



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:06 PM GMT

PDB ID : 4BIY
Title : Crystal structure of CpxAHDC (monoclinic form 2)
Authors : Mechaly, A.E.; Sassoon, N.; Betton, J.M.; Alzari, P.M.
Deposited on : 2013-04-13
Resolution : 3.30 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
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

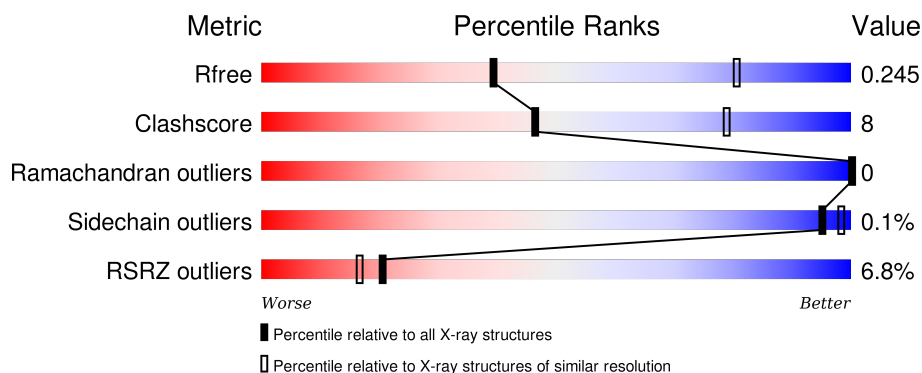
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 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	298	<div> <div>7%</div> <div>66%</div> <div>10%</div> <div>23%</div> </div>
1	B	298	<div> <div>7%</div> <div>61%</div> <div>13%</div> <div>26%</div> </div>
1	C	298	<div> <div>3%</div> <div>64%</div> <div>12%</div> <div>23%</div> </div>
1	D	298	<div> <div>10%</div> <div>60%</div> <div>12%</div> <div>28%</div> </div>

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
3	SO4	C	1457	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7134 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 SENSOR PROTEIN CPXA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1797	1125	323	344	5			
1	B	221	Total	C	N	O	S	0	0	0
			1756	1102	316	333	5			
1	C	228	Total	C	N	O	S	0	0	0
			1797	1125	323	344	5			
1	D	216	Total	C	N	O	S	0	0	0
			1710	1070	308	327	5			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	MET	-	EXPRESSION TAG	UNP P0AE82
A	161	GLY	-	EXPRESSION TAG	UNP P0AE82
A	162	SER	-	EXPRESSION TAG	UNP P0AE82
A	163	SER	-	EXPRESSION TAG	UNP P0AE82
A	164	HIS	-	EXPRESSION TAG	UNP P0AE82
A	165	HIS	-	EXPRESSION TAG	UNP P0AE82
A	166	HIS	-	EXPRESSION TAG	UNP P0AE82
A	167	HIS	-	EXPRESSION TAG	UNP P0AE82
A	168	HIS	-	EXPRESSION TAG	UNP P0AE82
A	169	HIS	-	EXPRESSION TAG	UNP P0AE82
A	170	SER	-	EXPRESSION TAG	UNP P0AE82
A	171	SER	-	EXPRESSION TAG	UNP P0AE82
A	172	GLY	-	EXPRESSION TAG	UNP P0AE82
A	173	LEU	-	EXPRESSION TAG	UNP P0AE82
A	174	VAL	-	EXPRESSION TAG	UNP P0AE82
A	175	PRO	-	EXPRESSION TAG	UNP P0AE82
A	176	ARG	-	EXPRESSION TAG	UNP P0AE82
A	177	GLY	-	EXPRESSION TAG	UNP P0AE82
A	178	SER	-	EXPRESSION TAG	UNP P0AE82
A	179	HIS	-	EXPRESSION TAG	UNP P0AE82
A	180	MET	-	EXPRESSION TAG	UNP P0AE82

