



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:38 PM UTC

PDB ID : 2ZYL / pdb_00002zyl
Title : Crystal structure of 3-ketosteroid-9- α -hydroxylase (KshA) from M. tuberculosis
Authors : D'Angelo, I.; Capyk, J.; Strynadka, N.; Eltis, L.
Deposited on : 2009-01-27
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

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

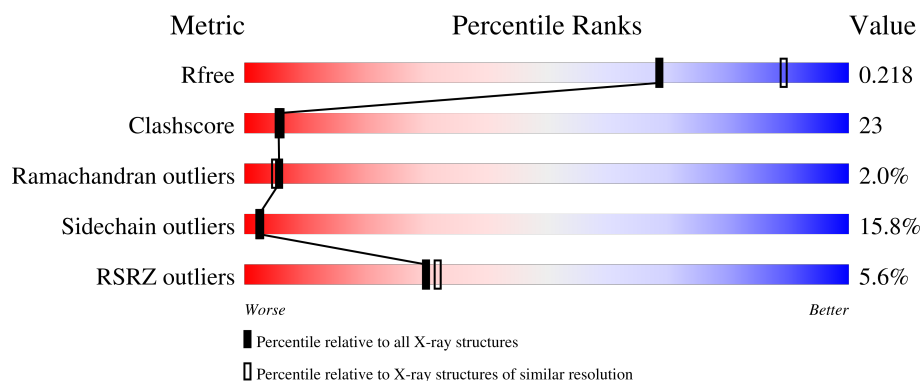
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 ≥ 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	386	5% 57% 25% 9% 7%

2 Entry composition [i](#)

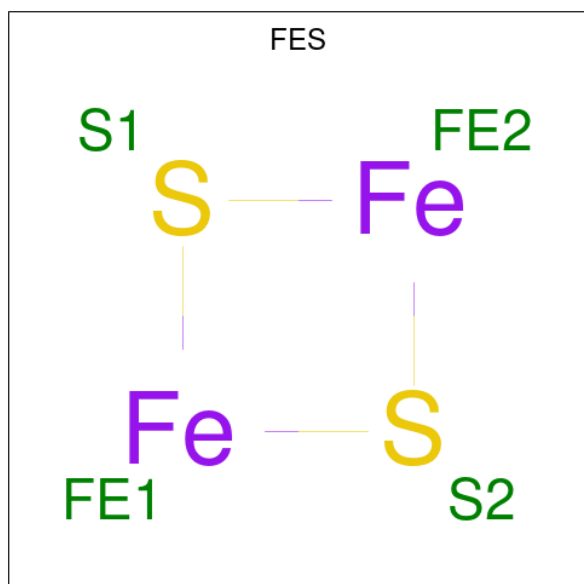
There are 5 unique types of molecules in this entry. The entry contains 3094 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 POSSIBLE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	359	2916	1857	509	537	13	0	0	0

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	4	2	2	0	0

- Molecule 3 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Na 1	0	0

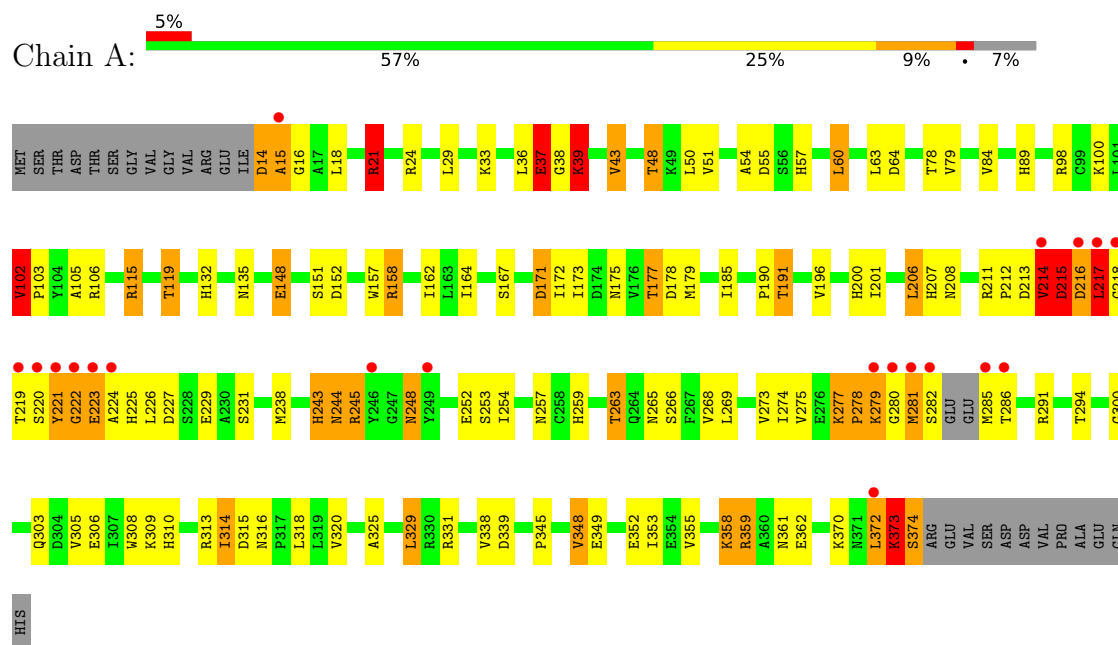
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total 172	O 172	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: POSSIBLE OXIDOREDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.20Å 116.20Å 81.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.85 – 2.30 19.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.85-2.30) 99.7 (19.85-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.235 (Not available) , 0.218	Depositor DCC
R_{free} test set	1417 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3094	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 3.87% 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: FE2, FES, NA

