



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:28 AM GMT

PDB ID : 3IK4
Title : CRYSTAL STRUCTURE OF mandelate racemase/muconate lactonizing protein from *Herpetosiphon aurantiacus*
Authors : Patskovsky, Y.; Toro, R.; Dickey, M.; Iizuka, M.; Sauder, J.M.; Gerlt, J.A.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-08-05
Resolution : 2.10 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

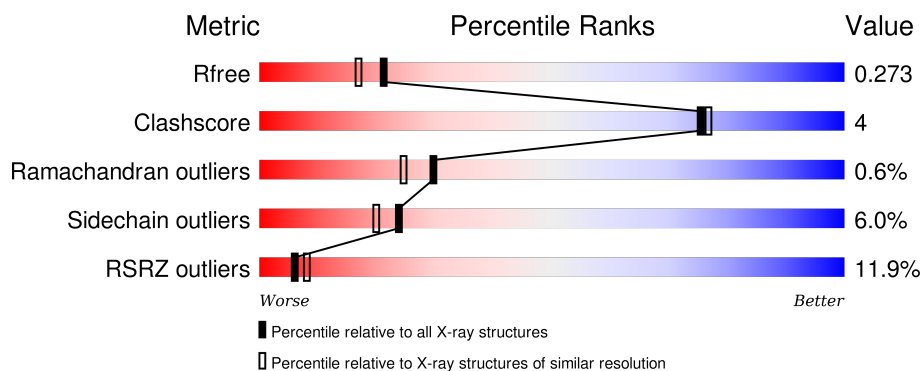
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	365	<div> <div>4%</div> <div>85%</div> <div>9%</div> <div>• •</div> </div>
1	B	365	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>• •</div> </div>
1	C	365	<div> <div>22%</div> <div>86%</div> <div>8%</div> <div>• •</div> </div>
1	D	365	<div> <div>18%</div> <div>85%</div> <div>9%</div> <div>• 5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10543 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 Mandelate racemase/muconate lactonizing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	4	0
			2574	1625	450	483	16			
1	B	358	Total	C	N	O	S	0	5	0
			2625	1658	459	492	16			
1	C	349	Total	C	N	O	S	0	4	0
			2556	1611	448	481	16			
1	D	348	Total	C	N	O	S	0	1	0
			2535	1598	443	478	16			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP A9B055
A	0	SER	-	expression tag	UNP A9B055
A	1	LEU	-	expression tag	UNP A9B055
A	356	GLU	-	expression tag	UNP A9B055
A	357	GLY	-	expression tag	UNP A9B055
A	358	HIS	-	expression tag	UNP A9B055
A	359	HIS	-	expression tag	UNP A9B055
A	360	HIS	-	expression tag	UNP A9B055
A	361	HIS	-	expression tag	UNP A9B055
A	362	HIS	-	expression tag	UNP A9B055
A	363	HIS	-	expression tag	UNP A9B055
B	-1	MET	-	expression tag	UNP A9B055
B	0	SER	-	expression tag	UNP A9B055
B	1	LEU	-	expression tag	UNP A9B055
B	356	GLU	-	expression tag	UNP A9B055
B	357	GLY	-	expression tag	UNP A9B055
B	358	HIS	-	expression tag	UNP A9B055
B	359	HIS	-	expression tag	UNP A9B055
B	360	HIS	-	expression tag	UNP A9B055
B	361	HIS	-	expression tag	UNP A9B055
B	362	HIS	-	expression tag	UNP A9B055

