S4TZM6
D	31	GLY	-	expression tag	UNP S4TZM6
D	32	ARG	-	expression tag	UNP S4TZM6
D	33	GLY	-	expression tag	UNP S4TZM6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	34	SER	-	expression tag	UNP S4TZM6
C	1	MET	-	expression tag	UNP S4TZM6
C	2	GLY	-	expression tag	UNP S4TZM6
C	3	SER	-	expression tag	UNP S4TZM6
C	4	SER	-	expression tag	UNP S4TZM6
C	5	HIS	-	expression tag	UNP S4TZM6
C	6	HIS	-	expression tag	UNP S4TZM6
C	7	HIS	-	expression tag	UNP S4TZM6
C	8	HIS	-	expression tag	UNP S4TZM6
C	9	HIS	-	expression tag	UNP S4TZM6
C	10	HIS	-	expression tag	UNP S4TZM6
C	11	SER	-	expression tag	UNP S4TZM6
C	12	SER	-	expression tag	UNP S4TZM6
C	13	GLY	-	expression tag	UNP S4TZM6
C	14	LEU	-	expression tag	UNP S4TZM6
C	15	VAL	-	expression tag	UNP S4TZM6
C	16	PRO	-	expression tag	UNP S4TZM6
C	17	ARG	-	expression tag	UNP S4TZM6
C	18	GLY	-	expression tag	UNP S4TZM6
C	19	SER	-	expression tag	UNP S4TZM6
C	20	HIS	-	expression tag	UNP S4TZM6
C	21	MET	-	expression tag	UNP S4TZM6
C	22	ALA	-	expression tag	UNP S4TZM6
C	23	SER	-	expression tag	UNP S4TZM6
C	24	MET	-	expression tag	UNP S4TZM6
C	25	THR	-	expression tag	UNP S4TZM6
C	26	GLY	-	expression tag	UNP S4TZM6
C	27	GLY	-	expression tag	UNP S4TZM6
C	28	GLN	-	expression tag	UNP S4TZM6
C	29	GLN	-	expression tag	UNP S4TZM6
C	30	MET	-	expression tag	UNP S4TZM6
C	31	GLY	-	expression tag	UNP S4TZM6
C	32	ARG	-	expression tag	UNP S4TZM6
C	33	GLY	-	expression tag	UNP S4TZM6
C	34	SER	-	expression tag	UNP S4TZM6
E	1	MET	-	expression tag	UNP S4TZM6
E	2	GLY	-	expression tag	UNP S4TZM6
E	3	SER	-	expression tag	UNP S4TZM6
E	4	SER	-	expression tag	UNP S4TZM6
E	5	HIS	-	expression tag	UNP S4TZM6
E	6	HIS	-	expression tag	UNP S4TZM6
E	7	HIS	-	expression tag	UNP S4TZM6

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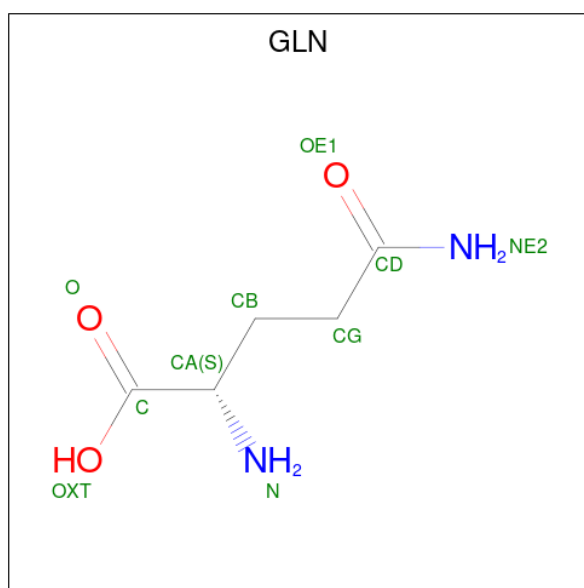
Chain	Residue	Modelled	Actual	Comment	Reference
E	8	HIS	-	expression tag	UNP S4TZM6
E	9	HIS	-	expression tag	UNP S4TZM6
E	10	HIS	-	expression tag	UNP S4TZM6
E	11	SER	-	expression tag	UNP S4TZM6
E	12	SER	-	expression tag	UNP S4TZM6
E	13	GLY	-	expression tag	UNP S4TZM6
E	14	LEU	-	expression tag	UNP S4TZM6