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	1.47	16/3004 (0.5%)	1.42	26/4079 (0.6%)

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	A	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	VAL	CA-CB	6.96	1.62	1.54
1	A	316	ASN	CA-C	6.64	1.60	1.53
1	A	15	ALA	CA-CB	-6.58	1.44	1.53
1	A	102	VAL	CA-CB	6.06	1.60	1.53
1	A	314	ILE	CA-CB	5.96	1.60	1.53
1	A	201	ILE	CA-CB	5.74	1.61	1.54
1	A	320	VAL	CA-C	5.53	1.57	1.52
1	A	79	VAL	CA-C	5.49	1.59	1.52
1	A	313	ARG	CA-C	-5.32	1.46	1.52
1	A	355	VAL	CA-CB	5.22	1.60	1.54
1	A	268	VAL	CA-CB	5.13	1.60	1.54
1	A	185	ILE	CA-CB	5.12	1.60	1.54
1	A	21	ARG	CB-CG	-5.11	1.37	1.52
1	A	171	ASP	CB-CG	5.07	1.64	1.52
1	A	84	VAL	CA-CB	5.05	1.61	1.54
1	A	106	ARG	N-CA	-5.03	1.40	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ALA	N-CA-C	12.29	128.20	108.41
1	A	37	GLU	N-CA-C	10.63	124.11	109.54
1	A	348	VAL	CB-CA-C	9.22	119.30	110.63
1	A	178	ASP	N-CA-C	9.10	123.76	108.20
1	A	244	ASN	N-CA-C	8.17	122.15	110.14
1	A	222	GLY	N-CA-C	-7.65	99.46	112.77
1	A	102	VAL	CB-CA-C	6.74	118.99	111.04
1	A	277	LYS	CA-C-N	6.74	127.10	119.83
1	A	277	LYS	C-N-CA	6.74	127.10	119.83
1	A	21	ARG	CB-CA-C	-6.62	97.18	110.30
1	A	215	ASP	N-CA-C	6.32	124.27	110.80
1	A	36	LEU	CA-C-N	-6.27	113.84	122.87
1	A	36	LEU	C-N-CA	-6.27	113.84	122.87
1	A	158	ARG	N-CA-C	-5.90	99.67	109.46
1	A	358	LYS	N-CA-C	5.83	117.31	111.07
1	A	179	MET	N-CA-CB	-5.69	101.82	110.07
1	A	177	THR	N-CA-CB	-5.54	103.23	110.88
1	A	43	VAL	N-CA-C	5.50	116.04	108.12
1	A	177	THR	N-CA-C	-5.49	106.49	114.12
1	A	278	PRO	CB-CA-C	-5.36	104.88	111.64
1	A	135	ASN	CA-C-N	-5.23	115.00	120.38
1	A	135	ASN	C-N-CA	-5.23	115.00	120.38
1	A	243	HIS	CA-C-N	-5.12	113.89	123.05
1	A	243	HIS	C-N-CA	-5.12	113.89	123.05
1	A	39	LYS	CA-C-N	-5.06	115.35	120.31
1	A	39	LYS	C-N-CA	-5.06	115.35	120.31

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ASP	Peptide
1	A	214	VAL	Peptide
1	A	37	GLU	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	2916	0	2752	133	0
2	A	4	0	0	1	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	172	0	0	35	0
All	All	3094	0	2752	133	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 23.

