



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:13 AM GMT

PDB ID : 2G4O
Title : anomalous substructure of 3-ISOPROPYLMALATE DEHYDROGENASE
Authors : Mueller-Dieckmann, C.; Weiss, M.S.
Deposited on : 2006-02-22
Resolution : 2.00 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

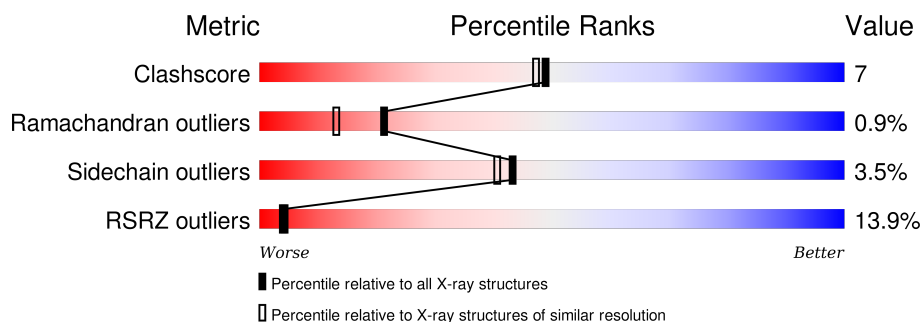
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	337	<div> <div>23%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	B	337	<div> <div>18%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
1	C	337	<div> <div>7%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	D	337	<div> <div>8%</div> <div>86%</div> <div>13%</div> <div>.</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	CL	A	804	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10587 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 3-isopropylmalate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	4	0
			2515	1570	462	476	7			
1	B	337	Total	C	N	O	S	0	2	0
			2505	1565	458	475	7			
1	C	337	Total	C	N	O	S	0	2	0
			2511	1567	462	476	6			
1	D	337	Total	C	N	O	S	0	2	0
			2507	1565	461	475	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P95313
A	1A	SER	-	CLONING ARTIFACT	UNP P95313
B	1	MET	-	INITIATING METHIONINE	UNP P95313
B	1A	SER	-	CLONING ARTIFACT	UNP P95313
C	1	MET	-	INITIATING METHIONINE	UNP P95313
C	1A	SER	-	CLONING ARTIFACT	UNP P95313
D	1	MET	-	INITIATING METHIONINE	UNP P95313
D	1A	SER	-	CLONING ARTIFACT	UNP P95313

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	3	Total	Cl	0	0
			3	3		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	145	Total	O	0	0
			145	145		
4	B	88	Total	O	0	0
			88	88		
4	C	162	Total	O	0	0
			162	162		

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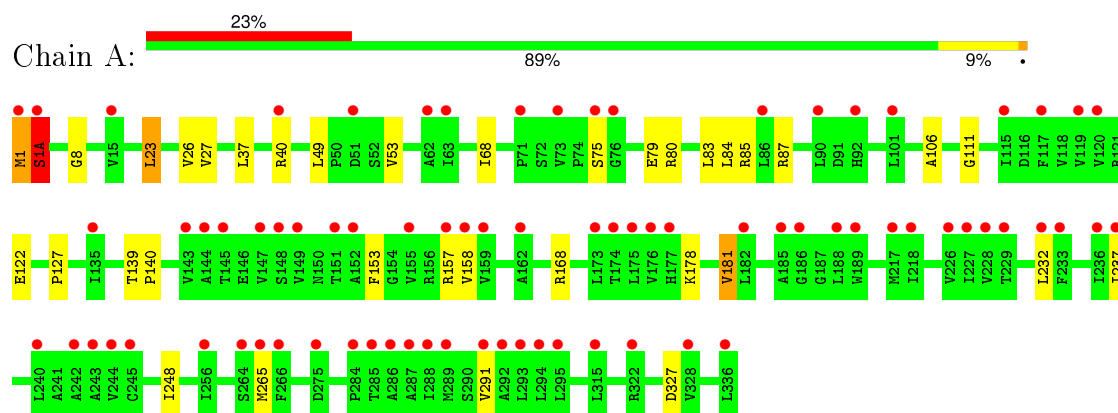
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	138	Total 138	O 138	0	0