E	15	VAL	-	expression tag	UNP S4TZM6
E	16	PRO	-	expression tag	UNP S4TZM6
E	17	ARG	-	expression tag	UNP S4TZM6
E	18	GLY	-	expression tag	UNP S4TZM6
E	19	SER	-	expression tag	UNP S4TZM6
E	20	HIS	-	expression tag	UNP S4TZM6
E	21	MET	-	expression tag	UNP S4TZM6
E	22	ALA	-	expression tag	UNP S4TZM6
E	23	SER	-	expression tag	UNP S4TZM6
E	24	MET	-	expression tag	UNP S4TZM6
E	25	THR	-	expression tag	UNP S4TZM6
E	26	GLY	-	expression tag	UNP S4TZM6
E	27	GLY	-	expression tag	UNP S4TZM6
E	28	GLN	-	expression tag	UNP S4TZM6
E	29	GLN	-	expression tag	UNP S4TZM6
E	30	MET	-	expression tag	UNP S4TZM6
E	31	GLY	-	expression tag	UNP S4TZM6
E	32	ARG	-	expression tag	UNP S4TZM6
E	33	GLY	-	expression tag	UNP S4TZM6
E	34	SER	-	expression tag	UNP S4TZM6
F	1	MET	-	expression tag	UNP S4TZM6
F	2	GLY	-	expression tag	UNP S4TZM6
F	3	SER	-	expression tag	UNP S4TZM6
F	4	SER	-	expression tag	UNP S4TZM6
F	5	HIS	-	expression tag	UNP S4TZM6
F	6	HIS	-	expression tag	UNP S4TZM6
F	7	HIS	-	expression tag	UNP S4TZM6
F	8	HIS	-	expression tag	UNP S4TZM6
F	9	HIS	-	expression tag	UNP S4TZM6
F	10	HIS	-	expression tag	UNP S4TZM6
F	11	SER	-	expression tag	UNP S4TZM6
F	12	SER	-	expression tag	UNP S4TZM6
F	13	GLY	-	expression tag	UNP S4TZM6
F	14	LEU	-	expression tag	UNP S4TZM6
F	15	VAL	-	expression tag	UNP S4TZM6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	16	PRO	-	expression tag	UNP S4TZM6
F	17	ARG	-	expression tag	UNP S4TZM6
F	18	GLY	-	expression tag	UNP S4TZM6
F	19	SER	-	expression tag	UNP S4TZM6
F	20	HIS	-	expression tag	UNP S4TZM6
F	21	MET	-	expression tag	UNP S4TZM6
F	22	ALA	-	expression tag	UNP S4TZM6
F	23	SER	-	expression tag	UNP S4TZM6
F	24	MET	-	expression tag	UNP S4TZM6
F	25	THR	-	expression tag	UNP S4TZM6
F	26	GLY	-	expression tag	UNP S4TZM6
F	27	GLY	-	expression tag	UNP S4TZM6
F	28	GLN	-	expression tag	UNP S4TZM6
F	29	GLN	-	expression tag	UNP S4TZM6
F	30	MET	-	expression tag	UNP S4TZM6
F	31	GLY	-	expression tag	UNP S4TZM6
F	32	ARG	-	expression tag	UNP S4TZM6
F	33	GLY	-	expression tag	UNP S4TZM6
F	34	SER	-	expression tag	UNP S4TZM6

- Molecule 2 is GLUTAMINE (CCD ID: GLN) (formula: $C_5H_{10}N_2O_3$).