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Chain	Residue	Modelled	Actual	Comment	Reference
B	363	HIS	-	expression tag	UNP A9B055
C	-1	MET	-	expression tag	UNP A9B055
C	0	SER	-	expression tag	UNP A9B055
C	1	LEU	-	expression tag	UNP A9B055
C	356	GLU	-	expression tag	UNP A9B055
C	357	GLY	-	expression tag	UNP A9B055
C	358	HIS	-	expression tag	UNP A9B055
C	359	HIS	-	expression tag	UNP A9B055
C	360	HIS	-	expression tag	UNP A9B055
C	361	HIS	-	expression tag	UNP A9B055
C	362	HIS	-	expression tag	UNP A9B055
C	363	HIS	-	expression tag	UNP A9B055
D	-1	MET	-	expression tag	UNP A9B055
D	0	SER	-	expression tag	UNP A9B055
D	1	LEU	-	expression tag	UNP A9B055
D	356	GLU	-	expression tag	UNP A9B055
D	357	GLY	-	expression tag	UNP A9B055
D	358	HIS	-	expression tag	UNP A9B055
D	359	HIS	-	expression tag	UNP A9B055
D	360	HIS	-	expression tag	UNP A9B055
D	361	HIS	-	expression tag	UNP A9B055
D	362	HIS	-	expression tag	UNP A9B055
D	363	HIS	-	expression tag	UNP A9B055

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

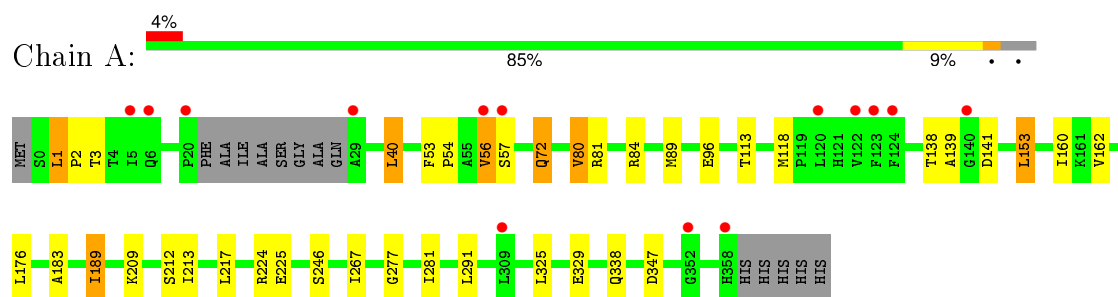
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	90	Total	O	0	0
			90	90		
4	B	91	Total	O	0	0
			91	91		
4	C	30	Total	O	0	0
			30	30		
4	D	26	Total	O	0	0
			26	26		

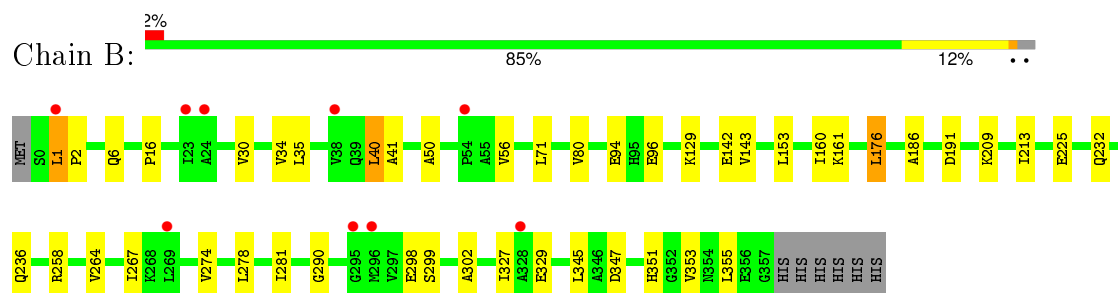
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

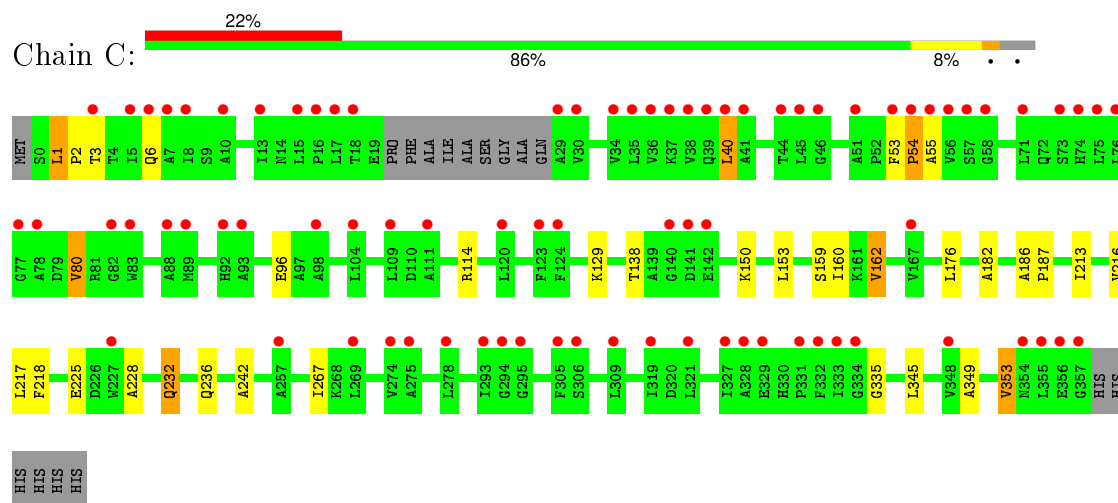
- Molecule 1: Mandelate racemase/muconate lactonizing protein