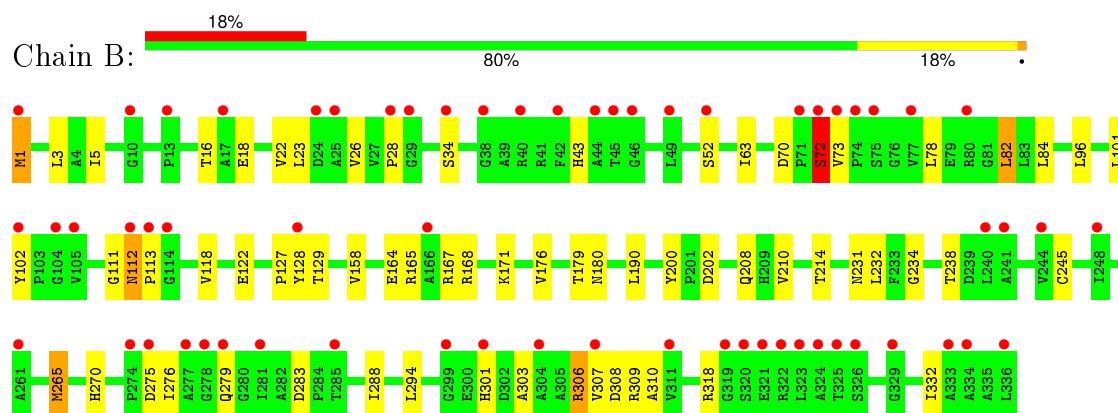
3 Residue-property plots

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.

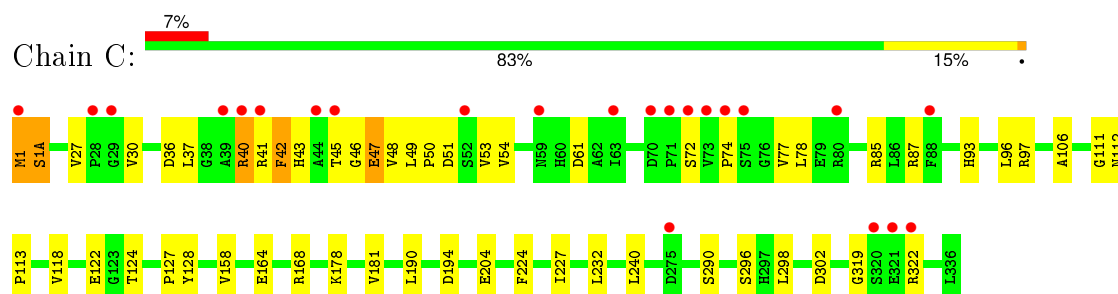
• Molecule 1: 3-isopropylmalate dehydrogenase



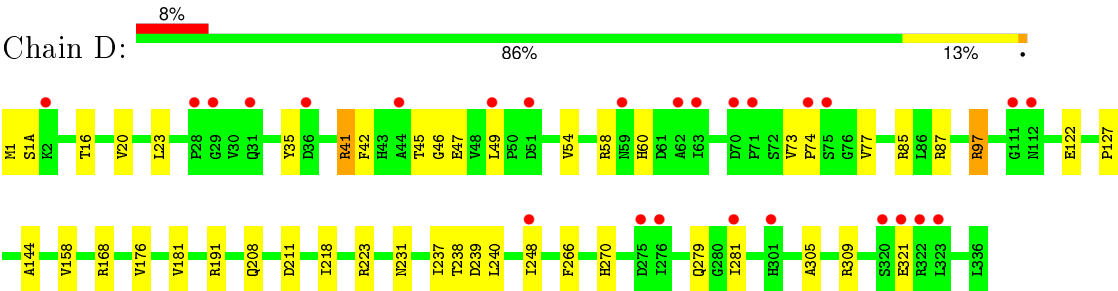
• Molecule 1: 3-isopropylmalate dehydrogenase



