Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:08 pm BST

PDB ID	:	1HKW
Title	:	MYCOBACTERIUM DIAMINOPIMELATE DICARBOXYLASE (LysA)
Authors	:	Gokulan, K.; Rupp, B.; Pavelka Jr, M.S.; Jacobs Jr, W.R.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2003-03-11
Resolution	:	2.80 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 following versions of software and data (see references ①) were used in the production of this report:

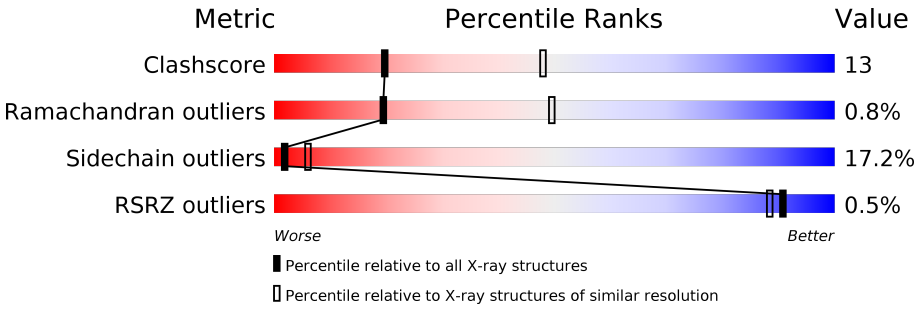
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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 <=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	453	67% 26% 5%
1	B	453	% 63% 26% 9%

2 Entry composition

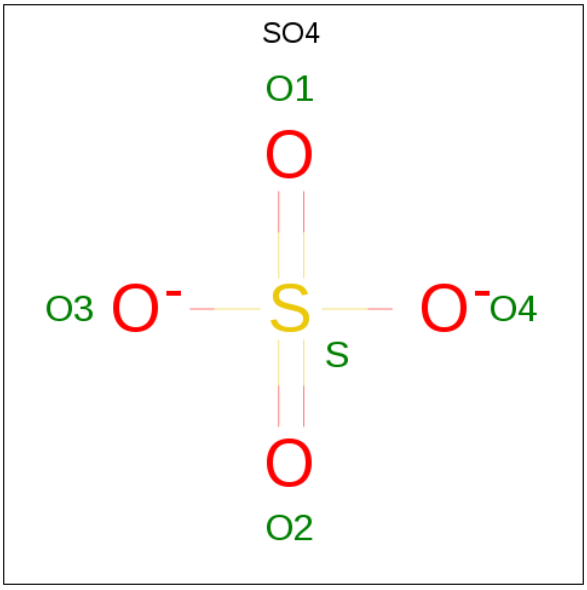
There are 3 unique types of molecules in this entry. The entry contains 6865 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIAMINOPIMELATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	Se	0	0	0
			3330	2089	591	639	7	4			
1	B	444	Total	C	N	O	S	Se	0	0	0
			3311	2079	585	636	7	4			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

