



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 10:47 PM EDT

PDB ID : 1HKW / pdb_00001hkw
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

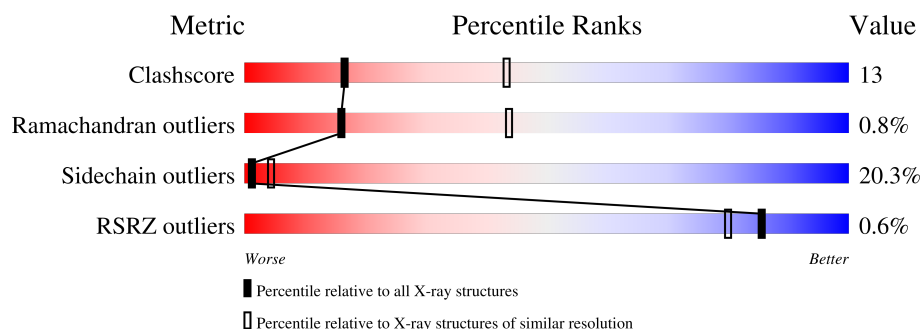
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	453	
1	B	453	

2 Entry composition [i](#)

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 (CCD ID: SO4) (formula: O₄S).



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		

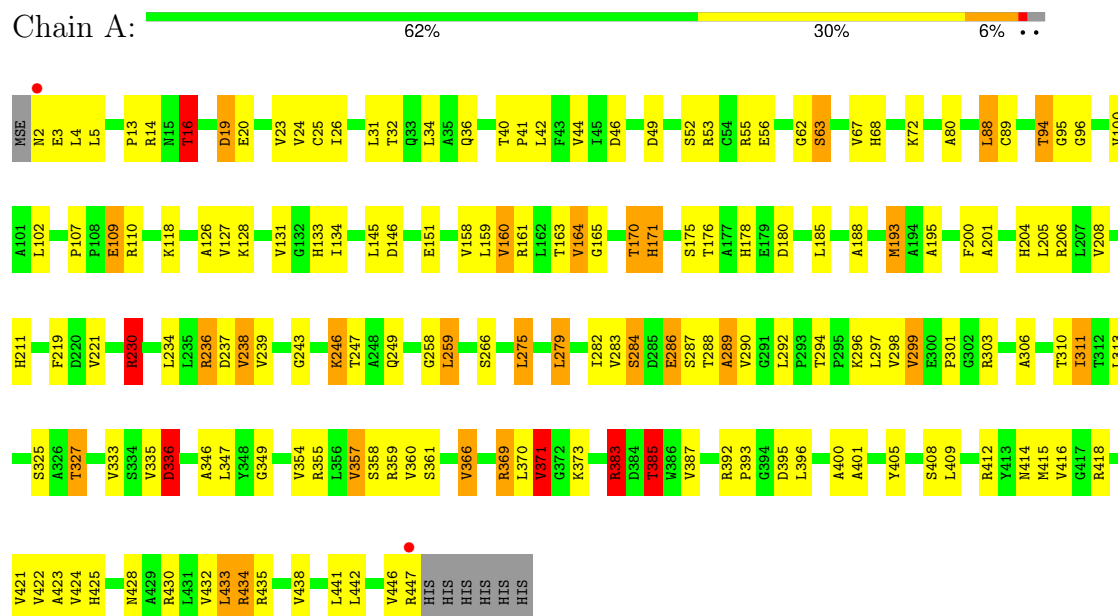
- Molecule 3 is water.

