



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:40 AM UTC

PDB ID : 6JFB / pdb_00006jfb
Title : Crystal structure of human pyruvate kinase M2 isoform
Authors : Chen, T.J.; Wang, W.C.
Deposited on : 2019-02-08
Resolution : 2.12 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

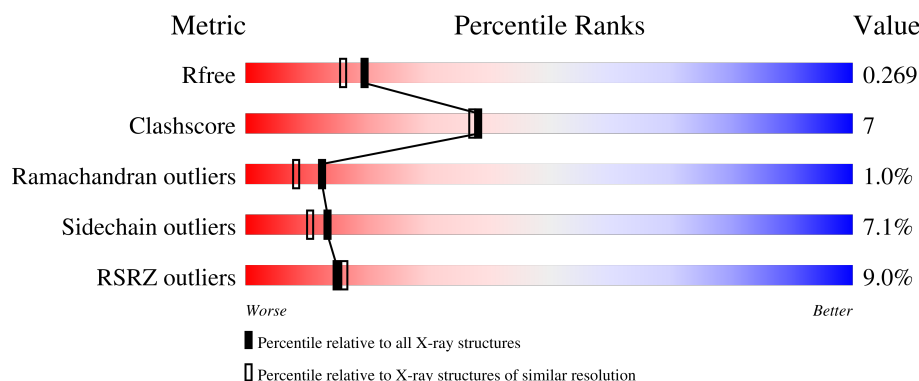
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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 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	552	9% 76% 16% • 5%
1	B	552	6% 76% 16% • 6%
1	C	552	7% 76% 16% • 5%
1	D	552	12% 76% 15% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16478 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 Pyruvate kinase PKM Isoform M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			3997	2515	708	749	25			
1	B	521	Total	C	N	O	S	0	0	0
			3994	2513	707	749	25			
1	C	523	Total	C	N	O	S	0	0	0
			4006	2520	709	752	25			
1	D	516	Total	C	N	O	S	0	0	0
			3950	2485	701	740	24			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P14618
A	-19	GLY	-	expression tag	UNP P14618
A	-18	SER	-	expression tag	UNP P14618
A	-17	SER	-	expression tag	UNP P14618
A	-16	HIS	-	expression tag	UNP P14618
A	-15	HIS	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	SER	-	expression tag	UNP P14618
A	-9	SER	-	expression tag	UNP P14618
A	-8	GLY	-	expression tag	UNP P14618
A	-7	LEU	-	expression tag	UNP P14618
A	-6	VAL	-	expression tag	UNP P14618
A	-5	PRO	-	expression tag	UNP P14618
A	-4	ARG	-	expression tag	UNP P14618
A	-3	GLY	-	expression tag	UNP P14618
A	-2	SER	-	expression tag	UNP P14618
A	-1	HIS	-	expression tag	UNP P14618
A	0	MET	-	expression tag	UNP P14618

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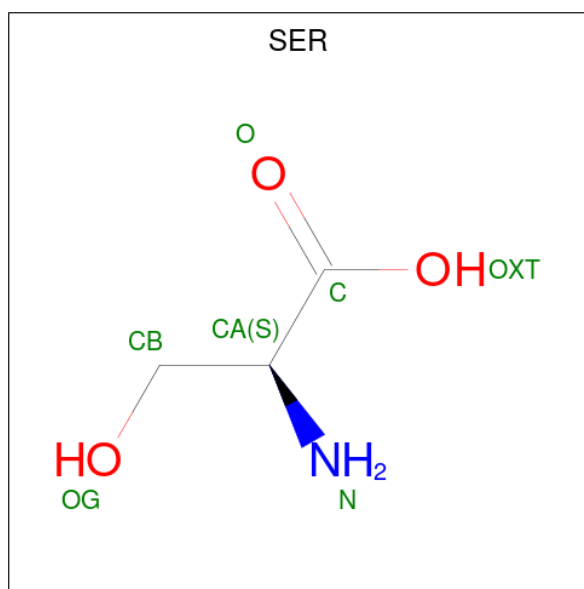
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP P14618
B	-19	GLY	-	expression tag	UNP P14618
B	-18	SER	-	expression tag	UNP P14618
B	-17	SER	-	expression tag	UNP P14618
B	-16	HIS	-	expression tag	UNP P14618
B	-15	HIS	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	SER	-	expression tag	UNP P14618
B	-9	SER	-	expression tag	UNP P14618
B	-8	GLY	-	expression tag	UNP P14618
B	-7	LEU	-	expression tag	UNP P14618
B	-6	VAL	-	expression tag	UNP P14618
B	-5	PRO	-	expression tag	UNP P14618
B	-4	ARG	-	expression tag	UNP P14618
B	-3	GLY	-	expression tag	UNP P14618
B	-2	SER	-	expression tag	UNP P14618
B	-1	HIS	-	expression tag	UNP P14618
B	0	MET	-	expression tag	UNP P14618
C	-20	MET	-	expression tag	UNP P14618
C	-19	GLY	-	expression tag	UNP P14618
C	-18	SER	-	expression tag	UNP P14618
C	-17	SER	-	expression tag	UNP P14618
C	-16	HIS	-	expression tag	UNP P14618
C	-15	HIS	-	expression tag	UNP P14618
C	-14	HIS	-	expression tag	UNP P14618
C	-13	HIS	-	expression tag	UNP P14618
C	-12	HIS	-	expression tag	UNP P14618
C	-11	HIS	-	expression tag	UNP P14618
C	-10	SER	-	expression tag	UNP P14618
C	-9	SER	-	expression tag	UNP P14618
C	-8	GLY	-	expression tag	UNP P14618
C	-7	LEU	-	expression tag	UNP P14618
C	-6	VAL	-	expression tag	UNP P14618
C	-5	PRO	-	expression tag	UNP P14618
C	-4	ARG	-	expression tag	UNP P14618
C	-3	GLY	-	expression tag	UNP P14618
C	-2	SER	-	expression tag	UNP P14618
C	-1	HIS	-	expression tag	UNP P14618
C	0	MET	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP P14618
D	-19	GLY	-	expression tag	UNP P14618
D	-18	SER	-	expression tag	UNP P14618
D	-17	SER	-	expression tag	UNP P14618
D	-16	HIS	-	expression tag	UNP P14618
D	-15	HIS	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	SER	-	expression tag	UNP P14618
D	-9	SER	-	expression tag	UNP P14618
D	-8	GLY	-	expression tag	UNP P14618
D	-7	LEU	-	expression tag	UNP P14618
D	-6	VAL	-	expression tag	UNP P14618
D	-5	PRO	-	expression tag	UNP P14618
D	-4	ARG	-	expression tag	UNP P14618
D	-3	GLY	-	expression tag	UNP P14618
D	-2	SER	-	expression tag	UNP P14618
D	-1	HIS	-	expression tag	UNP P14618
D	0	MET	-	expression tag	UNP P14618

- Molecule 2 is SERINE (CCD ID: SER) (formula: $C_3H_7NO_3$).