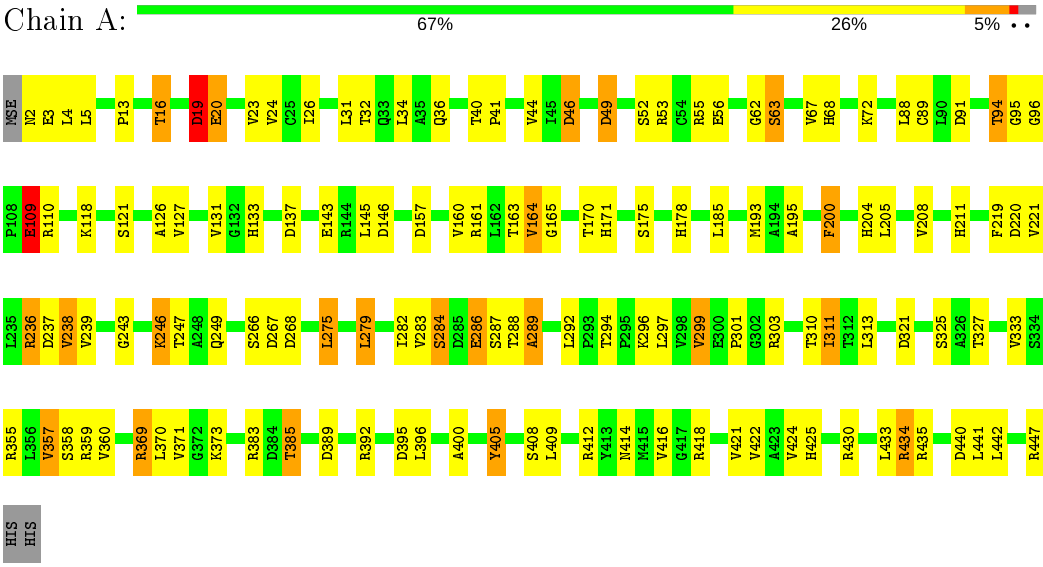
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	121	Total O 121 121	0	0
3	B	93	Total O 93 93	0	0

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 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.

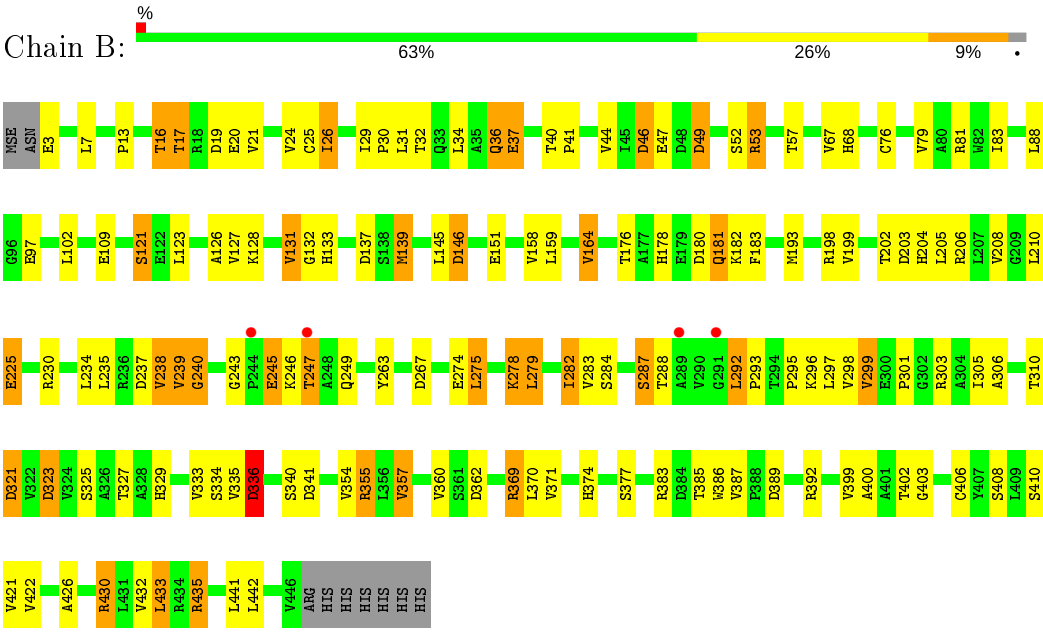
- Molecule 1: DIAMINOPIMELATE DECARBOXYLASE

Chain A:



- Molecule 1: DIAMINOPIMELATE DECARBOXYLASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	111.56Å 111.56Å 237.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 81.34 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.80) 100.0 (81.34-2.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.42 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.193 , 0.248 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 25.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6865	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 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4

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	1.37	14/3388 (0.4%)	0.99	15/4614 (0.3%)
1	B	1.40	24/3369 (0.7%)	0.97	13/4589 (0.3%)
All	All	1.38	38/6757 (0.6%)	0.98	28/9203 (0.3%)