All (133) 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:280:GLY:HA2	1:A:281:MET:CB	1.47	1.40
1:A:280:GLY:CA	1:A:281:MET:HB2	1.61	1.30
1:A:286:THR:HA	5:A:462:HOH:O	1.33	1.28
1:A:282:SER:HB2	5:A:494:HOH:O	1.33	1.23
1:A:217:LEU:HD22	1:A:218:GLY:N	1.58	1.18
1:A:222:GLY:O	1:A:223:GLU:HB3	1.49	1.06
1:A:64:ASP:OD1	1:A:115:ARG:NH1	1.91	1.03
1:A:280:GLY:N	1:A:281:MET:HE3	1.72	1.03
1:A:217:LEU:HD22	1:A:218:GLY:H	1.20	1.00
1:A:15:ALA:HB1	1:A:315:ASP:H	1.23	1.00
1:A:100:LYS:HE2	5:A:438:HOH:O	1.61	1.00
1:A:280:GLY:HA2	1:A:281:MET:HB3	1.44	0.99
1:A:280:GLY:HA2	1:A:281:MET:HB2	0.99	0.99
1:A:374:SER:HB2	5:A:558:HOH:O	1.68	0.92
1:A:263:THR:HG22	1:A:265:ASN:H	1.32	0.92
1:A:217:LEU:CD2	1:A:218:GLY:N	2.33	0.91
1:A:217:LEU:CD2	1:A:218:GLY:H	1.84	0.90
1:A:171:ASP:HB3	5:A:481:HOH:O	1.71	0.90
1:A:38:GLY:HA2	5:A:473:HOH:O	1.73	0.87
1:A:280:GLY:CA	1:A:281:MET:CB	2.29	0.84
1:A:285:MET:HA	5:A:494:HOH:O	1.76	0.83
1:A:39:LYS:HE2	5:A:461:HOH:O	1.79	0.82
1:A:158:ARG:HH12	1:A:291:ARG:HG2	1.44	0.82
1:A:60:LEU:O	1:A:119:THR:HG21	1.79	0.82
1:A:285:MET:HG2	1:A:286:THR:H	1.46	0.81
1:A:158:ARG:HD2	1:A:294:THR:HG21	1.63	0.81
1:A:243:HIS:HD2	1:A:252:GLU:OE1	1.62	0.81
1:A:285:MET:HG3	5:A:526:HOH:O	1.80	0.81
1:A:248:ASN:HB3	5:A:429:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:GLY:N	1:A:281:MET:CE	2.43	0.80
1:A:216:ASP:O	1:A:222:GLY:CA	2.30	0.79
1:A:223:GLU:CG	1:A:223:GLU:O	2.30	0.78
1:A:265:ASN:HB2	5:A:470:HOH:O	1.83	0.77
1:A:359:ARG:HB3	5:A:532:HOH:O	1.84	0.76
1:A:285:MET:CG	1:A:286:THR:H	2.00	0.75
1:A:374:SER:HB2	5:A:440:HOH:O	1.87	0.73
1:A:238:MET:HE3	5:A:512:HOH:O	1.88	0.72
1:A:280:GLY:N	1:A:281:MET:HB2	2.05	0.70
1:A:54:ALA:HB2	1:A:60:LEU:HD13	1.73	0.69
1:A:15:ALA:CB	1:A:315:ASP:H	2.02	0.68
1:A:151:SER:O	5:A:560:HOH:O	2.11	0.68
1:A:229:GLU:OE1	1:A:243:HIS:HE1	1.76	0.68
1:A:15:ALA:HB1	1:A:315:ASP:N	2.05	0.67
1:A:211:ARG:HB2	1:A:214:VAL:CG2	2.24	0.67
1:A:200:HIS:HE1	5:A:431:HOH:O	1.79	0.66
1:A:238:MET:HE2	1:A:257:ASN:HB3	1.77	0.65
1:A:238:MET:CE	5:A:512:HOH:O	2.42	0.65
1:A:223:GLU:O	1:A:223:GLU:HG2	1.95	0.65
1:A:224:ALA:HA	1:A:245:ARG:O	1.97	0.65
1:A:217:LEU:CG	1:A:218:GLY:H	2.05	0.64
1:A:218:GLY:HA3	1:A:219:THR:C	2.20	0.64
1:A:216:ASP:N	1:A:216:ASP:OD1	2.30	0.63
1:A:38:GLY:CA	5:A:473:HOH:O	2.37	0.63
1:A:102:VAL:HG22	1:A:105:ALA:CB	2.29	0.63
1:A:191:THR:CG2	5:A:547:HOH:O	2.46	0.62
1:A:345:PRO:O	1:A:349:GLU:HG2	1.99	0.61
1:A:216:ASP:O	1:A:222:GLY:HA3	2.00	0.61
1:A:280:GLY:CA	1:A:281:MET:HE3	2.31	0.61
1:A:222:GLY:O	1:A:223:GLU:CB	2.32	0.61
1:A:215:ASP:HB2	5:A:525:HOH:O	2.00	0.60
1:A:280:GLY:H	1:A:281:MET:CE	2.12	0.60
1:A:175:ASN:ND2	1:A:308:TRP:HE1	1.99	0.60
1:A:207:HIS:HD2	1:A:227:ASP:OD1	1.83	0.60
1:A:14:ASP:HB3	1:A:16:GLY:N	2.16	0.59
1:A:211:ARG:HD2	1:A:213:ASP:OD2	2.03	0.59
1:A:102:VAL:HG22	1:A:105:ALA:HB3	1.85	0.57
1:A:216:ASP:O	1:A:222:GLY:HA2	2.02	0.57
1:A:98:ARG:HB2	1:A:100:LYS:HE3	1.84	0.57
1:A:24:ARG:NH2	1:A:338:VAL:O	2.37	0.57
