



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:28 PM UTC

PDB ID : 1TWI / pdb_00001twi
Title : Crystal structure of Diaminopimelate Decarboxylase from *M. jannaschii* in co-complex with L-lysine
Authors : Rajashankar, K.R.; Ray, S.S.; Bonanno, J.B.; Pinho, M.G.; He, G.; De Lencastre, H.; Tomasz, A.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-07-01
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

<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

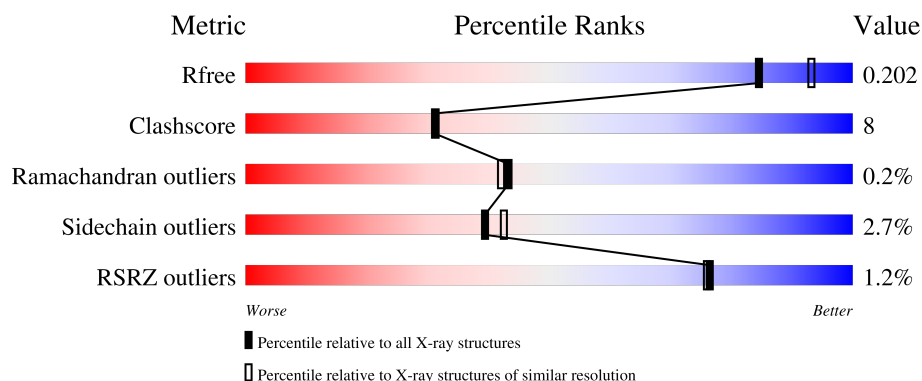
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	434	 82% 17% .
1	B	434	 78% 19% .
1	C	434	 83% 15% .
1	D	434	 81% 17% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15128 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	434	Total	C	N	O	S	0	0	0
			3395	2166	568	640	21			
1	B	434	Total	C	N	O	S	0	0	0
			3395	2166	568	640	21			
1	C	434	Total	C	N	O	S	0	0	0
			3395	2166	568	640	21			
1	D	434	Total	C	N	O	S	0	0	0
			3395	2166	568	640	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	initiating methionine	UNP Q58497
B	15	MET	-	initiating methionine	UNP Q58497
C	15	MET	-	initiating methionine	UNP Q58497
D	15	MET	-	initiating methionine	UNP Q58497

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).

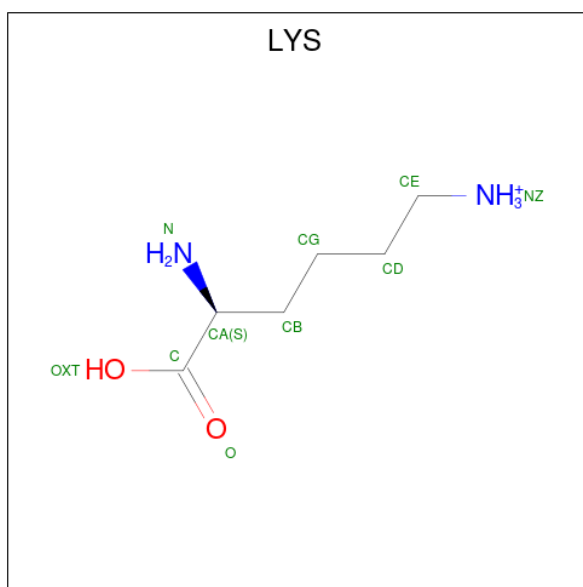


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			10	6	2	2		
4	D	1	Total	C	N	O	0	0
			10	6	2	2		
4	D	1	Total	C	N	O	0	0
			10	6	2	2		
4	D	1	Total	C	N	O	0	0
			10	6	2	2		
4	D	1	Total	C	N	O	0	0
			10	6	2	2		
4	D	1	Total	C	N	O	0	0
			10	6	2	2		

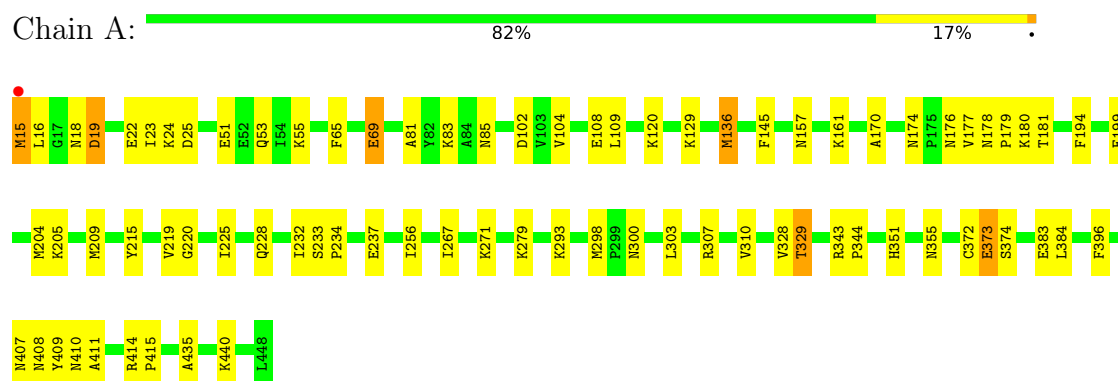
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	369	Total	O	0	0
			369	369		
5	B	301	Total	O	0	0
			301	301		
5	C	370	Total	O	0	0
			370	370		
5	D	383	Total	O	0	0
			383	383		