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Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLU	-	EXPRESSION TAG	UNP P0AE82
A	182	ASN	-	EXPRESSION TAG	UNP P0AE82
A	183	LEU	-	EXPRESSION TAG	UNP P0AE82
A	184	TYR	-	EXPRESSION TAG	UNP P0AE82
A	185	PHE	-	EXPRESSION TAG	UNP P0AE82
A	186	GLN	-	EXPRESSION TAG	UNP P0AE82
A	187	GLY	-	EXPRESSION TAG	UNP P0AE82
A	228	VAL	MET	CONFLICT	UNP P0AE82
B	160	MET	-	EXPRESSION TAG	UNP P0AE82
B	161	GLY	-	EXPRESSION TAG	UNP P0AE82
B	162	SER	-	EXPRESSION TAG	UNP P0AE82
B	163	SER	-	EXPRESSION TAG	UNP P0AE82
B	164	HIS	-	EXPRESSION TAG	UNP P0AE82
B	165	HIS	-	EXPRESSION TAG	UNP P0AE82
B	166	HIS	-	EXPRESSION TAG	UNP P0AE82
B	167	HIS	-	EXPRESSION TAG	UNP P0AE82
B	168	HIS	-	EXPRESSION TAG	UNP P0AE82
B	169	HIS	-	EXPRESSION TAG	UNP P0AE82
B	170	SER	-	EXPRESSION TAG	UNP P0AE82
B	171	SER	-	EXPRESSION TAG	UNP P0AE82
B	172	GLY	-	EXPRESSION TAG	UNP P0AE82
B	173	LEU	-	EXPRESSION TAG	UNP P0AE82
B	174	VAL	-	EXPRESSION TAG	UNP P0AE82
B	175	PRO	-	EXPRESSION TAG	UNP P0AE82
B	176	ARG	-	EXPRESSION TAG	UNP P0AE82
B	177	GLY	-	EXPRESSION TAG	UNP P0AE82
B	178	SER	-	EXPRESSION TAG	UNP P0AE82
B	179	HIS	-	EXPRESSION TAG	UNP P0AE82
B	180	MET	-	EXPRESSION TAG	UNP P0AE82
B	181	GLU	-	EXPRESSION TAG	UNP P0AE82
B	182	ASN	-	EXPRESSION TAG	UNP P0AE82
B	183	LEU	-	EXPRESSION TAG	UNP P0AE82
B	184	TYR	-	EXPRESSION TAG	UNP P0AE82
B	185	PHE	-	EXPRESSION TAG	UNP P0AE82
B	186	GLN	-	EXPRESSION TAG	UNP P0AE82
B	187	GLY	-	EXPRESSION TAG	UNP P0AE82
B	228	VAL	MET	CONFLICT	UNP P0AE82
C	160	MET	-	EXPRESSION TAG	UNP P0AE82
C	161	GLY	-	EXPRESSION TAG	UNP P0AE82
C	162	SER	-	EXPRESSION TAG	UNP P0AE82
C	163	SER	-	EXPRESSION TAG	UNP P0AE82
C	164	HIS	-	EXPRESSION TAG	UNP P0AE82

