Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 05:11 AM EDT

PDB ID	:	6S8S
Title	:	Extended structure of the human DDX6 C-terminal domain in complex with an EDC3 FDF peptide
Authors	:	Peter, D.; Valkov, E.
Deposited on	:	2019-07-10
Resolution	:	2.21 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 (i) 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 (i)) were used in the production of this report:

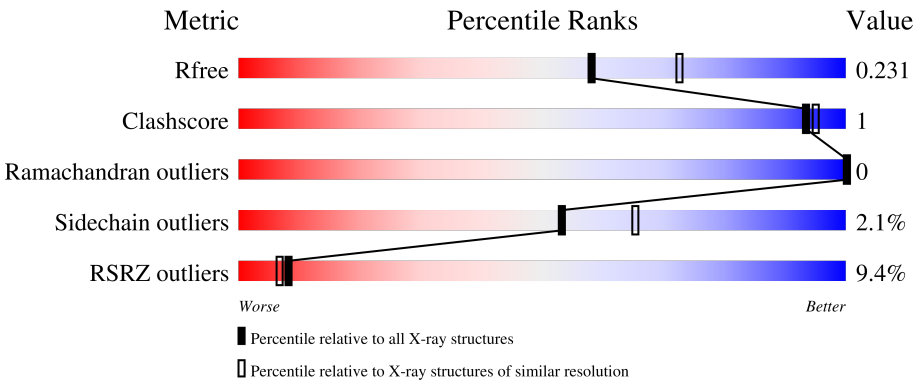
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 <=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	5%, 83%, •, 13%
1	C	193	6%, 87%, • •, 10%
2	B	44	20%, 82%, •, 16%
2	D	44	20%, 73%, 5%, 7%, 16%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3775 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 Probable ATP-dependent RNA helicase DDX6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	168	1381	880	250	245	6	0	0	0
1	C	173	1419	903	255	255	6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	GLY	-	expression tag	UNP P26196
A	281	PRO	-	expression tag	UNP P26196
A	282	GLN	-	expression tag	UNP P26196
A	283	ASP	-	expression tag	UNP P26196
C	280	GLY	-	expression tag	UNP P26196
C	281	PRO	-	expression tag	UNP P26196
C	282	GLN	-	expression tag	UNP P26196
C	283	ASP	-	expression tag	UNP P26196

- 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	37	301	193	39	69	0	0	0
2	D	37	301	193	39	69	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	185	GLY	-	expression tag	UNP Q96F86
B	186	PRO	-	expression tag	UNP Q96F86
B	187	HIS	-	expression tag	UNP Q96F86
B	188	MET	-	expression tag	UNP Q96F86

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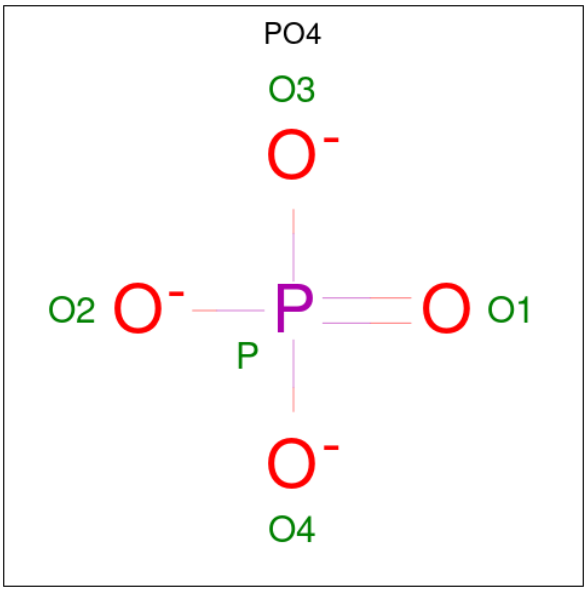
Chain	Residue	Modelled	Actual	Comment	Reference
B	189	ALA	-	expression tag	UNP Q96F86
B	190	ASP	-	expression tag	UNP Q96F86
B	191	LEU	-	expression tag	UNP Q96F86
D	185	GLY	-	expression tag	UNP Q96F86
D	186	PRO	-	expression tag	UNP Q96F86
D	187	HIS	-	expression tag	UNP Q96F86
D	188	MET	-	expression tag	UNP Q96F86
D	189	ALA	-	expression tag	UNP Q96F86
D	190	ASP	-	expression tag	UNP Q96F86
D	191	LEU	-	expression tag	UNP Q96F86