1:A:217:LEU:HD22	1:A:218:GLY:CA	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ARG:HD2	5:A:411:HOH:O	2.06	0.56
1:A:225:HIS:O	1:A:244:ASN:HB2	2.07	0.55
1:A:64:ASP:CG	1:A:115:ARG:NH1	2.64	0.54
1:A:238:MET:HE2	1:A:257:ASN:CB	2.38	0.54
1:A:217:LEU:HD22	1:A:219:THR:HA	1.88	0.54
1:A:14:ASP:HB3	1:A:15:ALA:C	2.34	0.53
1:A:373:LYS:C	5:A:440:HOH:O	2.51	0.53
1:A:263:THR:HB	1:A:266:SER:OG	2.08	0.53
1:A:191:THR:HG22	5:A:547:HOH:O	2.08	0.53
1:A:279:LYS:C	1:A:281:MET:HE3	2.33	0.53
1:A:212:PRO:O	1:A:217:LEU:HB2	2.10	0.52
1:A:325:ALA:HB2	1:A:353:ILE:HG21	1.92	0.52
1:A:374:SER:CB	5:A:558:HOH:O	2.40	0.52
1:A:259:HIS:HE1	5:A:400:HOH:O	1.91	0.52
1:A:285:MET:HG2	1:A:286:THR:N	2.22	0.51
1:A:372:LEU:C	1:A:374:SER:H	2.19	0.51
1:A:216:ASP:O	1:A:217:LEU:O	2.30	0.50
1:A:329:LEU:HD12	5:A:432:HOH:O	2.11	0.49
1:A:280:GLY:H	1:A:281:MET:HE2	1.78	0.49
1:A:285:MET:CG	1:A:286:THR:N	2.71	0.49
1:A:15:ALA:CB	1:A:314:ILE:HA	2.43	0.48
1:A:119:THR:HG23	5:A:553:HOH:O	2.13	0.48
1:A:214:VAL:O	1:A:216:ASP:N	2.37	0.48
1:A:374:SER:C	5:A:471:HOH:O	2.55	0.48
1:A:102:VAL:HG22	1:A:105:ALA:HB2	1.96	0.47
1:A:281:MET:HB3	1:A:286:THR:HG22	1.96	0.47
1:A:359:ARG:CD	5:A:411:HOH:O	2.62	0.47
1:A:300:GLY:O	1:A:303:GLN:HG2	2.14	0.47
1:A:21:ARG:NH2	1:A:339:ASP:OD2	2.34	0.47
1:A:217:LEU:O	1:A:222:GLY:N	2.48	0.47
1:A:259:HIS:HD2	5:A:406:HOH:O	1.96	0.47
1:A:223:GLU:O	1:A:223:GLU:HG3	2.13	0.46
1:A:211:ARG:CB	1:A:214:VAL:HG22	2.46	0.46
1:A:14:ASP:HB3	1:A:16:GLY:H	1.80	0.46
1:A:57:HIS:HE1	5:A:439:HOH:O	1.98	0.46
1:A:277:LYS:HA	1:A:278:PRO:HD3	1.70	0.45
1:A:102:VAL:HA	1:A:103:PRO:HD3	1.82	0.45
1:A:217:LEU:CD2	1:A:219:THR:HA	2.46	0.45
1:A:21:ARG:HG2	1:A:132:HIS:CG	2.52	0.45
1:A:200:HIS:CD2	1:A:200:HIS:H	2.34	0.44
1:A:281:MET:HB3	1:A:286:THR:CG2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:VAL:HG12	1:A:309:LYS:HD2	1.99	0.44
1:A:98:ARG:HD2	5:A:438:HOH:O	2.17	0.44
1:A:211:ARG:HB2	1:A:214:VAL:HG22	2.00	0.43
1:A:196:VAL:HG22	1:A:352:GLU:HG2	1.99	0.43
1:A:190:PRO:O	1:A:361:ASN:ND2	2.46	0.43
1:A:157:TRP:CE3	1:A:274:ILE:HG23	2.54	0.43
1:A:98:ARG:NH2	5:A:559:HOH:O	2.45	0.43
1:A:211:ARG:CB	1:A:214:VAL:CG2	2.96	0.43
1:A:215:ASP:CB	5:A:525:HOH:O	2.64	0.43
1:A:89:HIS:HB2	2:A:451:FES:S2	2.59	0.42
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.89	0.41
1:A:206:LEU:HD13	1:A:208:ASN:HB2	2.02	0.41
1:A:359:ARG:O	1:A:362:GLU:HG2	2.20	0.41
1:A:253:SER:HB3	1:A:275:VAL:HG12	2.02	0.41
1:A:281:MET:HB2	1:A:281:MET:HE3	1.76	0.41
1:A:148:GLU:HG2	1:A:254:ILE:HD12	2.01	0.41
1:A:162:ILE:HG21	1:A:162:ILE:HD13	1.87	0.41
1:A:231:SER:O	1:A:238:MET:HA	2.21	0.41
1:A:172:ILE:HD13	1:A:172:ILE:HG21	1.85	0.41
1:A:48:THR:HG21	5:A:556:HOH:O	2.21	0.41
1:A:243:HIS:CD2	1:A:252:GLU:OE1	2.55	0.41
1:A:306:GLU:O	1:A:310:HIS:HD2	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	355/386 (92%)	337 (95%)	11 (3%)	7 (2%)	6 5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	215	ASP
1	A	217	LEU
1	A	223	GLU
1	A	281	MET
1	A	221	TYR
1	A	373	LYS