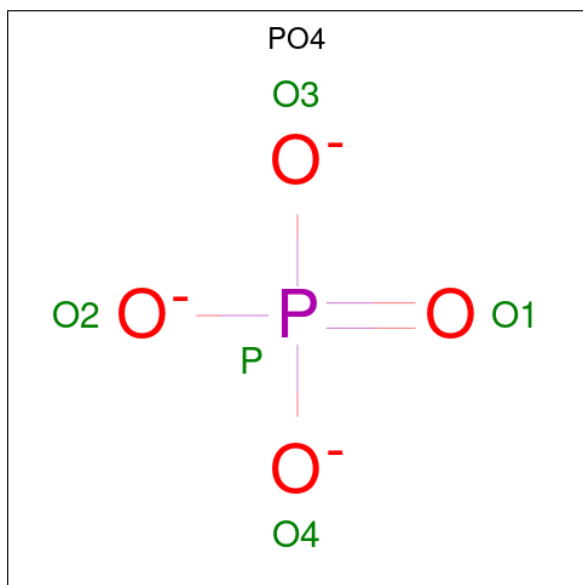
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	3	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			7	3	1	3		
2	C	1	Total	C	N	O	0	0
			7	3	1	3		
2	D	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O P	0	0
			5	4 1		
3	B	1	Total	O P	0	0
			5	4 1		
3	C	1	Total	O P	0	0
			5	4 1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	88	Total	O	0	0
			88	88		
4	B	156	Total	O	0	0
			156	156		
4	C	134	Total	O	0	0
			134	134		

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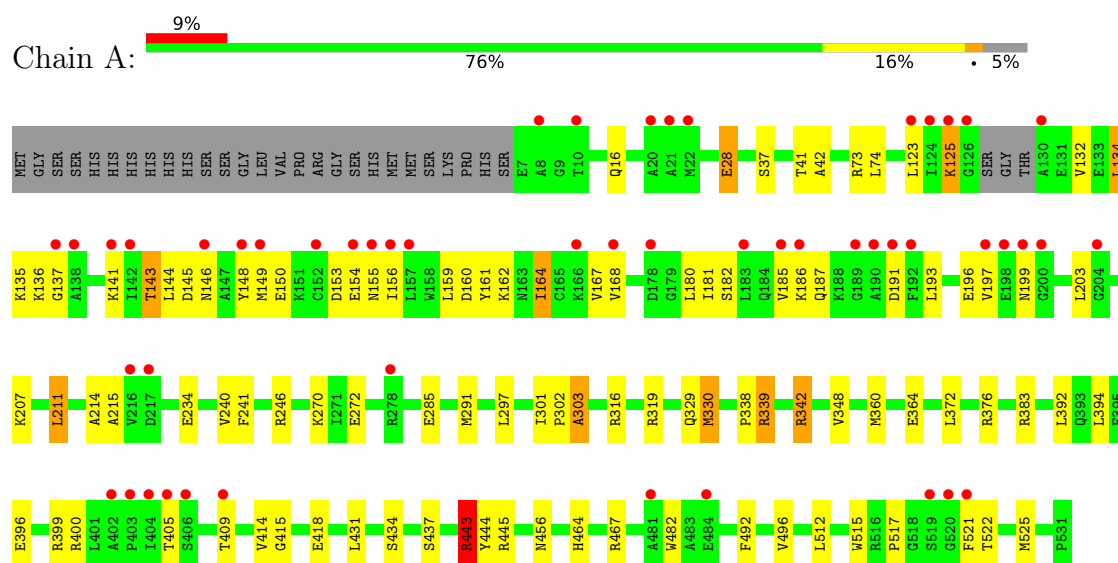
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	110	Total	O	0	0
			110	110		

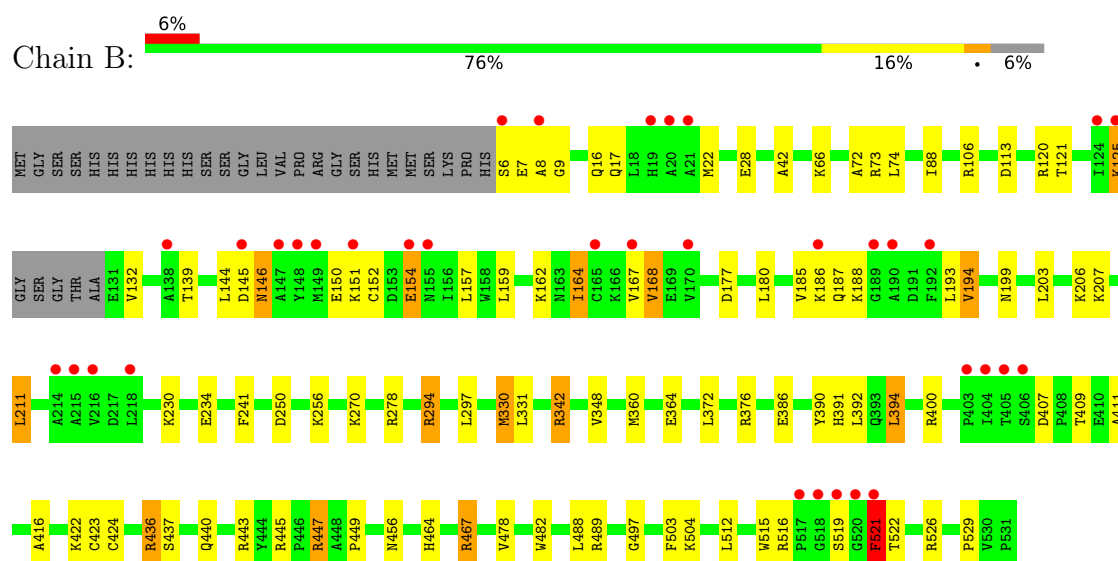
3 Residue-property plots [i](#)

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.