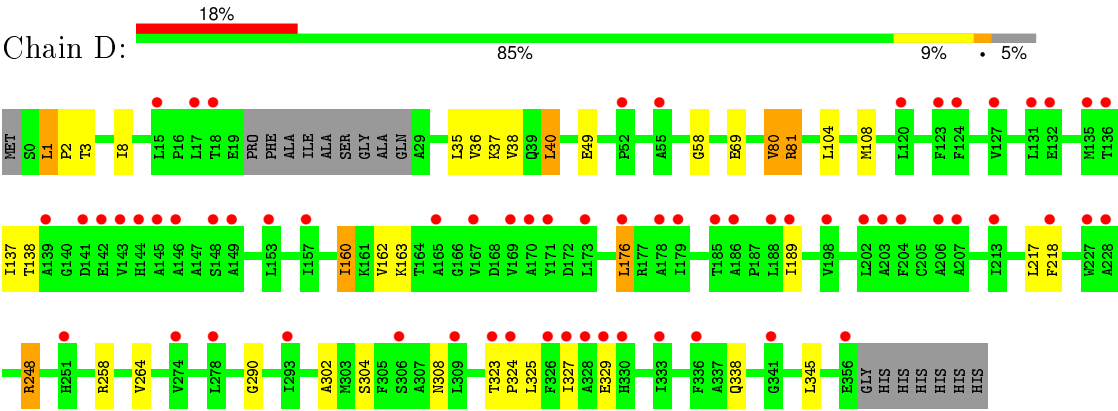
- Molecule 1: Mandelate racemase/muconate lactonizing protein



- Molecule 1: Mandelate racemase/muconate lactonizing protein



- Molecule 1: Mandelate racemase/muconate lactonizing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.03Å 93.34Å 85.91Å 90.00° 112.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 33.17 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.10) 98.1 (33.17-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.217 , 0.275 0.216 , 0.273	Depositor DCC
R_{free} test set	2148 reflections (3.12%)	DCC
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.9	EDS
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 73692 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10543	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: GOL, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/2628	0.63	0/3563
1	B	0.46	0/2683	0.65	2/3638 (0.1%)
1	C	0.37	0/2609	0.59	0/3537
1	D	0.38	0/2579	0.58	0/3498
All	All	0.43	0/10499	0.61	2/14236 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258[A]	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	258[B]	ARG	NE-CZ-NH1	5.23	122.91	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2574	0	2607	24	0
1	B	2625	0	2665	18	0
1	C	2556	0	2583	15	0
1	D	2535	0	2554	24	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
4	A	90	0	0	1	0
4	B	91	0	0	1	0
4	C	30	0	0	0	0
4	D	26	0	0	0	0
All	All	10543	0	10425	81	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 4.

