



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:29 PM UTC

PDB ID : 8IAS / pdb_00008ias
Title : Crystal structure of Streptococcus pneumoniae pyruvate kinase
Authors : Nakashima, R.; Taguchi, A.
Deposited on : 2023-02-09
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

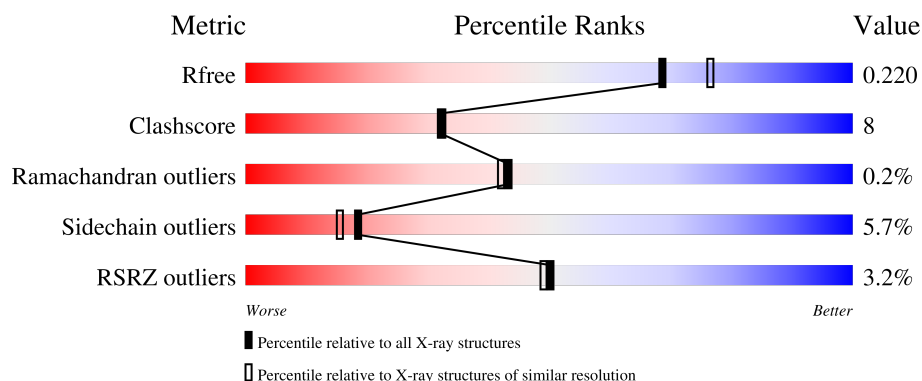
1 Overall quality at a glance

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	521	0% 84% 11% ...
1	B	521	3% 79% 15% ...
1	C	521	3% 80% 14% ...
1	D	521	5% 74% 20% ...

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16233 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	0	0
			3832	2394	663	759	16			
1	B	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	C	500	Total	C	N	O	S	0	0	0
			3832	2394	663	759	16			
1	D	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8DQ84
A	-18	GLY	-	expression tag	UNP Q8DQ84
A	-17	SER	-	expression tag	UNP Q8DQ84
A	-16	SER	-	expression tag	UNP Q8DQ84
A	-15	HIS	-	expression tag	UNP Q8DQ84
A	-14	HIS	-	expression tag	UNP Q8DQ84
A	-13	HIS	-	expression tag	UNP Q8DQ84
A	-12	HIS	-	expression tag	UNP Q8DQ84
A	-11	HIS	-	expression tag	UNP Q8DQ84
A	-10	HIS	-	expression tag	UNP Q8DQ84
A	-9	SER	-	expression tag	UNP Q8DQ84
A	-8	SER	-	expression tag	UNP Q8DQ84
A	-7	GLY	-	expression tag	UNP Q8DQ84
A	-6	LEU	-	expression tag	UNP Q8DQ84
A	-5	VAL	-	expression tag	UNP Q8DQ84
A	-4	PRO	-	expression tag	UNP Q8DQ84
A	-3	ARG	-	expression tag	UNP Q8DQ84
A	-2	GLY	-	expression tag	UNP Q8DQ84
A	-1	SER	-	expression tag	UNP Q8DQ84
A	0	HIS	-	expression tag	UNP Q8DQ84
B	1	MET	-	initiating methionine	UNP Q8DQ84

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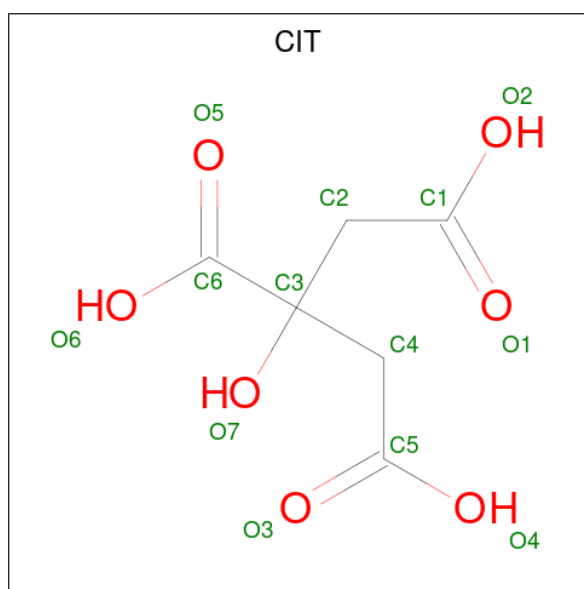
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	GLY	-	expression tag	UNP Q8DQ84
B	3	SER	-	expression tag	UNP Q8DQ84
B	4	SER	-	expression tag	UNP Q8DQ84
B	5	HIS	-	expression tag	UNP Q8DQ84
B	6	HIS	-	expression tag	UNP Q8DQ84
B	7	HIS	-	expression tag	UNP Q8DQ84
B	8	HIS	-	expression tag	UNP Q8DQ84
B	9	HIS	-	expression tag	UNP Q8DQ84
B	10	HIS	-	expression tag	UNP Q8DQ84
B	11	SER	-	expression tag	UNP Q8DQ84
B	12	SER	-	expression tag	UNP Q8DQ84
B	13	GLY	-	expression tag	UNP Q8DQ84
B	14	LEU	-	expression tag	UNP Q8DQ84
B	15	VAL	-	expression tag	UNP Q8DQ84
B	16	PRO	-	expression tag	UNP Q8DQ84
B	17	ARG	-	expression tag	UNP Q8DQ84
B	18	GLY	-	expression tag	UNP Q8DQ84
B	19	SER	-	expression tag	UNP Q8DQ84
B	20	HIS	-	expression tag	UNP Q8DQ84
C	1	MET	-	initiating methionine	UNP Q8DQ84
C	2	GLY	-	expression tag	UNP Q8DQ84
C	3	SER	-	expression tag	UNP Q8DQ84
C	4	SER	-	expression tag	UNP Q8DQ84
C	5	HIS	-	expression tag	UNP Q8DQ84
C	6	HIS	-	expression tag	UNP Q8DQ84
C	7	HIS	-	expression tag	UNP Q8DQ84
C	8	HIS	-	expression tag	UNP Q8DQ84
C	9	HIS	-	expression tag	UNP Q8DQ84
C	10	HIS	-	expression tag	UNP Q8DQ84
C	11	SER	-	expression tag	UNP Q8DQ84
C	12	SER	-	expression tag	UNP Q8DQ84
C	13	GLY	-	expression tag	UNP Q8DQ84
C	14	LEU	-	expression tag	UNP Q8DQ84
C	15	VAL	-	expression tag	UNP Q8DQ84
C	16	PRO	-	expression tag	UNP Q8DQ84
C	17	ARG	-	expression tag	UNP Q8DQ84
C	18	GLY	-	expression tag	UNP Q8DQ84
C	19	SER	-	expression tag	UNP Q8DQ84
C	20	HIS	-	expression tag	UNP Q8DQ84
D	1	MET	-	initiating methionine	UNP Q8DQ84
D	2	GLY	-	expression tag	UNP Q8DQ84
D	3	SER	-	expression tag	UNP Q8DQ84

