



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 01:18 pm GMT

PDB ID : 2WAX  
Title : Structure of the human DDX6 C-terminal domain in complex with an EDC3-FDF peptide  
Authors : Tritschler, F.; Weichenrieder, O.  
Deposited on : 2009-02-18  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

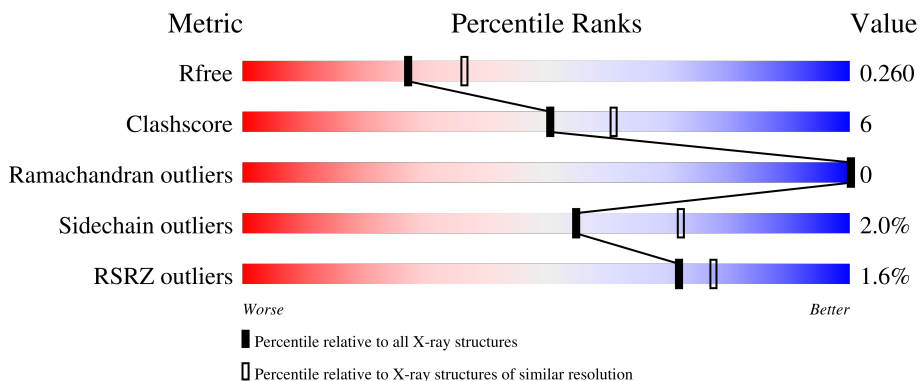
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	193	
1	C	193	
2	B	44	
2	D	44	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3497 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.

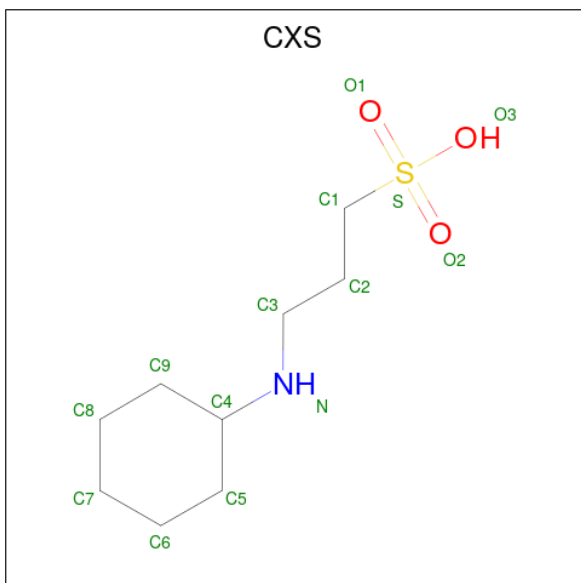
- Molecule 1 is a protein called ATP-DEPENDENT RNA HELICASE DDX6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	161	Total 1322	C 843	N 235	O 238	S 6	0	0	0
1	C	165	Total 1348	C 859	N 242	O 241	S 6	0	0	0

- Molecule 2 is a protein called ENHANCER OF MRNA-DECAPPING PROTEIN 3.

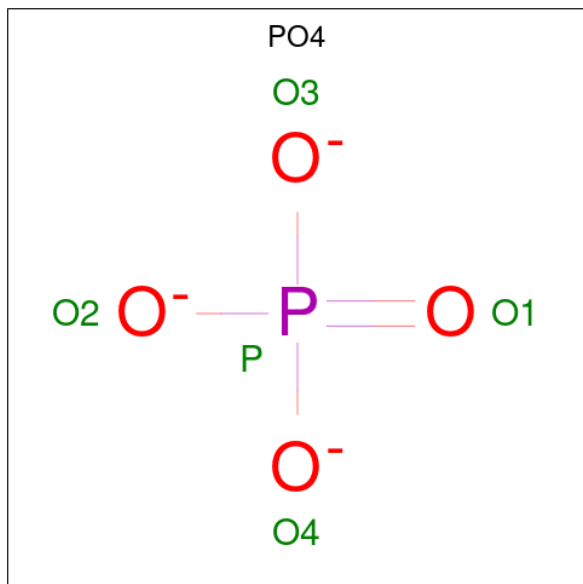
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	30	Total 246	C 158	N 32	O 56	0	0	0
2	D	28	Total 228	C 148	N 30	O 50	0	0	0

- Molecule 3 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula: C<sub>9</sub>H<sub>19</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
3	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
3	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
3	C	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
3	C	1	Total	C	N	O	S	0	1
			28	18	2	6	2		
3	D	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 5 is water.