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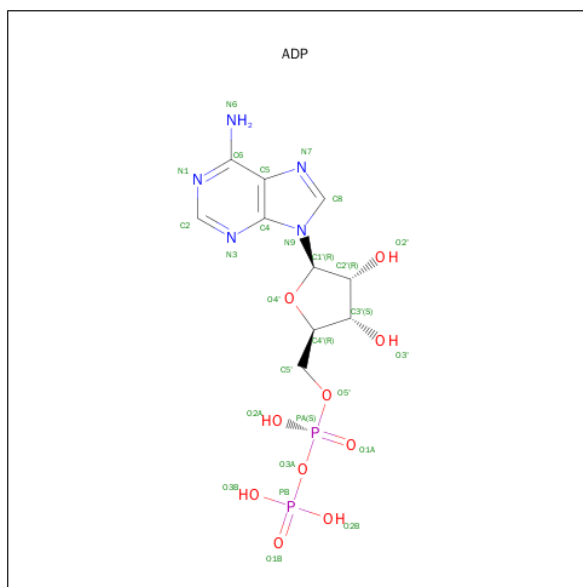
Chain	Residue	Modelled	Actual	Comment	Reference
C	165	HIS	-	EXPRESSION TAG	UNP P0AE82
C	166	HIS	-	EXPRESSION TAG	UNP P0AE82
C	167	HIS	-	EXPRESSION TAG	UNP P0AE82
C	168	HIS	-	EXPRESSION TAG	UNP P0AE82
C	169	HIS	-	EXPRESSION TAG	UNP P0AE82
C	170	SER	-	EXPRESSION TAG	UNP P0AE82
C	171	SER	-	EXPRESSION TAG	UNP P0AE82
C	172	GLY	-	EXPRESSION TAG	UNP P0AE82
C	173	LEU	-	EXPRESSION TAG	UNP P0AE82
C	174	VAL	-	EXPRESSION TAG	UNP P0AE82
C	175	PRO	-	EXPRESSION TAG	UNP P0AE82
C	176	ARG	-	EXPRESSION TAG	UNP P0AE82
C	177	GLY	-	EXPRESSION TAG	UNP P0AE82
C	178	SER	-	EXPRESSION TAG	UNP P0AE82
C	179	HIS	-	EXPRESSION TAG	UNP P0AE82
C	180	MET	-	EXPRESSION TAG	UNP P0AE82
C	181	GLU	-	EXPRESSION TAG	UNP P0AE82
C	182	ASN	-	EXPRESSION TAG	UNP P0AE82
C	183	LEU	-	EXPRESSION TAG	UNP P0AE82
C	184	TYR	-	EXPRESSION TAG	UNP P0AE82
C	185	PHE	-	EXPRESSION TAG	UNP P0AE82
C	186	GLN	-	EXPRESSION TAG	UNP P0AE82
C	187	GLY	-	EXPRESSION TAG	UNP P0AE82
C	228	VAL	MET	CONFLICT	UNP P0AE82
D	160	MET	-	EXPRESSION TAG	UNP P0AE82
D	161	GLY	-	EXPRESSION TAG	UNP P0AE82
D	162	SER	-	EXPRESSION TAG	UNP P0AE82
D	163	SER	-	EXPRESSION TAG	UNP P0AE82
D	164	HIS	-	EXPRESSION TAG	UNP P0AE82
D	165	HIS	-	EXPRESSION TAG	UNP P0AE82
D	166	HIS	-	EXPRESSION TAG	UNP P0AE82
D	167	HIS	-	EXPRESSION TAG	UNP P0AE82
D	168	HIS	-	EXPRESSION TAG	UNP P0AE82
D	169	HIS	-	EXPRESSION TAG	UNP P0AE82
D	170	SER	-	EXPRESSION TAG	UNP P0AE82
D	171	SER	-	EXPRESSION TAG	UNP P0AE82
D	172	GLY	-	EXPRESSION TAG	UNP P0AE82
D	173	LEU	-	EXPRESSION TAG	UNP P0AE82
D	174	VAL	-	EXPRESSION TAG	UNP P0AE82
D	175	PRO	-	EXPRESSION TAG	UNP P0AE82
D	176	ARG	-	EXPRESSION TAG	UNP P0AE82
D	177	GLY	-	EXPRESSION TAG	UNP P0AE82

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Chain	Residue	Modelled	Actual	Comment	Reference
D	178	SER	-	EXPRESSION TAG	UNP P0AE82
D	179	HIS	-	EXPRESSION TAG	UNP P0AE82
D	180	MET	-	EXPRESSION TAG	UNP P0AE82
D	181	GLU	-	EXPRESSION TAG	UNP P0AE82
D	182	ASN	-	EXPRESSION TAG	UNP P0AE82
D	183	LEU	-	EXPRESSION TAG	UNP P0AE82
D	184	TYR	-	EXPRESSION TAG	UNP P0AE82
D	185	PHE	-	EXPRESSION TAG	UNP P0AE82
D	186	GLN	-	EXPRESSION TAG	UNP P0AE82
D	187	GLY	-	EXPRESSION TAG	UNP P0AE82
D	228	VAL	MET	CONFLICT	UNP P0AE82