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Chain	Residue	Modelled	Actual	Comment	Reference
D	4	SER	-	expression tag	UNP Q8DQ84
D	5	HIS	-	expression tag	UNP Q8DQ84
D	6	HIS	-	expression tag	UNP Q8DQ84
D	7	HIS	-	expression tag	UNP Q8DQ84
D	8	HIS	-	expression tag	UNP Q8DQ84
D	9	HIS	-	expression tag	UNP Q8DQ84
D	10	HIS	-	expression tag	UNP Q8DQ84
D	11	SER	-	expression tag	UNP Q8DQ84
D	12	SER	-	expression tag	UNP Q8DQ84
D	13	GLY	-	expression tag	UNP Q8DQ84
D	14	LEU	-	expression tag	UNP Q8DQ84
D	15	VAL	-	expression tag	UNP Q8DQ84
D	16	PRO	-	expression tag	UNP Q8DQ84
D	17	ARG	-	expression tag	UNP Q8DQ84
D	18	GLY	-	expression tag	UNP Q8DQ84
D	19	SER	-	expression tag	UNP Q8DQ84
D	20	HIS	-	expression tag	UNP Q8DQ84

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

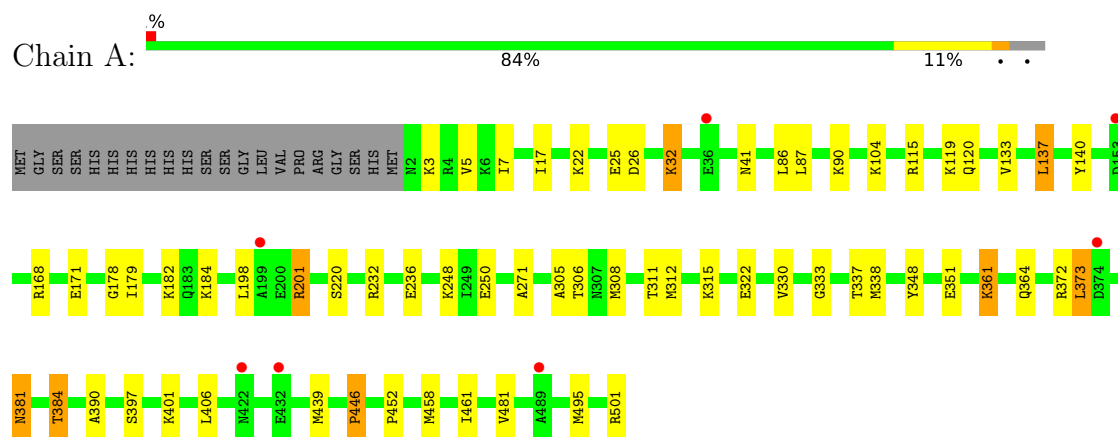
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	254	Total	O	0	0
			254	254		
4	B	223	Total	O	0	0
			223	223		
4	C	189	Total	O	0	0
			189	189		
4	D	191	Total	O	0	0
			191	191		

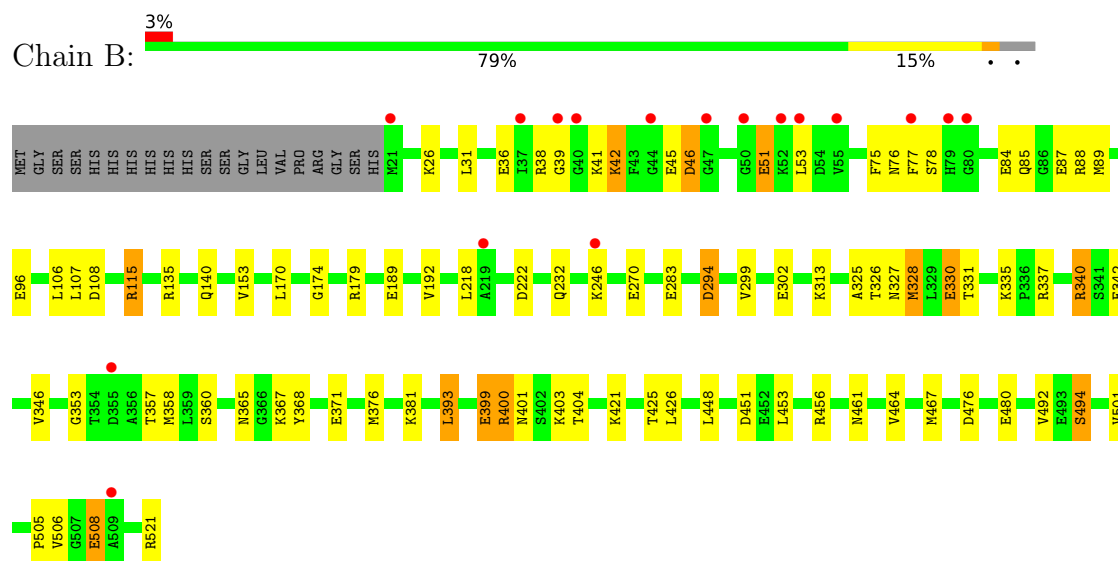
3 Residue-property plots [i](#)

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.

