



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:39 PM GMT

PDB ID : 4D0U
Title : Crystal structure of the fiber head domain of the Atadenovirus snake adenovirus 1, selenomethionine-derivative
Authors : Singh, A.K.; van Raaij, M.J.
Deposited on : 2014-04-30
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

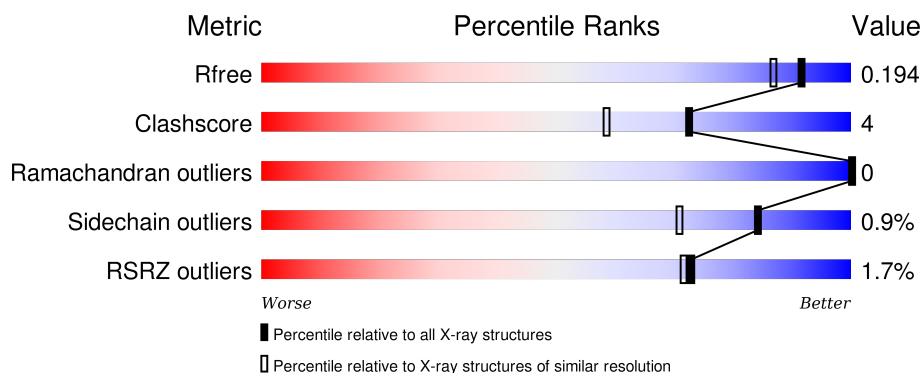
1 Overall quality at a glance

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}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	145	 73% 26%
1	B	145	 67% 6% 28%
1	C	145	 66% 7% 27%
1	D	145	 68% 6% 26%

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
2	PE8	A	1345	-	-	-	X
2	PE8	D	1346	-	-	-	X
3	SO4	B	1345	-	-	X	-
3	SO4	B	1346	-	-	X	-
3	SO4	C	1345	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3927 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	108	Total	C	N	O	Se	0	5	0
			837	534	133	168	2			
1	B	105	Total	C	N	O	Se	0	5	0
			812	519	128	163	2			
1	C	106	Total	C	N	O	Se	0	8	0
			837	535	132	168	2			
1	D	108	Total	C	N	O	Se	0	6	0
			837	532	133	170	2			

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	GLY	-	EXPRESSION TAG	UNP A9CB96
A	202	SER	-	EXPRESSION TAG	UNP A9CB96
A	203	SER	-	EXPRESSION TAG	UNP A9CB96
A	204	HIS	-	EXPRESSION TAG	UNP A9CB96
A	205	HIS	-	EXPRESSION TAG	UNP A9CB96
A	206	HIS	-	EXPRESSION TAG	UNP A9CB96
A	207	HIS	-	EXPRESSION TAG	UNP A9CB96
A	208	HIS	-	EXPRESSION TAG	UNP A9CB96
A	209	HIS	-	EXPRESSION TAG	UNP A9CB96
A	210	SER	-	EXPRESSION TAG	UNP A9CB96
A	211	SER	-	EXPRESSION TAG	UNP A9CB96
A	212	GLY	-	EXPRESSION TAG	UNP A9CB96
A	213	LEU	-	EXPRESSION TAG	UNP A9CB96
A	214	VAL	-	EXPRESSION TAG	UNP A9CB96
A	215	PRO	-	EXPRESSION TAG	UNP A9CB96
A	216	ARG	-	EXPRESSION TAG	UNP A9CB96
A	217	GLY	-	EXPRESSION TAG	UNP A9CB96
A	218	SER	-	EXPRESSION TAG	UNP A9CB96
A	219	HIS	-	EXPRESSION TAG	UNP A9CB96
A	220	MSE	-	EXPRESSION TAG	UNP A9CB96
A	221	ALA	-	EXPRESSION TAG	UNP A9CB96