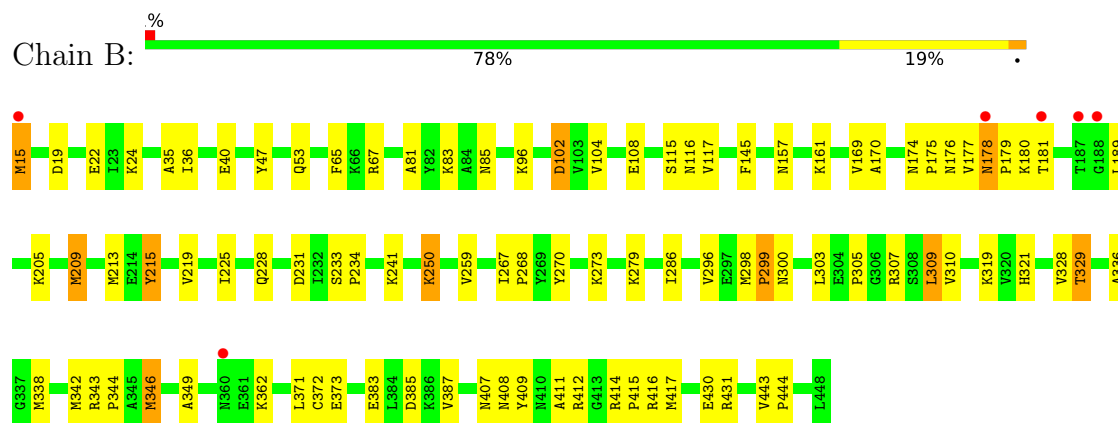
3 Residue-property plots

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.

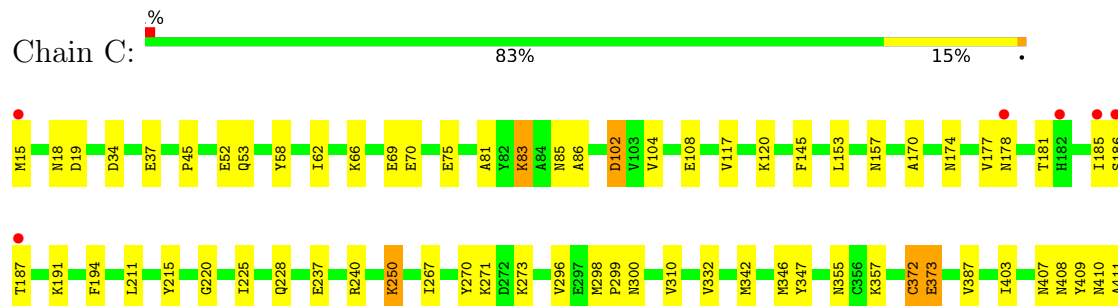
• Molecule 1: Diaminopimelate decarboxylase



• Molecule 1: Diaminopimelate decarboxylase

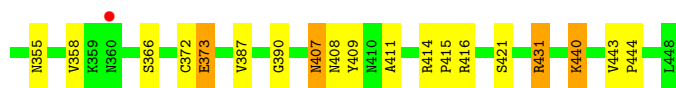
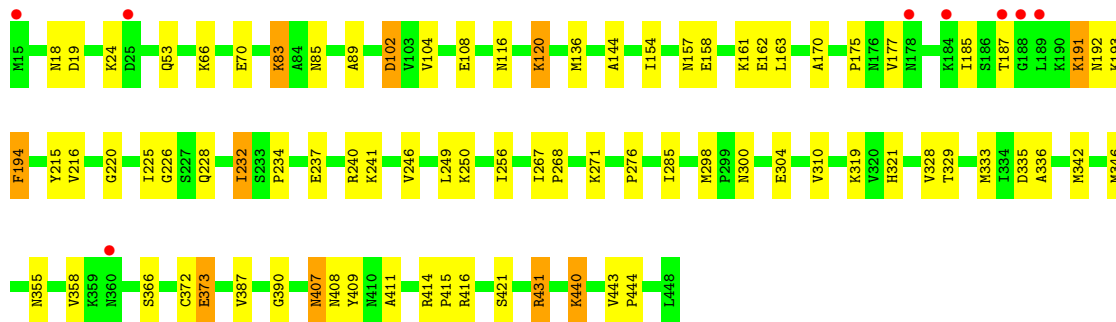
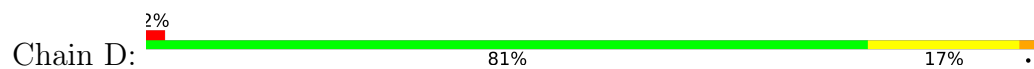


• Molecule 1: Diaminopimelate decarboxylase





• Molecule 1: Diaminopimelate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.24Å 147.07Å 89.39Å 90.00° 97.25° 90.00°	Depositor
Resolution (Å)	29.25 – 2.00 29.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.25-2.00) 98.5 (29.25-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.56 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.157 , 0.202 0.157 , 0.202	Depositor DCC
R_{free} test set	6043 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15128	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.11	3/3452 (0.1%)	1.17	15/4654 (0.3%)
1	B	1.04	4/3452 (0.1%)	1.16	18/4654 (0.4%)
1	C	1.09	2/3452 (0.1%)	1.17	14/4654 (0.3%)
1	D	1.15	7/3452 (0.2%)	1.22	18/4654 (0.4%)
All	All	1.10	16/13808 (0.1%)	1.18	65/18616 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	333	MET	SD-CE	6.67	1.96	1.79
1	D	285	ILE	CA-CB	6.33	1.61	1.54
1	C	86	ALA	CA-CB	6.16	1.61	1.53
1	D	342	MET	SD-CE	6.08	1.94	1.79
1	B	209	MET	SD-CE	5.92	1.94	1.79
1	D	444	PRO	CA-C	5.89	1.55	1.51
1	A	435	ALA	CA-CB	5.86	1.62	1.53
1	C	185	ILE	CA-CB	-5.58	1.47	1.54
1	A	204	MET	SD-CE	5.53	1.93	1.79
1	A	136	MET	SD-CE	-5.52	1.65	1.79
1	D	154	ILE	CA-CB	5.36	1.60	1.54
1	B	15	MET	SD-CE	5.34	1.93	1.79
1	D	136	MET	SD-CE	-5.29	1.66	1.79
1	B	338	MET	SD-CE	5.27	1.92	1.79
1	B	444	PRO	CA-C	5.17	1.55	1.52
1	D	358	VAL	CA-CB	5.01	1.60	1.54

