



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:36 AM UTC

PDB ID : 1IDC / pdb_00001idc
Title : ISOCITRATE DEHYDROGENASE FROM E.COLI (MUTANT K230M),
STEADY-STATE INTERMEDIATE COMPLEX DETERMINED BY LAUE
CRYSTALLOGRAPHY
Authors : Bolduc, J.M.; Dyer, D.H.; Scott, W.G.; Singer, P.; Sweet, R.M.; Koshland
Junior, D.E.; Stoddard, B.L.
Deposited on : 1995-01-18
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

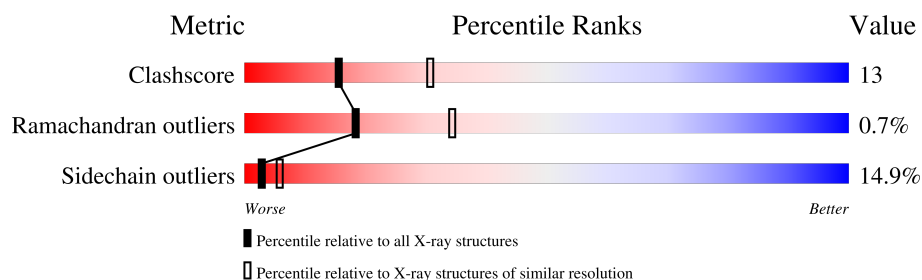
1 Overall quality at a glance

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)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	416	

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	OXS	A	418	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3231 atoms, of which 22 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 ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	414	3217	2034	22	537	605	19	30	0	0

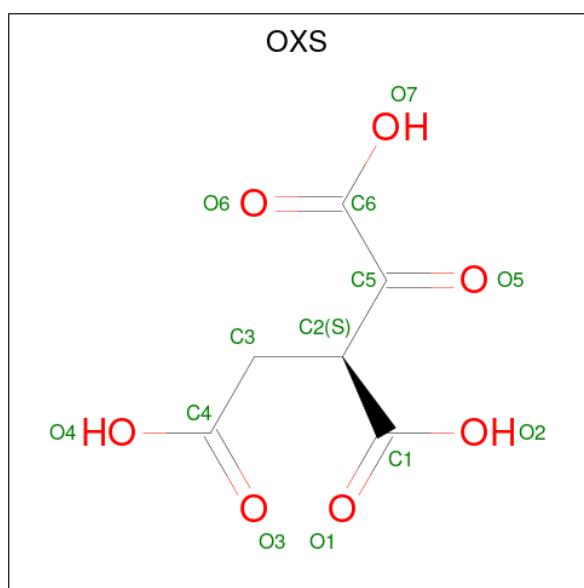
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	MET	LYS	engineered mutation	UNP P08200

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2-OXALOSUCCINIC ACID (CCD ID: OXS) (formula: C₆H₆O₇).