• Molecule 1: 3-isopropylmalate dehydrogenase



● Molecule 1: 3-isopropylmalate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.57Å 98.58Å 184.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 19.28 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.00) 100.0 (19.28-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.209 , 0.260 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 97028 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10587	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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, 0.375 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, CL

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	0.94	0/2567	0.93	4/3495 (0.1%)
1	B	0.85	1/2556 (0.0%)	0.83	0/3481
1	C	1.03	0/2559	0.89	0/3485
1	D	0.99	1/2559 (0.0%)	0.92	7/3485 (0.2%)
All	All	0.95	2/10241 (0.0%)	0.89	11/13946 (0.1%)

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	B	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	245	CYS	CB-SG	-6.53	1.71	1.82
1	D	144	ALA	CA-CB	-5.21	1.41	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	97[A]	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	D	97[B]	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	D	239	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	168	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	A	80	ARG	NE-CZ-NH1	6.13	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	D	191	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	211	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	191	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	327	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	D	223	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	MET	Peptide
1	D	46	GLY	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	2515	0	2506	39	0
1	B	2505	0	2513	61	0
1	C	2511	0	2516	35	0
1	D	2507	0	2513	25	0
2	A	5	0	0	0	0
2	D	5	0	0	0	0
3	A	3	0	0	0	0
3	B	1	0	0	1	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	145	0	0	10	0
4	B	88	0	0	16	2
4	C	162	0	0	10	1
4	D	138	0	0	2	1
All	All	10587	0	10048	145	2

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 7.