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	443	VAL	CA-C-N	9.58	126.66	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	443	VAL	C-N-CA	9.58	126.66	119.66
1	D	310	VAL	N-CA-C	9.46	123.02	113.47
1	D	415	PRO	N-CA-C	9.18	124.07	111.22
1	C	310	VAL	N-CA-C	8.32	121.68	113.53
1	B	310	VAL	N-CA-C	8.19	121.56	113.53
1	D	300	ASN	N-CA-C	-7.70	99.64	110.50
1	B	415	PRO	N-CA-C	7.29	121.42	111.22
1	C	170	ALA	N-CA-C	-7.26	99.50	109.95
1	D	170	ALA	N-CA-C	-7.06	99.00	109.81
1	A	310	VAL	N-CA-C	6.99	120.38	113.53
1	C	117	VAL	N-CA-C	-6.77	102.81	108.63
1	D	372	CYS	N-CA-C	6.74	120.96	112.87
1	B	145	PHE	N-CA-C	-6.71	98.30	109.24
1	A	415	PRO	N-CA-C	6.70	120.59	111.22
1	C	225	ILE	N-CA-C	6.66	121.42	113.22
1	A	225	ILE	N-CA-C	6.64	121.38	113.22
1	C	300	ASN	N-CA-C	-6.63	101.15	110.50
1	B	443	VAL	CA-C-N	6.48	124.33	119.66
1	B	443	VAL	C-N-CA	6.48	124.33	119.66
1	C	415	PRO	N-CA-C	6.38	120.64	111.13
1	A	170	ALA	N-CA-C	-6.33	100.83	110.14
1	D	387	VAL	N-CA-C	6.32	117.68	108.58
1	B	219	VAL	N-CA-C	6.19	119.72	113.47
1	B	385	ASP	N-CA-C	-6.17	101.28	110.23
1	B	169	VAL	N-CA-C	6.16	116.99	108.12
1	B	342	MET	N-CA-C	6.07	120.69	113.28
1	C	355	ASN	N-CA-C	-6.04	99.82	109.96
1	A	219	VAL	CB-CA-C	-6.00	104.14	110.62
1	B	170	ALA	N-CA-C	-5.92	101.44	110.14
1	C	174	ASN	CA-C-N	5.92	125.87	119.78
1	C	174	ASN	C-N-CA	5.92	125.87	119.78
1	D	366	SER	N-CA-C	-5.90	100.56	109.95
1	D	194	PHE	N-CA-C	5.88	119.68	110.32
1	B	387	VAL	N-CA-C	5.88	117.05	108.58
1	A	355	ASN	N-CA-C	-5.85	100.13	109.96
1	A	23	ILE	N-CA-C	-5.83	99.35	107.80
1	D	355	ASN	N-CA-C	-5.81	100.20	109.96
1	C	372	CYS	N-CA-C	5.81	119.47	112.38
1	D	144	ALA	N-CA-C	5.78	117.31	108.52
1	C	220	GLY	N-CA-C	5.74	118.97	110.42
1	D	336	ALA	N-CA-C	-5.69	101.28	110.32
1	B	215	TYR	N-CA-C	5.67	119.51	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	ASN	N-CA-C	-5.58	102.63	110.50
1	A	194	PHE	N-CA-C	5.56	118.75	110.52
1	B	300	ASN	N-CA-C	-5.53	102.70	110.50
1	C	145	PHE	N-CA-C	-5.53	100.29	109.46
1	A	145	PHE	N-CA-C	-5.50	100.33	109.46
1	D	225	ILE	N-CA-C	5.36	121.27	113.39
1	B	225	ILE	N-CA-C	5.30	121.18	113.39
1	D	342	MET	N-CA-C	5.29	119.74	113.28
1	C	342	MET	N-CA-C	5.29	119.72	113.16
1	B	117	VAL	N-CA-C	-5.24	103.81	108.95
1	B	346	MET	N-CA-C	5.24	118.14	111.69
1	B	336	ALA	N-CA-C	-5.24	101.99	110.32
1	A	199	GLU	N-CA-C	5.20	116.95	111.28
1	C	194	PHE	N-CA-C	5.19	118.57	110.32
1	A	174	ASN	CA-C-N	5.18	125.47	119.92
1	A	174	ASN	C-N-CA	5.18	125.47	119.92
1	D	89	ALA	N-CA-C	-5.18	105.72	111.36
1	A	396	PHE	N-CA-C	5.14	117.50	110.55
1	B	35	ALA	N-CA-C	5.14	116.88	111.28
1	D	246	VAL	N-CA-C	-5.11	105.40	110.62
1	D	102	ASP	N-CA-C	-5.07	99.53	108.20
1	A	19	ASP	N-CA-C	5.00	119.01	113.01

There are no chirality outliers.

There are no planarity outliers.

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	3395	0	3457	59	0
1	B	3395	0	3457	69	0
1	C	3395	0	3457	55	0
1	D	3395	0	3457	55	0
2	A	16	0	7	2	0
2	B	16	0	7	2	0
2	C	16	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	16	0	7	2	0
3	C	1	0	0	0	0
4	D	60	0	72	16	0
5	A	369	0	0	10	0
5	B	301	0	0	11	0
5	C	370	0	0	9	0
5	D	383	0	0	8	0
All	All	15128	0	13929	226	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 8.