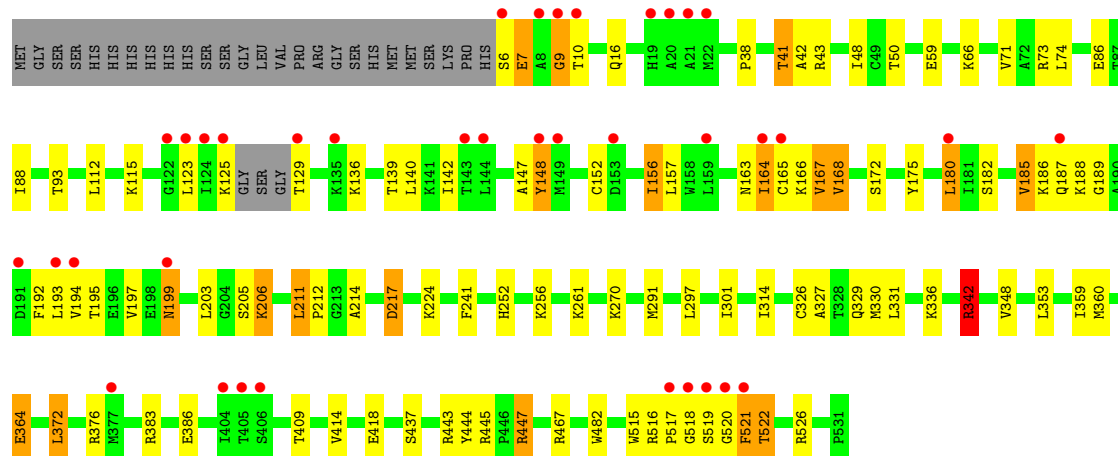
• Molecule 1: Pyruvate kinase PKM Isoform M2



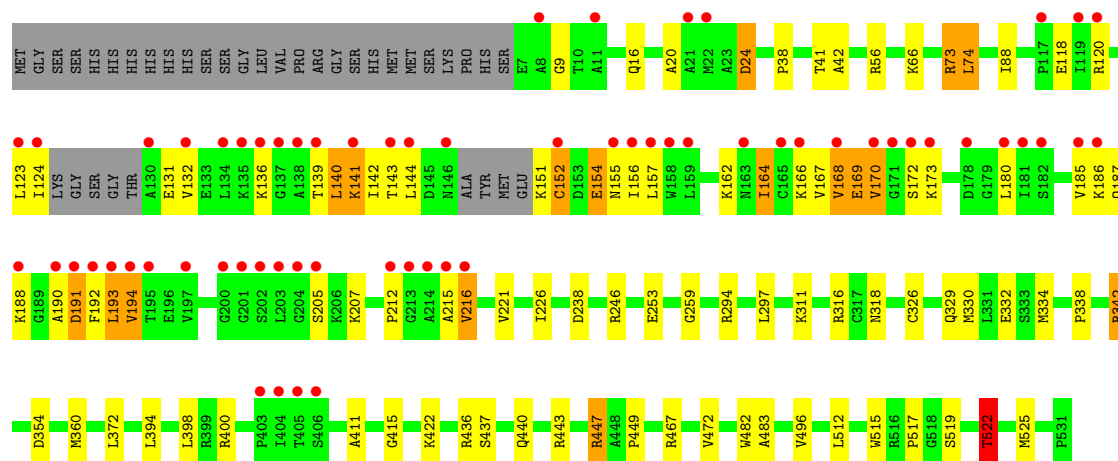
• Molecule 1: Pyruvate kinase PKM Isoform M2



• Molecule 1: Pyruvate kinase PKM Isoform M2



Chain D: 12% 76% 15% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.76Å 152.57Å 94.41Å 90.00° 97.88° 90.00°	Depositor
Resolution (Å)	29.96 – 2.12 29.96 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.96-2.12) 90.9 (29.96-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.192 , 0.251 (Not available) , 0.269	Depositor DCC
R_{free} test set	6128 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.1	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	0.94	EDS
Total number of atoms	16478	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: PO4

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	0.91	2/4061 (0.0%)	1.09	3/5483 (0.1%)
1	B	0.94	4/4058 (0.1%)	1.05	4/5479 (0.1%)
1	C	0.97	3/4070 (0.1%)	1.08	2/5496 (0.0%)
1	D	0.91	0/4012	1.09	6/5417 (0.1%)
All	All	0.93	9/16201 (0.1%)	1.08	15/21875 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	6
1	C	0	5
1	D	0	6
All	All	0	26

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	ALA	C-O	-6.59	1.16	1.24
1	B	529	PRO	C-O	-6.01	1.16	1.23
1	C	86	GLU	C-O	-5.76	1.17	1.24
1	C	270	LYS	C-O	5.62	1.30	1.24
1	B	488	LEU	C-O	-5.57	1.17	1.24
1	A	464	HIS	CE1-NE2	5.26	1.37	1.32
1	B	478	VAL	C-O	-5.14	1.19	1.24
1	A	431	LEU	N-CA	5.11	1.52	1.46
1	C	93	THR	C-O	-5.05	1.18	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	GLU	CB-CA-C	-6.75	98.15	110.63
1	A	456	ASN	CB-CA-C	6.05	117.04	110.08
1	D	522	THR	CB-CA-C	6.01	121.51	111.30
1	D	259	GLY	CA-C-N	5.94	128.16	120.44
1	D	259	GLY	C-N-CA	5.94	128.16	120.44
1	D	238	ASP	CA-CB-CG	-5.75	106.85	112.60
1	C	38	PRO	O-C-N	-5.64	118.50	121.15
1	D	38	PRO	N-CA-CB	5.59	106.13	103.22
1	B	456	ASN	CB-CA-C	5.52	115.63	110.17
1	A	160	ASP	CA-CB-CG	5.48	118.08	112.60
1	D	318	ASN	CA-CB-CG	5.46	118.06	112.60
1	B	250	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	154	GLU	CB-CG-CD	5.37	121.72	112.60
1	B	521	PHE	CA-CB-CG	5.20	119.00	113.80
1	C	364	GLU	CB-CA-C	-5.16	101.91	110.68

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	ARG	Sidechain
1	A	316	ARG	Sidechain
1	A	339	ARG	Sidechain
1	A	376	ARG	Sidechain
1	A	383	ARG	Sidechain
1	A	400	ARG	Sidechain
1	A	443	ARG	Sidechain
1	A	445	ARG	Sidechain
1	A	467	ARG	Sidechain
1	B	294	ARG	Sidechain
1	B	400	ARG	Sidechain
1	B	445	ARG	Sidechain
1	B	447	ARG	Sidechain
1	B	467	ARG	Sidechain
1	B	489	ARG	Sidechain
1	C	342	ARG	Sidechain
1	C	376	ARG	Sidechain
1	C	43	ARG	Sidechain
1	C	445	ARG	Sidechain
1	C	447	ARG	Sidechain
1	D	316	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	400	ARG	Sidechain
1	D	447	ARG	Sidechain
1	D	467	ARG	Sidechain
1	D	56	ARG	Sidechain
1	D	73	ARG	Sidechain