All (81) 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:1:LEU:HB2	1:D:2:PRO:HD2	1.47	0.95
1:B:1:LEU:HB3	1:B:2:PRO:HD2	1.64	0.78
1:D:1:LEU:CB	1:D:2:PRO:HD2	2.14	0.77
1:B:267[B]:ILE:HD13	1:B:281:ILE:HG13	1.72	0.72
1:D:248:ARG:NH1	1:D:248:ARG:HG3	2.08	0.69
1:D:1:LEU:HB2	1:D:2:PRO:CD	2.23	0.68
1:D:81:ARG:HH11	1:D:81:ARG:HG3	1.60	0.66
1:A:1:LEU:CD1	1:A:81:ARG:HH22	2.08	0.65
1:C:1:LEU:HB3	1:C:2:PRO:HD2	1.80	0.64
1:D:248:ARG:HH11	1:D:248:ARG:HG3	1.63	0.64
1:D:248:ARG:HH11	1:D:248:ARG:CG	2.12	0.62
1:A:1:LEU:HD11	1:A:81:ARG:HH22	1.64	0.62
1:A:84[A]:ARG:NH2	4:A:420:HOH:O	2.32	0.61
1:A:267[A]:ILE:HD11	1:A:291:LEU:HD22	1.83	0.61
1:C:40:LEU:HD21	1:C:80:VAL:HG11	1.83	0.61
1:A:1:LEU:HB2	1:A:2:PRO:HD2	1.83	0.60
1:D:1:LEU:CB	1:D:2:PRO:CD	2.78	0.59
1:A:189:ILE:HD13	1:A:217:LEU:HD23	1.87	0.57
1:A:267[A]:ILE:CD1	1:A:291:LEU:HD22	2.36	0.55
1:A:277:GLY:O	1:A:281:ILE:HG13	2.06	0.55
1:A:1:LEU:HD23	1:A:1:LEU:H	1.71	0.54
1:D:49:GLU:HB3	1:D:302:ALA:HB2	1.90	0.54
1:D:325:LEU:HD11	1:D:338:GLN:HE22	1.72	0.53
1:D:81:ARG:NH1	1:D:81:ARG:HG3	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ARG:HA	1:C:349:ALA:HB1	1.94	0.50
1:A:1:LEU:N	1:A:1:LEU:HD23	2.26	0.50
1:A:153:LEU:HD12	1:A:183:ALA:HB1	1.93	0.49
1:B:96[B]:GLU:CD	1:B:96[B]:GLU:H	2.15	0.49
1:B:351:HIS:O	4:B:444:HOH:O	2.20	0.49
1:B:176:LEU:HD13	1:B:213:ILE:HG21	1.95	0.48
1:C:217:LEU:HD11	1:C:242:ALA:HB2	1.95	0.48
1:B:34:VAL:HB	1:B:50:ALA:HB3	1.95	0.48
1:B:16:PRO:HA	1:B:30:VAL:HG22	1.96	0.48
1:A:96[B]:GLU:H	1:A:96[B]:GLU:CD	2.18	0.47
1:A:1:LEU:CD1	1:A:81:ARG:NH2	2.75	0.47
1:C:1:LEU:HB3	1:C:2:PRO:CD	2.43	0.47
1:D:323:THR:N	1:D:324:PRO:CD	2.77	0.47
1:B:35:LEU:HD21	1:B:355:LEU:HD11	1.95	0.47
1:A:176:LEU:HD13	1:A:213:ILE:HG21	1.96	0.47
1:C:150:LYS:HG2	1:C:182:ALA:HB1	1.97	0.47
1:B:1:LEU:O	1:B:41:ALA:HB3	2.15	0.47
1:D:3:THR:HG21	1:D:81:ARG:HD3	1.97	0.46
1:B:161[B]:LYS:HE3	1:B:191:ASP:HB2	1.97	0.46
1:D:189:ILE:HG23	1:D:217:LEU:HB3	1.96	0.46
1:A:1:LEU:O	1:A:3:THR:N	2.49	0.46
1:A:72:GLN:HE21	1:A:72:GLN:HB2	1.62	0.45