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

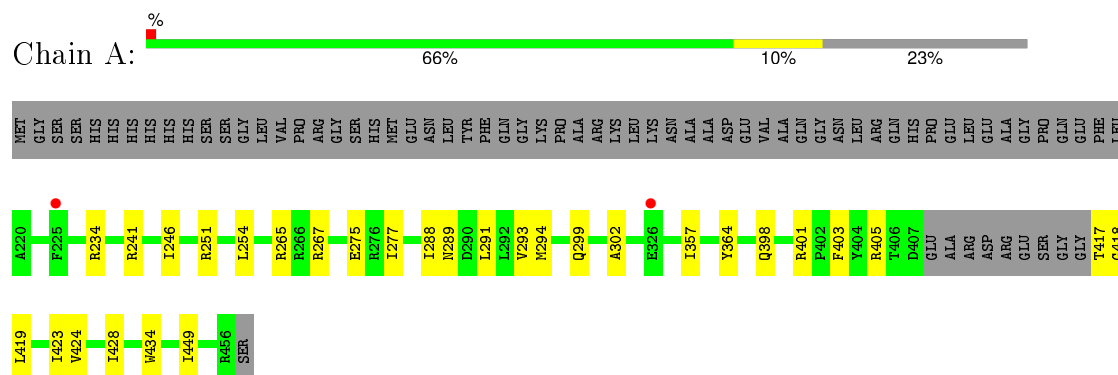


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

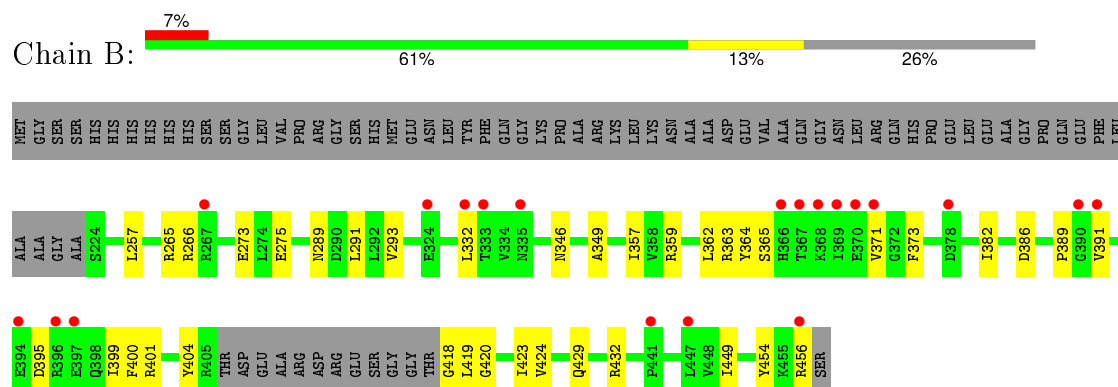
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