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	3997	0	4079	55	0
1	B	3994	0	4076	65	1
1	C	4006	0	4088	60	0
1	D	3950	0	4033	57	1
2	A	7	0	4	0	0
2	B	7	0	4	1	0
2	C	7	0	4	0	0
2	D	7	0	4	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	88	0	0	1	0
4	B	156	0	0	0	0
4	C	134	0	0	4	0
4	D	110	0	0	2	0
All	All	16478	0	16292	221	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (221) 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:372:LEU:HD11	1:B:376:ARG:CZ	1.85	1.07
1:C:330:MET:HE3	1:C:348:VAL:HG22	1.31	1.07
1:A:339:ARG:NH1	1:B:199:ASN:HD21	1.56	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ARG:HH21	1:B:443:ARG:HH12	1.12	0.97
1:A:330:MET:HE2	1:A:348:VAL:HG22	1.48	0.95
1:D:294:ARG:NH2	1:D:330:MET:HE3	1.82	0.94
1:B:436:ARG:HH21	1:B:443:ARG:NH1	1.67	0.93
1:D:330:MET:HA	1:D:330:MET:HE2	1.52	0.89
1:A:339:ARG:HH11	1:B:199:ASN:HD21	0.91	0.88
1:B:330:MET:CE	1:B:330:MET:HA	2.07	0.84
1:D:167:VAL:HG21	1:D:215:ALA:O	1.78	0.83
1:C:330:MET:CE	1:C:348:VAL:HG22	2.11	0.81
1:A:339:ARG:HH11	1:B:199:ASN:ND2	1.76	0.80
1:D:294:ARG:NH2	1:D:330:MET:CE	2.44	0.79
1:A:16:GLN:HE21	1:A:42:ALA:H	1.29	0.79
1:C:437:SER:OG	1:C:522:THR:HG21	1.82	0.79
1:B:330:MET:HE2	1:B:348:VAL:HG22	1.68	0.76
1:C:41:THR:HG22	1:C:42:ALA:O	1.85	0.75
1:D:124:ILE:HA	1:D:152:CYS:SG	2.27	0.74
1:B:330:MET:HA	1:B:330:MET:HE3	1.68	0.73
1:D:144:LEU:HD21	1:D:164:ILE:HD11	1.71	0.72
1:B:8:ALA:HB3	1:B:106:ARG:HH12	1.55	0.71
1:C:482:TRP:CH2	1:C:515:TRP:O	2.44	0.70
1:D:16:GLN:HE22	1:D:449:PRO:HD3	1.57	0.70
1:A:153:ASP:O	1:A:155:ASN:N	2.25	0.69
1:A:339:ARG:NH1	1:B:199:ASN:ND2	2.37	0.69
1:B:9:GLY:HA3	1:B:66:LYS:HB3	1.74	0.68
1:B:436:ARG:NH2	1:B:443:ARG:HH12	1.90	0.68
1:B:187:GLN:HB3	1:B:194:VAL:HG13	1.75	0.68
1:B:22:MET:HE3	1:B:447:ARG:HD3	1.77	0.67
1:A:330:MET:HA	1:A:330:MET:HE3	1.76	0.66
1:C:329:GLN:OE1	1:D:342:ARG:NH2	2.28	0.66
1:D:294:ARG:HH21	1:D:330:MET:HE3	1.59	0.66
1:A:16:GLN:HE21	1:A:42:ALA:N	1.93	0.64
1:C:327:ALA:HB1	1:C:360:MET:HE2	1.79	0.64
1:D:168:VAL:HG13	1:D:185:VAL:HG11	1.79	0.64
1:A:342:ARG:HD2	1:B:294:ARG:HB3	1.79	0.64
1:D:124:ILE:HD12	1:D:205:SER:OG	1.98	0.64
1:B:372:LEU:C	1:B:372:LEU:HD13	2.23	0.63
1:B:464:HIS:HD1	2:B:601:SER:N	1.97	0.63
1:D:141:LYS:HA	1:D:193:LEU:O	2.00	0.62
1:B:372:LEU:HD11	1:B:376:ARG:NE	2.13	0.61
1:B:168:VAL:O	1:B:188:LYS:HE3	2.00	0.61
1:D:187:GLN:HB3	1:D:194:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:LEU:CD1	1:B:376:ARG:CZ	2.73	0.61
1:C:168:VAL:HG22	1:C:172:SER:CB	2.31	0.60
1:C:482:TRP:CZ3	1:C:515:TRP:O	2.55	0.60
1:A:161:TYR:O	1:A:164:ILE:HG13	2.02	0.59
1:B:8:ALA:HB3	1:B:106:ARG:NH1	2.18	0.58
1:D:120:ARG:HA	1:D:207:LYS:O	2.04	0.58
1:D:151:LYS:C	1:D:152:CYS:SG	2.86	0.58
1:A:159:LEU:HD11	1:A:164:ILE:CD1	2.34	0.58
1:A:144:LEU:HD12	1:A:164:ILE:HD12	1.86	0.58
1:B:145:ASP:O	1:B:146:ASN:HB2	2.03	0.58
1:B:125:LYS:HA	1:B:150:GLU:O	2.05	0.57
1:D:190:ALA:O	1:D:191:ASP:HB2	2.03	0.57
1:B:372:LEU:HD11	1:B:376:ARG:NH1	2.17	0.57
1:A:137:GLY:O	1:A:197:VAL:HB	2.06	0.56
1:B:74:LEU:HD11	1:B:88:ILE:CG1	2.34	0.56
1:B:416:ALA:HB2	1:B:512:LEU:HD11	1.87	0.56
1:C:516:ARG:HB3	1:C:517:PRO:HD2	1.88	0.56
1:B:8:ALA:CB	1:B:106:ARG:HH12	2.18	0.56
1:A:134:LEU:HD23	1:A:203:LEU:HD12	1.88	0.56
1:A:414:VAL:HG22	1:A:444:TYR:CZ	2.41	0.55
1:D:124:ILE:HG13	1:D:152:CYS:SG	2.46	0.55
1:B:121:THR:HB	1:B:157:LEU:HD11	1.88	0.55
1:A:73:ARG:HD2	1:A:360:MET:SD	2.46	0.55
1:D:9:GLY:HA3	1:D:66:LYS:HB3	1.89	0.55
1:A:159:LEU:HD11	1:A:164:ILE:HD11	1.87	0.55
1:B:390:TYR:O	1:B:394:LEU:HD13	2.07	0.55
1:D:216:VAL:O	1:D:246:ARG:NH1	2.40	0.55
1:D:330:MET:HA	1:D:330:MET:CE	2.29	0.55
1:C:192:PHE:C	1:C:193:LEU:HD22	2.32	0.55
1:C:185:VAL:HA	1:C:195:THR:HG22	1.89	0.55
1:A:270:LYS:HE2	1:A:272:GLU:OE1	2.07	0.54
1:A:134:LEU:CD1	1:A:197:VAL:HG21	2.37	0.54
1:B:330:MET:HA	1:B:330:MET:HE2	1.86	0.54
1:C:206:LYS:O	1:C:206:LYS:HG2	2.07	0.54
1:A:434:SER:OG	3:A:602:PO4:O3	2.20	0.53
1:D:41:THR:HG22	1:D:42:ALA:O	2.08	0.53
1:D:173:LYS:O	1:D:212:PRO:HD3	2.08	0.53
1:C:175:TYR:HE2	1:C:212:PRO:HG2	1.74	0.53
1:C:152:CYS:SG	1:C:157:LEU:HD12	2.49	0.53
1:A:182:SER:HB3	1:A:199:ASN:HB2	1.90	0.53
1:A:482:TRP:HB2	1:A:517:PRO:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:GLU:CD	1:C:467:ARG:HH22	2.17	0.52
1:B:409:THR:HB	1:B:440:GLN:HE22	1.75	0.52
1:C:73:ARG:HD2	1:C:360:MET:SD	2.50	0.52
1:A:319:ARG:O	1:A:443:ARG:NH2	2.43	0.52
1:C:372:LEU:HB2	4:C:823:HOH:O	2.10	0.52
1:B:372:LEU:CD1	1:B:376:ARG:NH1	2.72	0.52
1:A:16:GLN:NE2	1:A:42:ALA:H	2.05	0.52
1:D:512:LEU:HD12	1:D:512:LEU:N	2.25	0.52
1:B:168:VAL:O	1:B:188:LYS:CE	2.58	0.51
1:C:147:ALA:O	1:C:148:TYR:CG	2.62	0.51
1:A:338:PRO:HG2	1:A:339:ARG:NH1	2.25	0.51
1:B:411:ALA:HA	1:D:422:LYS:HE3	1.93	0.51
1:D:142:ILE:HA	1:D:157:LEU:O	2.11	0.51
1:A:144:LEU:HD12	1:A:164:ILE:CD1	2.40	0.51
1:A:392:LEU:O	1:A:396:GLU:HG2	2.10	0.51
1:C:74:LEU:HD11	1:C:88:ILE:CG1	2.41	0.51
1:B:386:GLU:CD	1:B:467:ARG:HH22	2.19	0.50
1:C:409:THR:HG23	1:C:521:PHE:HB3	1.92	0.50
1:B:521:PHE:N	1:B:521:PHE:CD2	2.80	0.50
1:C:437:SER:OG	1:C:522:THR:CG2	2.55	0.50
1:C:59:GLU:HG2	4:C:820:HOH:O	2.11	0.50