All (226) 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:C:270:TYR:HB2	1:C:273:LYS:HE2	1.48	0.96
1:B:430:GLU:HG2	5:B:1559:HOH:O	1.76	0.86
1:A:407:ASN:HD22	1:A:409:TYR:H	1.24	0.85
1:C:414:ARG:HH12	1:D:408:ASN:HD22	1.25	0.85
1:B:47:TYR:HB2	1:B:417:MET:HG2	1.57	0.85
1:B:407:ASN:HD22	1:B:409:TYR:H	1.25	0.84
1:A:83:LYS:HE2	5:A:1795:HOH:O	1.78	0.83
1:D:407:ASN:HD22	1:D:409:TYR:H	1.26	0.82
1:C:373:GLU:OE1	4:D:1605:LYS:HG2	1.80	0.81
1:C:187:THR:O	1:C:191:LYS:HG2	1.81	0.80
1:A:414:ARG:HH12	1:B:408:ASN:HD22	1.30	0.80
1:D:187:THR:HG22	1:D:191:LYS:HD3	1.64	0.80
1:C:414:ARG:HH12	1:D:408:ASN:ND2	1.80	0.79
1:A:81:ALA:HB1	1:A:83:LYS:HE3	1.63	0.79
1:A:228:GLN:HE22	1:A:267:ILE:H	1.32	0.77
1:B:228:GLN:HE22	1:B:267:ILE:H	1.31	0.77
1:D:373:GLU:OE2	4:D:1603:LYS:HG2	1.84	0.77
1:B:83:LYS:HE2	5:B:1504:HOH:O	1.84	0.76
1:C:408:ASN:ND2	1:D:414:ARG:HH12	1.83	0.76
1:A:328:VAL:HG13	1:A:329:THR:HG23	1.66	0.76
1:A:408:ASN:HD22	1:B:414:ARG:HH12	1.33	0.76
5:A:1554:HOH:O	1:B:321:HIS:HD2	1.69	0.75
1:A:440:LYS:HE3	5:B:1710:HOH:O	1.86	0.75
1:C:407:ASN:HD22	1:C:409:TYR:H	1.36	0.74
1:A:414:ARG:HH12	1:B:408:ASN:ND2	1.85	0.74
1:C:228:GLN:HE22	1:C:267:ILE:H	1.33	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:TYR:HB2	1:B:273:LYS:HE3	1.70	0.74
1:C:416:ARG:HG3	1:C:431:ARG:HB3	1.70	0.74
1:A:328:VAL:HG22	1:A:329:THR:HG22	1.70	0.73
1:D:187:THR:O	1:D:191:LYS:HG2	1.88	0.72
1:C:408:ASN:HD22	1:D:414:ARG:HH12	1.37	0.72
1:D:228:GLN:HE22	1:D:267:ILE:H	1.39	0.70
1:D:187:THR:CG2	1:D:191:LYS:HD3	2.20	0.70
4:D:1606:LYS:HE2	5:D:1955:HOH:O	1.91	0.70
1:A:120:LYS:HG2	5:A:1692:HOH:O	1.92	0.69
1:A:25:ASP:HB3	5:A:1724:HOH:O	1.92	0.69
1:D:120:LYS:HG2	5:D:1818:HOH:O	1.93	0.69
1:A:408:ASN:ND2	1:B:414:ARG:HH12	1.91	0.69
1:C:414:ARG:NH1	1:D:408:ASN:HD22	1.90	0.68
1:A:372:CYS:H	1:A:410:ASN:HD21	1.42	0.66
1:A:178:ASN:HB3	1:A:181:THR:OG1	1.95	0.66
1:C:357:LYS:HE2	5:C:1748:HOH:O	1.94	0.66
1:A:329:THR:HG21	5:B:1578:HOH:O	1.95	0.65
1:D:19:ASP:H	1:D:53:GLN:HE22	1.42	0.65
1:C:157:ASN:HD21	1:C:215:TYR:H	1.42	0.65
1:D:83:LYS:HE3	5:D:1608:HOH:O	1.97	0.65
1:B:178:ASN:HD21	1:B:180:LYS:HB2	1.63	0.64
1:D:177:VAL:HG13	1:D:237:GLU:HG2	1.79	0.64
1:A:19:ASP:H	1:A:53:GLN:HE22	1.43	0.64
1:D:177:VAL:HG13	1:D:237:GLU:CG	2.28	0.64
1:A:307:ARG:HH22	4:D:1601:LYS:HB2	1.64	0.63
1:B:362:LYS:HD2	1:B:383:GLU:CD	2.24	0.63
1:D:431:ARG:HD2	1:D:431:ARG:C	2.24	0.62
4:D:1605:LYS:HE3	5:D:1850:HOH:O	1.99	0.62
1:B:416:ARG:HG3	1:B:431:ARG:HB3	1.82	0.62
1:A:157:ASN:HD21	1:A:215:TYR:H	1.46	0.62
1:B:15:MET:HB2	5:B:1685:HOH:O	1.99	0.62
1:B:81:ALA:HB1	1:B:83:LYS:HE3	1.81	0.61
1:C:177:VAL:HG23	1:C:237:GLU:HG2	1.82	0.61
1:D:157:ASN:HD21	1:D:215:TYR:H	1.49	0.61
1:B:157:ASN:HD21	1:B:215:TYR:H	1.49	0.61
1:C:34:ASP:OD1	1:C:37:GLU:HG3	2.01	0.61
1:A:407:ASN:ND2	1:A:409:TYR:H	1.99	0.59
1:D:232:ILE:HD13	1:D:276:PRO:HB3	1.84	0.59
1:B:19:ASP:H	1:B:53:GLN:HE22	1.50	0.59
1:C:83:LYS:HZ2	1:C:104:VAL:HG11	1.68	0.59
1:C:108:GLU:HG3	1:D:411:ALA:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ARG:NH2	4:D:1601:LYS:HB2	2.18	0.58
1:D:407:ASN:ND2	1:D:409:TYR:H	1.99	0.58
1:C:346:MET:HG2	1:C:347:TYR:CZ	2.39	0.58
1:A:108:GLU:HG3	1:B:411:ALA:HB3	1.86	0.58
1:D:185:ILE:HG13	1:D:234:PRO:HB3	1.86	0.58
1:B:329:THR:CG2	5:B:1544:HOH:O	2.51	0.57
1:B:343:ARG:NH2	1:B:349:ALA:HB1	2.18	0.57
1:D:321:HIS:HE1	1:D:335:ASP:OD2	1.87	0.57
5:C:1924:HOH:O	1:D:440:LYS:HE3	2.03	0.57