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	1
1	B	1	1
All	All	1	2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	ARG	NE-CZ	8.10	1.43	1.33
1	B	400	ALA	C-O	8.08	1.38	1.23
1	A	400	ALA	C-O	7.79	1.38	1.23
1	A	143	GLU	CD-OE1	7.00	1.33	1.25
1	A	109	GLU	CD-OE2	6.77	1.33	1.25
1	A	143	GLU	CG-CD	6.38	1.61	1.51
1	B	336	ASP	CB-CG	-6.38	1.38	1.51
1	B	418	ARG	NE-CZ	6.23	1.41	1.33
1	B	225	GLU	CD-OE2	6.20	1.32	1.25
1	A	336	ASP	CB-CG	-6.20	1.38	1.51
1	B	335	VAL	CB-CG1	-6.20	1.39	1.52
1	B	323	ASP	CB-CG	6.18	1.64	1.51
1	A	405	TYR	CD2-CE2	-6.16	1.30	1.39
1	B	37	GLU	CD-OE1	6.15	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	VAL	CB-CG2	-6.11	1.40	1.52
1	B	245	GLU	CG-CD	6.10	1.61	1.51
1	B	36	GLN	CG-CD	6.05	1.65	1.51
1	B	89	CYS	CB-SG	-6.02	1.72	1.82
1	B	121	SER	CB-OG	-5.98	1.34	1.42
1	A	143	GLU	CD-OE2	5.89	1.32	1.25
1	B	36	GLN	CD-NE2	5.88	1.47	1.32
1	B	410	SER	CB-OG	-5.82	1.34	1.42
1	A	335	VAL	CB-CG1	-5.62	1.41	1.52
1	B	53	ARG	CZ-NH1	-5.53	1.25	1.33
1	A	238	VAL	CB-CG1	-5.46	1.41	1.52
1	B	274	GLU	CD-OE1	5.38	1.31	1.25
1	B	81	ARG	CD-NE	5.31	1.55	1.46
1	A	289	ALA	C-O	5.29	1.33	1.23
1	A	121	SER	CB-OG	-5.22	1.35	1.42
1	A	20	GLU	CG-CD	5.22	1.59	1.51
1	A	230	ARG	CZ-NH1	-5.21	1.26	1.33
1	B	139	MSE	SE-CE	5.11	2.25	1.95
1	B	263	TYR	CB-CG	-5.11	1.44	1.51
1	B	199	VAL	C-O	5.09	1.33	1.23
1	B	296	LYS	CD-CE	5.05	1.63	1.51
1	B	410	SER	CA-CB	-5.03	1.45	1.52
1	B	81	ARG	CG-CD	5.02	1.64	1.51
1	A	3	GLU	CD-OE2	5.01	1.31	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	288	THR	C-N-CA	-8.89	99.48	121.70
1	B	389	ASP	CB-CG-OD2	8.13	125.62	118.30
1	A	46	ASP	CB-CG-OD2	7.36	124.93	118.30
1	A	389	ASP	CB-CG-OD2	7.36	124.92	118.30
1	A	220	ASP	CB-CG-OD2	7.17	124.75	118.30
1	A	440	ASP	CB-CG-OD2	7.13	124.72	118.30
1	B	49	ASP	CB-CG-OD2	7.01	124.61	118.30
1	A	19	ASP	CB-CG-OD2	6.95	124.55	118.30
1	A	49	ASP	CB-CG-OD2	6.83	124.45	118.30
1	B	146	ASP	CB-CG-OD2	6.82	124.44	118.30
1	A	267	ASP	CB-CG-OD2	6.45	124.10	118.30
1	B	341	ASP	CB-CG-OD2	6.42	124.08	118.30
1	B	323	ASP	CB-CG-OD2	5.94	123.65	118.30
1	B	180	ASP	CB-CG-OD2	5.92	123.63	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289	ALA	CA-C-O	-5.91	107.70	120.10
1	A	157	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	137	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	321	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	267	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	137	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	321	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	131	VAL	C-N-CA	-5.49	110.77	122.30
1	A	268	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	2	ASN	CB-CA-C	5.33	121.06	110.40
1	A	91	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	418	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	B	46	ASP	CB-CG-OD2	5.20	122.97	118.30
1	B	362	ASP	CB-CG-OD2	5.01	122.81	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	385	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	ALA	Mainchain
1	B	399	VAL	Peptide