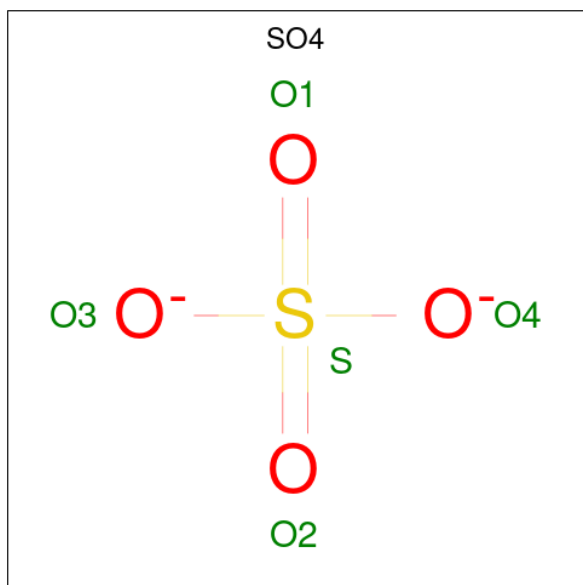
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	5	2	2		
2	B	1	Total	C	N	O	0	0
			9	5	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			9	5	2	2		
2	E	1	Total	C	N	O	0	0
			9	5	2	2		
2	F	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

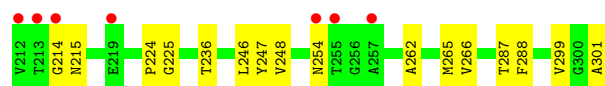
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		

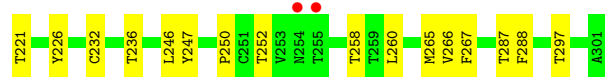
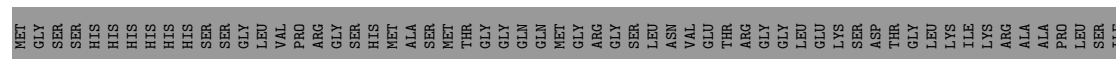
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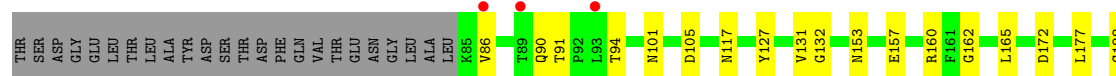
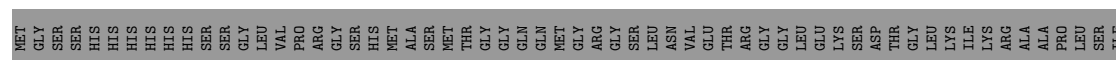
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	58	Total 58	O 58	0	0
4	D	40	Total 40	O 40	0	0
4	C	61	Total 61	O 61	0	0
4	E	25	Total 25	O 25	0	0
4	F	18	Total 18	O 18	0	0



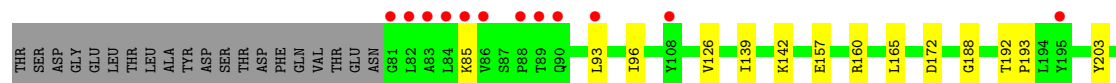
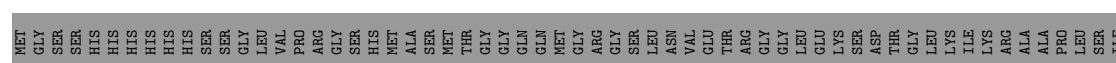
• Molecule 1: Fiber protein



• Molecule 1: Fiber protein



• Molecule 1: Fiber protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.52Å 63.24Å 165.81Å 90.00° 93.54° 90.00°	Depositor
Resolution (Å)	29.88 – 2.75 29.88 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.88-2.75) 98.9 (29.88-2.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.72Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.192 , 0.232 0.194 , 0.233	Depositor DCC
R_{free} test set	2903 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtrriage
Anisotropy	0.114	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10245	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3989e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.40	0/1704	0.67	2/2335 (0.1%)
1	B	0.39	0/1681	0.62	2/2306 (0.1%)
1	C	0.40	0/1690	0.62	2/2317 (0.1%)
1	D	0.38	0/1732	0.60	2/2373 (0.1%)
1	E	0.33	0/1690	0.57	2/2317 (0.1%)
1	F	0.33	0/1715	0.54	0/2351
All	All	0.37	0/10212	0.61	10/13999 (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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	237	THR	CA-C-N	-8.43	104.90	121.41
1	A	237	THR	C-N-CA	-8.43	104.90	121.41
1	D	157	GLU	CA-C-N	-6.87	107.22	123.16
1	D	157	GLU	C-N-CA	-6.87	107.22	123.16
1	C	157	GLU	CA-C-N	-6.43	109.18	122.82