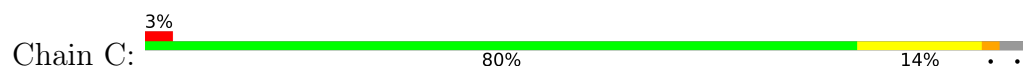
• Molecule 1: Pyruvate kinase

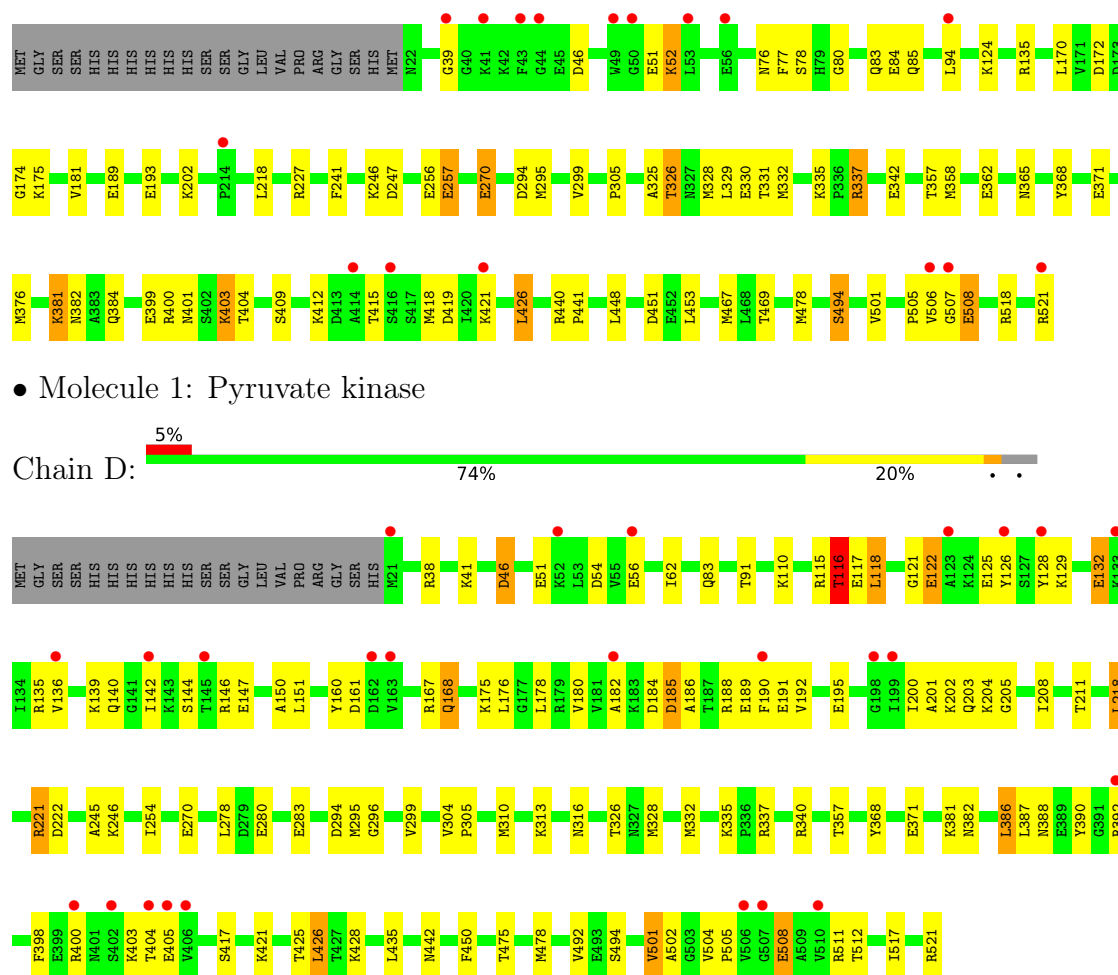


• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.09Å 84.70Å 107.01Å 101.22° 96.82° 91.42°	Depositor
Resolution (Å)	49.07 – 2.00 49.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.07-2.00) 76.2 (49.07-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.178 , 0.215 0.185 , 0.220	Depositor DCC
R_{free} test set	8420 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16233	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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: CIT, GOL

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	1.01	1/3877 (0.0%)	1.27	2/5228 (0.0%)
1	B	0.99	0/3885	1.28	3/5238 (0.1%)
1	C	0.96	2/3877 (0.1%)	1.27	0/5228
1	D	0.99	0/3885	1.28	1/5238 (0.0%)
All	All	0.99	3/15524 (0.0%)	1.28	6/20932 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	446	PRO	C-O	-6.33	1.17	1.23
1	C	440	ARG	N-CA	5.19	1.50	1.46
1	C	305	PRO	C-O	-5.09	1.17	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	THR	CA-CB-OG1	-6.08	100.48	109.60
1	B	360	SER	O-C-N	5.95	125.23	120.83
1	B	330	GLU	CB-CG-CD	5.42	121.81	112.60
1	D	116	THR	CB-CA-C	5.29	118.69	109.65
1	A	384	THR	CB-CA-C	5.26	119.14	110.88
1	A	25	GLU	CB-CA-C	5.14	120.00	109.76