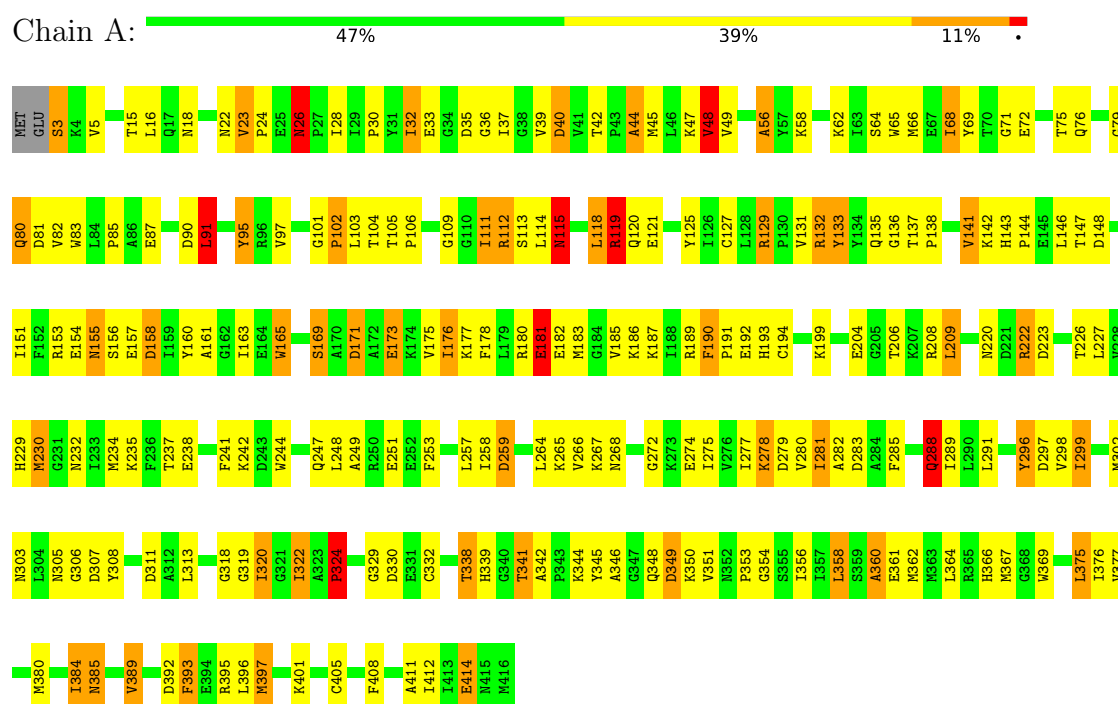
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: ISOCITRATE DEHYDROGENASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.10Å 105.10Å 150.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3231	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.17	9/3256 (0.3%)	2.15	139/4404 (3.2%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	HIS	CD2-NE2	-7.28	1.29	1.37
1	A	193	HIS	CD2-NE2	-7.00	1.30	1.37
1	A	143	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	366	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	339	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	324	PRO	CA-CB	-5.67	1.45	1.53
1	A	48	VAL	CA-CB	5.45	1.62	1.54
1	A	190	PHE	CA-CB	5.34	1.60	1.53
1	A	68	ILE	CA-CB	5.23	1.61	1.54