1	C	157	GLU	C-N-CA	-6.43	109.18	122.82
1	E	157	GLU	CA-C-N	-5.89	111.13	123.20
1	E	157	GLU	C-N-CA	-5.89	111.13	123.20
1	B	157	GLU	CA-C-N	-5.16	113.03	122.12
1	B	157	GLU	C-N-CA	-5.16	113.03	122.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	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	1656	0	1607	23	0
1	B	1632	0	1573	23	0
1	C	1641	0	1586	24	0
1	D	1684	0	1629	27	0
1	E	1641	0	1586	42	0
1	F	1666	0	1616	24	0
2	A	9	0	7	1	0
2	B	9	0	7	1	0
2	D	9	0	7	1	0
2	E	9	0	7	2	0
2	F	9	0	7	1	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	D	15	0	0	0	0
4	A	53	0	0	3	0
4	B	58	0	0	1	0
4	C	61	0	0	1	0
4	D	40	0	0	2	0
4	E	25	0	0	3	0
4	F	18	0	0	1	0
All	All	10245	0	9632	150	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 8.

All (150) 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:D:79:GLU:HG2	1:D:85:LYS:HD3	1.51	0.93
1:E:165:LEU:HB2	1:E:263:ILE:HB	1.66	0.77
1:A:248:VAL:HG22	1:A:265:MET:HE2	1.67	0.77
1:D:301:ALA:OXT	2:D:401:GLN:N	2.19	0.76
1:E:301:ALA:OXT	2:E:401:GLN:N	2.20	0.75
1:B:87:SER:H	1:B:88:PRO:HD3	1.54	0.72
1:D:189:ASP:OD2	1:D:190:SER:N	2.23	0.72
1:E:172:ASP:OD1	4:E:501:HOH:O	2.08	0.71
1:F:255:THR:HG22	1:F:257:ALA:H	1.55	0.71
1:D:78:THR:OG1	4:D:501:HOH:O	2.14	0.66
1:A:301:ALA:OXT	2:A:401:GLN:N	2.29	0.65
1:A:101:ASN:HD22	1:A:106:SER:HB3	1.61	0.65
1:C:171:ARG:NH1	1:C:191:ASN:OD1	2.30	0.64
1:E:94:THR:HG23	1:E:131:VAL:HG12	1.79	0.64
1:C:236:THR:HG23	1:C:288:PHE:H	1.64	0.62
1:D:248:VAL:HG22	1:D:265:MET:HE2	1.81	0.61
1:F:301:ALA:OXT	2:F:401:GLN:N	2.33	0.61
1:E:90:GLN:OE1	1:F:188:GLY:N	2.33	0.61
1:E:91:THR:HA	1:F:93:LEU:HD11	1.83	0.60
1:D:106:SER:OG	1:D:107:GLY:N	2.33	0.60
1:E:214:GLY:O	4:E:502:HOH:O	2.16	0.59
1:E:212:VAL:HG21	1:E:255:THR:H	1.67	0.59
1:F:255:THR:CG2	1:F:257:ALA:H	2.16	0.59
1:D:247:TYR:HB2	1:D:266:VAL:HG13	1.85	0.58
1:A:83:ALA:HA	1:A:88:PRO:HD3	1.86	0.57
1:D:84:LEU:HD22	1:D:85:LYS:H	1.68	0.57
1:E:117:ASN:HA	1:E:215:ASN:ND2	2.20	0.57
1:E:208:VAL:HG22	1:E:224:PRO:HD2	1.86	0.57
1:D:236:THR:HG23	1:D:288:PHE:H	1.67	0.57
1:E:188:GLY:HA3	1:E:192:THR:HG21	1.87	0.57
1:C:150:THR:HG22	4:C:504:HOH:O	2.04	0.57
1:E:172:ASP:OD2	1:E:258:THR:OG1	2.24	0.56