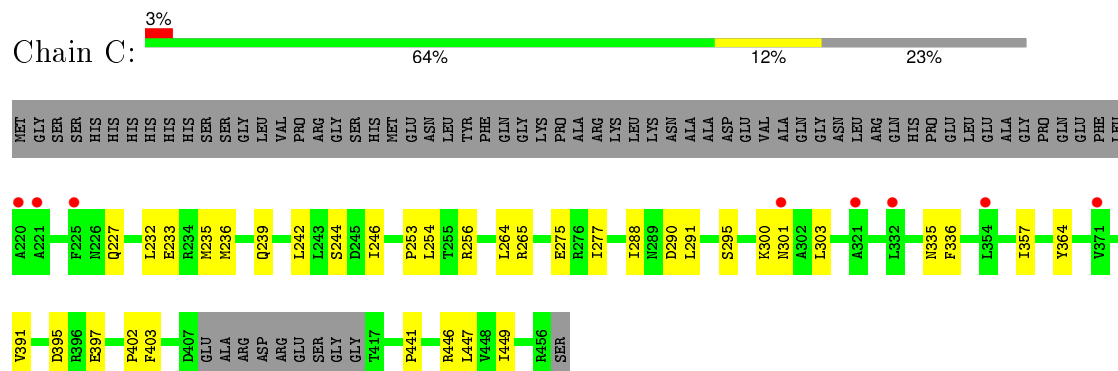
• Molecule 1: SENSOR PROTEIN CPXA



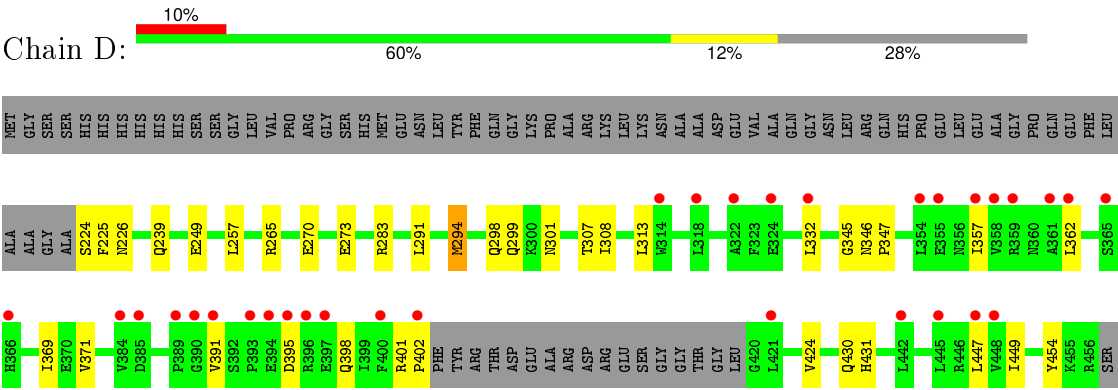
• Molecule 1: SENSOR PROTEIN CPXA



• Molecule 1: SENSOR PROTEIN CPXA



● Molecule 1: SENSOR PROTEIN CPXA



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.75Å 139.11Å 114.08Å 90.00° 99.19° 90.00°	Depositor
Resolution (Å)	47.74 – 3.30 47.74 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.74-3.30) 98.9 (47.74-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.200 , 0.219 0.226 , 0.245	Depositor DCC
R_{free} test set	1082 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	84.3	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 21081 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7134	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ADP

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	0.49	0/1827	0.67	0/2475
1	B	0.51	0/1786	0.67	0/2418
1	C	0.46	0/1827	0.65	0/2475
1	D	0.52	0/1738	0.69	1/2354 (0.0%)
All	All	0.49	0/7178	0.67	1/9722 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	225	PHE	C-N-CA	5.41	135.21	121.70