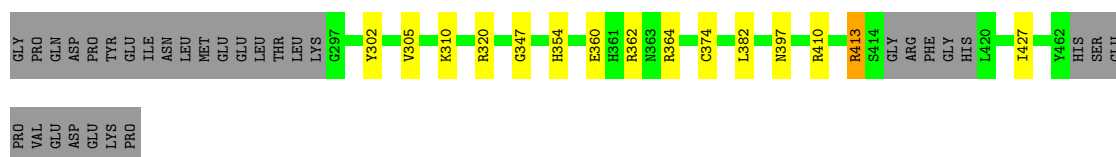
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total 103	O 103	0	0
5	B	24	Total 24	O 24	0	0
5	C	79	Total 79	O 79	0	0
5	D	29	Total 29	O 29	0	0

### 3 Residue-property plots

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.

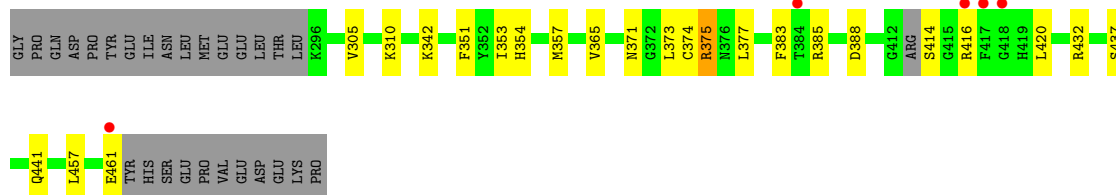
#### • Molecule 1: ATP-DEPENDENT RNA HELICASE DDX6

Chain A: 



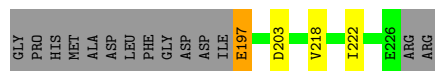
#### • Molecule 1: ATP-DEPENDENT RNA HELICASE DDX6

Chain C: 



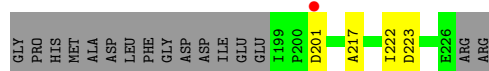
#### • Molecule 2: ENHANCER OF MRNA-DECAPPING PROTEIN 3

Chain B: 



#### • Molecule 2: ENHANCER OF MRNA-DECAPPING PROTEIN 3

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.63Å 47.85Å 65.78Å 90.00° 96.35° 90.00°	Depositor
Resolution (Å)	46.08 – 2.30 46.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.08-2.30) 98.4 (46.09-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.4.0066	Depositor
R, $R_{free}$	0.190 , 0.260 0.189 , 0.260	Depositor DCC
$R_{free}$ test set	1202 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtrriage
Anisotropy	0.130	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3497	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CXS, PO4