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	VAL	N-CA-CB	-11.50	92.25	111.23
1	A	56	ALA	N-CA-C	10.19	121.97	111.07
1	A	235	LYS	N-CA-C	9.14	122.39	111.33
1	A	115	ASN	OD1-CG-ND2	-8.83	113.77	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	TYR	CA-C-O	-8.54	111.50	120.55
1	A	193	HIS	CB-CG-CD2	-8.51	120.14	131.20
1	A	40	ASP	CA-CB-CG	8.50	121.10	112.60
1	A	392	ASP	CA-CB-CG	8.25	120.85	112.60
1	A	69	TYR	O-C-N	8.00	132.55	123.27
1	A	283	ASP	CA-CB-CG	7.73	120.33	112.60
1	A	141	VAL	N-CA-CB	-7.64	97.42	112.24
1	A	339	HIS	CB-CG-CD2	-7.59	121.33	131.20
1	A	385	ASN	OD1-CG-ND2	-7.59	115.01	122.60
1	A	389	VAL	CB-CA-C	7.23	123.14	111.29
1	A	23	VAL	CA-C-O	7.19	123.39	119.15
1	A	155	ASN	N-CA-C	7.18	122.72	113.88
1	A	220	ASN	CA-CB-CG	7.16	119.76	112.60
1	A	230	MET	N-CA-C	-7.07	101.86	111.55
1	A	102	PRO	N-CA-C	7.02	122.24	111.15
1	A	32	ILE	N-CA-C	-6.99	98.51	108.58
1	A	288	GLN	OE1-CD-NE2	-6.96	115.64	122.60
1	A	349	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	341	THR	N-CA-C	6.86	121.48	113.18
1	A	393	PHE	CA-CB-CG	6.77	120.57	113.80
1	A	101	GLY	CA-C-N	6.70	126.74	119.90
1	A	101	GLY	C-N-CA	6.70	126.74	119.90
1	A	190	PHE	CA-C-N	6.66	126.44	119.05
1	A	190	PHE	C-N-CA	6.66	126.44	119.05
1	A	330	ASP	N-CA-CB	-6.66	101.74	110.59
1	A	279	ASP	CA-CB-CG	6.63	119.23	112.60
1	A	95	TYR	CA-CB-CG	-6.63	101.96	113.90
1	A	141	VAL	CB-CA-C	6.53	120.52	111.38
1	A	342	ALA	N-CA-C	6.47	124.11	109.81
1	A	249	ALA	CA-C-N	6.46	129.23	120.44
1	A	249	ALA	C-N-CA	6.46	129.23	120.44
1	A	111	ILE	N-CA-CB	-6.45	104.56	111.46
1	A	338	THR	O-C-N	-6.43	114.04	122.59
1	A	176	ILE	CA-C-O	-6.35	114.44	121.17
1	A	193	HIS	CB-CG-ND1	6.34	132.21	122.70
1	A	238	GLU	CA-C-N	6.29	127.10	119.99
1	A	238	GLU	C-N-CA	6.29	127.10	119.99
1	A	223	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	65	TRP	CG-CD2-CE3	6.17	140.07	133.90
1	A	185	VAL	CA-C-O	6.16	127.86	120.65
1	A	288	GLN	CG-CD-NE2	6.11	125.56	116.40
1	A	291	LEU	N-CA-C	6.08	120.87	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ILE	CB-CG1-CD1	-6.07	101.05	113.80
1	A	384	ILE	N-CA-C	-6.07	104.83	110.53
1	A	105	THR	CA-C-O	-6.05	113.75	119.55
1	A	322	ILE	N-CA-C	-6.02	106.86	113.43
1	A	369	TRP	CA-C-N	6.00	128.61	120.38
1	A	369	TRP	C-N-CA	6.00	128.61	120.38
1	A	115	ASN	CB-CG-ND2	5.97	125.36	116.40
1	A	90	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	125	TYR	N-CA-C	5.91	117.72	111.28
1	A	251	GLU	CA-CB-CG	5.89	125.88	114.10
1	A	332	CYS	O-C-N	-5.89	116.69	122.99
1	A	384	ILE	CA-C-O	-5.86	114.54	121.05
1	A	208	ARG	CA-CB-CG	5.85	125.79	114.10
1	A	83	TRP	CG-CD2-CE3	5.84	139.74	133.90
1	A	76	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	26	ASN	CA-CB-CG	5.82	118.42	112.60
1	A	47	LYS	CA-C-O	-5.82	114.89	121.00
1	A	283	ASP	O-C-N	-5.82	115.42	122.22
1	A	163	ILE	N-CA-C	-5.79	98.09	106.88
1	A	173	GLU	N-CA-C	5.75	117.55	111.28
1	A	282	ALA	CA-C-O	-5.75	112.28	120.51
1	A	80	GLN	N-CA-C	5.74	120.02	113.19
1	A	360	ALA	N-CA-C	-5.73	105.03	111.28
1	A	237	THR	CA-CB-OG1	-5.68	101.07	109.60
1	A	366	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	A	244	TRP	CG-CD2-CE3	5.66	139.56	133.90