All (145) 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:B:34:SER:HA	4:B:887:HOH:O	1.32	1.29
1:A:79:GLU:OE2	1:B:180:ASN:ND2	1.90	1.04
1:B:101:LEU:HD23	4:B:889:HOH:O	1.61	0.98
1:B:43:HIS:HE2	1:B:72:SER:HG	1.09	0.93
1:B:127:PRO:O	4:B:878:HOH:O	1.88	0.90
1:B:23:LEU:HA	4:B:881:HOH:O	1.72	0.89
1:B:43:HIS:NE2	1:B:72:SER:OG	2.06	0.88
1:A:127:PRO:CD	4:A:940:HOH:O	2.24	0.86
1:C:127:PRO:HD2	4:C:959:HOH:O	1.75	0.84
1:C:72:SER:OG	4:C:907:HOH:O	1.96	0.81
1:B:306:ARG:O	1:B:308:ASP:N	2.14	0.79
1:A:127:PRO:HD2	4:A:940:HOH:O	1.81	0.79
1:C:43:HIS:NE2	4:C:907:HOH:O	2.11	0.74
1:A:127:PRO:HD3	4:A:940:HOH:O	1.87	0.74
1:C:1:MET:O	1:C:61:ASP:OD2	2.05	0.74
1:D:127:PRO:O	4:D:941:HOH:O	2.07	0.73
1:C:127:PRO:CD	4:C:959:HOH:O	2.34	0.73
1:A:153:PHE:O	1:A:157[A]:ARG:HG3	1.91	0.71
1:B:113:PRO:O	4:B:889:HOH:O	2.08	0.71
1:A:79:GLU:OE2	1:B:180:ASN:HB2	1.93	0.69
1:B:101:LEU:O	4:B:835:HOH:O	2.09	0.69
1:A:181:VAL:HG22	1:B:128:TYR:HA	1.74	0.69
1:C:36:ASP:OD1	1:C:40:ARG:HB3	1.94	0.68
1:A:248:ILE:O	4:A:866:HOH:O	2.11	0.68
1:B:232:LEU:HD23	1:B:232:LEU:C	2.15	0.67
1:A:1:MET:O	1:A:1(A):SER:HB2	1.94	0.66
1:B:171:LYS:HD3	1:B:202:ASP:HB2	1.78	0.66
1:C:302:ASP:HB3	4:C:956:HOH:O	1.97	0.65
1:A:106:ALA:HB2	1:C:111:GLY:HA2	1.79	0.65
1:C:194:ASP:OD1	4:C:878:HOH:O	2.15	0.63
1:A:23:LEU:HD22	1:A:291:VAL:HG13	1.79	0.63
1:A:127:PRO:HA	4:A:937:HOH:O	1.98	0.63
1:C:49:LEU:HD11	1:C:54:VAL:HG22	1.79	0.63
1:D:16:THR:O	1:D:20:VAL:HG23	1.99	0.63
1:A:127:PRO:O	4:A:938:HOH:O	2.16	0.62
1:B:128:TYR:HB2	1:B:231:ASN:OD1	2.00	0.62
1:B:122:GLU:HG2	1:B:158:VAL:HG21	1.82	0.62
1:B:167:ARG:O	1:B:171:LYS:NZ	2.32	0.61
1:D:45:THR:HB	1:D:47:GLU:HG3	1.82	0.61
1:A:79:GLU:CD	1:B:180:ASN:HD22	2.00	0.60
1:B:210:VAL:O	1:B:214:THR:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ARG:O	1:D:45:THR:OG1	2.19	0.60
1:B:310:ALA:HB1	1:B:332:ILE:O	2.02	0.60
1:B:102:TYR:C	4:B:874:HOH:O	2.40	0.60
1:B:127:PRO:C	1:B:129:THR:H	2.05	0.59
1:A:127:PRO:CA	4:A:937:HOH:O	2.50	0.59
1:A:49:LEU:HD23	1:A:85:ARG:HG2	1.83	0.59
1:B:3:LEU:HD23	1:B:5:ILE:HD11	1.85	0.59
1:A:75:SER:HA	4:A:933:HOH:O	2.01	0.58