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	0.92	1/1346 (0.1%)	0.86	0/1815
1	C	0.88	0/1373	0.83	0/1849
2	B	0.87	0/251	0.83	0/340
2	D	1.02	0/233	0.93	1/316 (0.3%)
All	All	0.91	1/3203 (0.0%)	0.85	1/4320 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	CYS	CB-SG	-6.54	1.71	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	223	ASP	CB-CG-OD1	5.93	123.64	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1322	0	1328	11	0
1	C	1348	0	1354	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	246	0	211	4	0
2	D	228	0	199	2	0
3	A	42	0	57	2	0
3	C	42	0	57	7	0
3	D	14	0	19	0	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	A	103	0	0	4	0
5	B	24	0	0	1	0
5	C	79	0	0	3	0
5	D	29	0	0	1	0
All	All	3497	0	3225	37	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (37) 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)
3:C:1463[A]:CXS:H12	3:C:1463[A]:CXS:H4	1.52	0.91
3:C:1463[A]:CXS:H12	3:C:1463[A]:CXS:C4	2.17	0.75
2:B:197:GLU:HA	2:B:197:GLU:OE1	1.94	0.66
3:C:1463[A]:CXS:O3	5:C:2078:HOH:O	2.13	0.65
1:C:420:LEU:HD22	1:C:457:LEU:O	1.99	0.62
1:C:354:HIS:CE1	1:C:357:MET:HG3	2.40	0.56
1:A:302:TYR:HB2	1:A:427:ILE:HG13	1.88	0.55
3:A:1465:CXS:H4	5:A:2015:HOH:O	2.07	0.55
2:B:197:GLU:N	5:B:2002:HOH:O	2.41	0.54
1:C:432:ARG:HG3	2:D:222:ILE:HD11	1.90	0.54
3:C:1463[A]:CXS:H22	5:C:2077:HOH:O	2.07	0.54
1:C:388:ASP:OD2	1:C:416:ARG:NH1	2.41	0.53
1:A:364:ARG:NH1	5:A:2033:HOH:O	2.46	0.48
1:A:354:HIS:O	1:A:362:ARG:HD3	2.13	0.48
1:C:371:ASN:HB2	1:C:373:LEU:HD13	1.96	0.48
2:D:217:ALA:HA	5:D:2019:HOH:O	2.13	0.47
1:C:385:ARG:O	1:C:414:SER:HB2	2.15	0.47
1:C:420:LEU:HD22	1:C:457:LEU:C	2.35	0.47
1:A:320:ARG:HD2	2:B:203:ASP:OD2	2.16	0.45
1:A:413:ARG:NH2	5:A:2061:HOH:O	2.48	0.45
1:A:347:GLY:HA3	3:C:1463[A]:CXS:H61	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:LYS:HA	1:C:342:LYS:HD3	1.79	0.44
1:A:397:ASN:OD1	1:A:410:ARG:HD3	2.16	0.44
3:C:1463[B]:CXS:H21	5:C:2077:HOH:O	2.18	0.44
1:C:437:SER:O	1:C:441:GLN:HG3	2.18	0.43
1:C:357:MET:HB3	1:C:357:MET:HE3	1.63	0.43
1:C:374:CYS:SG	1:C:375:ARG:N	2.91	0.43
1:A:302:TYR:HB2	1:A:427:ILE:CG1	2.49	0.42
1:A:360:GLU:O	1:A:364:ARG:HG3	2.19	0.42
1:A:413:ARG:H	1:A:413:ARG:HG2	1.65	0.41
2:B:218:VAL:O	2:B:222:ILE:HG13	2.20	0.41
1:C:305:VAL:HG21	1:C:310:LYS:HG2	2.03	0.41
1:A:305:VAL:HG21	1:A:310:LYS:HG2	2.03	0.41
1:C:351:PHE:HB3	1:C:365:VAL:CG1	2.51	0.41
1:C:353:ILE:HG12	1:C:377:LEU:HD11	2.02	0.41
3:A:1465:CXS:H32	5:A:2015:HOH:O	2.21	0.40
1:C:375:ARG:HD3	3:C:1463[B]:CXS:H71	2.04	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	157/193 (81%)	152 (97%)	5 (3%)	0	100	100
1	C	161/193 (83%)	152 (94%)	9 (6%)	0	100	100
2	B	28/44 (64%)	28 (100%)	0	0	100	100
2	D	26/44 (59%)	26 (100%)	0	0	100	100
All	All	372/474 (78%)	358 (96%)	14 (4%)	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	147/176 (84%)	145 (99%)	2 (1%)	67	81
1	C	149/176 (85%)	146 (98%)	3 (2%)	55	72
2	B	26/37 (70%)	25 (96%)	1 (4%)	33	47
2	D	24/37 (65%)	23 (96%)	1 (4%)	30	42
All	All	346/426 (81%)	339 (98%)	7 (2%)	55	72

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	382	LEU
1	A	413	ARG
2	B	197	GLU
1	C	375	ARG
1	C	383	PHE
1	C	461	GLU
2	D	201	ASP

Sometimes 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 monosaccharides in this entry.