1	A	119	ARG	NE-CZ-NH1	5.65	127.15	121.50
1	A	237	THR	CA-CB-CG2	5.63	120.08	110.50
1	A	401	LYS	N-CA-C	-5.63	100.52	109.76
1	A	158	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	339	HIS	CB-CG-ND1	5.59	131.08	122.70
1	A	298	VAL	N-CA-CB	-5.57	102.88	110.56
1	A	329	GLY	N-CA-C	-5.55	106.13	112.79
1	A	348	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	A	268	ASN	CA-C-N	5.53	125.89	119.47
1	A	268	ASN	C-N-CA	5.53	125.89	119.47
1	A	376	ILE	CA-C-O	-5.52	115.00	120.85
1	A	389	VAL	CG1-CB-CG2	5.49	122.87	110.80
1	A	171	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	305	ASN	CA-CB-CG	5.47	118.07	112.60
1	A	289	ILE	CA-CB-CG2	-5.46	101.22	110.50
1	A	83	TRP	CE2-CD2-CG	-5.45	100.66	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	HIS	CB-CG-CD2	-5.45	124.11	131.20
1	A	132	ARG	CB-CG-CD	-5.45	98.78	111.30
1	A	247	GLN	OE1-CD-NE2	-5.40	117.20	122.60
1	A	44	ALA	N-CA-C	-5.39	104.85	111.75
1	A	91	LEU	N-CA-C	5.39	117.15	111.28
1	A	266	VAL	N-CA-C	-5.36	100.72	108.71
1	A	238	GLU	O-C-N	5.36	127.66	122.09
1	A	220	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	A	26	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	A	156	SER	N-CA-C	5.34	119.64	113.18
1	A	308	TYR	CA-C-N	5.34	127.48	120.60
1	A	308	TYR	C-N-CA	5.34	127.48	120.60
1	A	146	LEU	N-CA-C	-5.33	106.55	113.16
1	A	83	TRP	CB-CG-CD1	-5.32	118.93	126.90
1	A	330	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	414	GLU	CA-CB-CG	5.31	124.71	114.10
1	A	227	LEU	O-C-N	-5.30	117.04	123.13
1	A	175	VAL	N-CA-C	-5.29	105.34	110.42
1	A	133	TYR	O-C-N	-5.28	116.52	123.02
1	A	392	ASP	N-CA-C	5.27	117.94	111.82
1	A	303	ASN	CB-CG-ND2	-5.27	108.49	116.40
1	A	39	VAL	CA-C-O	-5.27	114.93	120.57
1	A	169	SER	N-CA-C	-5.25	103.75	110.53
1	A	230	MET	CG-SD-CE	5.25	112.44	100.90
1	A	56	ALA	O-C-N	-5.22	116.69	122.07
1	A	275	ILE	N-CA-C	-5.21	102.01	108.89
1	A	71	GLY	O-C-N	5.21	127.91	122.86
1	A	384	ILE	CA-CB-CG2	-5.20	101.66	110.50
1	A	165	TRP	CE2-CD2-CG	-5.17	100.99	107.20
1	A	277	ILE	CB-CG1-CD1	5.17	124.67	113.80
1	A	157	GLU	CA-CB-CG	5.17	124.44	114.10
1	A	342	ALA	O-C-N	-5.17	115.37	121.32
1	A	259	ASP	O-C-N	-5.16	115.72	122.59
1	A	278	LYS	N-CA-C	-5.16	101.98	109.31
1	A	311	ASP	CA-C-O	-5.15	115.09	120.55
1	A	204	GLU	N-CA-C	-5.13	105.60	111.14
1	A	229	HIS	O-C-N	-5.12	117.75	123.48
1	A	384	ILE	CA-CB-CG1	5.11	119.09	110.40
1	A	142	LYS	CA-C-N	-5.08	117.00	123.15
1	A	142	LYS	C-N-CA	-5.08	117.00	123.15
1	A	268	ASN	CA-CB-CG	5.08	117.68	112.60
1	A	285	PHE	CA-CB-CG	-5.07	108.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	TRP	CB-CG-CD1	-5.06	119.32	126.90
1	A	181	GLU	CA-CB-CG	5.05	124.20	114.10
1	A	244	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	A	307	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	199	LYS	CB-CG-CD	-5.04	99.72	111.30
1	A	299	ILE	CB-CG1-CD1	5.04	124.38	113.80
1	A	165	TRP	CG-CD2-CE3	5.03	138.93	133.90
1	A	142	LYS	O-C-N	-5.02	116.43	122.15
1	A	3	SER	N-CA-C	-5.02	96.95	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	TYR	Sidechain
1	A	345	TYR	Sidechain
1	A	95	TYR	Sidechain

