



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:16 PM UTC

PDB ID : 1VZ4 / pdb_00001vz4
Title : Fe-Succinate Complex of AtsK
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Deposited on : 2004-05-14
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

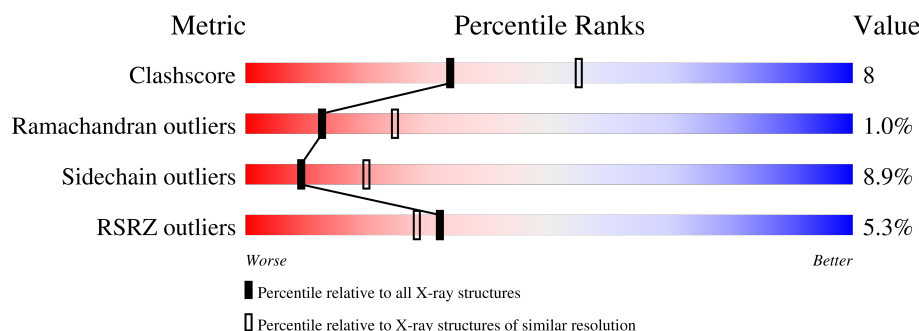
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	301	5% 52% 25% 5% 17%
1	D	301	4% 64% 18% • • 14%

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	SIN	A	1300	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3937 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.

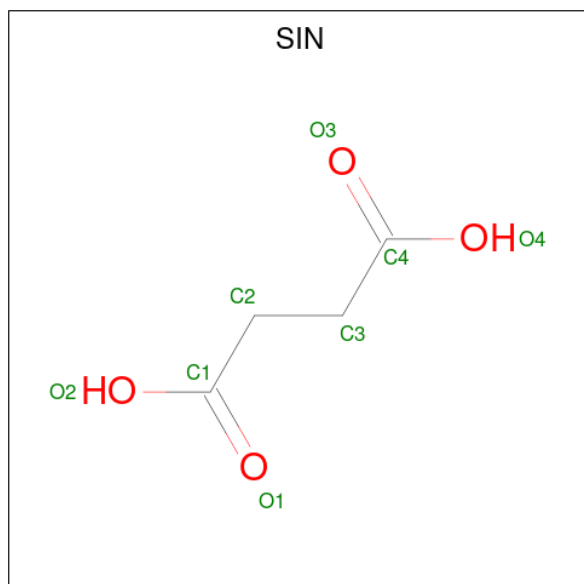
- Molecule 1 is a protein called PUTATIVE ALKYL SULFATASE ATSK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	0	0	0
			1896	1200	347	349			
1	D	259	Total	C	N	O	0	0	0
			1975	1250	359	366			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		
3	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	D	28	Total	O	0	0
			28	28		

● Molecule 1: PUTATIVE ALKYL SULFATASE ATSK



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.84Å 141.00Å 160.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.50) 95.5 (50.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.227 , 0.287 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	1.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3937	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIN, FE2