## 5.6 Ligand geometry

11 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
4	PO4	A	1467	-	4,4,4	0.98	0	6,6,6	0.86	0
3	CXS	C	1463[A]	-	14,14,14	2.09	1 (7%)	18,18,18	1.63	4 (22%)
4	PO4	A	1466	-	4,4,4	0.82	0	6,6,6	0.92	0
3	CXS	A	1464	-	14,14,14	1.96	1 (7%)	18,18,18	2.47	7 (38%)
3	CXS	A	1465	-	14,14,14	2.02	1 (7%)	18,18,18	1.77	5 (27%)
3	CXS	C	1463[B]	-	14,14,14	2.20	1 (7%)	18,18,18	1.31	2 (11%)
3	CXS	D	1227	-	14,14,14	1.84	1 (7%)	18,18,18	1.84	5 (27%)
4	PO4	C	1464	-	4,4,4	0.91	0	6,6,6	1.12	0
4	PO4	B	1227	-	4,4,4	0.84	0	6,6,6	0.54	0
3	CXS	A	1463	-	14,14,14	1.94	1 (7%)	18,18,18	1.49	4 (22%)
3	CXS	C	1462	-	14,14,14	2.18	2 (14%)	18,18,18	1.38	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CXS	C	1463[A]	-	-	6/8/16/16	0/1/1/1
3	CXS	A	1464	-	-	4/8/16/16	0/1/1/1
3	CXS	A	1465	-	-	1/8/16/16	0/1/1/1
3	CXS	C	1463[B]	-	-	6/8/16/16	0/1/1/1
3	CXS	D	1227	-	-	0/8/16/16	0/1/1/1
3	CXS	A	1463	-	-	2/8/16/16	0/1/1/1
3	CXS	C	1462	-	-	5/8/16/16	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1463[B]	CXS	C1-S	-7.72	1.66	1.77
3	C	1463[A]	CXS	C1-S	-7.46	1.66	1.77
3	C	1462	CXS	C1-S	-7.27	1.67	1.77
3	A	1465	CXS	C1-S	-6.79	1.67	1.77
3	A	1463	CXS	C1-S	-6.69	1.68	1.77
3	A	1464	CXS	C1-S	-6.65	1.68	1.77
3	D	1227	CXS	C1-S	-6.29	1.68	1.77
3	C	1462	CXS	O2-S	2.17	1.51	1.45

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1464	CXS	C3-N-C4	6.37	126.66	114.14
3	D	1227	CXS	C3-N-C4	5.23	124.41	114.14
3	A	1464	CXS	O3-S-C1	4.97	113.80	105.77
3	C	1463[A]	CXS	O3-S-C1	3.90	112.07	105.77
3	A	1465	CXS	C6-C5-C4	3.85	118.35	111.11
3	C	1462	CXS	O2-S-C1	3.83	111.53	106.92
3	A	1463	CXS	O2-S-C1	3.70	111.37	106.92
3	C	1463[A]	CXS	O2-S-C1	3.32	110.92	106.92
3	A	1463	CXS	O3-S-C1	3.26	111.04	105.77
3	A	1465	CXS	O1-S-C1	3.14	110.69	106.92
3	A	1464	CXS	O2-S-C1	2.99	110.52	106.92
3	C	1463[A]	CXS	C3-N-C4	2.97	119.97	114.14
3	A	1463	CXS	C3-N-C4	2.97	119.97	114.14
3	A	1465	CXS	C3-N-C4	2.89	119.82	114.14
3	C	1463[B]	CXS	O1-S-C1	2.81	110.30	106.92
3	C	1463[B]	CXS	C3-N-C4	2.75	119.53	114.14
3	D	1227	CXS	O3-S-C1	2.68	110.11	105.77
3	A	1465	CXS	C9-C4-C5	2.63	115.37	110.82
3	A	1464	CXS	C9-C4-C5	2.50	115.15	110.82
3	D	1227	CXS	O3-S-O2	-2.50	105.18	111.27
3	D	1227	CXS	O2-S-C1	2.37	109.77	106.92
3	A	1464	CXS	C8-C9-C4	2.25	115.34	111.11
3	A	1464	CXS	O3-S-O2	-2.24	105.80	111.27
3	A	1463	CXS	O2-S-O1	-2.21	106.31	113.95
3	A	1465	CXS	O2-S-C1	2.19	109.55	106.92
3	A	1464	CXS	C6-C5-C4	2.12	115.09	111.11
3	C	1463[A]	CXS	O3-S-O2	-2.08	106.20	111.27
3	D	1227	CXS	C2-C1-S	-2.05	110.11	113.25
3	C	1462	CXS	C2-C1-S	-2.03	110.13	113.25