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	3330	0	3315	79	0
1	B	3311	0	3296	99	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
3	A	121	0	0	7	0
3	B	93	0	0	4	0
All	All	6865	0	6611	168	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 (168) 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:139:MSE:SE	1:B:139:MSE:CE	2.25	1.34
1:B:13:PRO:O	1:B:16:THR:HG22	1.61	0.99
1:A:26:ILE:HD11	1:A:44:VAL:HG12	1.52	0.91
1:A:369:ARG:HG2	1:A:383:ARG:O	1.71	0.91
1:A:26:ILE:HD11	1:A:44:VAL:CG1	2.05	0.85
1:A:418:ARG:HH12	1:B:418:ARG:HH12	1.28	0.81
1:B:24:VAL:HB	1:B:357:VAL:HG22	1.63	0.80
1:A:283:VAL:O	1:A:287:SER:HB2	1.81	0.80
1:A:16:THR:HB	1:A:26:ILE:HG22	1.67	0.77
1:A:284:SER:OG	1:A:294:THR:HG21	1.86	0.74
1:B:385:THR:HG22	1:B:386:TRP:H	1.52	0.72
1:B:41:PRO:HG3	1:B:336:ASP:HB3	1.69	0.72
1:A:193:MSE:HE3	1:A:237:ASP:HB3	1.72	0.71
1:B:13:PRO:O	1:B:16:THR:CG2	2.39	0.71
1:B:68:HIS:CD2	1:B:89:CYS:HB2	2.27	0.69
1:A:24:VAL:HB	1:A:357:VAL:HG22	1.74	0.69
1:B:17:THR:HB	3:B:2006:HOH:O	1.93	0.68
1:A:358:SER:HB3	1:A:396:LEU:HB2	1.76	0.68
1:A:286:GLU:HG3	3:A:2082:HOH:O	1.93	0.67
1:B:198:ARG:HG3	1:B:198:ARG:O	1.95	0.67
1:B:126:ALA:O	1:B:131:VAL:HG13	1.95	0.67
1:B:193:MSE:HE3	1:B:237:ASP:HB3	1.77	0.67
1:A:164:VAL:HG22	1:A:230:ARG:HB3	1.77	0.66
1:B:354:VAL:CG1	1:B:385:THR:HG21	2.27	0.65
1:A:359:ARG:NH1	1:A:395:ASP:OD1	2.30	0.65
1:A:303:ARG:NH2	2:A:500:SO4:O3	2.30	0.65
1:B:164:VAL:HG22	1:B:230:ARG:HB3	1.78	0.65
1:B:333:VAL:HG22	1:B:370:LEU:HD12	1.79	0.65
1:A:246:LYS:HE2	1:A:249:GLN:OE1	1.98	0.64
1:B:299:VAL:HG13	1:B:301:PRO:HD3	1.79	0.64
1:A:418:ARG:NH1	1:B:418:ARG:HH12	1.95	0.64
1:B:369:ARG:HH11	1:B:369:ARG:HG3	1.62	0.64
1:A:193:MSE:CE	1:A:237:ASP:HB3	2.28	0.64
1:A:299:VAL:HG13	1:A:301:PRO:HD3	1.79	0.63
1:B:243:GLY:O	1:B:247:THR:HG23	1.98	0.63
1:B:288:THR:HG23	3:B:2056:HOH:O	1.98	0.63
1:B:47:GLU:OE1	1:B:430:ARG:NH1	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ILE:HD11	1:B:44:VAL:HG11	1.83	0.61