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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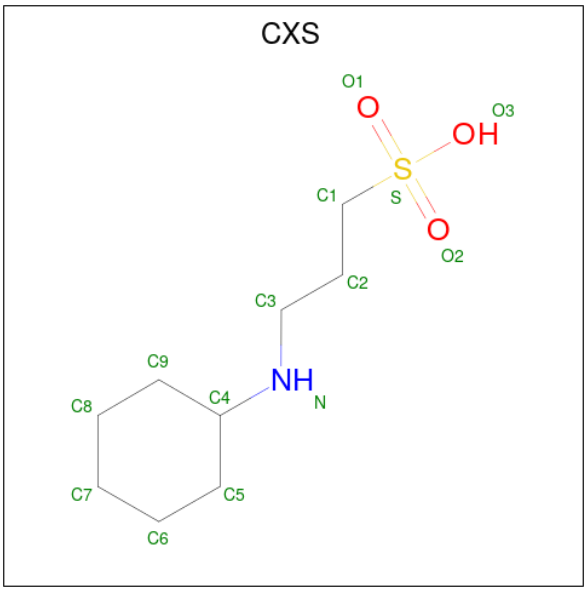
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula: $C_9H_{19}NO_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 14 9 1 3 1	0	0
4	A	1	Total C N O S 14 9 1 3 1	0	0
4	A	1	Total C N O S 14 9 1 3 1	0	0
4	C	1	Total C N O S 14 9 1 3 1	0	0
4	C	1	Total C N O S 14 9 1 3 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	98	Total O 98 98	0	0

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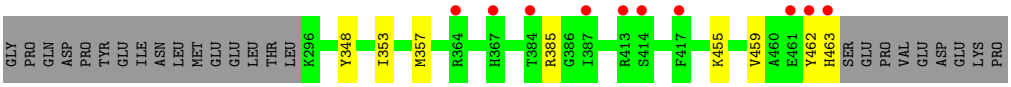
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	31	31	31	0	0
			Total	O		
5	C	99	99	99	0	0
			Total	O		
5	D	30	30	30	0	0

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.

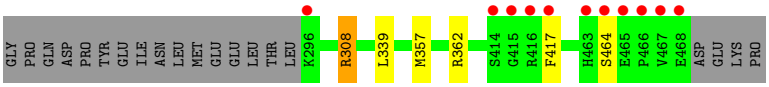
• Molecule 1: Probable ATP-dependent RNA helicase DDX6

Chain A:



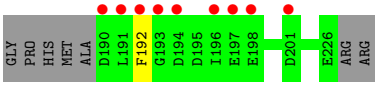
• Molecule 1: Probable ATP-dependent RNA helicase DDX6

Chain C:



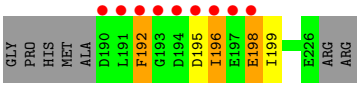
• Molecule 2: Enhancer of mRNA-decapping protein 3

Chain B:



• Molecule 2: Enhancer of mRNA-decapping protein 3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	172.43Å 47.88Å 65.76Å 90.00° 96.34° 90.00°	Depositor
Resolution (Å)	25.31 – 2.21 42.84 – 2.21	Depositor EDS
% Data completeness (in resolution range)	95.6 (25.31-2.21) 95.6 (42.84-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.179 , 0.226 0.187 , 0.231	Depositor DCC
R_{free} test set	1315 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3775	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, CXS

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	0.53	0/1409	0.67	0/1899
1	C	0.52	0/1448	0.68	0/1953
2	B	0.50	0/307	0.59	0/416
2	D	0.49	0/307	0.66	0/416
All	All	0.52	0/3471	0.67	0/4684

There are no bond length outliers.

There are no bond angle outliers.

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	1381	0	1384	4	0
1	C	1419	0	1417	4	0
2	B	301	0	257	0	0
2	D	301	0	257	3	0
3	A	25	0	0	0	0
3	C	15	0	0	0	0
3	D	5	0	0	0	0
4	A	42	0	54	1	0
4	C	28	0	37	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	98	0	0	0	0
5	B	31	0	0	0	0
5	C	99	0	0	0	0
5	D	30	0	0	0	0
All	All	3775	0	3406	10	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 1.