1:A:325:LEU:HD11	1:A:338:GLN:HE22	1.80	0.45
1:A:56:VAL:HB	1:A:57:SER:H	1.54	0.45
1:C:228:ALA:O	1:C:232[B]:GLN:HG2	2.16	0.44
1:A:40:LEU:HD21	1:A:80:VAL:HG11	2.00	0.44
1:B:40:LEU:HD21	1:B:80:VAL:HG11	2.00	0.44
1:B:299:SER:HA	1:B:327:ILE:HD12	1.99	0.44
1:D:137:ILE:HD12	1:D:160:ILE:HD13	2.00	0.44
1:A:53:PHE:HA	1:A:54:PRO:HD3	1.76	0.43
1:D:138:THR:HG22	1:D:163:LYS:HD3	2.01	0.43
1:B:71:LEU:HD21	1:B:94:GLU:HB2	2.01	0.43
1:D:324:PRO:HA	1:D:327:ILE:HD12	2.01	0.43
1:D:36:VAL:HG11	1:D:104:LEU:HD23	2.01	0.42
1:B:153:LEU:HD11	1:B:186:ALA:HB2	2.01	0.42
1:C:153:LEU:HD11	1:C:186:ALA:HB2	2.00	0.42
1:C:176:LEU:HD13	1:C:213:ILE:HG21	2.00	0.42
1:A:113:THR:HB	1:A:118:MET:O	2.20	0.42
1:B:298:GLU:HB3	1:B:302:ALA:HB3	2.01	0.42
1:B:1:LEU:HB3	1:B:2:PRO:CD	2.39	0.42
1:B:264:VAL:HG22	1:B:290:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:LEU:HD23	1:D:176:LEU:HA	1.96	0.42
1:A:224:ARG:HG3	1:A:246:SER:HA	2.01	0.41
1:D:304:SER:O	1:D:308:ASN:ND2	2.51	0.41
1:D:264:VAL:HG22	1:D:290:GLY:HA3	2.02	0.41
1:C:335:GLY:HA2	1:C:353:VAL:HG12	2.02	0.41
1:D:40:LEU:HD21	1:D:80:VAL:HG11	2.03	0.41
1:A:1:LEU:HD12	1:A:81:ARG:NH2	2.36	0.41
1:C:3:THR:HB	1:C:80:VAL:HG12	2.03	0.41
1:C:53:PHE:HA	1:C:54:PRO:HD2	1.78	0.41
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.92	0.41
1:B:274:VAL:O	1:B:278:LEU:HG	2.22	0.40
1:C:162:VAL:HG11	1:C:176:LEU:HD21	2.04	0.40
1:C:129:LYS:HB2	1:C:345:LEU:HB2	2.02	0.40
1:C:159:SER:HB3	1:C:187:PRO:HG2	2.02	0.40
1:D:308:ASN:HA	1:D:345:LEU:HD21	2.04	0.40
1:D:8:ILE:HG12	1:D:38:VAL:HG12	2.03	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	351/365 (96%)	331 (94%)	17 (5%)	3 (1%)	21	15
1	B	361/365 (99%)	345 (96%)	15 (4%)	1 (0%)	46	45
1	C	349/365 (96%)	329 (94%)	17 (5%)	3 (1%)	21	15
1	D	345/365 (94%)	328 (95%)	16 (5%)	1 (0%)	46	45
All	All	1406/1460 (96%)	1333 (95%)	65 (5%)	8 (1%)	30	24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1	LEU
1	C	54	PRO
1	C	55	ALA
1	D	58	GLY
1	A	56	VAL
1	A	139	ALA
1	C	6	GLN
1	A	138	THR