1:B:526:ARG:HD3	1:D:515:TRP:HB2	1.94	0.49
1:D:294:ARG:HD2	1:D:326:CYS:SG	2.52	0.49
1:C:148:TYR:CG	1:C:156:ILE:HD11	2.48	0.49
1:C:314:ILE:HD11	1:C:326:CYS:SG	2.52	0.49
1:A:159:LEU:HD11	1:A:164:ILE:HG12	1.93	0.49
1:D:124:ILE:HG22	1:D:124:ILE:O	2.12	0.49
1:B:16:GLN:HE21	1:B:42:ALA:H	1.60	0.49
1:C:163:ASN:O	1:C:164:ILE:C	2.55	0.49
1:A:330:MET:HA	1:A:330:MET:CE	2.41	0.48
1:A:146:ASN:C	1:A:148:TYR:H	2.21	0.48
1:C:217:ASP:C	1:C:217:ASP:OD2	2.56	0.48
1:B:113:ASP:OD1	1:B:270:LYS:NZ	2.39	0.48
1:C:125:LYS:HB2	4:C:791:HOH:O	2.13	0.48
1:B:516:ARG:HH11	1:D:483:ALA:HB3	1.78	0.48
1:C:252:HIS:CD2	4:C:829:HOH:O	2.67	0.48
1:B:74:LEU:HD11	1:B:88:ILE:HG13	1.96	0.47
1:C:330:MET:HE2	1:C:359:ILE:CG2	2.43	0.47
1:D:221:VAL:HG12	1:D:226:ILE:HG13	1.97	0.47
1:C:330:MET:HE2	1:C:359:ILE:HG23	1.96	0.47
1:D:143:THR:HG21	1:D:156:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LEU:HD11	1:B:164:ILE:HG12	1.96	0.47
1:B:16:GLN:HE22	1:B:449:PRO:HD3	1.79	0.47
1:D:437:SER:HA	1:D:440:GLN:HE21	1.80	0.47
1:D:132:VAL:HG21	1:D:152:CYS:O	2.14	0.47
1:D:141:LYS:N	1:D:155:ASN:O	2.30	0.47
1:A:515:TRP:HB2	1:C:526:ARG:HD3	1.95	0.47
1:B:22:MET:HE1	1:B:391:HIS:H	1.80	0.47
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.50	0.47
1:A:167:VAL:HG21	1:A:215:ALA:C	2.39	0.47
1:A:241:PHE:CD2	1:A:291:MET:HE1	2.49	0.47
1:C:16:GLN:HE21	1:C:42:ALA:H	1.62	0.47
1:C:241:PHE:CD2	1:C:291:MET:HE1	2.49	0.47
1:D:140:LEU:N	1:D:154:GLU:O	2.49	0.46
1:A:132:VAL:HG11	1:A:153:ASP:HA	1.98	0.46
1:A:167:VAL:HG21	1:A:215:ALA:O	2.15	0.46
1:B:331:LEU:O	1:B:364:GLU:HG2	2.15	0.46
1:C:175:TYR:CE2	1:C:212:PRO:HG2	2.50	0.46
1:C:211:LEU:HB3	1:C:214:ALA:HB3	1.98	0.46
1:D:169:GLU:O	1:D:170:VAL:C	2.58	0.46
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.98	0.46
1:B:73:ARG:HD2	1:B:360:MET:SD	2.55	0.46
1:C:167:VAL:HG13	1:C:214:ALA:HB1	1.98	0.46
1:A:399:ARG:NH1	1:A:418:GLU:OE2	2.49	0.46
1:C:414:VAL:HG22	1:C:444:TYR:CZ	2.50	0.46
1:D:73:ARG:HD2	1:D:360:MET:SD	2.56	0.46
1:B:422:LYS:CE	1:D:411:ALA:HA	2.46	0.46
1:A:144:LEU:HD11	1:A:162:LYS:O	2.15	0.46
1:C:6:SER:O	1:C:7:GLU:C	2.58	0.46
1:D:398:LEU:HD13	1:D:443:ARG:O	2.16	0.45
1:B:516:ARG:HH11	1:D:483:ALA:CB	2.29	0.45
1:B:241:PHE:HB3	1:B:270:LYS:HD2	1.99	0.45
1:C:136:LYS:HA	1:C:197:VAL:HG12	1.98	0.45
1:D:187:GLN:HB3	1:D:194:VAL:CG2	2.45	0.45
1:C:142:ILE:HA	1:C:157:LEU:O	2.17	0.45
1:C:50:THR:OG1	1:C:73:ARG:HD3	2.15	0.45
1:D:24:ASP:HB2	4:D:736:HOH:O	2.17	0.45
1:D:311:LYS:NZ	1:D:354:ASP:OD1	2.48	0.45
1:A:148:TYR:CD2	1:A:156:ILE:CD1	3.01	0.45
1:A:414:VAL:HG22	1:A:444:TYR:CE2	2.52	0.45
1:B:159:LEU:HD11	1:B:164:ILE:HD11	1.99	0.45
1:C:168:VAL:HG22	1:C:172:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD11	1:A:164:ILE:CG1	2.47	0.44
1:A:159:LEU:HD12	1:A:159:LEU:C	2.43	0.44
1:C:74:LEU:HD11	1:C:88:ILE:HG12	2.00	0.44
1:C:188:LYS:HD2	1:C:189:GLY:O	2.18	0.44
1:C:48:ILE:HG12	1:C:71:VAL:HB	1.99	0.44
1:B:159:LEU:HD11	1:B:164:ILE:CD1	2.47	0.44
1:D:482:TRP:HB2	1:D:517:PRO:HG3	2.00	0.44
1:D:118:GLU:HB3	1:D:120:ARG:HH11	1.83	0.44
1:C:353:LEU:CD1	1:D:311:LYS:HE3	2.48	0.43
1:B:139:THR:HG22	1:B:186:LYS:NZ	2.34	0.43
1:C:330:MET:HE3	1:C:348:VAL:CG2	2.24	0.43
1:A:211:LEU:HB3	1:A:214:ALA:HB3	2.00	0.43
1:B:437:SER:OG	1:B:522:THR:HG23	2.18	0.43
1:C:9:GLY:HA2	1:C:66:LYS:HB3	2.01	0.43
1:C:115:LYS:HD3	1:C:224:LYS:HD3	2.01	0.43
1:C:182:SER:HB3	1:C:199:ASN:HB2	2.00	0.43
1:C:518:GLY:O	1:C:520:GLY:N	2.51	0.43
1:B:416:ALA:CB	1:B:512:LEU:HD11	2.49	0.43
1:C:112:LEU:C	1:C:112:LEU:HD23	2.43	0.43
1:D:74:LEU:HD11	1:D:88:ILE:HG13	2.01	0.43
1:D:142:ILE:O	1:D:192:PHE:HA	2.18	0.43
1:B:120:ARG:HA	1:B:207:LYS:O	2.19	0.42
1:B:144:LEU:HD23	1:B:164:ILE:CD1	2.49	0.42
1:C:342:ARG:HD3	1:D:329:GLN:OE1	2.19	0.42
1:A:492:PHE:O	1:A:496:VAL:HG23	2.19	0.42
1:C:331:LEU:O	1:C:364:GLU:HG2	2.19	0.42
1:A:409:THR:HG22	1:A:522:THR:H	1.84	0.42
1:C:165:CYS:SG	1:C:193:LEU:HD21	2.60	0.42
1:C:123:LEU:HD13	1:C:205:SER:HB3	2.01	0.42
1:D:20:ALA:HB3	1:D:447:ARG:HH22	1.84	0.41
1:D:168:VAL:CG1	1:D:185:VAL:HG11	2.50	0.41
1:D:522:THR:HG23	4:D:772:HOH:O	2.20	0.41
1:A:409:THR:HG22	1:A:522:THR:N	2.35	0.41
1:B:159:LEU:C	1:B:159:LEU:HD12	2.45	0.41
1:D:334:MET:HE3	1:D:338:PRO:C	2.45	0.41
1:D:136:LYS:HD3	1:D:136:LYS:C	2.45	0.41
1:B:482:TRP:CZ3	1:B:515:TRP:O	2.73	0.41
1:A:186:LYS:HE3	1:A:196:GLU:N	2.35	0.41
1:D:415:GLY:HA3	1:D:525:MET:HE1	2.02	0.41
1:B:422:LYS:HE3	1:D:411:ALA:HA	2.02	0.41
1:A:164:ILE:HG23	1:A:211:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:HG3	4:A:761:HOH:O	2.21	0.41
1:A:132:VAL:HG21	1:A:153:ASP:HA	2.02	0.41
1:A:41:THR:HG22	1:A:42:ALA:O	2.21	0.41
1:B:423:CYS:O	1:B:424:CYS:C	2.64	0.41
1:C:180:LEU:O	1:C:180:LEU:HD13	2.20	0.41
1:A:415:GLY:HA3	1:A:525:MET:HE1	2.03	0.41
1:B:164:ILE:HG23	1:B:211:LEU:HD21	2.03	0.40
1:C:383:ARG:O	1:C:386:GLU:HB2	2.22	0.40
1:A:329:GLN:OE1	1:B:342:ARG:NH2	2.46	0.40
1:C:386:GLU:OE2	1:C:467:ARG:NH2	2.36	0.40
1:A:302:PRO:O	1:A:303:ALA:C	2.64	0.40
1:B:152:CYS:SG	1:B:157:LEU:HD12	2.61	0.40
1:A:143:THR:OG1	1:A:144:LEU:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ARG:NH2	1:D:166:LYS:O[1_556]	2.12	0.08