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	3832	0	3876	39	0
1	B	3840	0	3885	65	0
1	C	3832	0	3876	49	0
1	D	3840	0	3885	101	0
2	B	13	0	5	0	0
2	D	13	0	5	1	0
3	D	6	0	8	0	0
4	A	254	0	0	2	0
4	B	223	0	0	2	0
4	C	189	0	0	3	0
4	D	191	0	0	3	0
All	All	16233	0	15540	246	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 (246) 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:77:PHE:CZ	1:B:89:MET:HE1	1.80	1.15
1:B:494:SER:HB2	1:B:521:ARG:OXT	1.50	1.11
1:B:77:PHE:HZ	1:B:89:MET:HE1	1.02	1.11
1:D:116:THR:HG22	1:D:203:GLN:N	1.68	1.08
1:B:39:GLY:HA3	1:B:51:GLU:HG2	1.32	1.08
1:D:139:LYS:HD3	1:D:142:ILE:HD11	1.36	1.03
1:D:116:THR:HG21	1:D:201:ALA:O	1.58	1.02
1:B:328:MET:HE3	1:B:346:VAL:HG22	1.38	1.01
1:D:126:TYR:CG	1:D:146:ARG:HG3	1.97	0.99
1:D:139:LYS:CD	1:D:142:ILE:HD11	1.93	0.98
1:C:328:MET:CE	1:C:357:THR:HB	1.96	0.95
1:B:302:GLU:HG3	1:D:382:ASN:ND2	1.85	0.92
1:D:139:LYS:HB3	1:D:142:ILE:CD1	2.02	0.89
1:D:404:THR:HG22	1:D:435:LEU:HD12	1.54	0.89
1:B:77:PHE:CZ	1:B:89:MET:CE	2.56	0.89
1:B:39:GLY:HA3	1:B:51:GLU:CG	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:TYR:CD1	1:D:146:ARG:HG3	2.12	0.84
1:C:328:MET:HE1	1:C:357:THR:HB	1.58	0.82
1:D:126:TYR:CE1	1:D:146:ARG:HB2	2.13	0.82
1:A:306:THR:HG22	4:A:642:HOH:O	1.81	0.79
1:D:404:THR:HG22	1:D:435:LEU:CD1	2.12	0.79
1:A:120:GLN:HE22	1:A:133:VAL:H	1.31	0.77
1:D:116:THR:CG2	1:D:203:GLN:N	2.47	0.77
1:B:77:PHE:HZ	1:B:89:MET:CE	1.91	0.77
1:C:505:PRO:HG2	1:C:508:GLU:HB2	1.65	0.76
1:C:328:MET:HE1	1:C:357:THR:CB	2.14	0.76
1:B:96:GLU:OE1	1:B:456:ARG:NH1	2.20	0.75
1:B:39:GLY:CA	1:B:51:GLU:HG2	2.13	0.74
1:B:340:ARG:HG2	1:B:340:ARG:HH11	1.53	0.72
1:D:62:ILE:HD12	1:D:91:THR:HG22	1.71	0.71
1:D:116:THR:HG22	1:D:204:LYS:H	1.55	0.71
1:B:340:ARG:HE	1:D:296:GLY:HA3	1.56	0.70
1:A:308:MET:CE	1:A:337:THR:HB	2.22	0.70
1:B:76:ASN:HD21	1:B:78:SER:HB2	1.55	0.70
1:D:116:THR:HG22	1:D:202:LYS:C	2.18	0.69
1:D:388:ASN:HD21	1:D:442:ASN:ND2	1.90	0.69
1:D:126:TYR:CD1	1:D:146:ARG:CG	2.76	0.69
1:D:404:THR:CG2	1:D:435:LEU:HD12	2.23	0.68
1:B:115:ARG:HD2	4:B:890:HOH:O	1.94	0.68
1:B:327:ASN:HD22	1:D:340:ARG:HD2	1.59	0.68
1:B:140:GLN:HE22	1:B:153:VAL:H	1.42	0.67
1:D:501:VAL:HG13	1:D:512:THR:HG21	1.77	0.67
1:B:476:ASP:O	1:B:480:GLU:HG3	1.94	0.67
1:D:116:THR:HG23	1:D:202:LYS:HA	1.77	0.66
1:C:328:MET:HE3	1:C:357:THR:HB	1.75	0.66
1:B:328:MET:HE2	1:B:376:MET:HE2	1.78	0.65
1:D:116:THR:CG2	1:D:202:LYS:C	2.69	0.65
1:D:182:ALA:O	1:D:191:GLU:N	2.25	0.65
1:C:401:ASN:HB3	4:C:617:HOH:O	1.97	0.65
1:B:107:LEU:C	1:B:107:LEU:HD23	2.22	0.65
1:B:77:PHE:HA	1:B:85:GLN:NE2	2.13	0.64
1:B:218:LEU:HB3	1:B:222:ASP:HB2	1.79	0.64
1:D:139:LYS:HB3	1:D:142:ILE:HD12	1.77	0.64
1:B:26:LYS:HE2	1:B:461:ASN:O	1.99	0.63
1:C:337:ARG:HB2	1:C:337:ARG:HH21	1.62	0.63
1:C:80:GLY:HA3	1:C:84:GLU:OE2	1.99	0.62
1:D:421:LYS:CG	1:D:492:VAL:HG12	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:MET:HE1	1:C:357:THR:CG2	2.29	0.62
1:B:340:ARG:HH11	1:B:340:ARG:CG	2.13	0.62
1:D:126:TYR:CE1	1:D:146:ARG:CB	2.83	0.61
1:A:333:GLY:HA3	1:A:373:LEU:HD22	1.82	0.61
1:B:77:PHE:CE2	1:B:89:MET:CE	2.83	0.61
1:C:328:MET:HE3	1:C:376:MET:HE2	1.83	0.61
1:C:328:MET:CE	1:C:357:THR:CB	2.74	0.61
1:D:116:THR:CG2	1:D:204:LYS:H	2.14	0.61
1:D:421:LYS:HG2	1:D:492:VAL:HG12	1.83	0.61
1:C:448:LEU:HD23	1:C:467:MET:HB3	1.82	0.60
1:C:403:LYS:HE3	1:D:517:ILE:O	2.02	0.60
1:D:129:LYS:O	1:D:132:GLU:HB2	2.02	0.60
1:D:110:LYS:HD3	1:D:221:ARG:CZ	2.33	0.59
1:A:372:ARG:HD2	1:A:372:ARG:O	2.03	0.59
1:A:390:ALA:HB1	1:A:495:MET:HE1	1.84	0.59
1:B:421:LYS:HG2	1:B:492:VAL:HG12	1.85	0.58
1:C:328:MET:HE3	1:C:376:MET:CE	2.33	0.58
1:C:399:GLU:HG3	1:C:399:GLU:O	2.03	0.58
1:A:120:GLN:NE2	1:A:133:VAL:H	1.98	0.58
1:A:361:LYS:O	1:A:364:GLN:HG2	2.03	0.58
1:B:107:LEU:HD23	1:B:108:ASP:N	2.18	0.58
1:C:94:LEU:HD12	1:C:94:LEU:O	2.03	0.58