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	256/262 (98%)	241 (94%)	15 (6%)	24	20
1	B	260/262 (99%)	244 (94%)	16 (6%)	23	19
1	C	254/262 (97%)	239 (94%)	15 (6%)	24	20
1	D	251/262 (96%)	236 (94%)	15 (6%)	24	20
All	All	1021/1048 (97%)	960 (94%)	61 (6%)	24	20

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	40	LEU
1	A	72	GLN
1	A	80	VAL
1	A	89	MET
1	A	141	ASP
1	A	153	LEU
1	A	160	ILE
1	A	162	VAL
1	A	189	ILE
1	A	209	LYS
1	A	212	SER
1	A	225	GLU
1	A	329	GLU

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Mol	Chain	Res	Type
1	A	347	ASP
1	B	6	GLN
1	B	40	LEU
1	B	56	VAL
1	B	129	LYS
1	B	142	GLU
1	B	143	VAL
1	B	160	ILE
1	B	176	LEU
1	B	209	LYS
1	B	225	GLU
1	B	232	GLN
1	B	236	GLN
1	B	329	GLU
1	B	345	LEU
1	B	347	ASP
1	B	353	VAL
1	C	1	LEU
1	C	40	LEU
1	C	80	VAL
1	C	96	GLU
1	C	138	THR
1	C	160	ILE
1	C	162	VAL
1	C	216	VAL
1	C	218	PHE
1	C	225	GLU
1	C	232[A]	GLN
1	C	232[B]	GLN
1	C	236	GLN
1	C	267	ILE
1	C	353	VAL
1	D	1	LEU
1	D	35	LEU
1	D	37	LYS
1	D	40	LEU
1	D	69	GLU
1	D	80	VAL
1	D	81	ARG
1	D	108	MET
1	D	160	ILE
1	D	162	VAL

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Mol	Chain	Res	Type
1	D	176	LEU
1	D	218	PHE
1	D	248	ARG
1	D	258	ARG
1	D	329	GLU