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	3195	22	3218	85	0
2	A	1	0	0	0	0
3	A	13	0	3	5	0
All	All	3209	22	3221	85	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 13.

All (85) 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:160:TYR:OH	3:A:418:OXs:O1	1.71	1.07
1:A:160:TYR:OH	3:A:418:OXs:C1	2.17	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ILE:HG12	1:A:265:LYS:HG2	1.57	0.85
1:A:160:TYR:HH	3:A:418:OXS:C1	1.89	0.83
1:A:127:CYS:HB2	1:A:155:ASN:ND2	2.01	0.76
1:A:153:ARG:HB2	1:A:306:GLY:HA3	1.69	0.74
1:A:30:PRO:HA	1:A:66:MET:O	1.95	0.66
1:A:127:CYS:HB2	1:A:155:ASN:HD21	1.60	0.65
1:A:182:GLU:HG3	1:A:183:MET:HE2	1.77	0.65
1:A:324:PRO:HB3	1:A:358:LEU:HB3	1.78	0.65
1:A:37:ILE:HG21	1:A:351:VAL:HG11	1.80	0.63
1:A:114:LEU:O	1:A:118:LEU:HD12	2.00	0.62
1:A:32:ILE:HG13	1:A:68:ILE:HG13	1.82	0.62
1:A:112:ARG:HG3	1:A:112:ARG:HH11	1.67	0.60
1:A:354:GLY:O	1:A:358:LEU:HB2	2.02	0.59
1:A:395:ARG:HG3	1:A:396:LEU:HG	1.84	0.59
1:A:106:PRO:HG2	1:A:111:ILE:HD13	1.84	0.58
1:A:176:ILE:HG21	1:A:191:PRO:HB3	1.85	0.58
1:A:49:VAL:HG21	1:A:360:ALA:HB1	1.85	0.58
1:A:178:PHE:CZ	1:A:183:MET:HE3	2.39	0.58
1:A:26:ASN:HA	1:A:62:LYS:O	2.04	0.58
1:A:30:PRO:HD2	1:A:97:VAL:O	2.05	0.56
1:A:45:MET:HB2	1:A:356:ILE:HG23	1.88	0.56
1:A:36:GLY:HA3	1:A:341:THR:HB	1.86	0.56
1:A:115:ASN:O	1:A:119:ARG:HD3	2.05	0.56
1:A:15:THR:HB	1:A:22:ASN:HB3	1.89	0.55
1:A:354:GLY:HA2	1:A:380:MET:HE1	1.89	0.54
1:A:319:GLY:CA	1:A:322:ILE:HG22	2.39	0.53
1:A:206:THR:HG21	1:A:241:PHE:HA	1.90	0.53
1:A:23:VAL:HG12	1:A:24:PRO:O	2.08	0.53
1:A:138:PRO:O	1:A:318:GLY:HA3	2.09	0.52
1:A:206:THR:HG23	1:A:241:PHE:CD2	2.45	0.52
1:A:349:ASP:OD1	1:A:405:CYS:HB3	2.09	0.52
1:A:319:GLY:HA3	1:A:322:ILE:HG22	1.92	0.52
1:A:75:THR:HA	1:A:79:GLY:O	2.10	0.51
1:A:411:ALA:HA	1:A:414:GLU:HG2	1.92	0.51
1:A:320:ILE:H	1:A:320:ILE:HD12	1.77	0.50
1:A:288:GLN:HE21	1:A:288:GLN:HA	1.77	0.50
1:A:177:LYS:O	1:A:181:GLU:HG3	2.11	0.50
1:A:129:ARG:HH21	1:A:338:THR:HB	1.75	0.49
1:A:120:GLN:NE2	1:A:161:ALA:HA	2.27	0.49
1:A:265:LYS:HD2	1:A:274:GLU:HB3	1.94	0.49
1:A:358:LEU:HD22	1:A:380:MET:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLN:HE22	1:A:161:ALA:HA	1.78	0.49
1:A:154:GLU:HA	1:A:209:LEU:HD13	1.94	0.48
1:A:361:GLU:HG3	1:A:377:VAL:HG23	1.96	0.48
1:A:35:ASP:OD1	1:A:72:GLU:HB3	2.13	0.48
1:A:296:TYR:HB3	1:A:299:ILE:HD11	1.95	0.48
1:A:160:TYR:OH	3:A:418:OXS:O2	2.31	0.47
1:A:169:SER:O	1:A:173:GLU:HB2	2.14	0.47
1:A:226:THR:HG23	1:A:280:VAL:HG12	1.96	0.46
1:A:23:VAL:HG21	1:A:367:MET:O	2.15	0.46
1:A:106:PRO:CG	1:A:111:ILE:HD13	2.45	0.46
1:A:393:PHE:HB3	1:A:397:MET:HE3	1.97	0.46
1:A:408:PHE:CE2	1:A:412:ILE:HD11	2.51	0.46
1:A:37:ILE:HG22	1:A:346:ALA:HA	1.97	0.46
1:A:232:ASN:H	1:A:281:ILE:HD11	1.81	0.46
1:A:384:ILE:HD13	1:A:384:ILE:HG21	1.71	0.46
1:A:44:ALA:O	1:A:48:VAL:HG13	2.16	0.45
1:A:82:VAL:CG1	1:A:85:PRO:HG3	2.46	0.45
1:A:248:LEU:HD21	1:A:253:PHE:HE1	1.81	0.45
1:A:49:VAL:HG13	1:A:364:LEU:HD11	1.99	0.45
1:A:182:GLU:HG3	1:A:183:MET:CE	2.44	0.45
1:A:133:TYR:CD1	1:A:144:PRO:HB2	2.52	0.45
1:A:5:VAL:HG21	1:A:91:LEU:HD21	1.98	0.45
1:A:112:ARG:HG3	1:A:112:ARG:NH1	2.31	0.44
1:A:56:ALA:HB2	1:A:375:LEU:HD22	2.00	0.44
1:A:132:ARG:HA	1:A:147:THR:O	2.17	0.44
1:A:362:MET:HB3	1:A:362:MET:HE2	1.83	0.44
1:A:45:MET:HE3	1:A:45:MET:HB3	1.92	0.43
1:A:190:PHE:O	1:A:194:CYS:HB2	2.17	0.43
1:A:158:ASP:OD2	1:A:302:MET:HB3	2.18	0.43
1:A:258:ILE:CG1	1:A:265:LYS:HG2	2.39	0.43
1:A:353:PRO:O	1:A:356:ILE:HG22	2.19	0.43
1:A:191:PRO:O	1:A:194:CYS:HB3	2.19	0.43
1:A:226:THR:CG2	1:A:280:VAL:HG12	2.49	0.43
1:A:113:SER:OG	3:A:418:OXS:O4	2.36	0.42
1:A:267:LYS:HE3	1:A:272:GLY:CA	2.49	0.42
1:A:136:GLY:O	1:A:138:PRO:HD3	2.20	0.42
1:A:253:PHE:CD1	1:A:253:PHE:N	2.88	0.42
1:A:165:TRP:CD1	1:A:171:ASP:HB3	2.55	0.41
1:A:28:ILE:HA	1:A:64:SER:O	2.20	0.41
1:A:102:PRO:HB2	1:A:341:THR:HG22	2.02	0.41
1:A:222:ARG:HB3	1:A:297:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLY:C	1:A:111:ILE:HD12	2.47	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	412/416 (99%)	378 (92%)	31 (8%)	3 (1%)	18 34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	ASP
1	A	131	VAL
1	A	18	ASN