1:A:109:GLU:HG3	3:A:2033:HOH:O	2.00	0.61
1:B:385:THR:HG22	1:B:386:TRP:N	2.16	0.60
1:B:238:VAL:HG23	1:B:247:THR:CG2	2.33	0.59
1:B:354:VAL:HG12	1:B:385:THR:HG21	1.84	0.59
1:A:425:HIS:CE1	3:A:2114:HOH:O	2.56	0.58
1:A:243:GLY:O	1:A:247:THR:HG23	2.03	0.57
1:B:146:ASP:OD2	1:B:204:HIS:HB2	2.05	0.57
1:B:176:THR:HG22	1:B:178:HIS:H	1.69	0.57
1:B:181:GLN:NE2	1:B:183:PHE:H	2.03	0.56
1:B:235:LEU:O	1:B:238:VAL:HG22	2.06	0.56
1:A:193:MSE:CE	1:A:237:ASP:CB	2.84	0.56
1:A:26:ILE:HD11	1:A:44:VAL:HG11	1.87	0.56
1:B:146:ASP:OD2	1:B:202:THR:HB	2.05	0.56
1:B:225:GLU:HA	1:B:282:ILE:HD12	1.87	0.56
1:B:16:THR:HA	1:B:26:ILE:HG22	1.87	0.55
1:B:224:PHE:HB3	1:B:279:LEU:HD11	1.89	0.54
1:B:225:GLU:HA	1:B:282:ILE:CD1	2.37	0.54
1:B:193:MSE:CE	1:B:237:ASP:HB3	2.37	0.54
1:A:421:VAL:HB	1:A:433:LEU:HB2	1.89	0.54
1:B:94:THR:HG23	1:B:95:GLY:N	2.23	0.54
1:B:176:THR:HG22	1:B:178:HIS:N	2.23	0.54
1:B:76:CYS:SG	1:B:79:VAL:HG23	2.48	0.54
1:B:49:ASP:OD1	1:B:53:ARG:NH2	2.42	0.53
1:A:405:TYR:O	1:A:409:LEU:HD12	2.09	0.52
1:B:420:ALA:HB2	1:B:435:ARG:HB3	1.90	0.52
1:A:236:ARG:O	1:A:239:VAL:HG12	2.10	0.52
1:A:13:PRO:O	1:A:16:THR:CG2	2.58	0.52
1:B:13:PRO:CG	1:B:311:ILE:HD13	2.39	0.52
1:A:178:HIS:HD2	1:B:325:SER:HA	1.76	0.51
1:B:432:VAL:HG12	1:B:433:LEU:HD13	1.93	0.51
1:A:13:PRO:O	1:A:16:THR:HG22	2.10	0.51
1:B:369:ARG:NH1	1:B:369:ARG:HG3	2.22	0.51
1:A:146:ASP:OD2	1:A:204:HIS:HB2	2.12	0.50
1:A:41:PRO:HG3	1:A:336:ASP:HB3	1.93	0.50
1:B:238:VAL:HG23	1:B:247:THR:HG21	1.94	0.50
1:B:283:VAL:O	1:B:287:SER:HB2	2.12	0.50
1:B:340:SER:HB3	1:B:374:HIS:CE1	2.45	0.50
1:B:421:VAL:HB	1:B:433:LEU:HB2	1.94	0.50
1:A:275:LEU:HD22	1:A:279:LEU:HD22	1.93	0.50
1:A:171:HIS:CE1	1:A:219:PHE:HB3	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:SER:OG	1:A:294:THR:HA	2.12	0.49
1:B:25:CYS:SG	1:B:30:PRO:HA	2.52	0.49
1:B:16:THR:HB	1:B:26:ILE:HG22	1.93	0.49
1:A:354:VAL:HG12	1:A:385:THR:HG21	1.94	0.49
1:A:94:THR:CG2	1:A:96:GLY:H	2.25	0.49
1:A:94:THR:HG22	1:A:96:GLY:H	1.78	0.49