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

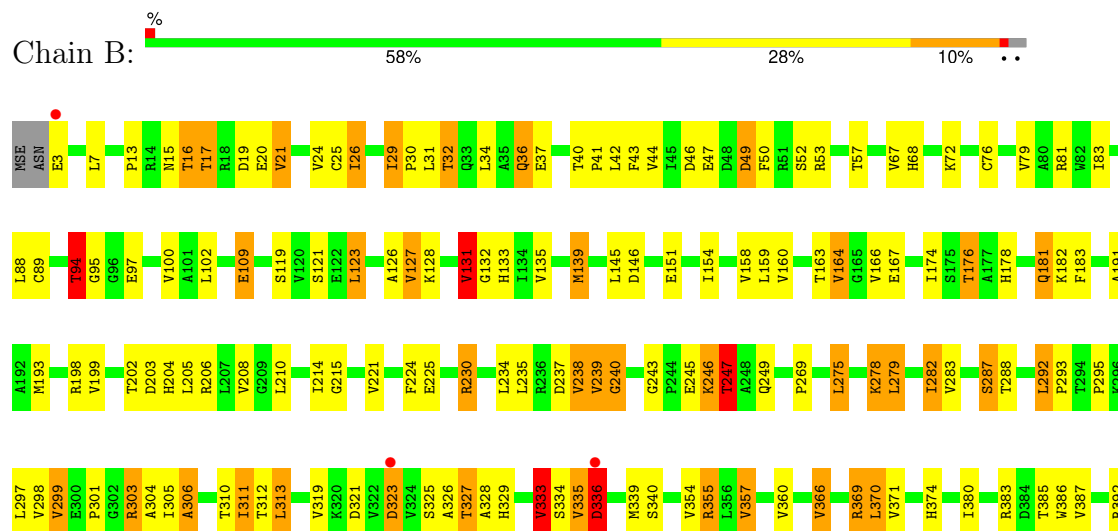
3 Residue-property plots

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

• Molecule 1: DIAMINOPIMELATE DECARBOXYLASE



• Molecule 1: DIAMINOPIMELATE DECARBOXYLASE





4 Data and refinement statistics

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 25.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.80) 99.8 (25.00-2.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.31 , 25.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.75	38/3388 (1.1%)	1.20	16/4614 (0.3%)
1	B	1.83	60/3369 (1.8%)	1.15	12/4589 (0.3%)
All	All	1.79	98/6757 (1.5%)	1.17	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 (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	400	ALA	C-O	11.81	1.38	1.23
1	A	400	ALA	C-O	11.02	1.38	1.24
1	B	139	MSE	SE-CE	10.05	2.25	1.95
1	B	81	ARG	NE-CZ	9.58	1.43	1.33
1	B	199	VAL	C-O	9.25	1.33	1.23
1	A	193	MSE	SE-CE	-8.81	1.69	1.95
1	B	176	THR	CA-C	-8.64	1.42	1.52
1	A	171	HIS	N-CA	8.46	1.55	1.46
1	A	298	VAL	C-O	-8.09	1.15	1.24
1	A	176	THR	CA-C	-7.75	1.43	1.52
1	A	385	THR	CA-CB	7.66	1.64	1.53
1	B	418	ARG	NE-CZ	7.37	1.41	1.33
1	B	430	ARG	C-O	-7.12	1.15	1.24
1	B	166	VAL	C-O	-7.11	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	29	ILE	CA-CB	-7.06	1.45	1.54
1	B	247	THR	CA-CB	6.96	1.65	1.53
1	B	36	GLN	CD-NE2	6.80	1.47	1.33
1	B	440	ASP	C-O	-6.76	1.16	1.24
1	B	135	VAL	CA-C	-6.72	1.45	1.52
1	A	238	VAL	CA-CB	6.69	1.63	1.54
1	B	416	VAL	C-O	-6.65	1.16	1.24
1	B	81	ARG	CD-NE	6.59	1.55	1.46
1	B	422	VAL	N-CA	-6.57	1.38	1.46
1	B	328	ALA	CA-CB	-6.56	1.43	1.53
1	B	327	THR	CA-C	6.54	1.61	1.52
1	B	339	MSE	SE-CE	-6.49	1.75	1.95
1	A	160	VAL	CA-CB	6.46	1.62	1.54
1	B	366	VAL	CA-C	6.44	1.59	1.52
1	B	411	SER	CA-C	6.43	1.61	1.52
1	A	80	ALA	CA-CB	-6.41	1.43	1.53
1	B	191	ALA	CA-CB	-6.39	1.43	1.53
1	B	21	VAL	CA-CB	6.34	1.61	1.54
1	B	42	LEU	C-O	-6.32	1.16	1.23
1	A	423	ALA	CA-CB	-6.29	1.42	1.53
1	B	238	VAL	CA-CB	6.22	1.63	1.54
1	B	370	LEU	CA-C	-6.22	1.45	1.52
1	B	119	SER	C-O	6.16	1.32	1.23
1	B	21	VAL	CA-C	6.16	1.59	1.52
1	A	393	PRO	CA-C	-6.14	1.45	1.52
1	A	349	GLY	C-O	-6.12	1.17	1.24
1	B	319	VAL	C-O	-6.10	1.17	1.24
1	B	167	GLU	C-O	-6.04	1.17	1.24
1	B	131	VAL	CA-CB	6.03	1.62	1.54
1	B	333	VAL	CA-CB	5.99	1.61	1.54
1	B	380	ILE	CA-CB	-5.97	1.47	1.54
1	B	94	THR	CA-CB	-5.90	1.45	1.53
1	B	32	THR	CA-CB	-5.87	1.44	1.53
1	B	36	GLN	CD-OE1	5.84	1.34	1.23
1	B	415	MSE	SE-CE	5.84	2.12	1.95
1	B	15	ASN	N-CA	-5.78	1.40	1.46
1	A	180	ASP	C-O	-5.77	1.16	1.23
1	A	289	ALA	C-O	5.71	1.33	1.24
1	A	290	VAL	CA-CB	5.67	1.62	1.54
1	B	432	VAL	CA-CB	-5.66	1.48	1.55