1:B:5:ILE:HG23	4:B:873:HOH:O	2.03	0.58
1:A:79:GLU:OE2	1:B:180:ASN:CB	2.54	0.56
1:A:122:GLU:HG2	1:A:158:VAL:HG21	1.87	0.56
1:A:1:MET:O	1:A:1(A):SER:CB	2.53	0.56
1:B:63:ILE:HB	1:B:265[A]:MET:HG3	1.87	0.55
1:C:128:TYR:CG	1:D:181:VAL:HG11	2.42	0.55
1:C:93:HIS:HA	1:C:124:THR:HG23	1.88	0.54
1:C:27:VAL:O	1:C:30:VAL:HG23	2.08	0.54
1:B:16:THR:HG21	4:B:873:HOH:O	2.08	0.53
1:D:42:PHE:CD2	1:D:73:VAL:HG22	2.43	0.53
1:A:111:GLY:HA2	1:C:106:ALA:HB2	1.90	0.53
1:C:37:LEU:HD21	1:C:53:VAL:HG11	1.92	0.52
1:A:127:PRO:HB3	4:A:937:HOH:O	2.09	0.52
1:B:78:LEU:O	1:B:82:LEU:HB3	2.09	0.52
1:B:127:PRO:C	1:B:129:THR:N	2.62	0.51
1:D:305:ALA:O	1:D:309:ARG:HG2	2.10	0.51
1:C:128:TYR:CD1	1:D:181:VAL:HG11	2.45	0.51
1:C:232:LEU:C	1:C:232:LEU:HD23	2.30	0.51
1:A:8:GLY:O	1:A:40:ARG:NH2	2.44	0.51
1:C:36:ASP:OD1	1:C:40:ARG:CB	2.58	0.51
1:B:18:GLU:O	1:B:22:VAL:HG23	2.11	0.51
1:B:294:LEU:C	1:B:294:LEU:HD23	2.31	0.50
1:B:26:VAL:HG23	1:B:303:ALA:HB1	1.92	0.50
1:C:47:GLU:CD	1:C:48:VAL:H	2.15	0.50
1:B:5:ILE:HB	4:B:887:HOH:O	2.10	0.50
1:D:35:TYR:OH	1:D:60:HIS:NE2	2.40	0.50
1:A:26:VAL:HG23	1:A:27:VAL:HG23	1.93	0.50
1:D:42:PHE:O	1:D:45:THR:O	2.29	0.49
1:C:42:PHE:O	1:C:46:GLY:N	2.37	0.49
1:C:74:PRO:HG2	1:C:77:VAL:HG21	1.93	0.49
1:D:49:LEU:HD23	1:D:85:ARG:HG2	1.93	0.49
1:C:48:VAL:HG13	1:C:78:LEU:HD23	1.93	0.49
1:D:122:GLU:HG2	1:D:158:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:HD23	1:A:232:LEU:C	2.33	0.49
1:B:276:ILE:HA	1:B:279:GLN:NE2	2.29	0.48
1:B:306:ARG:HG3	4:B:891:HOH:O	2.13	0.48
1:A:178:LYS:HG3	1:A:181:VAL:HG12	1.95	0.48
1:A:178:LYS:HD3	4:B:892:HOH:O	2.14	0.47
1:C:204:GLU:OE2	4:C:905:HOH:O	2.20	0.47
1:B:164:GLU:OE2	1:B:200:TYR:OH	2.24	0.47
1:D:248:ILE:HD12	1:D:270:HIS:HA	1.96	0.47
1:A:181:VAL:CG1	1:B:128:TYR:CE1	2.98	0.46
1:B:270:HIS:CD2	4:B:850:HOH:O	2.68	0.46
1:D:127:PRO:HA	4:D:944:HOH:O	2.14	0.46
1:B:26:VAL:HG22	4:B:881:HOH:O	2.15	0.46
1:C:178:LYS:HG3	1:C:181:VAL:HG22	1.98	0.46
1:A:181:VAL:CG1	1:B:128:TYR:CD1	2.99	0.46
1:B:111:GLY:O	1:B:112:ASN:C	2.53	0.46
1:D:97[A]:ARG:NH2	1:D:238:THR:O	2.49	0.46
1:A:37:LEU:HD21	1:A:53:VAL:HG11	1.97	0.46
1:C:96:LEU:HD11	1:C:118:VAL:HG11	1.99	0.45