1:B:164:VAL:CG2	1:B:230:ARG:HB3	2.43	0.48
1:B:279:LEU:O	1:B:283:VAL:HG23	2.13	0.48
1:B:287:SER:OG	1:B:295:PRO:HD3	2.13	0.48
1:A:170:THR:HG23	1:A:219:PHE:CE2	2.48	0.48
1:A:371:VAL:HG13	1:B:182:LYS:HD2	1.94	0.48
1:B:310:THR:O	1:B:311:ILE:HD12	2.14	0.48
1:A:23:VAL:HG22	1:A:358:SER:O	2.15	0.47
1:A:24:VAL:CB	1:A:357:VAL:HG22	2.43	0.47
1:B:208:VAL:HG12	1:B:208:VAL:O	2.15	0.47
1:B:83:ILE:HG23	1:B:88:LEU:HB2	1.97	0.47
1:A:230:ARG:HG2	3:A:2055:HOH:O	2.14	0.47
1:B:385:THR:CG2	1:B:386:TRP:H	2.22	0.47
1:A:354:VAL:HG21	1:A:370:LEU:HD22	1.97	0.47
1:B:181:GLN:HE21	1:B:182:LYS:N	2.13	0.47
1:A:284:SER:HB3	3:A:2080:HOH:O	2.15	0.47
1:B:303:ARG:O	1:B:306:ALA:O	2.33	0.47
1:A:418:ARG:HH12	1:B:418:ARG:NH1	2.05	0.47
1:A:40:THR:HA	1:A:41:PRO:C	2.35	0.47
1:B:46:ASP:O	1:B:49:ASP:HB3	2.15	0.46
1:B:132:GLY:C	1:B:133:HIS:HD1	2.19	0.46
1:B:193:MSE:CE	1:B:237:ASP:CB	2.93	0.46
1:B:310:THR:HB	1:B:403:GLY:HA3	1.98	0.46
1:B:57:THR:HG22	1:B:67:VAL:HG21	1.98	0.45
1:B:369:ARG:HH11	1:B:369:ARG:CG	2.27	0.45
1:A:49:ASP:OD1	1:A:53:ARG:NH2	2.50	0.45
1:A:62:GLY:O	1:A:63:SER:HB2	2.17	0.45
1:A:68:HIS:CD2	1:A:89:CYS:HB2	2.51	0.45
1:A:238:VAL:HG12	1:A:247:THR:HG22	1.97	0.45
1:A:13:PRO:HD3	1:A:311:ILE:HD11	1.98	0.45
1:B:329:HIS:CE1	3:B:2067:HOH:O	2.69	0.45
1:B:68:HIS:HD2	1:B:89:CYS:HB2	1.80	0.45
1:A:126:ALA:O	1:A:131:VAL:HG13	2.17	0.44
1:A:171:HIS:CE1	1:A:219:PHE:CB	3.00	0.44
1:A:94:THR:HG23	1:A:95:GLY:N	2.32	0.44
1:B:239:VAL:HA	1:B:247:THR:HG21	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:THR:HB	1:B:403:GLY:CA	2.47	0.44
1:A:418:ARG:HD3	3:A:2113:HOH:O	2.16	0.44
1:B:159:LEU:N	1:B:159:LEU:HD12	2.32	0.44
1:B:303:ARG:NH2	2:B:501:SO4:O3	2.51	0.44
1:B:369:ARG:CG	1:B:383:ARG:O	2.65	0.44
3:A:2098:HOH:O	1:B:94:THR:HG23	2.18	0.44
1:A:89:CYS:HB3	1:A:110:ARG:O	2.18	0.44
1:B:355:ARG:NH2	3:B:2072:HOH:O	2.51	0.44
1:B:292:LEU:HD12	1:B:293:PRO:HD2	1.99	0.43
1:A:325:SER:HA	1:B:178:HIS:HD2	1.83	0.43
1:B:323:ASP:OD1	1:B:329:HIS:CD2	2.71	0.43