1:D:501:VAL:HG13	1:D:512:THR:CG2	2.33	0.58
1:B:331:THR:OG1	1:B:342:GLU:OE2	2.22	0.58
1:D:116:THR:CG2	1:D:202:LYS:HA	2.33	0.57
1:B:494:SER:CB	1:B:521:ARG:OXT	2.40	0.57
1:D:168:GLN:NE2	1:D:195:GLU:OE2	2.37	0.57
1:A:308:MET:HE3	1:A:337:THR:HB	1.87	0.56
1:D:140:GLN:NE2	1:D:151:LEU:O	2.35	0.56
1:C:80:GLY:CA	1:C:84:GLU:OE2	2.52	0.56
1:A:178:GLY:C	1:A:179:ILE:HD12	2.30	0.56
1:B:26:LYS:NZ	1:B:464:VAL:O	2.33	0.56
1:A:311:THR:HG23	1:A:322:GLU:OE1	2.05	0.55
1:B:368:TYR:HB3	1:B:371:GLU:HB2	1.88	0.55
1:C:337:ARG:HH21	1:C:337:ARG:CB	2.19	0.55
1:C:328:MET:HE1	1:C:357:THR:HG22	1.88	0.55
1:C:328:MET:HE2	1:C:358:MET:H	1.72	0.55
1:D:139:LYS:HD2	1:D:142:ILE:HD11	1.83	0.55
1:C:494:SER:OG	1:C:521:ARG:O	2.24	0.55
1:C:181:VAL:HG11	1:C:193:GLU:HG3	1.88	0.54
1:D:126:TYR:CD1	1:D:146:ARG:CB	2.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ALA:HB3	1:D:191:GLU:HB2	1.89	0.54
1:B:135:ARG:HD3	1:B:189:GLU:OE2	2.08	0.54
1:D:116:THR:HG22	1:D:204:LYS:N	2.22	0.54
1:D:139:LYS:HD3	1:D:142:ILE:CD1	2.22	0.54
1:D:46:ASP:OD2	1:D:46:ASP:N	2.29	0.54
1:D:328:MET:CE	1:D:357:THR:HB	2.38	0.54
1:A:3:LYS:HE2	1:A:7:ILE:HD12	1.90	0.53
1:C:326:THR:HG21	4:C:768:HOH:O	2.07	0.53
1:A:250:GLU:HG2	1:A:271:ALA:HB3	1.88	0.53
1:B:353:GLY:HA3	1:B:393:LEU:HD22	1.90	0.53
1:D:116:THR:CG2	1:D:202:LYS:CA	2.86	0.53
1:B:140:GLN:NE2	1:B:153:VAL:H	2.06	0.53
1:A:104:LYS:HD3	1:A:182:LYS:HE2	1.90	0.53
1:A:115:ARG:NH2	1:A:171:GLU:OE1	2.41	0.53
1:A:220:SER:HA	1:A:248:LYS:HD3	1.91	0.53
1:D:160:TYR:CE2	1:D:188:ARG:HA	2.44	0.53
1:D:182:ALA:O	1:D:191:GLU:HB2	2.09	0.53
1:B:399:GLU:HG2	1:B:401:ASN:HD21	1.75	0.52
1:D:116:THR:HG22	1:D:203:GLN:H	1.67	0.52
1:D:139:LYS:CD	1:D:142:ILE:CD1	2.80	0.52
1:A:312:MET:HA	1:A:315:LYS:O	2.10	0.52
1:D:110:LYS:HD3	1:D:221:ARG:NE	2.25	0.52
1:A:381:ASN:C	1:A:381:ASN:HD22	2.18	0.51
1:B:448:LEU:HD23	1:B:467:MET:HB3	1.90	0.51
1:D:368:TYR:HB3	1:D:371:GLU:HB2	1.92	0.51
1:D:421:LYS:HG3	1:D:492:VAL:HG12	1.92	0.51
1:D:128:TYR:N	1:D:128:TYR:CD2	2.79	0.51
2:D:601:CIT:H21	4:D:758:HOH:O	2.10	0.51
1:A:179:ILE:HD12	1:A:179:ILE:N	2.26	0.50
1:C:400:ARG:HD3	1:D:417:SER:OG	2.11	0.50
1:B:36:GLU:OE1	1:B:88:ARG:NE	2.37	0.50
1:D:115:ARG:HH11	1:D:205:GLY:N	2.09	0.50
1:A:140:TYR:CE2	1:A:168:ARG:HA	2.47	0.50
1:B:399:GLU:HG2	1:B:401:ASN:ND2	2.26	0.50
1:C:172:ASP:O	1:C:175:LYS:HD2	2.12	0.49
1:D:126:TYR:CD2	1:D:146:ARG:HG3	2.45	0.49
1:D:381:LYS:NZ	4:D:707:HOH:O	2.46	0.49
1:B:96:GLU:CD	1:B:456:ARG:HH12	2.17	0.49
1:C:325:ALA:C	1:C:326:THR:HG23	2.38	0.49
1:D:38:ARG:HB3	1:D:51:GLU:HB2	1.95	0.49
1:A:90:LYS:HD3	1:A:201:ARG:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ARG:HH21	1:D:175:LYS:HE3	1.78	0.48
1:B:106:LEU:HD23	1:B:106:LEU:C	2.39	0.48
1:C:329:LEU:O	1:C:362:GLU:HG2	2.13	0.48
1:C:451:ASP:OD1	1:C:453:LEU:HB2	2.14	0.48
1:D:144:SER:HG	1:D:150:ALA:H	1.53	0.48
1:C:135:ARG:HD3	1:C:189:GLU:OE2	2.14	0.48
1:D:126:TYR:O	1:D:128:TYR:HE2	1.97	0.48
1:D:180:VAL:HA	1:D:192:VAL:HG12	1.96	0.47
1:B:42:LYS:NZ	1:B:42:LYS:CB	2.76	0.47
1:D:117:GLU:HB2	1:D:150:ALA:O	2.13	0.47
1:A:406:LEU:HD22	1:A:458:MET:HG2	1.94	0.47
1:D:278:LEU:CD2	1:D:310:MET:HE3	2.45	0.47
1:C:381:LYS:O	1:C:384:GLN:HG2	2.15	0.47
1:D:332:MET:HA	1:D:335:LYS:O	2.15	0.47
1:D:494:SER:CB	1:D:521:ARG:OXT	2.62	0.47
1:B:115:ARG:CD	4:B:890:HOH:O	2.58	0.47
1:C:368:TYR:HB3	1:C:371:GLU:HB2	1.97	0.47
1:C:415:THR:O	1:C:418:MET:O	2.33	0.47
1:D:221:ARG:HG3	1:D:222:ASP:N	2.30	0.47
1:D:295:MET:O	1:D:299:VAL:HG22	2.14	0.47
1:B:270:GLU:HB3	1:B:294:ASP:HB3	1.97	0.47
1:B:328:MET:HE2	1:B:357:THR:HB	1.97	0.47
1:B:302:GLU:HG3	1:D:382:ASN:HD22	1.76	0.46
1:D:386:LEU:HD13	1:D:390:TYR:CE2	2.50	0.46
1:A:87:LEU:C	1:A:87:LEU:HD23	2.40	0.46
1:C:51:GLU:HA	1:C:51:GLU:OE1	2.15	0.46
1:D:386:LEU:HD13	1:D:390:TYR:CD2	2.50	0.46
1:D:136:VAL:HB	1:D:190:PHE:HB2	1.98	0.46