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	1797	0	1801	23	0
1	B	1756	0	1765	34	0
1	C	1797	0	1801	42	0
1	D	1710	0	1720	35	0
2	A	27	0	12	2	0
2	C	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	3	0
3	D	5	0	0	0	0
All	All	7134	0	7111	108	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 (108) 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:C:236:MET:HE1	1:D:239:GLN:NE2	1.70	1.06
1:C:236:MET:HE1	1:D:239:GLN:HE22	1.02	1.05
1:C:236:MET:HG3	1:C:303:LEU:HD11	1.49	0.91
1:C:446:ARG:NH2	3:C:1457:SO4:O4	2.03	0.90
1:C:236:MET:CE	1:D:239:GLN:HE22	1.91	0.82
1:B:419:LEU:HD22	1:B:423:ILE:HD11	1.63	0.79
1:D:308:ILE:HD11	1:D:347:PRO:HG3	1.67	0.77
1:C:235:MET:SD	1:D:299:GLN:HA	2.25	0.76
1:A:357:ILE:HD11	1:A:424:VAL:HG11	1.66	0.76
1:A:234:ARG:NH1	1:B:432:ARG:HE	1.86	0.73
1:C:441:PRO:HG2	3:C:1457:SO4:O1	1.88	0.72
1:C:232:LEU:O	1:C:236:MET:HG2	1.88	0.72
1:C:254:LEU:HD22	1:C:288:ILE:HD12	1.77	0.66
1:A:234:ARG:HH12	1:B:432:ARG:HE	1.42	0.66
1:B:363:ARG:HH22	1:B:418:GLY:HA2	1.65	0.62
1:A:254:LEU:HD22	1:A:288:ILE:HD12	1.82	0.61
1:B:265:ARG:HH22	1:B:275:GLU:HG3	1.65	0.61
1:C:253:PRO:HB3	1:D:283:ARG:HD3	1.83	0.61
1:C:236:MET:CE	1:D:239:GLN:OE1	2.50	0.60
1:A:294:MET:HG2	1:A:417:THR:HG21	1.83	0.60
1:A:357:ILE:HD13	1:A:449:ILE:HD11	1.84	0.59
1:C:236:MET:CE	1:D:239:GLN:NE2	2.56	0.59
1:C:236:MET:HE1	1:D:239:GLN:CD	2.21	0.58
1:C:265:ARG:HH22	1:C:275:GLU:HG3	1.69	0.57
1:B:400:PHE:O	1:B:401:ARG:HG3	2.04	0.57
1:C:277:ILE:HG23	1:D:257:LEU:HG	1.87	0.57
1:A:246:ILE:HG13	1:B:291:LEU:HD13	1.87	0.56
1:C:227:GLN:HE21	1:D:430:GLN:HE22	1.54	0.56
1:B:357:ILE:HD11	1:B:424:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ARG:HH22	1:A:275:GLU:HG3	1.71	0.55
1:B:401:ARG:HB2	1:B:404:TYR:OH	2.07	0.55
1:B:395:ASP:O	1:B:399:ILE:HG23	2.07	0.55
1:B:289:ASN:O	1:B:293:VAL:HG23	2.06	0.54
1:C:233:GLU:HG2	1:C:303:LEU:HD12	1.89	0.54
1:A:251:ARG:NH2	1:A:289:ASN:OD1	2.38	0.53
1:C:357:ILE:HD13	1:C:449:ILE:HD11	1.90	0.53
1:B:419:LEU:HD22	1:B:423:ILE:CD1	2.37	0.53
1:D:265:ARG:HH11	1:D:270:GLU:HG2	1.74	0.53
1:C:242:LEU:HD21	1:D:294:MET:HB2	1.91	0.52
1:D:357:ILE:HD13	1:D:449:ILE:HD11	1.91	0.52
1:B:365:SER:HB3	1:B:386:ASP:HB2	1.91	0.52
1:B:359:ARG:HA	1:B:362:LEU:HD12	1.91	0.51
1:C:402:PRO:HD2	1:D:249:GLU:HG3	1.92	0.51
1:C:239:GLN:HG3	1:D:298:GLN:OE1	2.11	0.51
1:C:264:LEU:HD13	1:D:273:GLU:HB2	1.93	0.51
1:D:398:GLN:HE22	1:D:401:ARG:HH11	1.59	0.51
1:A:277:ILE:HG23	1:B:257:LEU:HG	1.92	0.50
1:A:405:ARG:HG3	2:A:501:ADP:O3'	2.12	0.49
1:D:301:ASN:HB3	1:D:346:ASN:HD21	1.78	0.49
1:C:244:SER:HB2	1:C:295:SER:HB3	1.94	0.48
1:B:346:ASN:HD22	1:B:349:ALA:H	1.60	0.48
1:B:346:ASN:ND2	1:B:349:ALA:H	2.12	0.48
1:B:357:ILE:HD13	1:B:449:ILE:HD11	1.95	0.47
1:B:419:LEU:HD13	1:B:423:ILE:CD1	2.45	0.47
1:B:391:VAL:CG1	1:B:395:ASP:HB2	2.45	0.47
1:A:364:TYR:OH	2:A:501:ADP:H2'	2.15	0.47
1:C:227:GLN:HE21	1:D:430:GLN:NE2	2.14	0.46
1:C:364:TYR:OH	2:C:501:ADP:H2'	2.16	0.46
1:C:236:MET:CE	1:D:239:GLN:CD	2.83	0.46
1:D:308:ILE:HG21	1:D:313:LEU:HD13	1.98	0.46
1:C:336:PHE:CD2	1:C:336:PHE:N	2.83	0.46
1:C:256:ARG:HH12	1:D:283:ARG:CZ	2.29	0.46
1:B:346:ASN:HD22	1:B:349:ALA:HB2	1.80	0.46
1:C:290:ASP:HB2	1:C:403:PHE:CD1	2.49	0.46