1:B:283:ASP:OD1	1:B:283:ASP:C	2.55	0.45
1:C:97[B]:ARG:CZ	1:C:97[B]:ARG:HB3	2.47	0.45
1:C:194:ASP:CG	4:C:878:HOH:O	2.55	0.45
1:B:234:GLY:O	1:B:238:THR:HG23	2.17	0.45
1:A:265[B]:MET:HE3	4:A:935:HOH:O	2.16	0.44
1:A:106:ALA:HB2	1:C:111:GLY:CA	2.45	0.44
1:D:176:VAL:HA	1:D:208:GLN:O	2.18	0.44
1:B:73:VAL:HG21	1:B:78:LEU:HD11	2.00	0.44
1:A:79:GLU:OE2	1:B:180:ASN:CG	2.52	0.44
1:A:178:LYS:CG	1:A:181:VAL:HG12	2.47	0.44
1:A:181:VAL:HG11	1:B:128:TYR:CE1	2.53	0.44
1:B:101:LEU:HB3	4:B:889:HOH:O	2.17	0.43
1:C:47:GLU:OE2	1:C:47:GLU:HA	2.18	0.43
1:C:112:ASN:N	1:C:113:PRO:CD	2.82	0.43
1:B:101:LEU:CD2	4:B:889:HOH:O	2.39	0.43
1:C:224:PHE:CG	1:C:227:ILE:HD11	2.53	0.43
1:B:179:THR:HG21	1:B:190:LEU:HG	2.00	0.42
1:B:308:ASP:HB3	1:B:309:ARG:NH2	2.34	0.42
1:D:73:VAL:HG13	1:D:74:PRO:HD2	2.01	0.42
1:D:74:PRO:HG2	1:D:77:VAL:HG21	2.02	0.42
1:D:97[A]:ARG:HG3	1:D:238:THR:HG21	2.01	0.42
1:A:181:VAL:HG13	1:B:128:TYR:CD1	2.54	0.42
1:B:232:LEU:O	1:B:232:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:VAL:CG2	1:B:303:ALA:HB1	2.50	0.41
1:B:168:ARG:NH1	1:B:168:ARG:HB2	2.35	0.41
1:D:168:ARG:HG2	1:D:168:ARG:HH11	1.85	0.41
1:C:1:MET:HA	1:C:298:LEU:HD13	2.02	0.41
1:B:232:LEU:CD2	1:B:232:LEU:C	2.85	0.41
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.93	0.41
1:D:279:GLN:HB2	1:D:281:ILE:HD12	2.03	0.41
1:D:87:ARG:HH22	1:D:231:ASN:HD21	1.68	0.41
1:C:168[B]:ARG:NH2	4:C:962:HOH:O	2.53	0.41
1:B:294:LEU:O	1:B:294:LEU:HD23	2.20	0.41
1:A:139:THR:HB	1:A:140:PRO:HD2	2.03	0.41
1:D:54:VAL:HG12	1:D:58:ARG:NH1	2.36	0.41
1:D:266:PHE:CD2	1:D:266:PHE:N	2.88	0.41
1:B:96:LEU:HD11	1:B:118:VAL:HG11	2.03	0.41
1:B:176:VAL:HA	1:B:208:GLN:O	2.20	0.40
1:B:165:ARG:HD3	3:B:805:CL:CL	2.58	0.40
1:B:171:LYS:HB3	1:B:202:ASP:O	2.21	0.40
1:D:218:ILE:HD11	1:D:240:LEU:HD11	2.01	0.40
1:A:68:ILE:HG13	1:A:83:LEU:HD21	2.02	0.40
1:C:127:PRO:HD3	4:C:959:HOH:O	2.12	0.40
1:B:22:VAL:HG21	1:B:288:ILE:HG12	2.04	0.40
1:C:122:GLU:HG2	1:C:158:VAL:HG21	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:830:HOH:O	4:C:869:HOH:O[2_564]	1.61	0.59
4:B:856:HOH:O	4:D:913:HOH:O[2_564]	1.81	0.39