1:B:505:PRO:HG2	1:B:508:GLU:HG2	1.97	0.46
1:B:46:ASP:OD1	1:B:46:ASP:N	2.49	0.46
1:D:304:VAL:HB	1:D:305:PRO:HD3	1.97	0.46
1:D:504:VAL:HA	1:D:505:PRO:C	2.40	0.46
1:A:32:LYS:HD2	1:A:32:LYS:HA	1.70	0.46
1:A:184:LYS:HD3	1:A:184:LYS:HA	1.77	0.46
1:B:41:LYS:HA	1:B:45:GLU:OE2	2.16	0.46
1:A:305:ALA:HB1	1:A:338:MET:HE2	1.97	0.46
1:B:170:LEU:HB3	1:B:174:GLY:HA2	1.97	0.46
1:C:76:ASN:OD1	1:C:78:SER:HB2	2.16	0.46
1:B:107:LEU:C	1:B:107:LEU:CD2	2.89	0.45
1:C:241:PHE:N	1:C:270:GLU:OE2	2.49	0.45
1:D:126:TYR:CD1	1:D:146:ARG:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLY:CA	1:A:373:LEU:HD22	2.46	0.45
1:B:53:LEU:HD23	1:B:87:GLU:HB3	1.98	0.45
1:B:451:ASP:OD1	1:B:453:LEU:HB2	2.17	0.45
1:C:412:LYS:HD2	1:C:441:PRO:HA	1.98	0.45
1:A:348:TYR:HB3	1:A:351:GLU:HB2	1.97	0.45
1:D:185:ASP:OD1	1:D:185:ASP:N	2.50	0.45
1:D:426:LEU:HD11	1:D:450:PHE:CZ	2.51	0.45
1:D:478:MET:HE2	1:D:502:ALA:HB3	1.99	0.44
1:C:295:MET:O	1:C:299:VAL:HG22	2.18	0.44
1:D:126:TYR:O	1:D:128:TYR:CE2	2.70	0.44
1:D:83:GLN:H	1:D:83:GLN:NE2	2.15	0.44
1:B:84:GLU:O	1:B:87:GLU:HB2	2.18	0.44
1:A:308:MET:HE1	1:A:337:THR:HG22	1.99	0.44
1:C:426:LEU:HD22	1:C:478:MET:HG2	1.99	0.44
1:D:167:ARG:HD3	1:D:167:ARG:HA	1.84	0.44
1:B:84:GLU:OE2	1:B:88:ARG:NH2	2.46	0.44
1:D:135:ARG:HD3	1:D:189:GLU:OE2	2.17	0.43
1:B:38:ARG:HB3	1:B:51:GLU:HB3	2.00	0.43
1:B:36:GLU:CD	1:B:88:ARG:HE	2.25	0.43
1:D:316:ASN:ND2	1:D:398:PHE:HZ	2.16	0.43
1:D:245:ALA:HB2	1:D:280:GLU:HG3	2.00	0.43
1:A:17:ILE:HD11	1:A:41:ASN:HD21	1.83	0.43
1:B:31:LEU:HD12	1:B:75:PHE:CE1	2.53	0.43
1:B:179:ARG:O	1:B:192:VAL:HA	2.19	0.43
1:A:452:PRO:HB3	1:A:461:ILE:HD12	2.00	0.43
1:C:332:MET:HA	1:C:335:LYS:O	2.19	0.43
1:D:139:LYS:HB3	1:D:142:ILE:HD13	1.91	0.43
1:D:508:GLU:H	1:D:508:GLU:HG3	1.54	0.43
1:B:508:GLU:N	1:B:508:GLU:CD	2.77	0.43
1:A:501:ARG:NH2	4:A:620:HOH:O	2.52	0.43
1:C:39:GLY:N	1:C:52:LYS:O	2.44	0.42
1:C:331:THR:HG23	1:C:342:GLU:OE1	2.19	0.42
1:A:5:VAL:HG21	1:A:330:VAL:HG13	2.01	0.42
1:B:42:LYS:NZ	1:B:42:LYS:HB2	2.33	0.42
1:C:124:LYS:HD2	1:C:202:LYS:NZ	2.34	0.42
1:D:387:LEU:HD23	1:D:387:LEU:HA	1.81	0.42
1:B:85:GLN:OE1	1:B:85:GLN:HA	2.20	0.42
1:C:400:ARG:CZ	1:C:409:SER:OG	2.67	0.42
1:D:176:LEU:HD22	1:D:200:ILE:HG12	2.02	0.42
1:A:137:LEU:HD23	1:A:137:LEU:HA	1.84	0.42
1:D:208:ILE:HG22	1:D:211:THR:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HD23	1:A:86:LEU:C	2.45	0.42
1:C:227:ARG:HH22	1:C:257:GLU:CD	2.28	0.42
1:D:115:ARG:NH1	1:D:205:GLY:N	2.68	0.41
1:C:80:GLY:HA2	1:C:84:GLU:OE2	2.20	0.41
1:C:507:GLY:N	4:C:603:HOH:O	2.33	0.41
1:D:494:SER:OG	1:D:521:ARG:OXT	2.31	0.41
1:D:184:ASP:OD1	1:D:186:ALA:HB3	2.21	0.41
1:D:475:THR:OG1	1:D:504:VAL:HG13	2.20	0.41
1:D:218:LEU:HD11	1:D:254:ILE:HD11	2.03	0.41
1:A:308:MET:CE	1:A:337:THR:CB	2.96	0.41
1:C:77:PHE:CZ	1:C:85:GLN:HG3	2.56	0.41
1:D:178:LEU:HB3	1:D:192:VAL:HG21	2.02	0.41
1:C:418:MET:HE1	1:D:403:LYS:HB2	2.03	0.41
1:D:38:ARG:O	1:D:41:LYS:HB2	2.21	0.41
1:D:326:THR:HG21	4:D:871:HOH:O	2.20	0.40
1:A:397:SER:HB3	1:B:400:ARG:O	2.21	0.40
1:A:439:MET:HG3	1:A:446:PRO:HG2	2.02	0.40
1:B:325:ALA:HB1	1:B:358:MET:HE2	2.04	0.40
1:D:161:ASP:OD1	1:D:188:ARG:NH2	2.54	0.40
1:A:232:ARG:O	1:A:236:GLU:HG2	2.22	0.40
1:B:42:LYS:HB2	1:B:42:LYS:HZ2	1.87	0.40
1:C:170:LEU:HB3	1:C:174:GLY:HA2	2.02	0.40
1:D:116:THR:CG2	1:D:203:GLN:H	2.28	0.40
1:D:121:GLY:O	1:D:122:GLU:CB	2.70	0.40
1:D:118:LEU:HD12	1:D:118:LEU:HA	1.93	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	498/521 (96%)	489 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	499/521 (96%)	490 (98%)	8 (2%)	1 (0%)	43	42
1	C	498/521 (96%)	492 (99%)	5 (1%)	1 (0%)	43	42
1	D	499/521 (96%)	491 (98%)	7 (1%)	1 (0%)	43	42
All	All	1994/2084 (96%)	1962 (98%)	29 (2%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	508	GLU
1	B	326	THR
1	C	326	THR