1:A:414:ASN:HA	1:B:97:GLU:OE1	2.18	0.43
1:A:325:SER:HA	1:B:178:HIS:CD2	2.53	0.43
1:A:107:PRO:HG2	1:A:110:ARG:NH2	2.33	0.43
1:A:221:VAL:HG23	1:A:279:LEU:HD13	2.01	0.43
1:B:68:HIS:CE1	1:B:298:VAL:HG11	2.53	0.43
1:B:49:ASP:CG	1:B:53:ARG:HH21	2.21	0.43
1:B:275:LEU:HD22	1:B:275:LEU:O	2.18	0.43
1:A:20:GLU:H	1:A:20:GLU:CD	2.22	0.42
1:A:200:PHE:HA	1:A:200:PHE:HD1	1.73	0.42
1:B:298:VAL:CG1	1:B:299:VAL:N	2.81	0.42
1:B:369:ARG:HG2	1:B:383:ARG:O	2.18	0.42
1:A:161:ARG:HD2	1:A:211:HIS:ND1	2.35	0.42
1:B:41:PRO:O	1:B:435:ARG:NH2	2.53	0.42
1:B:298:VAL:HG12	1:B:299:VAL:N	2.34	0.42
1:A:175:SER:OG	1:A:230:ARG:NH2	2.48	0.42
1:B:402:THR:O	1:B:406:CYS:HB2	2.20	0.42
1:A:279:LEU:HA	1:A:279:LEU:HD12	1.94	0.42
1:B:278:LYS:O	1:B:282:ILE:HG23	2.20	0.42
1:B:354:VAL:HG13	1:B:385:THR:HG21	1.98	0.42
1:A:13:PRO:CG	1:A:311:ILE:HD13	2.50	0.42
1:A:67:VAL:CG1	1:A:88:LEU:HD13	2.49	0.42
1:B:29:ILE:HA	1:B:30:PRO:HD3	1.95	0.41
1:A:412:ARG:HA	1:A:416:VAL:O	2.21	0.41
1:A:165:GLY:O	1:A:175:SER:HA	2.21	0.41
1:A:359:ARG:NH1	1:A:395:ASP:CG	2.74	0.41
1:A:52:SER:O	1:A:56:GLU:HB2	2.20	0.41
1:B:239:VAL:O	1:B:240:GLY:C	2.59	0.41
1:A:178:HIS:CD2	1:B:325:SER:HA	2.56	0.41
1:A:19:ASP:HB2	1:A:23:VAL:N	2.35	0.41
1:B:21:VAL:HG22	1:B:21:VAL:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ILE:HG13	1:A:424:VAL:HG21	2.03	0.41
1:A:46:ASP:O	1:A:49:ASP:HB3	2.21	0.41
1:B:123:LEU:O	1:B:127:VAL:HG13	2.21	0.41
1:A:185:LEU:HD13	1:A:195:ALA:HB2	2.03	0.41
1:B:68:HIS:CD2	1:B:89:CYS:CB	3.00	0.41
1:A:236:ARG:HB3	1:A:236:ARG:CZ	2.51	0.40
1:A:371:VAL:CG1	1:B:182:LYS:HD2	2.52	0.40
1:B:210:LEU:HD11	1:B:235:LEU:CD2	2.51	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	444/453 (98%)	413 (93%)	28 (6%)	3 (1%)	22	53
1	B	442/453 (98%)	413 (93%)	25 (6%)	4 (1%)	17	46
All	All	886/906 (98%)	826 (93%)	53 (6%)	7 (1%)	19	49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	B	19	ASP
1	B	426	ALA
1	B	240	GLY
1	A	434	ARG
1	A	63	SER
1	B	109	GLU