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Chain	Residue	Modelled	Actual	Comment	Reference
A	222	SER	-	EXPRESSION TAG	UNP A9CB96
A	223	MSE	-	EXPRESSION TAG	UNP A9CB96
A	224	THR	-	EXPRESSION TAG	UNP A9CB96
A	225	GLY	-	EXPRESSION TAG	UNP A9CB96
A	226	GLY	-	EXPRESSION TAG	UNP A9CB96
A	227	GLN	-	EXPRESSION TAG	UNP A9CB96
A	228	GLN	-	EXPRESSION TAG	UNP A9CB96
A	229	MSE	-	EXPRESSION TAG	UNP A9CB96
A	230	GLY	-	EXPRESSION TAG	UNP A9CB96
A	231	ARG	-	EXPRESSION TAG	UNP A9CB96
A	232	GLY	-	EXPRESSION TAG	UNP A9CB96
A	233	SER	-	EXPRESSION TAG	UNP A9CB96
A	340	PHE	-	EXPRESSION TAG	UNP A9CB96
A	341	TYR	-	EXPRESSION TAG	UNP A9CB96
A	342	LEU	-	EXPRESSION TAG	UNP A9CB96
A	343	THR	-	EXPRESSION TAG	UNP A9CB96
A	344	GLU	-	EXPRESSION TAG	UNP A9CB96
A	345	LYS	-	EXPRESSION TAG	UNP A9CB96
A	323	MSE	LEU	ENGINEERED MUTATION	UNP A9CB96
A	325	MSE	LEU	ENGINEERED MUTATION	UNP A9CB96
B	201	GLY	-	EXPRESSION TAG	UNP A9CB96
B	202	SER	-	EXPRESSION TAG	UNP A9CB96
B	203	SER	-	EXPRESSION TAG	UNP A9CB96
B	204	HIS	-	EXPRESSION TAG	UNP A9CB96
B	205	HIS	-	EXPRESSION TAG	UNP A9CB96
B	206	HIS	-	EXPRESSION TAG	UNP A9CB96
B	207	HIS	-	EXPRESSION TAG	UNP A9CB96
B	208	HIS	-	EXPRESSION TAG	UNP A9CB96
B	209	HIS	-	EXPRESSION TAG	UNP A9CB96
B	210	SER	-	EXPRESSION TAG	UNP A9CB96
B	211	SER	-	EXPRESSION TAG	UNP A9CB96
B	212	GLY	-	EXPRESSION TAG	UNP A9CB96
B	213	LEU	-	EXPRESSION TAG	UNP A9CB96
B	214	VAL	-	EXPRESSION TAG	UNP A9CB96
B	215	PRO	-	EXPRESSION TAG	UNP A9CB96
B	216	ARG	-	EXPRESSION TAG	UNP A9CB96
B	217	GLY	-	EXPRESSION TAG	UNP A9CB96
B	218	SER	-	EXPRESSION TAG	UNP A9CB96
B	219	HIS	-	EXPRESSION TAG	UNP A9CB96
B	220	MSE	-	EXPRESSION TAG	UNP A9CB96
B	221	ALA	-	EXPRESSION TAG	UNP A9CB96
B	222	SER	-	EXPRESSION TAG	UNP A9CB96