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

Mol	Chain	Res	Type
1	A	72	GLN
1	A	181	GLN
1	A	232	GLN
1	A	330	HIS
1	B	236	GLN
1	B	285	GLN
1	B	313	ASN
1	D	72	GLN
1	D	232	GLN
1	D	330	HIS
1	D	338	GLN
1	D	344	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 6 ligands modelled in this entry, 4 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	GOL	B	364	-	5,5,5	0.35	0	5,5,5	0.30	0
3	GOL	C	364	-	5,5,5	0.37	0	5,5,5	0.32	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
3	GOL	B	364	-	-	0/4/4/4	0/0/0/0
3	GOL	C	364	-	-	0/4/4/4	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	351/365 (96%)	0.23	14 (3%) 42 51	18, 34, 58, 111	0
1	B	358/365 (98%)	0.10	9 (2%) 61 67	18, 36, 58, 74	0
1	C	349/365 (95%)	1.29	81 (23%) 1 1	23, 41, 79, 123	0
1	D	348/365 (95%)	0.93	64 (18%) 2 2	26, 43, 75, 94	0
All	All	1406/1460 (96%)	0.63	168 (11%) 6 8	18, 38, 70, 123	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	167	VAL	12.1
1	C	55	ALA	11.0
1	C	7	ALA	10.3
1	C	56	VAL	10.2
1	C	8	ILE	8.8
1	C	15	LEU	8.7
1	C	30	VAL	8.6
1	C	38	VAL	8.5
1	A	56	VAL	8.1
1	C	29	ALA	7.5
1	C	37	LYS	7.1
1	D	326	PHE	6.8
1	D	170	ALA	6.2
1	C	6	GLN	5.8
1	D	139	ALA	5.7
1	C	10	ALA	5.6
1	C	45	LEU	5.5
1	C	327	ILE	5.2
1	C	17	LEU	5.2
1	C	34	VAL	5.1
1	C	71	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	203	ALA	4.9
1	C	57	SER	4.9
1	A	20	PRO	4.9
1	D	176	LEU	4.9
1	D	145	ALA	4.9
1	C	40	LEU	4.8
1	D	171	TYR	4.8
1	C	328	ALA	4.7
1	C	73	SER	4.6
1	D	309	LEU	4.4
1	D	327	ILE	4.4
1	C	74	HIS	4.4
1	C	3	THR	4.4
1	C	355	LEU	4.3
1	C	16	PRO	4.2
1	D	179	ILE	4.0
1	A	140	GLY	4.0
1	C	5	ILE	4.0
1	D	356	GLU	4.0
1	C	35	LEU	3.9
1	D	178	ALA	3.9
1	C	89	MET	3.8
1	D	227	TRP	3.8
1	D	202	LEU	3.8
1	D	141	ASP	3.7
1	D	336	PHE	3.6
1	C	44	THR	3.6
1	C	54	PRO	3.6
1	C	92	HIS	3.5
1	D	148	SER	3.5
1	D	186	ALA	3.5
1	C	305	PHE	3.4
1	C	39	GLN	3.4
1	C	75	LEU	3.4
1	D	341	GLY	3.3
1	D	198	VAL	3.3
1	C	123	PHE	3.3
1	D	204	PHE	3.3
1	C	82	GLY	3.3
1	D	17	LEU	3.3
1	C	332	PHE	3.2
1	D	185	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	328	ALA	3.2
1	C	53	PHE	3.2
1	C	58	GLY	3.2
1	D	324	PRO	3.2
1	C	167	VAL	3.2
1	D	173	LEU	3.2
1	C	18	THR	3.1
1	C	140	GLY	3.1
1	C	46	GLY	3.1
1	C	274	VAL	3.1
1	D	143	VAL	3.1
1	C	104	LEU	3.0
1	D	323	THR	3.0
1	D	213	ILE	3.0
1	A	29	ALA	3.0
1	A	5	ILE	3.0
1	C	36	VAL	3.0
1	D	131	LEU	3.0
1	C	329	GLU	2.9
1	D	330	HIS	2.9
1	D	120	LEU	2.9
1	B	24	ALA	2.9
1	C	257	ALA	2.9
1	C	331	PRO	2.9
1	D	207	ALA	2.9
1	D	293	ILE	2.9
1	A	123	PHE	2.8
1	C	294	GLY	2.8
1	D	188	LEU	2.8
1	D	278	LEU	2.8
1	C	334	GLY	2.7
1	D	15	LEU	2.7
1	C	93	ALA	2.7
1	D	149	ALA	2.7
1	C	124	PHE	2.7
1	D	142	GLU	2.7
1	C	109	LEU	2.6
1	C	319	ILE	2.6
1	D	132	GLU	2.6
1	C	111	ALA	2.6
1	A	120	LEU	2.6
1	C	51	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	120	LEU	2.6
1	C	227	TRP	2.5
1	D	206	ALA	2.5
1	B	295	GLY	2.5
1	B	328	ALA	2.5
1	D	165	ALA	2.5
1	A	309	LEU	2.5
1	D	18	THR	2.5
1	D	329	GLU	2.5
1	D	274	VAL	2.5
1	D	55	ALA	2.4
1	C	348	VAL	2.4
1	C	98	ALA	2.4
1	A	6	GLN	2.4
1	C	309	LEU	2.4
1	C	321	LEU	2.4
1	C	78	ALA	2.4
1	C	333	ILE	2.4
1	C	306	SER	2.4
1	C	356	GLU	2.4
1	B	54	PRO	2.3
1	B	269	LEU	2.3
1	D	136	THR	2.3
1	C	269	LEU	2.3
1	D	52	PRO	2.3
1	C	88	ALA	2.3
1	D	189	ILE	2.3
1	D	306	SER	2.3
1	D	123	PHE	2.3
1	D	228	ALA	2.3
1	B	38	VAL	2.3
1	C	293	ILE	2.2
1	A	57	SER	2.2
1	D	124	PHE	2.2
1	D	146	ALA	2.2
1	C	77	GLY	2.2
1	D	333	ILE	2.2
1	D	153	LEU	2.2
1	A	124	PHE	2.2
1	C	295	GLY	2.2
1	A	122	VAL	2.2
1	A	352	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	357	GLY	2.1
1	B	23	ILE	2.1
1	D	251	HIS	2.1
1	C	142	GLU	2.1
1	C	13	ILE	2.1
1	C	278	LEU	2.1
1	C	41	ALA	2.1
1	D	135	MET	2.1
1	D	144	HIS	2.1
1	B	296	MET	2.1
1	B	1	LEU	2.1
1	D	218	PHE	2.1
1	C	141	ASP	2.1
1	D	127	VAL	2.1
1	D	169	VAL	2.1
1	D	157	ILE	2.0
1	C	76	LEU	2.0
1	C	275	ALA	2.0
1	C	83	TRP	2.0
1	A	358	HIS	2.0
1	C	354	ASN	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
2	K	B	365	1/1	0.87	0.21	1.68	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	K	D	364	1/1	0.84	0.17	0.65	67,67,67,67	1
2	K	A	364	1/1	0.89	0.12	0.21	37,37,37,37	1
3	GOL	B	364	6/6	0.91	0.16	-0.35	32,48,53,56	0
2	K	C	365	1/1	0.88	0.09	-1.19	48,48,48,48	1
3	GOL	C	364	6/6	0.91	0.15	-1.70	40,54,58,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.