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	518/552 (94%)	493 (95%)	20 (4%)	5 (1%)	12	8
1	B	517/552 (94%)	495 (96%)	16 (3%)	6 (1%)	10	6
1	C	519/552 (94%)	494 (95%)	20 (4%)	5 (1%)	12	8
1	D	510/552 (92%)	487 (96%)	18 (4%)	5 (1%)	12	8
All	All	2064/2208 (94%)	1969 (95%)	74 (4%)	21 (1%)	12	8

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	LYS
1	A	154	GLU
1	C	148	TYR
1	C	519	SER
1	D	140	LEU
1	D	170	VAL
1	A	521	PHE
1	B	7	GLU
1	B	146	ASN
1	B	206	LYS
1	B	519	SER
1	B	521	PHE
1	D	139	THR
1	D	191	ASP
1	D	519	SER
1	A	405	THR
1	C	7	GLU
1	C	10	THR
1	A	303	ALA
1	B	177	ASP
1	C	9	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	428/454 (94%)	393 (92%)	35 (8%)	10	8
1	B	429/454 (94%)	400 (93%)	29 (7%)	14	11
1	C	430/454 (95%)	399 (93%)	31 (7%)	13	10
1	D	424/454 (93%)	398 (94%)	26 (6%)	17	14
All	All	1711/1816 (94%)	1590 (93%)	121 (7%)	13	10