1:E:208:VAL:HG22	1:E:224:PRO:CD	2.36	0.56
1:E:212:VAL:HG21	1:E:255:THR:OG1	2.06	0.56
1:D:165:LEU:O	1:D:262:ALA:HB1	2.05	0.55
1:F:188:GLY:HA3	1:F:192:THR:HG21	1.88	0.55
1:D:246:LEU:HD11	1:D:265:MET:HB3	1.89	0.55
1:F:172:ASP:OD1	1:F:255:THR:HG21	2.07	0.55
1:F:247:TYR:HB2	1:F:266:VAL:HG13	1.88	0.55
1:B:247:TYR:HB2	1:B:266:VAL:HG13	1.87	0.54
1:E:201:ILE:O	1:E:204:THR:HG23	2.07	0.54
1:A:131:VAL:HG13	4:A:508:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LEU:HD11	1:A:253:VAL:HG11	1.89	0.53
1:A:128:LEU:HD23	1:A:137:GLY:HA3	1.91	0.53
1:C:236:THR:HG21	1:C:287:THR:HA	1.91	0.53
1:F:126:VAL:HG11	1:F:165:LEU:HD13	1.91	0.53
1:D:89:THR:C	1:D:91:THR:H	2.17	0.52
1:B:87:SER:N	1:B:88:PRO:HD3	2.24	0.52
1:C:236:THR:HG22	1:C:288:PHE:CD1	2.45	0.52
1:D:95:ARG:HH21	1:D:192:THR:HG22	1.75	0.51
1:E:86:VAL:O	1:E:86:VAL:HG13	2.09	0.51
1:E:153:ASN:HA	1:E:277:ASN:ND2	2.26	0.51
1:F:211:ALA:C	1:F:213:THR:H	2.19	0.51
1:B:203:TYR:O	1:B:207:ARG:HG2	2.09	0.51
1:B:301:ALA:OXT	2:B:401:GLN:N	2.44	0.50
1:C:203:TYR:CD1	1:C:250:PRO:HG2	2.46	0.50
1:A:90:GLN:NE2	4:A:501:HOH:O	2.36	0.50
1:E:198:ALA:HB3	1:E:261:ASN:HB3	1.94	0.50
1:E:203:TYR:O	1:E:207:ARG:HG2	2.11	0.50
1:A:117:ASN:HD22	1:A:215:ASN:HB3	1.77	0.50
1:E:212:VAL:CG2	1:E:255:THR:H	2.24	0.50
1:C:246:LEU:HD21	1:C:265:MET:HE2	1.94	0.49
1:A:265:MET:HE1	1:A:296:PHE:CZ	2.47	0.49
1:D:224:PRO:C	1:E:234:THR:HB	2.38	0.49
1:A:93:LEU:HD23	1:A:95:ARG:CZ	2.44	0.48
1:E:231:PHE:O	1:E:244:GLY:N	2.46	0.48
1:D:89:THR:HG23	4:D:517:HOH:O	2.13	0.48
1:C:246:LEU:HD11	1:C:265:MET:HE2	1.96	0.48
1:C:247:TYR:HB2	1:C:266:VAL:HG13	1.95	0.47
1:E:212:VAL:HG23	1:E:254:ASN:HB3	1.96	0.47
1:D:82:LEU:HB3	1:F:85:LYS:HD2	1.95	0.47
1:D:79:GLU:CG	1:D:85:LYS:HD3	2.35	0.47
1:D:199:ASN:HB2	1:D:299:VAL:HG12	1.95	0.47
1:C:128:LEU:HD23	1:C:137:GLY:HA3	1.97	0.47
1:E:226:TYR:CZ	1:F:232:CYS:HB2	2.49	0.47
1:B:90:GLN:O	4:B:501:HOH:O	2.19	0.47
1:A:117:ASN:ND2	1:A:215:ASN:HB3	2.29	0.47
1:D:225:GLY:HA2	1:E:232:CYS:O	2.14	0.46
1:E:192:THR:N	1:E:193:PRO:HD2	2.31	0.46
1:A:167:PRO:O	1:A:193:PRO:HB3	2.16	0.46
1:F:207:ARG:NH2	1:F:261:ASN:OD1	2.48	0.46
1:A:232:CYS:HB2	1:C:226:TYR:CZ	2.51	0.46