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Chain	Residue	Modelled	Actual	Comment	Reference
B	223	MSE	-	EXPRESSION TAG	UNP A9CB96
B	224	THR	-	EXPRESSION TAG	UNP A9CB96
B	225	GLY	-	EXPRESSION TAG	UNP A9CB96
B	226	GLY	-	EXPRESSION TAG	UNP A9CB96
B	227	GLN	-	EXPRESSION TAG	UNP A9CB96
B	228	GLN	-	EXPRESSION TAG	UNP A9CB96
B	229	MSE	-	EXPRESSION TAG	UNP A9CB96
B	230	GLY	-	EXPRESSION TAG	UNP A9CB96
B	231	ARG	-	EXPRESSION TAG	UNP A9CB96
B	232	GLY	-	EXPRESSION TAG	UNP A9CB96
B	233	SER	-	EXPRESSION TAG	UNP A9CB96
B	340	PHE	-	EXPRESSION TAG	UNP A9CB96
B	341	TYR	-	EXPRESSION TAG	UNP A9CB96
B	342	LEU	-	EXPRESSION TAG	UNP A9CB96
B	343	THR	-	EXPRESSION TAG	UNP A9CB96
B	344	GLU	-	EXPRESSION TAG	UNP A9CB96
B	345	LYS	-	EXPRESSION TAG	UNP A9CB96
B	323	MSE	LEU	ENGINEERED MUTATION	UNP A9CB96
B	325	MSE	LEU	ENGINEERED MUTATION	UNP A9CB96
C	201	GLY	-	EXPRESSION TAG	UNP A9CB96
C	202	SER	-	EXPRESSION TAG	UNP A9CB96
C	203	SER	-	EXPRESSION TAG	UNP A9CB96
C	204	HIS	-	EXPRESSION TAG	UNP A9CB96
C	205	HIS	-	EXPRESSION TAG	UNP A9CB96
C	206	HIS	-	EXPRESSION TAG	UNP A9CB96
C	207	HIS	-	EXPRESSION TAG	UNP A9CB96
C	208	HIS	-	EXPRESSION TAG	UNP A9CB96
C	209	HIS	-	EXPRESSION TAG	UNP A9CB96
C	210	SER	-	EXPRESSION TAG	UNP A9CB96
C	211	SER	-	EXPRESSION TAG	UNP A9CB96
C	212	GLY	-	EXPRESSION TAG	UNP A9CB96
C	213	LEU	-	EXPRESSION TAG	UNP A9CB96
C	214	VAL	-	EXPRESSION TAG	UNP A9CB96
C	215	PRO	-	EXPRESSION TAG	UNP A9CB96
C	216	ARG	-	EXPRESSION TAG	UNP A9CB96
C	217	GLY	-	EXPRESSION TAG	UNP A9CB96
C	218	SER	-	EXPRESSION TAG	UNP A9CB96
C	219	HIS	-	EXPRESSION TAG	UNP A9CB96
C	220	MSE	-	EXPRESSION TAG	UNP A9CB96
C	221	ALA	-	EXPRESSION TAG	UNP A9CB96
C	222	SER	-	EXPRESSION TAG	UNP A9CB96
C	223	MSE	-	EXPRESSION TAG	UNP A9CB96