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	1.72	21/1940 (1.1%)	1.54	18/2652 (0.7%)
1	D	1.68	15/2021 (0.7%)	1.49	14/2762 (0.5%)
All	All	1.70	36/3961 (0.9%)	1.51	32/5414 (0.6%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	111	VAL	CA-CB	10.92	1.69	1.54
1	A	76	GLY	N-CA	9.65	1.54	1.45
1	D	54	VAL	C-O	8.62	1.32	1.24
1	A	151	LEU	CA-C	8.14	1.63	1.52
1	D	219	ILE	CA-C	7.85	1.61	1.52
1	A	286	VAL	CA-C	7.39	1.60	1.52
1	D	80	ALA	CA-C	6.83	1.61	1.52
1	A	267	VAL	C-O	6.71	1.30	1.24
1	D	24	ILE	CG1-CD1	6.67	1.77	1.51
1	A	205	SER	CA-C	6.54	1.61	1.52
1	D	161	VAL	CA-CB	6.33	1.61	1.54
1	D	165	GLU	CA-C	6.33	1.61	1.52
1	A	167	ASP	N-CA	6.27	1.54	1.46
1	D	298	THR	CA-CB	6.22	1.63	1.53
1	D	211	GLN	CG-CD	6.17	1.67	1.52
1	A	103	ARG	N-CA	6.15	1.53	1.46
1	D	97	ASP	CA-C	5.97	1.60	1.52
1	A	167	ASP	CA-C	5.96	1.60	1.52
1	A	55	ILE	CA-C	-5.95	1.45	1.52
1	A	286	VAL	CA-CB	5.91	1.61	1.54
1	A	29	ARG	N-CA	5.89	1.52	1.45
1	A	149	GLU	CA-C	5.81	1.59	1.52
1	A	133	GLY	C-O	5.74	1.31	1.24
1	A	265	TYR	CE2-CZ	5.73	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	155	ALA	CA-CB	-5.72	1.44	1.53
1	A	227	SER	CA-C	5.71	1.60	1.52
1	D	81	HIS	C-O	5.62	1.34	1.23
1	A	134	ASP	CA-C	-5.51	1.45	1.53
1	A	250	GLU	N-CA	5.46	1.52	1.45
1	D	41	THR	CA-CB	5.27	1.61	1.53
1	A	227	SER	N-CA	5.24	1.52	1.46
1	A	244	THR	CA-C	5.22	1.59	1.52
1	D	265	TYR	C-O	-5.21	1.18	1.23
1	A	216	VAL	CA-CB	-5.21	1.47	1.53
1	A	266	ALA	C-O	-5.14	1.17	1.24
1	D	232	ALA	N-CA	-5.06	1.40	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ASP	N-CA-C	10.57	125.86	110.42
1	D	157	LYS	N-CA-C	-9.11	101.87	113.72
1	A	106	SER	N-CA-C	-7.13	97.79	108.99
1	D	166	TYR	N-CA-C	6.97	121.72	112.25
1	D	157	LYS	CB-CA-C	6.91	121.17	109.55
1	A	73	LYS	N-CA-C	-6.89	104.84	113.18
1	A	274	PRO	N-CD-CG	-6.32	93.72	103.20
1	A	166	TYR	N-CA-C	6.10	121.77	113.97
1	A	126	VAL	N-CA-C	-5.93	106.03	111.67
1	A	36	ASP	CB-CA-C	-5.88	102.00	111.28
1	D	80	ALA	N-CA-C	5.86	123.28	110.80
1	A	62	HIS	N-CA-C	-5.57	106.44	113.18
1	A	291	ASP	N-CA-C	-5.57	106.38	112.72
1	A	235	GLN	N-CA-C	5.56	118.11	111.71
1	D	97	ASP	N-CA-C	5.47	122.45	110.80
1	A	135	THR	OG1-CB-CG2	-5.47	98.36	109.30
1	D	197	PRO	N-CD-CG	-5.46	95.01	103.20
1	A	102	GLN	CA-C-N	5.43	131.45	122.33
1	A	102	GLN	C-N-CA	5.43	131.45	122.33
1	A	219	ILE	CB-CG1-CD1	-5.39	102.48	113.80
1	D	81	HIS	N-CA-C	5.24	125.67	111.00
1	A	42	VAL	N-CA-C	5.20	115.93	110.62
1	D	213	GLY	CA-C-O	-5.20	116.54	122.78
1	D	158	LEU	N-CA-C	5.19	118.21	110.52
1	A	197	PRO	N-CA-C	-5.18	103.14	111.38
1	A	229	HIS	N-CA-C	-5.18	105.08	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	152	ARG	N-CA-CB	5.10	117.71	110.06
1	D	167	ASP	N-CA-C	5.10	117.93	109.46
1	D	49	LEU	N-CA-C	5.09	116.51	111.07
1	D	60	GLN	CB-CA-C	-5.08	104.84	111.40
1	A	35	PRO	N-CD-CG	-5.05	95.63	103.20
1	D	237	HIS	N-CA-C	5.02	116.83	111.36

There are no chirality outliers.

There are no planarity outliers.