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	338/337 (100%)	323 (96%)	14 (4%)	1 (0%)	46	41
1	B	337/337 (100%)	310 (92%)	23 (7%)	4 (1%)	16	8
1	C	337/337 (100%)	317 (94%)	15 (4%)	5 (2%)	13	5
1	D	337/337 (100%)	319 (95%)	16 (5%)	2 (1%)	30	22
All	All	1349/1348 (100%)	1269 (94%)	68 (5%)	12 (1%)	21	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1(A)	SER
1	B	306	ARG
1	B	307	VAL
1	D	1(A)	SER
1	D	321	GLU
1	B	72	SER
1	C	40	ARG
1	C	42	PHE
1	B	28	PRO
1	C	1(A)	SER
1	C	50	PRO
1	C	319	GLY

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	260/257 (101%)	253 (97%)	7 (3%)	52	52
1	B	259/257 (101%)	247 (95%)	12 (5%)	33	28
1	C	259/257 (101%)	245 (95%)	14 (5%)	27	21
1	D	259/257 (101%)	255 (98%)	4 (2%)	72	75
All	All	1037/1028 (101%)	1000 (96%)	37 (4%)	43	39

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	1(A)	SER
1	A	23	LEU
1	A	84	LEU
1	A	87	ARG
1	A	181	VAL
1	A	237	ILE
1	B	1	MET
1	B	52	SER
1	B	70	ASP
1	B	72	SER
1	B	82	LEU
1	B	84	LEU
1	B	112	ASN
1	B	265[A]	MET
1	B	265[B]	MET
1	B	275	ASP
1	B	301	HIS
1	B	318	ARG
1	C	1	MET
1	C	1(A)	SER
1	C	41	ARG
1	C	45	THR
1	C	47	GLU
1	C	51	ASP
1	C	85	ARG
1	C	87	ARG
1	C	164	GLU
1	C	190	LEU
1	C	240	LEU
1	C	290	SER
1	C	296	SER
1	C	322	ARG
1	D	1	MET
1	D	23	LEU
1	D	41	ARG
1	D	237	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	31	GLN
1	B	60	HIS

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Mol	Chain	Res	Type
1	C	60	HIS
1	D	31	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 ⓘ