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/428 (96%)	397 (97%)	13 (3%)	34	35
1	B	411/428 (96%)	384 (93%)	27 (7%)	15	12
1	C	410/428 (96%)	384 (94%)	26 (6%)	16	13
1	D	411/428 (96%)	383 (93%)	28 (7%)	14	11
All	All	1642/1712 (96%)	1548 (94%)	94 (6%)	18	15

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	26	ASP
1	A	32	LYS
1	A	119	LYS
1	A	137	LEU
1	A	198	LEU
1	A	201	ARG
1	A	361	LYS

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Mol	Chain	Res	Type
1	A	373	LEU
1	A	381	ASN
1	A	384	THR
1	A	401	LYS
1	A	481	VAL
1	B	42	LYS
1	B	46	ASP
1	B	51	GLU
1	B	115	ARG
1	B	232	GLN
1	B	246	LYS
1	B	283	GLU
1	B	294	ASP
1	B	299	VAL
1	B	313	LYS
1	B	328	MET
1	B	330	GLU
1	B	335	LYS
1	B	340	ARG
1	B	365	ASN
1	B	367	LYS
1	B	381	LYS
1	B	393	LEU
1	B	399	GLU
1	B	400	ARG
1	B	403	LYS
1	B	404	THR
1	B	426	LEU
1	B	494	SER
1	B	501	VAL
1	B	506	VAL
1	B	508	GLU
1	C	46	ASP
1	C	52	LYS
1	C	83	GLN
1	C	218	LEU
1	C	246	LYS
1	C	247	ASP
1	C	256	GLU
1	C	257	GLU
1	C	270	GLU
1	C	294	ASP