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	279/333 (84%)	235 (84%)	44 (16%)	2 2

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	29	LEU
1	A	33	LYS
1	A	37	GLU
1	A	39	LYS
1	A	43	VAL
1	A	48	THR
1	A	50	LEU
1	A	60	LEU
1	A	63	LEU
1	A	78	THR
1	A	102	VAL
1	A	115	ARG
1	A	119	THR
1	A	148	GLU
1	A	152	ASP
1	A	164	ILE
1	A	167	SER
1	A	173	ILE
1	A	177	THR

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Mol	Chain	Res	Type
1	A	191	THR
1	A	206	LEU
1	A	214	VAL
1	A	216	ASP
1	A	217	LEU
1	A	220	SER
1	A	221	TYR
1	A	226	LEU
1	A	245	ARG
1	A	248	ASN
1	A	263	THR
1	A	269	LEU
1	A	273	VAL
1	A	279	LYS
1	A	318	LEU
1	A	329	LEU
1	A	331	ARG
1	A	348	VAL
1	A	358	LYS
1	A	359	ARG
1	A	370	LYS
1	A	372	LEU
1	A	373	LYS
1	A	374	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	132	HIS
1	A	175	ASN
1	A	200	HIS
1	A	207	HIS
1	A	208	ASN
1	A	225	HIS
1	A	240	ASN
1	A	243	HIS
1	A	259	HIS
1	A	265	ASN
1	A	365	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
2	FES	A	451	1	0,4,4	-	-	-		

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	FES	A	451	1	-	-	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	451	FES	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	359/386 (93%)	-0.11	20 (5%) 30 32	19, 36, 73, 110	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	THR	6.4
1	A	218	GLY	5.7
1	A	217	LEU	5.6
1	A	221	TYR	4.4
1	A	222	GLY	4.2
1	A	220	SER	4.0
1	A	246	TYR	3.9
1	A	285	MET	3.8
1	A	15	ALA	3.6
1	A	282	SER	3.0
1	A	249	TYR	2.9
1	A	286	THR	2.4
1	A	281	MET	2.4
1	A	279	LYS	2.3
1	A	224	ALA	2.3
1	A	372	LEU	2.3
1	A	214	VAL	2.2
1	A	280	GLY	2.2
1	A	223	GLU	2.1
1	A	216	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
4	NA	A	387	1/1	0.97	0.12	41,41,41,41	0
3	FE2	A	452	1/1	0.99	0.03	34,34,34,34	0
2	FES	A	451	4/4	0.99	0.03	26,29,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.