1	B	123	LEU	C-O	5.65	1.30	1.24
1	A	134	ILE	CA-CB	-5.64	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	385	THR	CA-C	-5.63	1.45	1.53
1	B	269	PRO	CA-C	-5.63	1.48	1.52
1	B	407	TYR	CA-C	5.63	1.60	1.52
1	A	383	ARG	C-O	-5.59	1.17	1.24
1	A	415	MSE	SE-CE	5.53	2.12	1.95
1	B	412	ARG	CA-C	-5.53	1.45	1.52
1	A	327	THR	CA-CB	5.51	1.63	1.54
1	A	401	ALA	CA-CB	-5.51	1.46	1.53
1	A	347	LEU	C-O	-5.48	1.17	1.24
1	B	336	ASP	CB-CG	-5.48	1.38	1.52
1	A	289	ALA	C-N	-5.45	1.26	1.33
1	B	304	ALA	CA-CB	-5.44	1.44	1.53
1	A	3	GLU	N-CA	5.43	1.53	1.46
1	B	437	THR	CA-C	-5.38	1.46	1.52
1	B	336	ASP	CG-OD1	5.37	1.35	1.25
1	B	246	LYS	CA-C	5.35	1.59	1.52
1	A	371	VAL	N-CA	-5.34	1.40	1.46
1	B	43	PHE	CA-C	-5.34	1.45	1.52
1	A	336	ASP	CB-CG	-5.33	1.38	1.52
1	A	336	ASP	CA-C	5.22	1.59	1.52
1	A	230	ARG	CZ-NH2	-5.21	1.26	1.33
1	B	312	THR	CA-CB	-5.17	1.46	1.53
1	B	36	GLN	CG-CD	5.17	1.65	1.52
1	A	133	HIS	N-CA	5.16	1.52	1.46
1	A	361	SER	CA-C	-5.14	1.46	1.52
1	A	201	ALA	C-O	-5.13	1.18	1.24
1	B	72	LYS	CA-C	5.13	1.59	1.52
1	B	401	ALA	CA-C	-5.09	1.47	1.53
1	A	16	THR	CA-CB	5.08	1.65	1.53
1	B	49	ASP	C-O	-5.08	1.18	1.24
1	B	135	VAL	C-O	-5.07	1.18	1.24
1	B	323	ASP	CB-CG	5.07	1.64	1.52
1	B	303	ARG	NE-CZ	-5.07	1.27	1.33
1	B	313	LEU	C-O	-5.06	1.17	1.24
1	A	346	ALA	C-O	-5.06	1.18	1.24
1	A	206	ARG	C-O	-5.05	1.18	1.24
1	A	14	ARG	C-O	-5.04	1.17	1.24
1	A	188	ALA	C-O	-5.04	1.17	1.24
1	B	43	PHE	C-O	-5.03	1.17	1.23
1	B	420	ALA	CA-CB	-5.02	1.45	1.53
1	A	366	VAL	CA-CB	-5.02	1.47	1.54
1	A	42	LEU	CA-C	5.00	1.58	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	THR	CA-C-N	-11.36	99.48	122.55
1	A	288	THR	C-N-CA	-11.36	99.48	122.55
1	B	432	VAL	CB-CA-C	-7.26	104.54	111.44
1	A	432	VAL	CB-CA-C	-6.85	104.72	111.30
1	A	400	ALA	CA-C-N	-6.77	112.28	123.04
1	A	400	ALA	C-N-CA	-6.77	112.28	123.04
1	A	289	ALA	CA-C-O	-6.44	107.70	119.36
1	B	306	ALA	CA-C-N	-5.94	112.54	121.87
1	B	306	ALA	C-N-CA	-5.94	112.54	121.87
1	B	269	PRO	O-C-N	5.81	123.88	121.15
1	A	2	ASN	CB-CA-C	5.77	121.06	110.10
1	A	306	ALA	N-CA-C	-5.76	103.05	110.19
1	A	25	CYS	CA-C-N	-5.73	115.16	123.06
1	A	25	CYS	C-N-CA	-5.73	115.16	123.06
1	B	335	VAL	CA-C-N	5.68	128.68	120.38
1	B	335	VAL	C-N-CA	5.68	128.68	120.38
1	B	214	ILE	N-CA-C	5.53	117.52	112.43
1	B	131	VAL	CA-C-N	-5.43	110.77	121.41
1	B	131	VAL	C-N-CA	-5.43	110.77	121.41
1	A	400	ALA	N-CA-C	5.31	120.03	113.50
1	A	327	THR	N-CA-C	-5.28	107.49	114.04
1	B	215	GLY	N-CA-C	5.28	118.19	110.63
1	B	428	ASN	N-CA-C	5.27	117.00	108.26
1	B	326	ALA	N-CA-C	-5.17	105.77	111.71
1	A	170	THR	OG1-CB-CG2	-5.13	99.04	109.30
1	A	159	LEU	CA-C-N	-5.03	116.62	123.10
1	A	159	LEU	C-N-CA	-5.03	116.62	123.10
1	A	201	ALA	N-CA-C	5.01	116.74	111.28