1:A:176:ASN:ND2	5:A:1756:HOH:O	2.37	0.57
1:B:319:LYS:NZ	5:B:1794:HOH:O	2.37	0.56
1:A:328:VAL:HG13	1:A:329:THR:CG2	2.35	0.56
1:C:177:VAL:HG11	1:C:186:SER:HA	1.87	0.56
5:C:1656:HOH:O	1:D:321:HIS:HD2	1.86	0.56
1:A:307:ARG:HH22	4:D:1601:LYS:CB	2.18	0.56
1:B:96:LYS:NZ	5:B:1673:HOH:O	2.39	0.56
1:A:177:VAL:HG13	1:A:237:GLU:HG2	1.88	0.55
1:A:411:ALA:HB3	1:B:108:GLU:HG3	1.89	0.55
1:B:279:LYS:HG2	5:B:1569:HOH:O	2.06	0.55
1:B:250:LYS:HG3	1:B:296:VAL:HG12	1.89	0.55
1:C:409:TYR:O	1:C:410:ASN:HB2	2.08	0.54
1:C:66:LYS:O	1:C:70:GLU:HG3	2.08	0.54
1:B:178:ASN:HD22	1:B:180:LYS:H	1.56	0.54
4:D:1604:LYS:N	5:D:1984:HOH:O	2.40	0.54
1:C:157:ASN:ND2	1:C:215:TYR:H	2.06	0.54
1:A:19:ASP:N	1:A:53:GLN:HE22	2.07	0.53
1:B:407:ASN:ND2	1:B:409:TYR:H	2.02	0.53
1:A:22:GLU:HG3	1:A:24:LYS:HG3	1.91	0.53
1:B:250:LYS:CG	1:B:296:VAL:HG12	2.38	0.53
1:B:36:ILE:O	1:B:40:GLU:HG3	2.09	0.53
1:B:267:ILE:HB	1:B:268:PRO:HD2	1.91	0.53
1:B:371:LEU:HD12	1:B:371:LEU:N	2.24	0.53
1:B:231:ASP:O	1:B:234:PRO:HD2	2.10	0.52
1:A:19:ASP:H	1:A:53:GLN:NE2	2.08	0.52
1:B:178:ASN:ND2	1:B:180:LYS:H	2.08	0.52
1:A:109:LEU:HD23	1:A:136:MET:HG2	1.92	0.52
1:C:298:MET:HA	1:C:298:MET:HE2	1.91	0.52
1:C:81:ALA:HB1	1:C:83:LYS:HE3	1.91	0.51
1:A:298:MET:HA	1:A:298:MET:HE2	1.92	0.51
1:B:115:SER:O	1:B:116:ASN:HB2	2.10	0.51
1:D:249:LEU:HD13	1:D:256:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1502:PLP:O4A	4:D:1602:LYS:NZ	2.42	0.51
1:B:298:MET:HE2	1:B:298:MET:HA	1.93	0.51
1:D:19:ASP:N	1:D:53:GLN:HE22	2.06	0.50
1:A:373:GLU:OE1	4:D:1602:LYS:HD3	2.12	0.50
4:D:1606:LYS:N	5:D:1965:HOH:O	2.43	0.50
1:B:177:VAL:O	1:B:179:PRO:HD3	2.11	0.50
1:C:177:VAL:CG1	1:C:186:SER:HA	2.39	0.50
1:A:83:LYS:HD2	2:A:1501:PLP:C4A	2.41	0.50
1:C:120:LYS:CE	5:C:1890:HOH:O	2.59	0.50
1:C:177:VAL:HG23	1:C:237:GLU:CG	2.41	0.50
1:A:157:ASN:ND2	1:A:215:TYR:H	2.10	0.50
1:D:421:SER:HA	5:D:1709:HOH:O	2.11	0.50
1:C:19:ASP:H	1:C:53:GLN:HE22	1.60	0.49
1:D:19:ASP:H	1:D:53:GLN:NE2	2.10	0.49
1:C:120:LYS:HE2	5:C:1890:HOH:O	2.12	0.49
1:B:19:ASP:N	1:B:53:GLN:HE22	2.10	0.49
1:A:414:ARG:NH1	1:B:408:ASN:HD22	2.06	0.49
1:B:178:ASN:HB3	1:B:181:THR:OG1	2.13	0.48
1:C:414:ARG:NH1	1:D:408:ASN:ND2	2.52	0.48
1:C:81:ALA:HB1	1:C:83:LYS:CE	2.42	0.48
1:C:411:ALA:HB3	1:D:108:GLU:HG3	1.94	0.48
1:D:319:LYS:HE3	1:D:390:GLY:HA2	1.96	0.48
1:A:279:LYS:HG3	5:A:1526:HOH:O	2.14	0.48
1:A:220:GLY:HA2	1:A:256:ILE:HG23	1.96	0.48
1:D:175:PRO:HB2	1:D:241:LYS:CB	2.44	0.48
1:A:161:LYS:HE3	5:A:1863:HOH:O	2.14	0.48
1:C:332:VAL:HG11	1:C:387:VAL:HG11	1.96	0.48
1:D:226:GLY:HA2	4:D:1606:LYS:HE3	1.96	0.48
1:A:328:VAL:C	1:A:329:THR:HG22	2.38	0.47
1:C:178:ASN:HB3	1:C:181:THR:OG1	2.14	0.47
1:B:259:VAL:HG23	1:B:299:PRO:HG3	1.96	0.47
1:B:307:ARG:HH22	4:D:1602:LYS:HB3	1.79	0.47
1:B:174:ASN:HA	1:B:189:LEU:HD22	1.96	0.47
1:B:83:LYS:HZ3	1:B:104:VAL:HG11	1.80	0.47
1:A:18:ASN:HD21	1:A:271:LYS:NZ	2.12	0.47
1:C:177:VAL:HG13	1:C:186:SER:HB2	1.97	0.47
1:D:157:ASN:HD22	1:D:216:VAL:HG13	1.80	0.47
1:C:18:ASN:HD21	1:C:271:LYS:NZ	2.12	0.46
1:C:250:LYS:HG3	1:C:296:VAL:HG12	1.96	0.46
1:C:250:LYS:CG	1:C:296:VAL:HG12	2.45	0.46
1:C:15:MET:N	1:C:18:ASN:HD22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:LYS:HE2	5:B:1555:HOH:O	2.15	0.46
1:C:403:ILE:CB	1:C:417:MET:HE1	2.46	0.46
1:C:407:ASN:HB3	1:D:407:ASN:HB3	1.97	0.46
1:B:83:LYS:HD2	2:B:1502:PLP:C4A	2.46	0.46
1:B:176:ASN:OD1	1:B:241:LYS:HD2	2.16	0.46
1:D:161:LYS:HG3	1:D:215:TYR:CZ	2.51	0.46