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	336/338 (99%)	286 (85%)	50 (15%)	3 6

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	16	LEU
1	A	26	ASN
1	A	33	GLU
1	A	40	ASP
1	A	42	THR
1	A	48	VAL
1	A	58	LYS
1	A	80	GLN
1	A	81	ASP
1	A	87	GLU
1	A	91	LEU
1	A	103	LEU
1	A	104	THR
1	A	112	ARG
1	A	115	ASN
1	A	118	LEU
1	A	119	ARG
1	A	121	GLU
1	A	129	ARG
1	A	135	GLN
1	A	137	THR
1	A	141	VAL
1	A	148	ASP
1	A	180	ARG
1	A	181	GLU
1	A	186	LYS
1	A	187	LYS
1	A	189	ARG
1	A	192	GLU
1	A	209	LEU
1	A	222	ARG
1	A	230	MET
1	A	234	MET
1	A	242	LYS
1	A	257	LEU
1	A	264	LEU
1	A	278	LYS
1	A	281	ILE
1	A	288	GLN
1	A	313	LEU
1	A	320	ILE
1	A	324	PRO

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Mol	Chain	Res	Type
1	A	344	LYS
1	A	350	LYS
1	A	358	LEU
1	A	375	LEU
1	A	385	ASN
1	A	389	VAL
1	A	397	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	120	GLN
1	A	155	ASN
1	A	288	GLN
1	A	348	GLN
1	A	366	HIS
1	A	385	ASN

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 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
3	OXS	A	418	2	12,12,12	4.83	6 (50%)	14,16,16	2.62	6 (42%)

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	OXS	A	418	2	-	2/15/16/16	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	418	OXS	O5-C5	-14.56	0.97	1.22
3	A	418	OXS	C2-C1	4.45	1.57	1.52
3	A	418	OXS	C2-C5	-3.65	1.46	1.53
3	A	418	OXS	C5-C6	-3.63	1.50	1.54
3	A	418	OXS	O4-C4	-2.66	1.22	1.30
3	A	418	OXS	O7-C6	-2.57	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	418	OXS	C2-C5-C6	-5.98	108.51	116.93
3	A	418	OXS	O5-C5-C6	4.74	126.63	119.35
3	A	418	OXS	O6-C6-C5	-3.86	117.23	122.15
3	A	418	OXS	C2-C3-C4	-3.07	108.44	112.97
3	A	418	OXS	O5-C5-C2	2.20	124.75	121.31
3	A	418	OXS	O4-C4-C3	2.02	120.29	114.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	418	OXS	C1-C2-C3-C4
3	A	418	OXS	C5-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	418	OXS	5	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.