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 ⓘ

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	81	0
1	B	3311	0	3296	100	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	171	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 (171) 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:O	1:B:198:ARG:HG3	1.95	0.67
1:B:126:ALA:O	1:B:131:VAL:HG13	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:26:ILE:HD11	1:B:44:VAL:HG11	1.83	0.61
1:B:47:GLU:OE1	1:B:430:ARG:NH1	2.33	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:76:CYS:SG	1:B:79:VAL:HG23	2.48	0.54
1:B:176:THR:HG22	1:B:178:HIS:N	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:40:THR:HA	1:A:41:PRO:C	2.35	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:132:GLY:C	1:B:133:HIS:HD1	2.19	0.51
1:B:369:ARG:HG3	1:B:369:ARG:NH1	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
1:A:287:SER:OG	1:A:294:THR:HA	2.12	0.49
1:B:16:THR:HB	1:B:26:ILE:HG22	1.93	0.49
1:B:25:CYS:SG	1:B:30:PRO:HA	2.52	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:A:354:VAL:HG12	1:A:385:THR:HG21	1.94	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:B:49:ASP:CG	1:B:53:ARG:HH21	2.21	0.48
1:A:20:GLU:CD	1:A:20:GLU:H	2.22	0.47
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:83:ILE:HG23	1:B:88:LEU:HB2	1.97	0.47
1:B:208:VAL:O	1:B:208:VAL:HG12	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:46:ASP:O	1:B:49:ASP:HB3	2.15	0.46
1:B:193:MSE:CE	1:B:237:ASP:CB	2.93	0.46
1:A:359:ARG:NH1	1:A:395:ASP:CG	2.74	0.46
1:B:239:VAL:O	1:B:240:GLY:C	2.59	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:68:HIS:HD2	1:B:89:CYS:HB2	1.80	0.45
1:B:329:HIS:CE1	3:B:2067:HOH:O	2.69	0.45
1:A:126:ALA:O	1:A:131:VAL:HG13	2.17	0.44
1:A:94:THR:HG23	1:A:95:GLY:N	2.32	0.44
1:A:171:HIS:CE1	1:A:219:PHE:CB	3.00	0.44
1:B:239:VAL:HA	1:B:247:THR:HG21	1.99	0.44
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
3:A:2098:HOH:O	1:B:94:THR:HG23	2.18	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
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:A:414:ASN:HA	1:B:97:GLU:OE1	2.18	0.43
1:B:323:ASP:OD1	1:B:329:HIS:CD2	2.71	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:275:LEU:HD22	1:B:275:LEU:O	2.18	0.43
1:A:200:PHE:HD1	1:A:200:PHE:HA	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:VAL:CG1	1:B:299:VAL:N	2.81	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:HD12	1:A:279:LEU:HA	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:52:SER:O	1:A:56:GLU:HB2	2.20	0.41
1:A:165:GLY:O	1:A:175:SER:HA	2.21	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:O	1:B:21:VAL:HG22	2.21	0.41
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:40:THR:OG1	1:A:336:ASP:OD2	2.39	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:CZ	1:A:236:ARG:HB3	2.51	0.40
1:A:258:GLY:O	1:A:259:LEU:C	2.64	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
1:B:49:ASP:O	1:B:50:PHE:C	2.63	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%)	18	47
1	B	442/453 (98%)	413 (93%)	25 (6%)	4 (1%)	14	41
All	All	886/906 (98%)	826 (93%)	53 (6%)	7 (1%)	16	44