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	1896	0	1804	35	0
1	D	1975	0	1882	23	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	4	0	0
3	D	8	0	4	0	0
4	A	20	0	0	0	0
4	D	28	0	0	3	0
All	All	3937	0	3694	58	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 (58) 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:24:ILE:CD1	1:D:24:ILE:CG1	1.77	1.57
1:D:153:GLU:HG2	4:D:2013:HOH:O	1.51	1.10
1:A:15:LEU:H	1:A:15:LEU:HD12	1.46	0.80
1:A:126:VAL:HG21	1:A:278:ARG:HG3	1.68	0.75
1:A:224:LEU:O	1:A:228:GLN:HG3	1.87	0.73
1:A:15:LEU:HD11	1:A:44:ALA:HB1	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ILE:CD1	1:D:24:ILE:CB	2.72	0.67
1:A:164:ASN:OD1	1:A:192:TYR:HB2	1.95	0.67
1:A:154:LEU:O	1:A:158:LEU:HG	1.97	0.65
1:D:42:VAL:HG13	1:D:75:LEU:HD23	1.80	0.62
1:D:121:SER:HB3	1:D:281:THR:HG22	1.81	0.61
1:D:242:GLU:OE1	1:D:242:GLU:N	2.29	0.61
1:A:111:VAL:HG12	1:A:114:VAL:HG22	1.83	0.61
1:D:164:ASN:OD1	1:D:192:TYR:HB2	2.02	0.58
1:D:122:ILE:HG12	1:D:256:ILE:HD12	1.87	0.57
1:D:50:VAL:O	1:D:53:LYS:HE3	2.05	0.56
1:A:97:ASP:C	1:A:102:GLN:HG3	2.30	0.56
1:D:229:HIS:HE1	4:D:2018:HOH:O	1.89	0.56
1:A:147:LEU:HB2	1:A:152:ARG:HG2	1.87	0.56
1:D:195:GLU:O	1:D:295:SER:HB3	2.05	0.56
1:A:33:LEU:HD22	1:A:71:PHE:CE1	2.42	0.55
1:A:146:GLU:OE2	1:A:237:HIS:ND1	2.25	0.54
1:A:287:PRO:HB2	1:A:295:SER:OG	2.07	0.54
1:D:123:LEU:HD11	1:D:277:VAL:HB	1.91	0.53
1:A:64:ASP:O	1:A:65:ASP:C	2.55	0.50
1:A:121:SER:HB2	1:A:257:TRP:CE2	2.47	0.50
1:A:54:VAL:HG23	1:A:257:TRP:HB3	1.95	0.48
1:D:111:VAL:HG13	1:D:118:PRO:HD2	1.96	0.48
1:D:205:SER:HB2	1:D:207:GLU:HG3	1.95	0.48
1:A:219:ILE:HG23	1:A:219:ILE:HD13	1.60	0.47
1:A:279:ARG:HD3	1:A:281:THR:HG23	1.95	0.47
1:A:144:TYR:O	1:A:145:GLN:C	2.58	0.47
1:D:285:GLU:H	1:D:285:GLU:CD	2.22	0.46
1:A:279:ARG:HD3	1:A:281:THR:CG2	2.46	0.46
1:A:46:GLN:O	1:A:50:VAL:HG23	2.15	0.46
1:A:126:VAL:CG2	1:A:278:ARG:HG3	2.43	0.46
1:A:111:VAL:O	1:A:114:VAL:HG22	2.16	0.45
1:A:38:ASP:O	1:A:40:ALA:N	2.49	0.45
1:D:27:GLU:OE2	1:D:58:ARG:HG3	2.16	0.45
1:D:97:ASP:CG	1:D:98:GLY:H	2.23	0.45
1:A:107:TRP:HB3	1:A:263:GLN:OE1	2.16	0.45
1:D:97:ASP:HB2	4:D:2003:HOH:O	2.17	0.45
1:A:123:LEU:HD11	1:A:277:VAL:CG2	2.47	0.45
1:D:76:GLY:O	1:D:78:PRO:HD3	2.17	0.45
1:A:62:HIS:HE2	1:A:63:LEU:HD13	1.82	0.44
1:A:58:ARG:O	1:A:60:GLN:HG2	2.17	0.43
1:A:76:GLY:O	1:A:78:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:NH1	1:A:271:GLY:O	2.51	0.43
1:D:107:TRP:CD1	1:D:265:TYR:HD1	2.38	0.42
1:D:122:ILE:HG12	1:D:256:ILE:CD1	2.48	0.42
1:A:111:VAL:HB	1:A:118:PRO:HD2	2.01	0.41
1:A:123:LEU:HD11	1:A:277:VAL:HG23	2.02	0.41
1:A:133:GLY:HA2	1:A:270:TYR:CD2	2.56	0.41
1:A:111:VAL:HG12	1:A:111:VAL:O	2.21	0.41
1:A:144:TYR:CE2	1:A:152:ARG:HD2	2.55	0.41
1:A:24:ILE:HG13	1:A:25:GLY:N	2.36	0.40
1:D:97:ASP:CG	1:D:98:GLY:N	2.79	0.40
1:D:105:ASN:HB3	1:D:266:ALA:O	2.21	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	241/301 (80%)	223 (92%)	15 (6%)	3 (1%)	10	20
1	D	251/301 (83%)	235 (94%)	14 (6%)	2 (1%)	16	31
All	All	492/602 (82%)	458 (93%)	29 (6%)	5 (1%)	12	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ALA
1	A	165	GLU
1	D	223	SER
1	A	80	ALA
1	D	80	ALA