1:B:265:MET:HE1	1:B:296:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:ASN:ND2	1:E:105:ASP:OD1	2.43	0.46
1:A:154:SER:HB2	1:A:159:ILE:HG13	1.97	0.46
1:B:175:ALA:HA	1:B:253:VAL:HG21	1.98	0.46
1:A:203:TYR:CD1	1:A:250:PRO:HG2	2.52	0.45
1:E:91:THR:HA	1:F:93:LEU:CD1	2.47	0.45
1:D:84:LEU:HD11	1:D:86:VAL:HB	1.98	0.45
1:F:192:THR:N	1:F:193:PRO:HD2	2.31	0.45
1:E:208:VAL:HG21	1:E:223:LEU:HD22	1.98	0.45
1:D:195:TYR:HA	1:D:301:ALA:HB3	1.99	0.45
1:A:91:THR:HG22	1:B:93:LEU:HD21	1.99	0.45
1:E:257:ALA:HA	4:E:518:HOH:O	2.15	0.45
1:C:258:THR:HB	1:C:260:LEU:HG	2.00	0.44
1:E:212:VAL:CG2	1:E:254:ASN:HB3	2.47	0.44
1:C:207:ARG:NH2	1:C:252:THR:HG21	2.32	0.44
1:E:117:ASN:ND2	1:E:215:ASN:OD1	2.39	0.44
1:B:247:TYR:HB2	1:B:266:VAL:CG1	2.47	0.44
1:B:128:LEU:HD23	1:B:137:GLY:HA3	1.99	0.44
1:C:87:SER:OG	1:C:90:GLN:HG3	2.17	0.44
1:B:93:LEU:HD12	1:B:95:ARG:HG2	1.98	0.44
1:D:132:GLY:O	1:E:127:TYR:OH	2.34	0.44
1:C:192:THR:N	1:C:193:PRO:HD2	2.32	0.43
1:D:214:GLY:O	1:D:215:ASN:C	2.61	0.43
1:C:95:ARG:HD2	1:C:195:TYR:HD2	1.83	0.43
1:F:142:LYS:NZ	4:F:503:HOH:O	2.47	0.43
1:A:117:ASN:ND2	4:A:506:HOH:O	2.51	0.43
1:B:111:PHE:HB3	1:B:178:SER:HA	2.01	0.43
1:B:226:TYR:CD1	1:B:226:TYR:C	2.97	0.43
1:E:247:TYR:HB2	1:E:266:VAL:HG13	2.00	0.43
1:E:301:ALA:O	2:E:401:GLN:HG3	2.18	0.43
1:F:157:GLU:H	1:F:157:GLU:HG3	1.59	0.43
1:B:87:SER:N	1:B:88:PRO:CD	2.82	0.43
1:F:126:VAL:HG22	1:F:139:ILE:HD12	2.01	0.43
1:B:129:THR:O	1:B:135:VAL:HA	2.19	0.42
1:D:236:THR:HG21	1:D:287:THR:HA	2.00	0.42
1:C:236:THR:HG22	1:C:288:PHE:CE1	2.54	0.42
1:B:248:VAL:HG22	1:B:265:MET:HE2	2.01	0.42
1:E:160:ARG:HA	1:E:267:PHE:O	2.19	0.42
1:B:209:ASN:HA	1:B:252:THR:HG22	2.00	0.42
1:E:132:GLY:HA2	1:F:96:ILE:HD11	2.01	0.42
1:D:209:ASN:OD1	1:D:254:ASN:HB3	2.19	0.42
1:C:171:ARG:HH21	1:C:171:ARG:HG3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:TYR:CZ	1:B:232:CYS:HB2	2.54	0.42
1:C:160:ARG:HA	1:C:267:PHE:O	2.20	0.42
1:F:203:TYR:CD1	1:F:250:PRO:HG2	2.55	0.42
1:A:189:ASP:N	1:A:189:ASP:OD2	2.52	0.42
1:C:219:GLU:HG2	1:C:221:THR:H	1.85	0.41
1:B:158:SER:HB3	1:B:269:ILE:O	2.19	0.41
1:C:157:GLU:H	1:C:157:GLU:HG3	1.51	0.41
1:E:265:MET:HE1	1:E:296:PHE:CZ	2.56	0.41
1:A:126:VAL:HG11	1:A:165:LEU:HD13	2.02	0.41