Of 8 ligands modelled in this entry, 6 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	$\# Z > 2$
2	SO4	A	802	-	4,4,4	0.52	0	6,6,6	0.64	0
2	SO4	D	801	-	4,4,4	0.24	0	6,6,6	0.61	0

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	SO4	A	802	-	-	0/0/0/0	0/0/0/0
2	SO4	D	801	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

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	337/337 (100%)	1.23	78 (23%) 1 1	37, 44, 54, 66	0
1	B	337/337 (100%)	1.02	61 (18%) 2 2	28, 56, 74, 88	0
1	C	337/337 (100%)	0.41	23 (6%) 20 22	26, 40, 72, 87	0
1	D	337/337 (100%)	0.30	26 (7%) 16 17	27, 42, 63, 75	0
All	All	1348/1348 (100%)	0.74	188 (13%) 4 4	26, 45, 69, 88	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	8.2
1	C	71	PRO	6.9
1	C	44	ALA	6.4
1	B	334	ALA	6.0
1	B	322	ARG	5.9
1	C	45	THR	5.4
1	B	320	SER	5.3
1	C	28	PRO	5.2
1	B	102	TYR	5.1
1	A	1	MET	5.0
1	D	322	ARG	5.0
1	A	75	SER	5.0
1	B	28	PRO	4.9
1	A	63	ILE	4.9
1	B	128	TYR	4.9
1	B	336	LEU	4.8
1	B	323	LEU	4.8
1	A	328	VAL	4.7
1	C	1	MET	4.6
1	D	320	SER	4.6
1	B	25	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	44	ALA	4.5
1	A	264	SER	4.5
1	C	74	PRO	4.5
1	B	278	GLY	4.5
1	B	324	ALA	4.5
1	B	274	PRO	4.5
1	C	75	SER	4.4
1	B	112	ASN	4.3
1	B	45	THR	4.3
1	B	311	VAL	4.3
1	D	29	GLY	4.3
1	D	275	ASP	4.3
1	A	228	VAL	4.3
1	A	284	PRO	4.2
1	A	294	LEU	4.2
1	C	73	VAL	4.1
1	A	73	VAL	4.1
1	B	244	VAL	4.1
1	B	321	GLU	4.1
1	A	291	VAL	4.1
1	C	320	SER	4.1
1	A	144	ALA	4.1
1	A	188	LEU	4.0
1	A	189	TRP	4.0
1	D	71	PRO	4.0
1	B	281	ILE	4.0
1	A	159	VAL	3.9
1	C	88	PHE	3.9
1	A	176	VAL	3.9
1	A	185	ALA	3.8
1	B	275	ASP	3.8
1	A	288	ILE	3.7
1	D	59	ASN	3.6
1	A	155	VAL	3.6
1	A	175	LEU	3.6
1	A	143	VAL	3.6
1	B	333	ALA	3.6
1	A	115	ILE	3.6
1	A	240	LEU	3.6
1	B	279	GLN	3.5
1	B	34	SER	3.4
1	B	44	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	75	SER	3.4
1	A	227	ILE	3.4
1	C	321	GLU	3.4
1	C	40	ARG	3.3
1	B	105	VAL	3.3
1	B	240	LEU	3.3
1	A	76	GLY	3.2
1	A	218	ILE	3.2
1	A	101	LEU	3.2
1	A	147	VAL	3.2
1	B	17	ALA	3.2
1	A	90	LEU	3.2
1	B	277	ALA	3.2
1	C	41	ARG	3.2
1	B	73	VAL	3.2
1	B	71	PRO	3.2
1	C	29	GLY	3.1
1	B	10	GLY	3.1
1	B	46	GLY	3.1
1	A	266	PHE	3.1
1	A	151	THR	3.1
1	A	322	ARG	3.1
1	A	287	ALA	3.0
1	A	285	THR	3.0
1	B	307	VAL	3.0
1	C	80	ARG	3.0
1	A	1(A)	SER	3.0
1	D	111	GLY	3.0
1	A	173	LEU	3.0
1	B	326	SER	3.0
1	B	301	HIS	3.0
1	A	149	VAL	3.0
1	C	72	SER	3.0
1	A	292	ALA	3.0
1	B	325	THR	2.9
1	A	119	VAL	2.9
1	A	244	VAL	2.9
1	D	321	GLU	2.9
1	B	77	VAL	2.9
1	D	74	PRO	2.9
1	A	229	THR	2.9
1	B	261	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	112	ASN	2.8
1	A	237	ILE	2.8
1	B	72	SER	2.8
1	B	166	ALA	2.8
1	C	52	SER	2.8
1	A	226	VAL	2.8
1	A	265[A]	MET	2.8
1	D	28	PRO	2.8
1	C	322	ARG	2.8
1	B	113	PRO	2.7
1	A	336	LEU	2.7
1	D	281	ILE	2.7
1	B	38	GLY	2.7
1	A	286	ALA	2.7
1	B	80	ARG	2.6
1	C	70	ASP	2.6
1	D	36	ASP	2.6
1	A	135	ILE	2.6
1	D	31	GLN	2.6
1	B	241	ALA	2.6
1	A	245	CYS	2.5
1	A	232	LEU	2.5
1	C	63	ILE	2.5
1	B	74	PRO	2.5
1	D	2	LYS	2.5
1	A	158	VAL	2.5
1	B	52	SER	2.5
1	C	39	ALA	2.5
1	A	86	LEU	2.5
1	A	157[A]	ARG	2.5
1	A	152	ALA	2.5
1	B	304	ALA	2.5
1	B	42	PHE	2.5
1	A	275	ASP	2.5
1	A	233	PHE	2.5
1	D	75	SER	2.5
1	B	319	GLY	2.4
1	A	293	LEU	2.4
1	A	289	MET	2.4
1	A	62	ALA	2.4
1	D	63	ILE	2.4
1	A	51	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	51	ASP	2.4
1	B	29	GLY	2.4
1	B	299	GLY	2.4
1	A	120	VAL	2.3
1	A	145	THR	2.3
1	A	186	GLY	2.3
1	A	236	ILE	2.3
1	C	59	ASN	2.3
1	A	71	PRO	2.3
1	A	177	HIS	2.3
1	A	242	ALA	2.3
1	D	323	LEU	2.3
1	B	24	ASP	2.3
1	A	15	VAL	2.3
1	B	248	ILE	2.3
1	B	49	LEU	2.3
1	B	329	GLY	2.2
1	D	301	HIS	2.3
1	B	40	ARG	2.2
1	A	243	ALA	2.2
1	A	217	MET	2.2
1	A	174	THR	2.2
1	B	114	GLY	2.2
1	D	276	ILE	2.2
1	C	275	ASP	2.2
1	A	148	SER	2.1
1	B	104	GLY	2.1
1	A	117	PHE	2.1
1	D	248	ILE	2.1
1	A	182	LEU	2.1
1	B	285	THR	2.1
1	A	40	ARG	2.1
1	A	256	ILE	2.1
1	D	62	ALA	2.1
1	A	315	LEU	2.1
1	A	162	ALA	2.1
1	A	295	LEU	2.0
1	D	49	LEU	2.0
1	A	92	HIS	2.0
1	B	13	PRO	2.0
1	D	70	ASP	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(Å ²)	Q<0.9
3	CL	A	804	1/1	0.94	0.22	2.49	27,27,27,27	1
2	SO4	A	802	5/5	0.95	0.15	-0.78	45,49,53,54	5
3	CL	A	803	1/1	0.96	0.17	-	35,35,35,35	1
3	CL	C	806	1/1	0.95	0.19	-	34,34,34,34	1
3	CL	A	807	1/1	0.79	0.74	-	53,53,53,53	1
3	CL	B	805	1/1	0.88	0.31	-	46,46,46,46	1
3	CL	D	808	1/1	0.96	0.24	-	32,32,32,32	1
2	SO4	D	801	5/5	0.92	0.15	-	46,47,50,56	5

6.5 Other polymers [i](#)

There are no such residues in this entry.