All (10) 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:455:LYS:HB2	1:A:463:HIS:HB2	1.54	0.89
1:C:357:MET:HE2	1:C:362:ARG:HG3	1.78	0.65
2:D:195:ASP:HB2	2:D:198:GLU:HB2	1.83	0.61
2:D:196:ILE:HA	2:D:199:ILE:HD12	1.90	0.52
1:C:308:ARG:HB2	1:C:308:ARG:CZ	2.45	0.46
1:A:353:ILE:HG22	1:A:357:MET:HE1	1.99	0.45
1:C:339:LEU:HB2	2:D:192:PHE:HZ	1.82	0.44
1:C:357:MET:HB3	1:C:357:MET:HE3	1.96	0.41
1:A:348:TYR:CD1	4:A:507:CXS:H71	2.56	0.40
1:A:459:VAL:HG12	1:A:462:TYR:HB2	2.04	0.40

There are no symmetry-related clashes.

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	166/193 (86%)	161 (97%)	5 (3%)	0	100 100
1	C	171/193 (89%)	167 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	35/44 (80%)	34 (97%)	1 (3%)	0	100	100
2	D	35/44 (80%)	34 (97%)	1 (3%)	0	100	100
All	All	407/474 (86%)	396 (97%)	11 (3%)	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	152/176 (86%)	151 (99%)	1 (1%)	84	91
1	C	157/176 (89%)	154 (98%)	3 (2%)	57	69
2	B	32/37 (86%)	31 (97%)	1 (3%)	40	50
2	D	32/37 (86%)	29 (91%)	3 (9%)	8	7
All	All	373/426 (88%)	365 (98%)	8 (2%)	53	65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	385	ARG
2	B	192	PHE
1	C	308	ARG
1	C	417	PHE
1	C	464	SER
2	D	192	PHE
2	D	196	ILE
2	D	198	GLU

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 (i)

14 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	PO4	C	501	-	4,4,4	2.52	2 (50%)	6,6,6	0.72	0
4	CXS	A	507	-	14,14,14	0.58	0	18,18,18	1.27	2 (11%)
4	CXS	C	504	-	14,14,14	0.57	0	18,18,18	0.78	0
4	CXS	A	508	-	14,14,14	0.28	0	18,18,18	0.90	1 (5%)
4	CXS	A	506	-	14,14,14	0.55	0	18,18,18	1.26	2 (11%)
3	PO4	C	502	-	4,4,4	2.57	1 (25%)	6,6,6	0.29	0
3	PO4	D	301	-	4,4,4	2.50	2 (50%)	6,6,6	0.89	0
3	PO4	A	504	-	4,4,4	2.00	1 (25%)	6,6,6	0.52	0
3	PO4	A	505	-	4,4,4	2.57	2 (50%)	6,6,6	0.91	0
3	PO4	A	503	-	4,4,4	2.58	3 (75%)	6,6,6	0.55	0
3	PO4	A	502	-	4,4,4	2.57	2 (50%)	6,6,6	0.69	0
3	PO4	A	501	-	4,4,4	2.54	3 (75%)	6,6,6	0.65	0
3	PO4	C	503	-	4,4,4	2.60	2 (50%)	6,6,6	0.56	0
4	CXS	C	505	-	14,14,14	0.29	0	18,18,18	1.05	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
4	CXS	A	507	-	-	4/8/16/16	0/1/1/1
4	CXS	A	508	-	-	1/8/16/16	0/1/1/1
4	CXS	A	506	-	-	1/8/16/16	0/1/1/1
4	CXS	C	504	-	-	0/8/16/16	0/1/1/1
4	CXS	C	505	-	-	4/8/16/16	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	505	PO4	P-O1	4.32	1.60	1.50
3	C	503	PO4	P-O1	4.29	1.60	1.50
3	A	502	PO4	P-O1	4.28	1.60	1.50
3	A	503	PO4	P-O1	4.26	1.60	1.50
3	C	502	PO4	P-O1	4.25	1.60	1.50
3	A	501	PO4	P-O1	4.18	1.60	1.50
3	C	501	PO4	P-O1	4.13	1.60	1.50
3	D	301	PO4	P-O1	4.12	1.60	1.50
3	A	503	PO4	P-O2	2.05	1.60	1.54
3	A	505	PO4	P-O4	2.04	1.60	1.54
3	A	504	PO4	P-O1	2.04	1.55	1.50
3	C	503	PO4	P-O3	2.03	1.60	1.54
3	A	501	PO4	P-O2	2.03	1.60	1.54
3	D	301	PO4	P-O3	2.02	1.60	1.54
3	A	503	PO4	P-O4	2.02	1.60	1.54
3	C	501	PO4	P-O2	2.02	1.60	1.54
3	A	502	PO4	P-O2	2.02	1.60	1.54
3	A	501	PO4	P-O4	2.01	1.60	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	506	CXS	C3-N-C4	4.21	122.29	114.18
4	A	507	CXS	C9-C4-N	3.78	129.46	110.56
4	C	505	CXS	C9-C4-N	2.91	125.10	110.56
4	A	507	CXS	O2-S-C1	-2.51	102.94	106.73
4	A	508	CXS	C3-N-C4	2.50	119.00	114.18
4	A	506	CXS	C9-C4-N	2.25	121.79	110.56
4	C	505	CXS	C2-C1-S	-2.19	109.88	113.25