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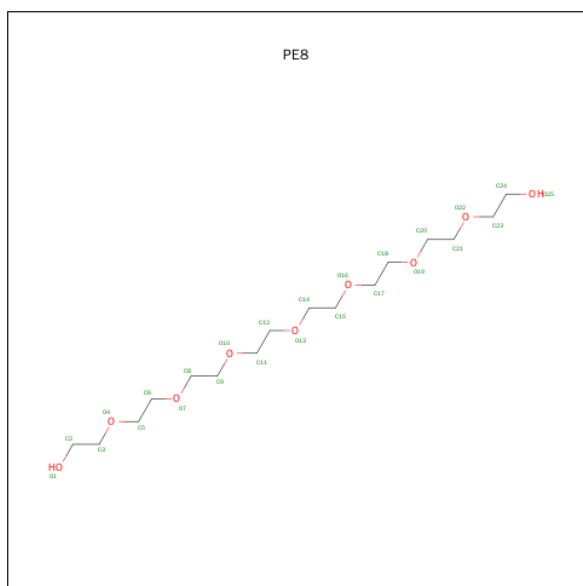
Chain	Residue	Modelled	Actual	Comment	Reference
C	224	THR	-	EXPRESSION TAG	UNP A9CB96
C	225	GLY	-	EXPRESSION TAG	UNP A9CB96
C	226	GLY	-	EXPRESSION TAG	UNP A9CB96
C	227	GLN	-	EXPRESSION TAG	UNP A9CB96
C	228	GLN	-	EXPRESSION TAG	UNP A9CB96
C	229	MSE	-	EXPRESSION TAG	UNP A9CB96
C	230	GLY	-	EXPRESSION TAG	UNP A9CB96
C	231	ARG	-	EXPRESSION TAG	UNP A9CB96
C	232	GLY	-	EXPRESSION TAG	UNP A9CB96
C	233	SER	-	EXPRESSION TAG	UNP A9CB96
C	340	PHE	-	EXPRESSION TAG	UNP A9CB96
C	341	TYR	-	EXPRESSION TAG	UNP A9CB96
C	342	LEU	-	EXPRESSION TAG	UNP A9CB96
C	343	THR	-	EXPRESSION TAG	UNP A9CB96
C	344	GLU	-	EXPRESSION TAG	UNP A9CB96
C	345	LYS	-	EXPRESSION TAG	UNP A9CB96
C	323	MSE	LEU	ENGINEERED MUTATION	UNP A9CB96
C	325	MSE	LEU	ENGINEERED MUTATION	UNP A9CB96
D	201	GLY	-	EXPRESSION TAG	UNP A9CB96
D	202	SER	-	EXPRESSION TAG	UNP A9CB96
D	203	SER	-	EXPRESSION TAG	UNP A9CB96
D	204	HIS	-	EXPRESSION TAG	UNP A9CB96
D	205	HIS	-	EXPRESSION TAG	UNP A9CB96
D	206	HIS	-	EXPRESSION TAG	UNP A9CB96
D	207	HIS	-	EXPRESSION TAG	UNP A9CB96
D	208	HIS	-	EXPRESSION TAG	UNP A9CB96
D	209	HIS	-	EXPRESSION TAG	UNP A9CB96
D	210	SER	-	EXPRESSION TAG	UNP A9CB96
D	211	SER	-	EXPRESSION TAG	UNP A9CB96
D	212	GLY	-	EXPRESSION TAG	UNP A9CB96
D	213	LEU	-	EXPRESSION TAG	UNP A9CB96
D	214	VAL	-	EXPRESSION TAG	UNP A9CB96
D	215	PRO	-	EXPRESSION TAG	UNP A9CB96
D	216	ARG	-	EXPRESSION TAG	UNP A9CB96
D	217	GLY	-	EXPRESSION TAG	UNP A9CB96
D	218	SER	-	EXPRESSION TAG	UNP A9CB96
D	219	HIS	-	EXPRESSION TAG	UNP A9CB96
D	220	MSE	-	EXPRESSION TAG	UNP A9CB96
D	221	ALA	-	EXPRESSION TAG	UNP A9CB96
D	222	SER	-	EXPRESSION TAG	UNP A9CB96
D	223	MSE	-	EXPRESSION TAG	UNP A9CB96
D	224	THR	-	EXPRESSION TAG	UNP A9CB96

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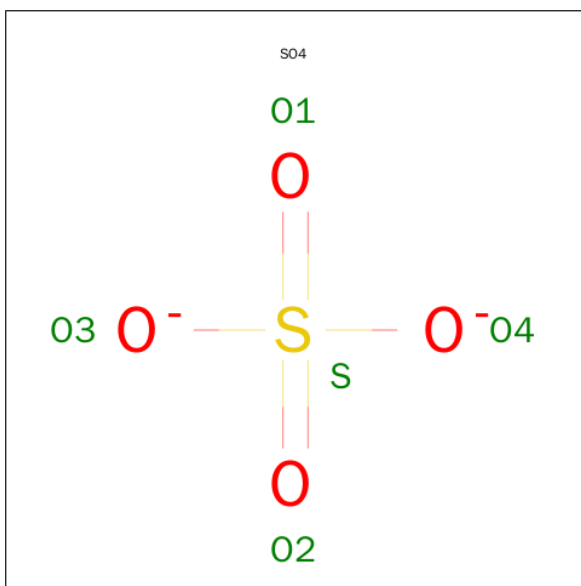
Chain	Residue	Modelled	Actual	Comment	Reference
D	225	GLY	-	EXPRESSION TAG	UNP A9CB96
D	226	GLY	-	EXPRESSION TAG	UNP A9CB96
D	227	GLN	-	EXPRESSION TAG	UNP A9CB96
D	228	GLN	-	EXPRESSION TAG	UNP A9CB96
D	229	MSE	-	EXPRESSION TAG	UNP A9CB96
D	230	GLY	-	EXPRESSION TAG	UNP A9CB96
D	231	ARG	-	EXPRESSION TAG	UNP A9CB96
D	232	GLY	-	EXPRESSION TAG	UNP A9CB96
D	233	SER	-	EXPRESSION TAG	UNP A9CB96
D	340	PHE	-	EXPRESSION TAG	UNP A9CB96
D	341	TYR	-	EXPRESSION TAG	UNP A9CB96
D	342	LEU	-	EXPRESSION TAG	UNP A9CB96
D	343	THR	-	EXPRESSION TAG	UNP A9CB96
D	344	GLU	-	EXPRESSION TAG	UNP A9CB96
D	345	LYS	-	EXPRESSION TAG	UNP A9CB96
D	323	MSE	LEU	ENGINEERED MUTATION	UNP A9CB96
D	325	MSE	LEU	ENGINEERED MUTATION	UNP A9CB96