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

Mol	Chain	Res	Type
1	A	28	GLU

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Mol	Chain	Res	Type
1	A	37	SER
1	A	74	LEU
1	A	123	LEU
1	A	125	LYS
1	A	134	LEU
1	A	135	LYS
1	A	136	LYS
1	A	141	LYS
1	A	143	THR
1	A	145	ASP
1	A	149	MET
1	A	150	GLU
1	A	164	ILE
1	A	168	VAL
1	A	180	LEU
1	A	181	ILE
1	A	185	VAL
1	A	187	GLN
1	A	191	ASP
1	A	193	LEU
1	A	207	LYS
1	A	211	LEU
1	A	234	GLU
1	A	240	VAL
1	A	285	GLU
1	A	297	LEU
1	A	301	ILE
1	A	330	MET
1	A	342	ARG
1	A	372	LEU
1	A	394	LEU
1	A	437	SER
1	A	443	ARG
1	A	512	LEU
1	B	6	SER
1	B	17	GLN
1	B	28	GLU
1	B	125	LYS
1	B	132	VAL
1	B	151	LYS
1	B	154	GLU
1	B	162	LYS

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Mol	Chain	Res	Type
1	B	164	ILE
1	B	167	VAL
1	B	168	VAL
1	B	180	LEU
1	B	185	VAL
1	B	193	LEU
1	B	194	VAL
1	B	203	LEU
1	B	211	LEU
1	B	230	LYS
1	B	234	GLU
1	B	256	LYS
1	B	297	LEU
1	B	330	MET
1	B	342	ARG
1	B	392	LEU
1	B	394	LEU
1	B	407	ASP
1	B	436	ARG
1	B	504	LYS
1	B	521	PHE
1	C	41	THR
1	C	129	THR
1	C	139	THR
1	C	140	LEU
1	C	156	ILE
1	C	164	ILE
1	C	166	LYS
1	C	167	VAL
1	C	168	VAL
1	C	180	LEU
1	C	185	VAL
1	C	186	LYS
1	C	187	GLN
1	C	194	VAL
1	C	199	ASN
1	C	203	LEU
1	C	206	LYS
1	C	211	LEU
1	C	217	ASP
1	C	256	LYS
1	C	261	LYS

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Mol	Chain	Res	Type
1	C	297	LEU
1	C	301	ILE
1	C	336	LYS
1	C	342	ARG
1	C	372	LEU
1	C	418	GLU
1	C	443	ARG
1	C	447	ARG
1	C	521	PHE
1	C	522	THR
1	D	24	ASP
1	D	74	LEU
1	D	123	LEU
1	D	131	GLU
1	D	141	LYS
1	D	152	CYS
1	D	154	GLU
1	D	162	LYS
1	D	164	ILE
1	D	168	VAL
1	D	169	GLU
1	D	172	SER
1	D	180	LEU
1	D	186	LYS
1	D	188	LYS
1	D	193	LEU
1	D	194	VAL
1	D	216	VAL
1	D	253	GLU
1	D	297	LEU
1	D	332	GLU
1	D	342	ARG
1	D	372	LEU
1	D	394	LEU
1	D	436	ARG
1	D	522	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	44	ASN

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Mol	Chain	Res	Type
1	A	146	ASN
1	A	252	HIS
1	A	378	GLN
1	B	16	GLN
1	B	146	ASN
1	B	155	ASN
1	B	199	ASN
1	B	378	GLN
1	B	440	GLN
1	B	458	GLN
1	B	479	GLN
1	C	16	GLN
1	C	17	GLN
1	C	19	HIS
1	C	29	HIS
1	C	146	ASN
1	C	163	ASN
1	C	187	GLN
1	C	252	HIS
1	C	378	GLN
1	C	393	GLN
1	C	440	GLN
1	C	479	GLN
1	D	16	GLN
1	D	29	HIS
1	D	155	ASN
1	D	163	ASN
1	D	210	ASN
1	D	378	GLN
1	D	393	GLN
1	D	440	GLN
1	D	458	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	SER	C	601	-	4,6,6	1.22	1 (25%)	2,7,7	1.11	0
3	PO4	A	602	-	4,4,4	1.03	0	6,6,6	1.19	0
3	PO4	B	602	-	4,4,4	0.64	0	6,6,6	1.49	1 (16%)
3	PO4	C	602	-	4,4,4	0.72	0	6,6,6	1.05	0
2	SER	B	601	-	4,6,6	1.17	0	2,7,7	1.55	1 (50%)
2	SER	D	601	-	4,6,6	0.91	0	2,7,7	1.14	0
2	SER	A	601	-	4,6,6	0.58	0	2,7,7	2.32	1 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SER	C	601	-	-	0/6/6/6	-
2	SER	B	601	-	-	0/6/6/6	-
2	SER	D	601	-	-	0/6/6/6	-
2	SER	A	601	-	-	0/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	SER	O-C	2.18	1.28	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	SER	OXT-C-O	-3.08	117.09	124.08
3	B	602	PO4	O4-P-O1	-2.26	102.95	110.95
2	B	601	SER	OXT-C-O	-2.05	119.42	124.08