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	506	CXS	C9-C4-N-C3
4	A	507	CXS	C9-C4-N-C3
4	C	505	CXS	C9-C4-N-C3
4	C	505	CXS	C1-C2-C3-N
4	A	507	CXS	C2-C1-S-O2
4	C	505	CXS	C2-C3-N-C4
4	A	507	CXS	C2-C1-S-O3
4	A	508	CXS	C2-C3-N-C4
4	C	505	CXS	C5-C4-N-C3
4	A	507	CXS	S-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	507	CXS	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 (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	168/193 (87%)	-0.00	10 (5%)	21	20	18, 31, 66, 118	0
1	C	173/193 (89%)	-0.03	11 (6%)	19	18	18, 28, 79, 103	0
2	B	37/44 (84%)	0.89	9 (24%)	0	0	21, 35, 106, 108	0
2	D	37/44 (84%)	1.14	9 (24%)	0	0	24, 35, 112, 114	0
All	All	415/474 (87%)	0.17	39 (9%)	8	7	18, 30, 89, 118	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	196	ILE	11.7
1	A	463	HIS	8.2
2	B	196	ILE	8.1
1	A	462	TYR	7.9
2	D	193	GLY	6.2
2	D	198	GLU	6.1
2	B	190	ASP	5.7
2	D	190	ASP	5.6
2	B	193	GLY	5.3
1	C	417	PHE	5.1
2	B	191	LEU	4.9
1	C	463	HIS	4.7
1	C	466	PRO	4.7
2	B	197	GLU	4.7
1	C	468	GLU	4.6
1	C	416	ARG	4.5
2	D	195	ASP	4.5
1	C	465	GLU	4.4
2	D	194	ASP	4.4
1	C	464	SER	4.4
2	D	197	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	192	PHE	4.1
1	A	367	HIS	3.9
1	A	387	ILE	3.6
1	C	467	VAL	3.6
2	B	201	ASP	3.4
1	A	417	PHE	3.4
1	C	415	GLY	3.3
1	C	296	LYS	3.3
1	C	414	SER	2.8
1	A	461	GLU	2.5
2	D	192	PHE	2.3
1	A	413	ARG	2.3
1	A	414	SER	2.3
2	D	191	LEU	2.2
2	B	198	GLU	2.2
2	B	194	ASP	2.1
1	A	384	THR	2.1
1	A	364	ARG	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, 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
4	CXS	A	508	14/14	0.56	0.35	78,88,109,109	0
4	CXS	A	507	14/14	0.79	0.21	43,53,84,85	0
3	PO4	A	503	5/5	0.80	0.34	106,107,107,108	0
4	CXS	C	504	14/14	0.80	0.21	44,57,83,83	0
3	PO4	A	502	5/5	0.84	0.34	80,81,83,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CXS	C	505	14/14	0.84	0.19	48,60,86,87	0
3	PO4	A	501	5/5	0.87	0.28	90,90,91,91	0
3	PO4	C	503	5/5	0.91	0.20	74,75,77,77	0
3	PO4	C	501	5/5	0.92	0.29	76,77,79,79	0
3	PO4	A	505	5/5	0.93	0.30	66,67,69,70	0
3	PO4	A	504	5/5	0.94	0.18	82,82,83,83	0
3	PO4	C	502	5/5	0.95	0.21	66,67,67,71	0
3	PO4	D	301	5/5	0.96	0.22	49,55,59,62	0
4	CXS	A	506	14/14	0.98	0.09	26,30,34,36	0

6.5 Other polymers (i)

There are no such residues in this entry.