1:D:193:LYS:HE3	1:D:194:PHE:CE1	2.51	0.45
1:C:102:ASP:OD1	1:C:102:ASP:C	2.59	0.45
1:C:240:ARG:NE	5:C:1791:HOH:O	2.49	0.45
1:A:407:ASN:HB3	1:B:407:ASN:HB3	1.99	0.45
1:D:18:ASN:HD21	1:D:271:LYS:NZ	2.14	0.45
1:D:175:PRO:HB2	1:D:241:LYS:HB3	1.97	0.45
1:A:51:GLU:HG2	1:A:55:LYS:HE2	1.98	0.45
1:D:158:GLU:O	1:D:162:GLU:HG3	2.17	0.45
1:C:240:ARG:HD2	5:C:1791:HOH:O	2.16	0.45
1:A:83:LYS:HD2	2:A:1501:PLP:O4A	2.16	0.45
1:B:412:ARG:NE	5:B:1546:HOH:O	2.33	0.45
1:C:83:LYS:HD2	2:C:1503:PLP:C4A	2.46	0.45
1:D:304:GLU:O	2:D:1504:PLP:H6	2.16	0.45
1:B:22:GLU:HG3	1:B:24:LYS:HG3	1.99	0.45
1:B:307:ARG:NH2	4:D:1602:LYS:HB3	2.32	0.44
1:D:298:MET:HE2	1:D:298:MET:HA	1.99	0.44
1:B:270:TYR:CB	1:B:273:LYS:HE3	2.45	0.44
1:C:66:LYS:HA	5:C:1838:HOH:O	2.16	0.44
1:A:328:VAL:HG22	1:A:328:VAL:O	2.16	0.44
1:B:102:ASP:OD1	1:B:102:ASP:C	2.60	0.44
1:B:373:GLU:CG	1:B:409:TYR:HE2	2.30	0.44
1:C:75:GLU:OE1	1:C:120:LYS:NZ	2.50	0.44
1:C:332:VAL:CG1	1:C:387:VAL:HG11	2.47	0.44
1:D:228:GLN:O	1:D:228:GLN:HG3	2.17	0.44
1:D:416:ARG:HG3	1:D:431:ARG:HB3	1.99	0.44
1:A:233:SER:HB3	1:A:234:PRO:HD3	2.00	0.44
1:C:403:ILE:HB	1:C:417:MET:HE1	2.00	0.44
1:A:293:LYS:HA	1:A:298:MET:HE3	1.99	0.44
1:B:19:ASP:H	1:B:53:GLN:NE2	2.14	0.44
1:C:83:LYS:HZ2	1:C:104:VAL:CG1	2.30	0.43
1:D:192:ASN:HB2	5:D:1822:HOH:O	2.18	0.43
1:D:66:LYS:O	1:D:70:GLU:HG3	2.17	0.43
1:B:233:SER:HB3	1:B:234:PRO:HD3	2.00	0.43
1:A:383:GLU:O	1:A:384:LEU:HD23	2.19	0.43
1:B:373:GLU:OE1	4:D:1601:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:PRO:HG2	1:B:309:LEU:HD22	2.00	0.43
1:C:45:PRO:HG2	1:C:415:PRO:HB3	2.01	0.43
1:B:205:LYS:O	1:B:209:MET:HG3	2.19	0.42
1:D:431:ARG:C	1:D:431:ARG:CD	2.91	0.42
1:C:58:TYR:CZ	1:C:62:ILE:HD11	2.54	0.42
1:A:65:PHE:CZ	1:A:303:LEU:HD11	2.55	0.42
1:A:69:GLU:HB2	5:A:1640:HOH:O	2.19	0.42
1:A:328:VAL:C	1:A:329:THR:CG2	2.92	0.42
1:B:175:PRO:HB2	1:B:241:LYS:HB3	2.01	0.42
1:B:343:ARG:HB2	1:B:344:PRO:HD3	2.00	0.42
1:D:104:VAL:HG22	1:D:104:VAL:O	2.20	0.42
1:B:65:PHE:CZ	1:B:303:LEU:HD11	2.55	0.42
1:C:372:CYS:SG	1:D:83:LYS:HD3	2.60	0.42
1:A:120:LYS:HE3	5:A:1692:HOH:O	2.20	0.41
1:A:104:VAL:HG22	1:A:108:GLU:OE1	2.19	0.41
1:A:179:PRO:HG2	1:A:180:LYS:NZ	2.35	0.41
1:B:67:ARG:HG3	1:B:286:ILE:HD13	2.02	0.41
4:D:1605:LYS:HD2	2:D:1504:PLP:O4A	2.20	0.41
1:B:228:GLN:NE2	1:B:228:GLN:HA	2.35	0.41
1:A:343:ARG:HB2	1:A:344:PRO:HD3	2.01	0.41
1:B:215:TYR:CD1	1:B:215:TYR:N	2.88	0.41
1:D:267:ILE:HB	1:D:268:PRO:HD2	2.02	0.41
1:B:328:VAL:HG12	1:B:329:THR:OG1	2.21	0.41
1:D:220:GLY:HA2	1:D:256:ILE:HG23	2.02	0.41
1:A:205:LYS:O	1:A:209:MET:HG3	2.21	0.41
1:A:328:VAL:O	1:A:329:THR:HG22	2.21	0.41
1:A:15:MET:HB2	5:A:1685:HOH:O	2.20	0.41
1:D:346:MET:HE2	1:D:346:MET:HB3	1.61	0.40
1:A:343:ARG:HD3	1:A:351:HIS:NE2	2.36	0.40
1:C:52:GLU:HG3	5:C:1790:HOH:O	2.22	0.40
1:D:232:ILE:HA	1:D:232:ILE:HD12	1.88	0.40
1:D:328:VAL:HG12	1:D:329:THR:OG1	2.21	0.40
1:B:346:MET:HE2	1:B:346:MET:HB3	1.92	0.40
1:C:211:LEU:HD23	1:C:211:LEU:HA	1.92	0.40
1:B:157:ASN:ND2	1:B:213:MET:HB3	2.37	0.40
1:B:161:LYS:HG3	1:B:215:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	432/434 (100%)	425 (98%)	6 (1%)	1 (0%)	43	42
1	B	432/434 (100%)	422 (98%)	9 (2%)	1 (0%)	43	42
1	C	432/434 (100%)	425 (98%)	6 (1%)	1 (0%)	43	42
1	D	432/434 (100%)	423 (98%)	8 (2%)	1 (0%)	43	42
All	All	1728/1736 (100%)	1695 (98%)	29 (2%)	4 (0%)	43	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	D	85	ASN
1	C	85	ASN
1	B	85	ASN