- Molecule 2 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: $C_{16}H_{34}O_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			25	16	9		
2	D	1	Total	C	O	0	0
			25	16	9		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	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	143	Total	O	0	0
			143	143		
4	B	130	Total	O	0	0
			130	130		
4	C	120	Total	O	0	0
			120	120		
4	D	141	Total	O	0	0
			141	141		

- Molecule 1: FIBER PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	149.54Å 149.54Å 149.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.33 – 1.60 29.33 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.33-1.60) 100.0 (29.33-1.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.47 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.158 , 0.189 0.164 , 0.194	Depositor DCC
R_{free} test set	2005 reflections (2.83%)	DCC
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.4	EDS
Estimated twinning fraction	0.019 for -l,-k,-h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 72960 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3927	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PE8, 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	0.56	0/865	0.74	0/1165
1	B	0.62	0/845	0.77	0/1138
1	C	0.60	0/875	0.76	1/1178 (0.1%)
1	D	0.63	0/871	0.78	0/1171
All	All	0.60	0/3456	0.76	1/4652 (0.0%)

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	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	342	LEU	CA-CB-CG	6.72	130.76	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	239	LYS	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	837	0	816	2	0
1	B	812	0	796	6	0
1	C	837	0	819	7	0
1	D	837	0	817	6	0
2	A	25	0	34	3	0
2	D	25	0	34	8	0
3	B	10	0	0	2	0
3	C	10	0	0	0	0
4	A	143	0	0	1	0
4	B	130	0	0	3	1
4	C	120	0	0	2	0
4	D	141	0	0	2	0
All	All	3927	0	3316	28	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 4.

All (28) 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:251[B]:ASP:OD1	4:D:2025:HOH:O	1.57	1.19
1:B:286:LYS:NZ	4:B:2055:HOH:O	1.82	1.11
1:A:265[A]:LEU:O	4:A:2035:HOH:O	1.71	1.07
3:B:1345:SO4:O1	3:B:1346:SO4:O4	1.73	0.94
1:C:315:ILE:HD12	2:D:1346:PE8:H121	1.57	0.85
1:D:313[B]:THR:HG23	2:D:1346:PE8:H201	1.61	0.80
3:B:1345:SO4:O2	3:B:1346:SO4:O2	1.93	0.79
1:D:326:GLU:OE1	2:D:1346:PE8:H142	1.86	0.76
1:C:271:ARG:HD3	4:C:2063:HOH:O	1.84	0.75
2:A:1345:PE8:H151	2:A:1345:PE8:H21	1.68	0.73
1:B:282:THR:HB	4:B:2052:HOH:O	1.96	0.66
2:D:1346:PE8:H21	2:D:1346:PE8:H151	1.80	0.63
2:A:1345:PE8:C2	2:A:1345:PE8:H151	2.32	0.59
1:B:271:ARG:HD3	4:B:2041:HOH:O	2.02	0.59
1:A:315:ILE:CD1	2:A:1345:PE8:H112	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:ARG:HD2	1:C:341:TYR:OH	2.09	0.51
1:C:243[A]:ASP:OD2	1:C:261:ARG:NH2	2.39	0.49
1:D:268:PHE:CE2	1:D:344:GLU:HG3	2.48	0.48
1:C:315:ILE:CD1	2:D:1346:PE8:H121	2.38	0.48
1:C:326:GLU:HB3	2:D:1346:PE8:H92	1.97	0.47
1:D:243:ASP:OD2	1:D:261:ARG:NH2	2.50	0.45
1:B:271:ARG:HD2	1:B:341:TYR:OH	2.16	0.45
1:C:243[B]:ASP:OD2	1:C:261:ARG:NH2	2.49	0.45
4:C:2104:HOH:O	2:D:1346:PE8:H231	2.17	0.44
1:B:256:PHE:HB3	1:B:258:PHE:CE2	2.54	0.43
2:D:1346:PE8:H62	4:D:2141:HOH:O	2.18	0.42
1:B:313[B]:THR:HG22	1:B:328:SER:HB3	2.01	0.42
1:D:244:ILE:HD11	1:D:292:GLU:HG2	2.01	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)
4:B:2123:HOH:O	4:B:2123:HOH:O[14_555]	2.04	0.16