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
3	A	602	PO4	1	0
2	B	601	SER	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	522/552 (94%)	0.52	51 (9%) 13 14	14, 30, 81, 116	0
1	B	521/552 (94%)	0.22	35 (6%) 24 26	11, 24, 64, 95	0
1	C	523/552 (94%)	0.36	37 (7%) 22 24	12, 26, 63, 92	0
1	D	516/552 (93%)	0.55	64 (12%) 8 9	14, 29, 90, 131	0
All	All	2082/2208 (94%)	0.41	187 (8%) 15 16	11, 27, 76, 131	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	ALA	6.0
1	D	130	ALA	5.9
1	B	189	GLY	5.7
1	D	404	ILE	5.4
1	A	190	ALA	5.4
1	B	124	ILE	5.3
1	A	404	ILE	5.0
1	B	519	SER	4.9
1	B	21	ALA	4.8
1	D	124	ILE	4.8
1	A	520	GLY	4.8
1	B	404	ILE	4.7
1	A	152	CYS	4.6
1	C	404	ILE	4.6
1	C	8	ALA	4.5
1	A	189	GLY	4.5
1	D	138	ALA	4.5
1	C	521	PHE	4.4
1	A	124	ILE	4.3
1	A	192	PHE	4.3
1	A	197	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	405	THR	4.2
1	D	132	VAL	4.2
1	D	139	THR	4.1
1	B	521	PHE	4.1
1	D	186	LYS	4.1
1	D	170	VAL	4.0
1	D	8	ALA	3.9
1	D	144	LEU	3.9
1	D	123	LEU	3.9
1	B	190	ALA	3.9
1	B	192	PHE	3.7
1	A	138	ALA	3.7
1	D	190	ALA	3.6
1	D	158	TRP	3.6
1	B	215	ALA	3.6
1	C	6	SER	3.6
1	C	20	ALA	3.5
1	D	159	LEU	3.5
1	A	185	VAL	3.5
1	B	20	ALA	3.5
1	A	403	PRO	3.5
1	B	154	GLU	3.5
1	A	519	SER	3.4
1	A	402	ALA	3.4
1	D	156	ILE	3.3
1	C	194	VAL	3.3
1	A	142	ILE	3.3
1	B	151	LYS	3.3
1	A	125	LYS	3.3
1	C	144	LEU	3.2
1	D	180	LEU	3.2
1	D	172	SER	3.2
1	D	213	GLY	3.1
1	D	197	VAL	3.1
1	C	406	SER	3.1
1	A	126	GLY	3.1
1	C	153	ASP	3.1
1	A	168	VAL	3.1
1	C	124	ILE	3.1
1	D	406	SER	3.1
1	D	181	ILE	3.1
1	D	173	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	157	LEU	3.0
1	D	185	VAL	3.0
1	A	137	GLY	3.0
1	D	200	GLY	3.0
1	A	521	PHE	3.0
1	C	125	LYS	3.0
1	A	481	ALA	3.0
1	D	146	ASN	3.0
1	C	193	LEU	3.0
1	A	154	GLU	3.0
1	A	155	ASN	3.0
1	A	10	THR	3.0
1	C	143	THR	3.0
1	D	403	PRO	3.0
1	C	519	SER	2.9
1	D	137	GLY	2.9
1	C	149	MET	2.9
1	A	123	LEU	2.9
1	B	6	SER	2.9
1	D	193	LEU	2.9
1	D	216	VAL	2.9
1	A	148	TYR	2.9
1	B	406	SER	2.9
1	A	204	GLY	2.8
1	D	214	ALA	2.8
1	C	10	THR	2.8
1	D	215	ALA	2.8
1	A	183	LEU	2.8
1	A	186	LYS	2.8
1	C	19	HIS	2.7
1	A	198	GLU	2.7
1	D	194	VAL	2.7
1	C	123	LEU	2.7
1	B	125	LYS	2.7
1	C	520	GLY	2.7
1	D	22	MET	2.7
1	D	155	ASN	2.7
1	A	178	ASP	2.6
1	C	159	LEU	2.6
1	D	192	PHE	2.6
1	A	191	ASP	2.6
1	A	156	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	165	CYS	2.6
1	C	164	ILE	2.6
1	C	517	PRO	2.6
1	A	406	SER	2.6
1	B	214	ALA	2.5
1	D	201	GLY	2.5
1	B	19	HIS	2.5
1	A	166	LYS	2.5
1	A	21	ALA	2.5
1	A	484	GLU	2.5
1	B	8	ALA	2.5
1	C	180	LEU	2.5
1	C	22	MET	2.5
1	C	518	GLY	2.5
1	A	146	ASN	2.5
1	B	405	THR	2.5
1	D	195	THR	2.5
1	B	155	ASN	2.5
1	B	145	ASP	2.4
1	D	178	ASP	2.4
1	D	135	LYS	2.4
1	D	204	GLY	2.4
1	B	170	VAL	2.4
1	A	199	ASN	2.4
1	B	149	MET	2.4
1	B	186	LYS	2.4
1	D	165	CYS	2.4
1	B	148	TYR	2.3
1	C	21	ALA	2.3
1	D	203	LEU	2.3
1	D	188	LYS	2.3
1	D	119	ILE	2.3
1	B	167	VAL	2.3
1	B	403	PRO	2.3
1	D	405	THR	2.3
1	C	405	THR	2.3
1	C	9	GLY	2.3
1	D	134	LEU	2.3
1	D	171	GLY	2.3
1	D	202	SER	2.3
1	C	129	THR	2.3
1	A	200	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	518	GLY	2.3
1	B	218	LEU	2.3
1	D	143	THR	2.2
1	A	149	MET	2.2
1	B	520	GLY	2.2
1	A	22	MET	2.2
1	A	157	LEU	2.2
1	C	148	TYR	2.2
1	D	182	SER	2.2
1	D	163	ASN	2.2
1	A	8	ALA	2.2
1	D	152	CYS	2.2
1	D	205	SER	2.2
1	D	166	LYS	2.2
1	B	138	ALA	2.1
1	D	11	ALA	2.1
1	D	136	LYS	2.1
1	C	187	GLN	2.1
1	B	216	VAL	2.1
1	A	278	ARG	2.1
1	A	20	ALA	2.1
1	D	21	ALA	2.1
1	B	165	CYS	2.1
1	C	377	MET	2.1
1	A	217	ASP	2.1
1	D	117	PRO	2.1
1	D	120	ARG	2.1
1	A	216	VAL	2.1
1	D	168	VAL	2.1
1	C	135	LYS	2.1
1	D	141	LYS	2.1
1	A	409	THR	2.1
1	C	122	GLY	2.1
1	B	147	ALA	2.1
1	D	191	ASP	2.0
1	B	517	PRO	2.0
1	D	212	PRO	2.0
1	A	141	LYS	2.0
1	C	199	ASN	2.0
1	C	191	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
3	PO4	A	602	5/5	0.80	0.16	35,44,59,65	0
2	SER	B	601	7/7	0.93	0.07	16,19,22,25	0
2	SER	C	601	7/7	0.93	0.09	21,23,24,26	0
2	SER	D	601	7/7	0.93	0.11	27,29,30,31	0
2	SER	A	601	7/7	0.93	0.11	23,24,28,33	0
3	PO4	B	602	5/5	0.94	0.14	33,40,43,45	0
3	PO4	C	602	5/5	0.94	0.10	28,35,39,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.