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	367/367 (100%)	358 (98%)	9 (2%)	42	45
1	B	367/367 (100%)	360 (98%)	7 (2%)	50	56
1	C	367/367 (100%)	360 (98%)	7 (2%)	50	56
1	D	367/367 (100%)	353 (96%)	14 (4%)	29	29
All	All	1468/1468 (100%)	1431 (98%)	37 (2%)	39	45

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

Mol	Chain	Res	Type
1	A	15	MET
1	A	16	LEU
1	A	69	GLU
1	A	102	ASP
1	A	129	LYS
1	A	232	ILE
1	A	329	THR
1	A	373	GLU
1	A	374	SER
1	B	102	ASP
1	B	178	ASN
1	B	250	LYS
1	B	299	PRO
1	B	309	LEU
1	B	329	THR
1	B	372	CYS
1	C	69	GLU
1	C	83	LYS
1	C	102	ASP
1	C	153	LEU
1	C	250	LYS
1	C	299	PRO
1	C	373	GLU
1	D	24	LYS
1	D	83	LYS
1	D	102	ASP
1	D	116	ASN
1	D	120	LYS
1	D	163	LEU
1	D	191	LYS
1	D	232	ILE
1	D	240	ARG
1	D	250	LYS
1	D	373	GLU
1	D	407	ASN
1	D	431	ARG
1	D	440	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	53	GLN
1	A	157	ASN
1	A	176	ASN
1	A	192	ASN
1	A	228	GLN
1	A	407	ASN
1	A	408	ASN
1	A	410	ASN
1	B	18	ASN
1	B	53	GLN
1	B	116	ASN
1	B	157	ASN
1	B	178	ASN
1	B	192	ASN
1	B	228	GLN
1	B	321	HIS
1	B	407	ASN
1	B	408	ASN
1	C	18	ASN
1	C	53	GLN
1	C	141	ASN
1	C	157	ASN
1	C	176	ASN
1	C	217	ASN
1	C	228	GLN
1	C	407	ASN
1	C	408	ASN
1	D	18	ASN
1	D	53	GLN
1	D	116	ASN
1	D	141	ASN
1	D	157	ASN
1	D	176	ASN
1	D	217	ASN
1	D	228	GLN
1	D	321	HIS
1	D	352	HIS
1	D	407	ASN
1	D	408	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z > 2$
4	LYS	D	1601	-	8,9,9	1.17	1 (12%)	7,10,10	1.00	0
4	LYS	D	1604	-	8,9,9	1.00	1 (12%)	7,10,10	0.75	0
4	LYS	D	1602	-	8,9,9	0.92	0	7,10,10	0.69	0
2	PLP	C	1503	4	16,16,16	2.44	5 (31%)	20,23,23	2.14	4 (20%)
4	LYS	D	1605	-	8,9,9	0.72	0	7,10,10	0.42	0
2	PLP	B	1502	-	16,16,16	1.60	1 (6%)	20,23,23	2.25	5 (25%)
4	LYS	D	1603	2	8,9,9	0.98	0	7,10,10	0.40	0
4	LYS	D	1606	-	8,9,9	0.82	0	7,10,10	0.70	0
2	PLP	A	1501	-	16,16,16	1.92	6 (37%)	20,23,23	2.15	4 (20%)
2	PLP	D	1504	-	16,16,16	2.86	6 (37%)	20,23,23	2.42	5 (25%)