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	111/145 (77%)	111 (100%)	0	0	100	100
1	B	108/145 (74%)	107 (99%)	1 (1%)	0	100	100
1	C	112/145 (77%)	111 (99%)	1 (1%)	0	100	100
1	D	112/145 (77%)	111 (99%)	1 (1%)	0	100	100
All	All	443/580 (76%)	440 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	91/111 (82%)	91 (100%)	0	100	100
1	B	89/111 (80%)	89 (100%)	0	100	100
1	C	92/111 (83%)	90 (98%)	2 (2%)	60	31
1	D	92/111 (83%)	91 (99%)	1 (1%)	80	63
All	All	364/444 (82%)	361 (99%)	3 (1%)	84	75

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

Mol	Chain	Res	Type
1	C	241	SER
1	C	242	LEU
1	D	243	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	PE8	A	1345	-	24,24,24	0.50	0	23,23,23	0.59	0
3	SO4	B	1345	3	4,4,4	0.25	0	6,6,6	0.14	0
3	SO4	B	1346	3	4,4,4	0.30	0	6,6,6	0.08	0
3	SO4	C	1345	3	4,4,4	0.22	0	6,6,6	0.28	0
3	SO4	C	1346	3	4,4,4	0.17	0	6,6,6	0.45	0
2	PE8	D	1346	-	24,24,24	0.55	0	23,23,23	0.56	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	PE8	A	1345	-	-	0/22/22/22	0/0/0/0
3	SO4	B	1345	3	-	0/0/0/0	0/0/0/0
3	SO4	B	1346	3	-	0/0/0/0	0/0/0/0
3	SO4	C	1345	3	-	0/0/0/0	0/0/0/0
3	SO4	C	1346	3	-	0/0/0/0	0/0/0/0
2	PE8	D	1346	-	-	0/22/22/22	0/0/0/0

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.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1345	PE8	3	0
3	B	1345	SO4	2	0
3	B	1346	SO4	2	0
2	D	1346	PE8	8	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	106/145 (73%)	-0.32	2 (1%) 70 68	8, 16, 31, 52	0
1	B	103/145 (71%)	-0.26	2 (1%) 70 68	8, 13, 28, 48	1 (0%)
1	C	104/145 (71%)	-0.30	1 (0%) 84 84	7, 12, 30, 49	0
1	D	106/145 (73%)	-0.41	2 (1%) 70 68	7, 12, 29, 50	0
All	All	419/580 (72%)	-0.32	7 (1%) 73 71	7, 13, 30, 52	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	SER	3.7
1	C	241	SER	3.5
1	D	238	SER	3.2
1	A	237	PRO	3.0
1	B	240	THR	3.0
1	D	345	LYS	2.7
1	B	253	GLY	2.7

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	PE8	D	1346	25/25	0.82	0.19	13.36	27,41,53,58	0
3	SO4	C	1345	5/5	0.89	0.14	7.84	7,8,9,9	5
2	PE8	A	1345	25/25	0.82	0.18	6.16	31,41,52,55	0
3	SO4	B	1346	5/5	0.94	0.09	-	9,10,10,10	5
3	SO4	C	1346	5/5	0.96	0.11	-	15,15,15,18	5
3	SO4	B	1345	5/5	0.99	0.07	-	9,10,10,10	5

6.5 Other polymers [i](#)

There are no such residues in this entry.