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	187/244 (77%)	170 (91%)	17 (9%)	9	19
1	D	196/244 (80%)	179 (91%)	17 (9%)	9	21
All	All	383/488 (78%)	349 (91%)	34 (9%)	9	20

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	24	ILE
1	A	32	LYS
1	A	43	GLU
1	A	61	THR
1	A	67	SER
1	A	118	PRO
1	A	145	GLN
1	A	149	GLU
1	A	163	SER
1	A	200	ARG
1	A	219	ILE
1	A	224	LEU
1	A	240	ARG
1	A	256	ILE
1	A	265	TYR
1	A	279	ARG
1	D	28	ILE
1	D	29	ARG
1	D	34	SER
1	D	43	GLU
1	D	53	LYS
1	D	63	LEU
1	D	67	SER
1	D	103	ARG
1	D	111	VAL
1	D	121	SER

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Mol	Chain	Res	Type
1	D	163	SER
1	D	211	GLN
1	D	223	SER
1	D	265	TYR
1	D	274	PRO
1	D	276	ILE
1	D	295	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	68	GLN
1	A	228	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	SIN	D	1302	2	7,7,7	1.65	2 (28%)	8,8,8	1.69	1 (12%)
3	SIN	A	1300	2	7,7,7	1.38	1 (14%)	8,8,8	2.19	3 (37%)

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	SIN	D	1302	2	-	2/5/5/5	-
3	SIN	A	1300	2	-	4/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1300	SIN	O1-C1	2.88	1.31	1.22
3	D	1302	SIN	C2-C1	2.50	1.56	1.50
3	D	1302	SIN	O4-C4	-2.11	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1300	SIN	O4-C4-C3	4.10	126.95	114.00
3	D	1302	SIN	O2-C1-O1	-3.56	114.18	123.33
3	A	1300	SIN	O3-C4-C3	-3.36	112.43	123.09
3	A	1300	SIN	C3-C2-C1	-2.12	108.04	113.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1300	SIN	O1-C1-C2-C3
3	A	1300	SIN	O2-C1-C2-C3
3	D	1302	SIN	C2-C3-C4-O3
3	D	1302	SIN	C2-C3-C4-O4
3	A	1300	SIN	C2-C3-C4-O3
3	A	1300	SIN	C2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

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

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	249/301 (82%)	0.62	16 (6%) 25 22	33, 52, 69, 86	0
1	D	259/301 (86%)	0.45	11 (4%) 40 36	36, 50, 68, 77	0
All	All	508/602 (84%)	0.53	27 (5%) 32 28	33, 51, 68, 86	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	TYR	4.0
1	A	81	HIS	3.7
1	D	166	TYR	3.3
1	D	81	HIS	3.3
1	A	165	GLU	3.2
1	A	13	LEU	3.2
1	A	102	GLN	3.1
1	D	300	LYS	3.1
1	D	98	GLY	3.0
1	A	291	ASP	3.0
1	A	192	TYR	3.0
1	D	80	ALA	2.9
1	D	211	GLN	2.9
1	D	13	LEU	2.8
1	A	93	LEU	2.8
1	D	85	PRO	2.6
1	A	79	VAL	2.5
1	A	224	LEU	2.5
1	D	91	ARG	2.4
1	A	169	ALA	2.4
1	D	192	TYR	2.3
1	A	214	HIS	2.3
1	A	298	THR	2.2
1	A	297	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	42	VAL	2.0
1	A	288	VAL	2.0
1	A	159	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SIN	A	1300	8/8	0.94	0.11	48,51,57,61	0
3	SIN	D	1302	8/8	0.95	0.12	43,51,54,55	0
2	FE2	A	1299	1/1	0.99	0.02	50,50,50,50	0
2	FE2	D	1301	1/1	1.00	0.02	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.