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
4	LYS	D	1601	-	-	3/9/9/9	-
4	LYS	D	1604	-	-	1/9/9/9	-
4	LYS	D	1602	-	-	2/9/9/9	-
2	PLP	C	1503	4	-	0/8/8/8	0/1/1/1
4	LYS	D	1605	-	-	2/9/9/9	-
2	PLP	B	1502	-	-	0/8/8/8	0/1/1/1
4	LYS	D	1603	2	-	2/9/9/9	-
4	LYS	D	1606	-	-	3/9/9/9	-
2	PLP	A	1501	-	-	0/8/8/8	0/1/1/1
2	PLP	D	1504	-	-	0/8/8/8	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1504	PLP	O4A-C4A	-7.11	0.96	1.21
2	C	1503	PLP	C4-C4A	4.68	1.57	1.46
2	D	1504	PLP	C4-C4A	4.66	1.57	1.46
2	B	1502	PLP	C4-C4A	4.53	1.57	1.46
2	A	1501	PLP	C4-C4A	4.51	1.57	1.46
2	C	1503	PLP	O4A-C4A	-4.41	1.06	1.21
2	D	1504	PLP	C2A-C2	4.29	1.57	1.50
2	C	1503	PLP	C3-C2	-4.11	1.36	1.41
2	C	1503	PLP	C2-N1	4.09	1.41	1.33
2	D	1504	PLP	C6-N1	3.25	1.41	1.34
2	D	1504	PLP	C4-C3	-3.08	1.36	1.41
2	A	1501	PLP	C2A-C2	3.06	1.55	1.50
2	A	1501	PLP	C2-N1	2.78	1.38	1.33
4	D	1604	LYS	OXT-C	-2.56	1.22	1.30
2	A	1501	PLP	C6-N1	2.56	1.39	1.34
4	D	1601	LYS	OXT-C	-2.32	1.23	1.30
2	D	1504	PLP	P-O1P	-2.29	1.43	1.50
2	A	1501	PLP	C4-C3	-2.23	1.37	1.41
2	C	1503	PLP	C6-N1	2.22	1.38	1.34
2	A	1501	PLP	P-O3P	-2.20	1.46	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1504	PLP	C4-C3-C2	8.24	124.78	120.14
2	C	1503	PLP	C4-C3-C2	7.20	124.19	120.14
2	A	1501	PLP	C4-C3-C2	6.41	123.75	120.14
2	B	1502	PLP	C2A-C2-C3	6.12	127.96	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1502	PLP	C4-C3-C2	5.09	123.01	120.14
2	A	1501	PLP	C2A-C2-C3	4.32	125.86	120.80
2	D	1504	PLP	C2A-C2-C3	4.22	125.74	120.80
2	A	1501	PLP	O4A-C4A-C4	-3.60	116.27	124.80
2	C	1503	PLP	O4A-C4A-C4	3.32	132.66	124.80
2	B	1502	PLP	O4A-C4A-C4	-3.25	117.09	124.80
2	C	1503	PLP	C2A-C2-C3	3.10	124.42	120.80
2	D	1504	PLP	O4A-C4A-C4	2.92	131.73	124.80
2	B	1502	PLP	C3-C2-N1	-2.91	117.29	120.96
2	A	1501	PLP	C3-C2-N1	-2.62	117.66	120.96
2	C	1503	PLP	O4P-C5A-C5	2.49	114.03	109.36
2	B	1502	PLP	O4P-C5A-C5	2.48	114.01	109.36
2	D	1504	PLP	O4P-C5A-C5	2.36	113.78	109.36
2	D	1504	PLP	C3-C2-N1	-2.23	118.14	120.96

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1606	LYS	N-CA-CB-CG
4	D	1602	LYS	CG-CD-CE-NZ
4	D	1601	LYS	CE-CD-CG-CB
4	D	1605	LYS	CE-CD-CG-CB
4	D	1603	LYS	CA-CB-CG-CD
4	D	1603	LYS	CE-CD-CG-CB
4	D	1606	LYS	C-CA-CB-CG
4	D	1601	LYS	N-CA-CB-CG
4	D	1605	LYS	N-CA-CB-CG
4	D	1606	LYS	CG-CD-CE-NZ
4	D	1602	LYS	O-C-CA-N
4	D	1604	LYS	OXT-C-CA-N
4	D	1601	LYS	O-C-CA-CB

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1601	LYS	4	0
4	D	1604	LYS	1	0
4	D	1602	LYS	4	0
2	C	1503	PLP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1605	LYS	3	0
2	B	1502	PLP	2	0
4	D	1603	LYS	1	0
4	D	1606	LYS	3	0
2	A	1501	PLP	2	0
2	D	1504	PLP	2	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, 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	434/434 (100%)	-0.64	1 (0%) 91 90	8, 15, 27, 33	0
1	B	434/434 (100%)	-0.33	6 (1%) 73 73	9, 18, 36, 42	0
1	C	434/434 (100%)	-0.58	6 (1%) 73 73	8, 15, 30, 40	0
1	D	434/434 (100%)	-0.54	8 (1%) 67 67	8, 15, 31, 39	0
All	All	1736/1736 (100%)	-0.52	21 (1%) 76 76	8, 15, 32, 42	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	188	GLY	3.2
1	D	25	ASP	3.1
1	D	187	THR	3.0
1	A	15	MET	3.0
1	D	189	LEU	2.7
1	D	184	LYS	2.5
1	D	360	ASN	2.3
1	D	188	GLY	2.3
1	B	178	ASN	2.3
1	C	15	MET	2.2
1	B	360	ASN	2.2
1	C	187	THR	2.2
1	D	178	ASN	2.2
1	C	182	HIS	2.2
1	C	178	ASN	2.2
1	D	15	MET	2.1
1	C	186	SER	2.1
1	C	185	ILE	2.1
1	B	181	THR	2.0
1	B	187	THR	2.0
1	B	15	MET	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 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
4	LYS	D	1601	10/10	0.74	0.15	34,35,37,42	0
4	LYS	D	1606	10/10	0.80	0.14	33,34,35,36	0
4	LYS	D	1602	10/10	0.81	0.14	33,34,35,36	0
4	LYS	D	1604	10/10	0.82	0.17	42,47,49,49	0
4	LYS	D	1605	10/10	0.88	0.12	25,28,38,39	0
4	LYS	D	1603	10/10	0.92	0.09	24,27,35,36	0
2	PLP	C	1503	16/16	0.97	0.05	11,12,17,26	0
2	PLP	D	1504	16/16	0.97	0.05	9,11,16,27	0
2	PLP	A	1501	16/16	0.97	0.06	9,12,15,31	0
2	PLP	B	1502	16/16	0.97	0.06	15,17,20,30	0
3	MG	C	1607	1/1	0.99	0.03	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.