1:B:404:TYR:HB2	1:B:420:GLY:HA2	1.98	0.45
1:D:357:ILE:HD11	1:D:424:VAL:HG11	1.98	0.45
1:D:362:LEU:HA	1:D:369:ILE:HD11	1.99	0.45
1:C:236:MET:HE2	1:C:236:MET:HB3	1.63	0.45
1:B:364:TYR:HB2	1:B:386:ASP:OD2	2.17	0.45
1:C:291:LEU:HD13	1:C:403:PHE:HZ	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ARG:HH11	1:A:418:GLY:N	2.15	0.44
1:C:290:ASP:HB2	1:C:403:PHE:CE1	2.53	0.44
1:B:419:LEU:CD2	1:B:423:ILE:HD11	2.42	0.43
1:D:391:VAL:CG1	1:D:395:ASP:HB2	2.49	0.43
1:B:373:PHE:CE2	1:B:382:ILE:HG12	2.52	0.43
1:C:244:SER:CB	1:C:295:SER:HB3	2.49	0.43
1:A:398:GLN:HG3	1:A:401:ARG:HH11	1.84	0.43
1:D:398:GLN:HE22	1:D:401:ARG:NH1	2.16	0.43
1:C:246:ILE:HG13	1:D:291:LEU:HD13	2.01	0.43
1:A:357:ILE:CD1	1:A:424:VAL:HG11	2.43	0.42
1:B:346:ASN:HD22	1:B:349:ALA:CB	2.32	0.42
1:D:307:THR:HG23	1:D:454:TYR:HD2	1.85	0.42
1:B:391:VAL:HG13	1:B:395:ASP:HB2	2.01	0.42
1:C:357:ILE:HG23	1:C:447:LEU:HD13	2.02	0.42
1:C:300:LYS:HG2	1:C:301:ASN:H	1.84	0.42
1:C:233:GLU:CG	1:C:303:LEU:HD12	2.50	0.42
1:C:391:VAL:CG1	1:C:395:ASP:HB2	2.50	0.42
1:A:419:LEU:O	1:A:423:ILE:HD12	2.20	0.41
1:B:332:LEU:HD11	1:B:371:VAL:HG23	2.02	0.41
1:A:299:GLN:HE21	1:A:302:ALA:HB2	1.85	0.41
1:C:441:PRO:CG	3:C:1457:SO4:O1	2.64	0.41
1:B:266:ARG:HH12	1:C:227:GLN:C	2.23	0.41
1:D:345:GLY:HA3	1:D:431:HIS:CD2	2.55	0.41
1:B:364:TYR:HB3	1:B:389:PRO:HD2	2.02	0.41
1:D:332:LEU:HD11	1:D:371:VAL:HG23	2.02	0.41
1:D:357:ILE:HG23	1:D:447:LEU:HD13	2.03	0.41
1:D:401:ARG:HA	1:D:402:PRO:HD2	1.94	0.41
1:A:291:LEU:HD13	1:A:403:PHE:HZ	1.86	0.41
1:A:434:TRP:HB3	1:C:397:GLU:CD	2.40	0.41
1:B:454:TYR:HE2	1:B:456:ARG:HE	1.68	0.41
1:A:289:ASN:O	1:A:293:VAL:HG23	2.21	0.40
1:C:335:ASN:HB2	1:C:336:PHE:CD2	2.56	0.40
1:A:241:ARG:NH2	1:B:429:GLN:OE1	2.54	0.40
1:D:224:SER:C	1:D:226:ASN:H	2.25	0.40
1:A:267:ARG:HD3	1:B:273:GLU:CD	2.41	0.40
1:A:424:VAL:O	1:A:428:ILE:HG12	2.22	0.40
1:D:301:ASN:HB3	1:D:346:ASN:ND2	2.37	0.40
1:B:363:ARG:NH2	1:B:418:GLY:HA2	2.32	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	224/298 (75%)	213 (95%)	11 (5%)	0	100	100
1	B	217/298 (73%)	209 (96%)	8 (4%)	0	100	100
1	C	224/298 (75%)	217 (97%)	7 (3%)	0	100	100
1	D	212/298 (71%)	206 (97%)	6 (3%)	0	100	100
All	All	877/1192 (74%)	845 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/251 (78%)	195 (100%)	0	100	100
1	B	192/251 (76%)	192 (100%)	0	100	100
1	C	195/251 (78%)	195 (100%)	0	100	100
1	D	188/251 (75%)	187 (100%)	1 (0%)	92	95
All	All	770/1004 (77%)	769 (100%)	1 (0%)	95	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	294	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
1	A	299	GLN
1	A	348	ASN
1	B	346	ASN
1	B	348	ASN
1	C	226	ASN
1	C	239	GLN
1	C	348	ASN
1	C	398	GLN
1	D	239	GLN
1	D	289	ASN
1	D	299	GLN
1	D	301	ASN
1	D	348	ASN
1	D	430	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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
3	SO4	A	1457	-	4,4,4	0.29	0	6,6,6	0.22	0
2	ADP	A	501	-	22,29,29	0.61	0	27,45,45	0.76	1 (3%)
3	SO4	B	1457	-	4,4,4	0.14	0	6,6,6	0.11	0
3	SO4	C	1457	-	4,4,4	1.14	1 (25%)	6,6,6	0.71	0
2	ADP	C	501	-	22,29,29	0.59	0	27,45,45	0.69	1 (3%)
3	SO4	D	1457	-	4,4,4	1.20	1 (25%)	6,6,6	1.00	1 (16%)