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	353/355 (99%)	295 (84%)	58 (16%)	2 7
1	B	351/355 (99%)	288 (82%)	63 (18%)	2 5
All	All	704/710 (99%)	583 (83%)	121 (17%)	2 6

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	LEU
1	A	16	THR
1	A	31	LEU
1	A	32	THR
1	A	34	LEU
1	A	36	GLN
1	A	55	ARG
1	A	72	LYS
1	A	94	THR
1	A	102	LEU
1	A	109	GLU
1	A	118	LYS
1	A	127	VAL
1	A	133	HIS
1	A	145	LEU
1	A	160	VAL
1	A	163	THR
1	A	164	VAL
1	A	200	PHE
1	A	205	LEU
1	A	208	VAL
1	A	230	ARG
1	A	234	LEU
1	A	236	ARG
1	A	246	LYS
1	A	266	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	275	LEU
1	A	279	LEU
1	A	282	ILE
1	A	284	SER
1	A	286	GLU
1	A	292	LEU
1	A	296	LYS
1	A	297	LEU
1	A	299	VAL
1	A	310	THR
1	A	311	ILE
1	A	313	LEU
1	A	327	THR
1	A	333	VAL
1	A	335	VAL
1	A	336	ASP
1	A	355	ARG
1	A	357	VAL
1	A	360	VAL
1	A	369	ARG
1	A	373	LYS
1	A	385	THR
1	A	392	ARG
1	A	408	SER
1	A	422	VAL
1	A	430	ARG
1	A	434	ARG
1	A	435	ARG
1	A	441	LEU
1	A	442	LEU
1	A	447	ARG
1	B	3	GLU
1	B	7	LEU
1	B	16	THR
1	B	17	THR
1	B	20	GLU
1	B	26	ILE
1	B	31	LEU
1	B	32	THR
1	B	34	LEU
1	B	36	GLN
1	B	37	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	40	THR
1	B	52	SER
1	B	94	THR
1	B	102	LEU
1	B	121	SER
1	B	128	LYS
1	B	145	LEU
1	B	151	GLU
1	B	158	VAL
1	B	164	VAL
1	B	181	GLN
1	B	203	ASP
1	B	205	LEU
1	B	206	ARG
1	B	221	VAL
1	B	234	LEU
1	B	239	VAL
1	B	245	GLU
1	B	246	LYS
1	B	247	THR
1	B	249	GLN
1	B	275	LEU
1	B	278	LYS
1	B	279	LEU
1	B	282	ILE
1	B	284	SER
1	B	287	SER
1	B	292	LEU
1	B	297	LEU
1	B	299	VAL
1	B	305	ILE
1	B	311	ILE
1	B	313	LEU
1	B	321	ASP
1	B	327	THR
1	B	334	SER
1	B	336	ASP
1	B	355	ARG
1	B	357	VAL
1	B	360	VAL
1	B	369	ARG
1	B	371	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	377	SER
1	B	387	VAL
1	B	392	ARG
1	B	408	SER
1	B	422	VAL
1	B	430	ARG
1	B	433	LEU
1	B	435	ARG
1	B	441	LEU
1	B	442	LEU

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

Mol	Chain	Res	Type
1	A	178	HIS
1	A	351	GLN
1	B	6	HIS
1	B	68	HIS
1	B	178	HIS
1	B	181	GLN
1	B	329	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	500	-	4,4,4	0.50	0	6,6,6	0.66	0
2	SO4	B	501	-	4,4,4	0.54	0	6,6,6	1.38	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	SO4	O4-S-O1	-2.31	97.24	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	SO4	1	0
2	B	501	SO4	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, 95^{th} 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	442/453 (97%)	-0.44	0 100 100	29, 39, 54, 70	0
1	B	440/453 (97%)	-0.23	4 (0%) 84 80	28, 39, 54, 71	0
All	All	882/906 (97%)	-0.34	4 (0%) 91 88	28, 39, 54, 71	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	PRO	2.5
1	B	289	ALA	2.1
1	B	291	GLY	2.1
1	B	247	THR	2.0

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

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
2	SO4	A	500	5/5	0.99	0.12	19,27,31,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	501	5/5	0.99	0.12	29,29,33,35	0

6.5 Other polymers (i)

There are no such residues in this entry.