1:E:199:ASN:HB2	1:E:300:GLY:O	2.20	0.41
1:E:210:LEU:HD22	1:E:216:PHE:HB2	2.01	0.41
1:F:160:ARG:HA	1:F:267:PHE:O	2.20	0.41
1:E:177:LEU:HD23	1:E:177:LEU:HA	1.83	0.41
1:F:250:PRO:HA	1:F:263:ILE:HA	2.03	0.41
1:B:209:ASN:OD1	1:B:252:THR:HG23	2.20	0.41
1:D:81:GLY:O	1:D:83:ALA:N	2.54	0.41
1:E:162:GLY:HA2	1:E:265:MET:O	2.20	0.41
1:B:89:THR:HG23	1:B:90:GLN:H	1.86	0.41
1:C:212:VAL:H	1:C:212:VAL:HG22	1.64	0.40
1:F:208:VAL:HG21	1:F:218:LYS:HG3	2.03	0.40
1:C:135:VAL:O	1:C:297:THR:HA	2.21	0.40
1:D:236:THR:HG22	1:D:288:PHE:CD2	2.57	0.40
1:F:142:LYS:HG3	1:F:290:LEU:HB2	2.03	0.40
1:B:226:TYR:CZ	1:C:232:CYS:HB2	2.56	0.40
1:A:99:MET:CE	1:A:167:PRO:HB3	2.50	0.40
1:A:101:ASN:ND2	1:A:106:SER:HB3	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	168/245 (69%)	167 (99%)	1 (1%)	78	88
1	B	166/245 (68%)	166 (100%)	0	100	100
1	C	178/245 (73%)	178 (100%)	0	100	100
1	D	182/245 (74%)	182 (100%)	0	100	100
1	E	178/245 (73%)	178 (100%)	0	100	100
1	F	180/245 (74%)	179 (99%)	1 (1%)	78	88
All	All	1052/1470 (72%)	1050 (100%)	2 (0%)	87	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	F	255	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	240	ASN
1	A	271	GLN
1	B	156	GLN
1	D	117	ASN
1	D	271	GLN
1	C	240	ASN
1	C	245	ASN
1	C	271	GLN
1	E	271	GLN
1	F	156	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
3	SO4	D	404	-	4,4,4	0.57	0	6,6,6	0.20	0
3	SO4	D	403	-	4,4,4	0.33	0	6,6,6	0.30	0
2	GLN	D	401	-	7,8,9	0.54	0	4,9,11	0.06	0
3	SO4	A	402	-	4,4,4	0.35	0	6,6,6	0.12	0
2	GLN	E	401	-	7,8,9	0.70	0	4,9,11	0.14	0
3	SO4	D	402	-	4,4,4	0.27	0	6,6,6	0.28	0
2	GLN	F	401	-	7,8,9	0.68	0	4,9,11	0.27	0
2	GLN	B	401	-	7,8,9	0.56	0	4,9,11	0.05	0
2	GLN	A	401	-	7,8,9	0.95	0	4,9,11	0.21	0
3	SO4	C	401	-	4,4,4	0.39	0	6,6,6	0.38	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	GLN	D	401	-	-	0/6/7/9	-
2	GLN	E	401	-	-	1/6/7/9	-
2	GLN	F	401	-	-	0/6/7/9	-
2	GLN	B	401	-	-	3/6/7/9	-
2	GLN	A	401	-	-	1/6/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GLN	O-C-CA-CB
2	B	401	GLN	C-CA-CB-CG
2	E	401	GLN	CA-CB-CG-CD
2	B	401	GLN	CA-CB-CG-CD
2	B	401	GLN	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	GLN	1	0
2	E	401	GLN	2	0
2	F	401	GLN	1	0