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 ⓘ

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%)	283 (80%)	70 (20%)	1	5
1	B	351/355 (99%)	278 (79%)	73 (21%)	1	4
All	All	704/710 (99%)	561 (80%)	143 (20%)	1	4

All (143) 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

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Mol	Chain	Res	Type
1	A	88	LEU
1	A	94	THR
1	A	100	VAL
1	A	102	LEU
1	A	109	GLU
1	A	118	LYS
1	A	127	VAL
1	A	128	LYS
1	A	145	LEU
1	A	151	GLU
1	A	158	VAL
1	A	160	VAL
1	A	163	THR
1	A	164	VAL
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	259	LEU
1	A	266	SER
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	366	VAL

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Mol	Chain	Res	Type
1	A	369	ARG
1	A	371	VAL
1	A	373	LYS
1	A	383	ARG
1	A	385	THR
1	A	387	VAL
1	A	392	ARG
1	A	408	SER
1	A	422	VAL
1	A	428	ASN
1	A	430	ARG
1	A	433	LEU
1	A	434	ARG
1	A	435	ARG
1	A	438	VAL
1	A	441	LEU
1	A	442	LEU
1	A	446	VAL
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
1	B	40	THR
1	B	52	SER
1	B	94	THR
1	B	100	VAL
1	B	102	LEU
1	B	109	GLU
1	B	121	SER
1	B	127	VAL
1	B	128	LYS
1	B	131	VAL
1	B	145	LEU
1	B	151	GLU

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Mol	Chain	Res	Type
1	B	154	ILE
1	B	158	VAL
1	B	160	VAL
1	B	163	THR
1	B	164	VAL
1	B	174	ILE
1	B	181	GLN
1	B	203	ASP
1	B	205	LEU
1	B	206	ARG
1	B	221	VAL
1	B	230	ARG
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	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	333	VAL
1	B	334	SER
1	B	335	VAL
1	B	336	ASP
1	B	355	ARG
1	B	357	VAL
1	B	360	VAL
1	B	366	VAL
1	B	369	ARG
1	B	371	VAL
1	B	387	VAL

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Mol	Chain	Res	Type
1	B	392	ARG
1	B	408	SER
1	B	418	ARG
1	B	422	VAL
1	B	433	LEU
1	B	435	ARG
1	B	441	LEU
1	B	442	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	66	ASN
1	A	68	HIS
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 ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	501	-	4,4,4	0.48	0	6,6,6	1.37	1 (16%)
2	SO4	A	500	-	4,4,4	0.54	0	6,6,6	0.59	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	501	SO4	O4-S-O1	-2.36	97.24	109.56

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	B	501	SO4	1	0
2	A	500	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	442/453 (97%)	-0.25	2 (0%) 87 82	29, 39, 54, 70	0
1	B	440/453 (97%)	-0.21	3 (0%) 84 77	28, 39, 54, 71	0
All	All	882/906 (97%)	-0.23	5 (0%) 85 80	28, 39, 54, 71	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ASN	3.0
1	B	323	ASP	2.6
1	B	336	ASP	2.5
1	B	3	GLU	2.4
1	A	447	ARG	2.4

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	500	5/5	0.99	0.04	19,27,31,34	0
2	SO4	B	501	5/5	0.99	0.04	29,29,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.