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Mol	Chain	Res	Type
1	C	330	GLU
1	C	337	ARG
1	C	365	ASN
1	C	381	LYS
1	C	382	ASN
1	C	403	LYS
1	C	404	THR
1	C	419	ASP
1	C	421	LYS
1	C	426	LEU
1	C	469	THR
1	C	494	SER
1	C	501	VAL
1	C	506	VAL
1	C	508	GLU
1	C	518	ARG
1	D	46	ASP
1	D	54	ASP
1	D	56	GLU
1	D	116	THR
1	D	118	LEU
1	D	122	GLU
1	D	125	GLU
1	D	132	GLU
1	D	147	GLU
1	D	168	GLN
1	D	185	ASP
1	D	218	LEU
1	D	221	ARG
1	D	246	LYS
1	D	270	GLU
1	D	283	GLU
1	D	294	ASP
1	D	313	LYS
1	D	337	ARG
1	D	386	LEU
1	D	392	ARG
1	D	400	ARG
1	D	405	GLU
1	D	425	THR
1	D	426	LEU
1	D	428	LYS

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Mol	Chain	Res	Type
1	D	501	VAL
1	D	511	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	362	ASN
1	A	381	ASN
1	A	422	ASN
1	B	76	ASN
1	B	140	GLN
1	B	210	ASN
1	B	316	ASN
1	B	327	ASN
1	B	382	ASN
1	C	79	HIS
1	C	83	GLN
1	C	210	ASN
1	C	262	HIS
1	C	272	GLN
1	C	382	ASN
1	D	83	GLN
1	D	210	ASN
1	D	273	GLN
1	D	316	ASN
1	D	382	ASN
1	D	388	ASN

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

3 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$
3	GOL	D	602	-	5,5,5	0.30	0	5,5,5	0.71	0
2	CIT	B	601	-	12,12,12	1.49	1 (8%)	17,17,17	1.36	3 (17%)
2	CIT	D	601	-	12,12,12	1.32	1 (8%)	17,17,17	1.11	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	602	-	-	4/4/4/4	-
2	CIT	B	601	-	-	0/16/16/16	-
2	CIT	D	601	-	-	0/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	CIT	C3-C6	3.89	1.57	1.53
2	D	601	CIT	C3-C6	2.74	1.56	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	CIT	O6-C6-C3	3.28	119.44	113.14
2	B	601	CIT	O5-C6-C3	-2.88	116.52	122.09
2	D	601	CIT	O5-C6-C3	-2.22	117.80	122.09
2	D	601	CIT	O6-C6-C3	2.13	117.22	113.14
2	B	601	CIT	O3-C5-C4	-2.02	117.22	122.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	602	GOL	O1-C1-C2-C3
3	D	602	GOL	C1-C2-C3-O3
3	D	602	GOL	O2-C2-C3-O3
3	D	602	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	CIT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	500/521 (95%)	-0.03	7 (1%) 73 73	22, 35, 54, 90	0
1	B	501/521 (96%)	0.17	17 (3%) 48 47	25, 38, 69, 124	0
1	C	500/521 (95%)	0.25	16 (3%) 50 49	24, 41, 73, 95	0
1	D	501/521 (96%)	0.26	25 (4%) 34 33	23, 39, 76, 98	0
All	All	2002/2084 (96%)	0.16	65 (3%) 50 49	22, 38, 69, 124	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	HIS	5.3
1	D	198	GLY	3.7
1	C	506	VAL	3.7
1	D	123	ALA	3.6
1	B	21	MET	3.5
1	B	39	GLY	3.3
1	B	50	GLY	3.3
1	B	44	GLY	3.2
1	D	392	ARG	3.1
1	D	145	THR	3.0
1	B	77	PHE	3.0
1	D	199	ILE	3.0
1	D	507	GLY	3.0
1	D	128	TYR	2.9
1	B	55	VAL	2.9
1	C	39	GLY	2.7
1	C	507	GLY	2.7
1	D	56	GLU	2.6
1	D	162	ASP	2.6
1	B	219	ALA	2.6
1	B	509	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	506	VAL	2.6
1	B	40	GLY	2.6
1	A	153	ASP	2.6
1	D	142	ILE	2.5
1	D	163	VAL	2.5
1	C	41	LYS	2.5
1	C	416	SER	2.5
1	B	37	ILE	2.5
1	B	80	GLY	2.5
1	B	246	LYS	2.5
1	C	521	ARG	2.5
1	C	44	GLY	2.5
1	D	404	THR	2.4
1	D	21	MET	2.4
1	D	133	LYS	2.4
1	C	50	GLY	2.4
1	A	422	ASN	2.4
1	A	199	ALA	2.3
1	A	374	ASP	2.3
1	B	53	LEU	2.3
1	D	400	ARG	2.3
1	B	52	LYS	2.2
1	B	47	GLY	2.2
1	D	136	VAL	2.2
1	A	36	GLU	2.2
1	C	421	LYS	2.2
1	C	49	TRP	2.2
1	D	182	ALA	2.1
1	D	126	TYR	2.1
1	B	355	ASP	2.1
1	D	190	PHE	2.1
1	A	489	ALA	2.1
1	C	53	LEU	2.1
1	D	52	LYS	2.1
1	D	406	VAL	2.1
1	C	43	PHE	2.1
1	D	510	VAL	2.1
1	A	432	GLU	2.0
1	C	56	GLU	2.0
1	C	94	LEU	2.0
1	D	405	GLU	2.0
1	D	402	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	414	ALA	2.0
1	C	214	PRO	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
2	CIT	D	601	13/13	0.88	0.10	45,62,71,71	0
3	GOL	D	602	6/6	0.89	0.10	39,49,52,52	0
2	CIT	B	601	13/13	0.93	0.08	41,51,58,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.