2	B	401	GLN	1	0
2	A	401	GLN	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	219/301 (72%)	-0.12	9 (4%) 41 39	29, 37, 77, 92	0
1	B	216/301 (71%)	-0.26	7 (3%) 50 48	28, 36, 65, 94	0
1	C	217/301 (72%)	-0.27	5 (2%) 61 59	27, 35, 64, 94	0
1	D	223/301 (74%)	0.17	22 (9%) 13 12	32, 43, 94, 119	0
1	E	217/301 (72%)	0.27	8 (3%) 45 42	36, 53, 83, 108	0
1	F	221/301 (73%)	0.33	15 (6%) 23 23	37, 51, 82, 110	0
All	All	1313/1806 (72%)	0.02	66 (5%) 34 34	27, 42, 79, 119	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	LEU	7.3
1	D	86	VAL	6.6
1	D	82	LEU	5.8
1	F	82	LEU	5.7
1	D	83	ALA	5.5
1	A	83	ALA	5.1
1	A	85	LYS	4.7
1	D	84	LEU	4.6
1	F	81	GLY	4.5
1	F	84	LEU	4.4
1	B	86	VAL	4.4
1	C	85	LYS	4.4
1	D	89	THR	4.4
1	D	188	GLY	4.3
1	F	214	GLY	4.1
1	A	90	GLN	4.1
1	D	85	LYS	4.0
1	F	195	TYR	4.0
1	B	116	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	83	ALA	3.9
1	E	213	THR	3.7
1	E	255	THR	3.7
1	D	214	GLY	3.6
1	D	88	PRO	3.5
1	E	86	VAL	3.4
1	A	255	THR	3.3
1	B	255	THR	3.3
1	C	195	TYR	3.3
1	D	255	THR	3.2
1	A	86	VAL	3.1
1	C	86	VAL	3.1
1	D	78	THR	3.0
1	A	89	THR	3.0
1	F	237	THR	2.9
1	F	85	LYS	2.8
1	E	93	LEU	2.8
1	F	108	TYR	2.8
1	D	254	ASN	2.7
1	C	254	ASN	2.6
1	A	84	LEU	2.6
1	D	81	GLY	2.6
1	F	89	THR	2.5
1	D	87	SER	2.5
1	D	212	VAL	2.5
1	D	213	THR	2.5
1	F	213	THR	2.5
1	F	86	VAL	2.5
1	F	93	LEU	2.4
1	D	257	ALA	2.4
1	B	189	ASP	2.3
1	B	88	PRO	2.3
1	D	158	SER	2.3
1	D	190	SER	2.3
1	F	88	PRO	2.3
1	D	116	GLN	2.3
1	B	87	SER	2.2
1	F	90	GLN	2.2
1	C	255	THR	2.2
1	D	195	TYR	2.2
1	E	256	GLY	2.2
1	A	219	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	89	THR	2.1
1	E	254	ASN	2.1
1	E	214	GLY	2.1
1	D	219	GLU	2.0
1	E	89	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(Å ²)	Q<0.9
3	SO4	D	404	5/5	0.60	0.19	56,63,70,110	0
2	GLN	E	401	9/10	0.69	0.18	68,72,83,85	0
2	GLN	A	401	9/10	0.78	0.20	41,54,78,81	0
2	GLN	F	401	9/10	0.81	0.16	55,68,75,77	0
2	GLN	D	401	9/10	0.81	0.15	57,67,85,89	0
2	GLN	B	401	9/10	0.88	0.14	45,46,74,76	0
3	SO4	C	401	5/5	0.93	0.12	47,51,57,66	0
3	SO4	D	403	5/5	0.95	0.08	51,54,58,67	0
3	SO4	D	402	5/5	0.96	0.08	54,55,59,59	0
3	SO4	A	402	5/5	0.97	0.06	38,45,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.