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	SO4	A	1457	-	-	0/0/0/0	0/0/0/0
2	ADP	A	501	-	-	0/12/32/32	0/3/3/3
3	SO4	B	1457	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1457	-	-	0/0/0/0	0/0/0/0
2	ADP	C	501	-	-	0/12/32/32	0/3/3/3
3	SO4	D	1457	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1457	SO4	O2-S	-2.21	1.39	1.47
3	C	1457	SO4	O2-S	-2.18	1.39	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ADP	O3A-PA-O5'	2.08	108.44	102.94
2	C	501	ADP	O3A-PA-O5'	2.08	108.45	102.94
3	D	1457	SO4	O4-S-O3	2.24	118.08	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ADP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1457	SO4	3	0
2	C	501	ADP	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	228/298 (76%)	0.10	2 (0%) 85 82	60, 92, 137, 161	0
1	B	221/298 (74%)	0.52	20 (9%) 12 9	48, 98, 155, 193	0
1	C	228/298 (76%)	0.28	8 (3%) 48 40	70, 105, 150, 182	0
1	D	216/298 (72%)	0.86	31 (14%) 3 3	55, 132, 189, 225	0
All	All	893/1192 (74%)	0.43	61 (6%) 20 17	48, 103, 164, 225	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	400	PHE	6.6
1	D	361	ALA	4.9
1	D	357	ILE	4.4
1	D	354	LEU	4.2
1	C	221	ALA	4.1
1	C	321	ALA	4.0
1	D	402	PRO	3.9
1	B	390	GLY	3.8
1	D	322	ALA	3.7
1	C	332	LEU	3.6
1	D	318	LEU	3.5
1	D	390	GLY	3.5
1	D	421	LEU	3.5
1	B	456	ARG	3.3
1	D	391	VAL	3.3
1	D	365	SER	3.3
1	D	397	GLU	3.3
1	B	335	ASN	3.2
1	D	366	HIS	3.2
1	C	225	PHE	3.1
1	D	362	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	358	VAL	3.0
1	D	359	ARG	3.0
1	D	385	ASP	2.9
1	B	366	HIS	2.9
1	D	389	PRO	2.8
1	B	394	GLU	2.7
1	B	371	VAL	2.7
1	B	332	LEU	2.7
1	B	391	VAL	2.6
1	A	326	GLU	2.6
1	D	442	LEU	2.6
1	C	371	VAL	2.6
1	B	367	THR	2.6
1	D	448	VAL	2.6
1	D	384	VAL	2.6
1	D	394	GLU	2.6
1	B	324	GLU	2.5
1	D	324	GLU	2.5
1	D	395	ASP	2.5
1	A	225	PHE	2.5
1	C	220	ALA	2.4
1	B	397	GLU	2.4
1	C	354	LEU	2.4
1	B	333	THR	2.4
1	C	301	ASN	2.4
1	B	447	LEU	2.3
1	B	368	LYS	2.3
1	B	267	ARG	2.3
1	D	314	TRP	2.3
1	D	355	GLU	2.3
1	B	369	ILE	2.3
1	D	396	ARG	2.3
1	B	396	ARG	2.3
1	B	378	ASP	2.2
1	B	370	GLU	2.2
1	D	447	LEU	2.2
1	D	393	PRO	2.2
1	D	445	LEU	2.2
1	B	441	PRO	2.0
1	D	332	LEU	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 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(\AA^2)	Q<0.9
3	SO4	B	1457	5/5	0.97	0.25	0.88	104,106,106,106	0
3	SO4	A	1457	5/5	0.95	0.27	0.49	101,102,103,105	0
2	ADP	C	501	27/27	0.95	0.20	-0.40	86,92,100,101	0
2	ADP	A	501	27/27	0.96	0.20	-0.41	71,77,87,89	0
3	SO4	C	1457	5/5	0.62	0.67	-	228,229,229,230	0
3	SO4	D	1457	5/5	0.67	0.44	-	210,210,210,212	0

6.5 Other polymers [i](#)

There are no such residues in this entry.