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1464	CXS	C1-C2-C3-N
3	A	1464	CXS	C5-C4-N-C3
3	C	1462	CXS	C2-C1-S-O1
3	C	1462	CXS	S-C1-C2-C3
3	C	1463[A]	CXS	C2-C1-S-O3
3	C	1463[B]	CXS	C2-C1-S-O2
3	C	1463[B]	CXS	C5-C4-N-C3
3	C	1462	CXS	C2-C1-S-O3
3	C	1463[B]	CXS	C2-C1-S-O3
3	C	1462	CXS	C1-C2-C3-N
3	C	1463[A]	CXS	C1-C2-C3-N
3	A	1465	CXS	S-C1-C2-C3
3	A	1463	CXS	C2-C3-N-C4
3	A	1464	CXS	C2-C3-N-C4
3	C	1463[A]	CXS	C2-C3-N-C4
3	C	1462	CXS	C2-C1-S-O2
3	C	1463[A]	CXS	C2-C1-S-O1
3	C	1463[A]	CXS	C2-C1-S-O2
3	C	1463[B]	CXS	C2-C1-S-O1
3	C	1463[A]	CXS	S-C1-C2-C3
3	C	1463[B]	CXS	S-C1-C2-C3
3	C	1463[B]	CXS	C1-C2-C3-N
3	A	1464	CXS	C9-C4-N-C3
3	A	1463	CXS	C2-C1-S-O2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1463[A]	CXS	5	0
3	A	1465	CXS	2	0
3	C	1463[B]	CXS	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	161/193 (83%)	-0.25	0 <b>100</b> <b>100</b>	11, 21, 35, 53	0
1	C	165/193 (85%)	-0.05	5 (3%) 50 57	14, 24, 51, 59	0
2	B	30/44 (68%)	-0.06	0 <b>100</b> <b>100</b>	22, 26, 56, 61	0
2	D	28/44 (63%)	0.03	1 (3%) 42 49	17, 23, 57, 59	0
All	All	384/474 (81%)	-0.13	6 (1%) 72 77	11, 23, 51, 61	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	418	GLY	3.2
1	C	416	ARG	3.0
1	C	461	GLU	2.9
2	D	201	ASP	2.8
1	C	417	PHE	2.6
1	C	384	THR	2.1

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CXS	A	1463	14/14	0.82	0.22	65,69,78,78	0
3	CXS	C	1462	14/14	0.85	0.17	26,38,58,58	0
3	CXS	A	1464	14/14	0.86	0.17	31,37,63,63	0
3	CXS	A	1465	14/14	0.87	0.17	43,48,69,69	0
4	PO4	C	1464	5/5	0.88	0.19	58,59,60,60	0
4	PO4	A	1467	5/5	0.92	0.21	59,60,61,62	0
3	CXS	C	1463[A]	14/14	0.93	0.18	38,40,41,43	14
3	CXS	C	1463[B]	14/14	0.93	0.18	15,18,30,31	14
4	PO4	A	1466	5/5	0.95	0.13	60,60,60,62	0
4	PO4	B	1227	5/5	0.97	0.23	54,56,58,59	0
3	CXS	D	1227	14/14	0.98	0.12	16,22,26,26	0

## 6.5 Other polymers

There are no such residues in this entry.