



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:10 AM UTC

PDB ID : 2JBM / pdb_00002jbm
Title : QPRTASE STRUCTURE FROM HUMAN
Authors : Liu, H.; Naismith, J.H.
Deposited on : 2006-12-08
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

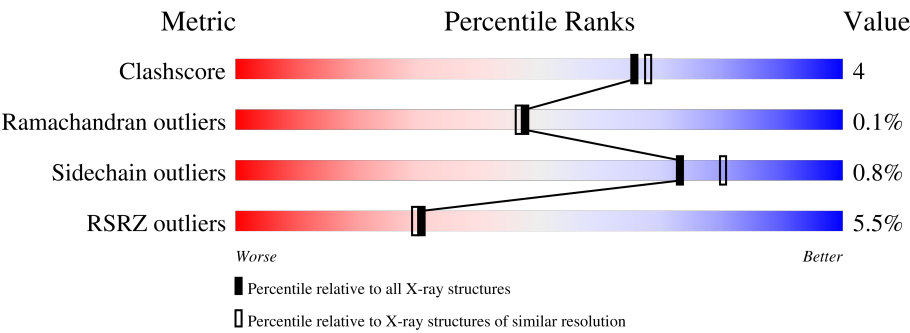
1 Overall quality at a glance i

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))
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	299	5% 87% 9%
1	B	299	10% 89% 7%
1	C	299	4% 88% 7%
1	D	299	5% 89% 6% 5%
1	E	299	9% 91% 6%
1	F	299	3% 88% 7% 5%

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Mol	Chain	Length	Quality of chain
1	G	299	
1	H	299	
1	I	299	
1	J	299	
1	K	299	
1	L	299	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SRT	A	401	-	X	-	-
2	SRT	C	401	-	X	-	-
2	SRT	D	401	-	X	-	-
2	SRT	F	401	-	X	-	-
2	SRT	J	401	-	X	-	-
2	SRT	K	401	-	X	-	-

2 Entry composition

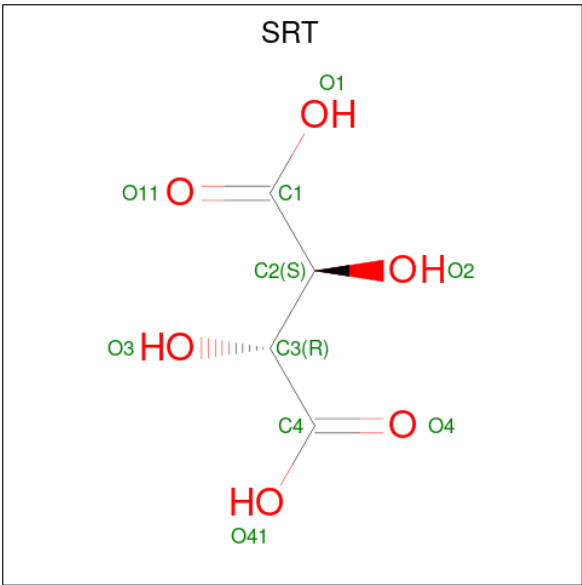
There are 3 unique types of molecules in this entry. The entry contains 28196 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	1
			2109	1343	366	390	10			
1	B	289	Total	C	N	O	S	0	0	1
			2101	1338	365	389	9			
1	C	286	Total	C	N	O	S	0	0	0
			2085	1329	361	385	10			
1	D	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			
1	E	289	Total	C	N	O	S	0	0	1
			2101	1338	365	389	9			
1	F	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			
1	G	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			
1	H	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			
1	I	289	Total	C	N	O	S	0	0	1
			2101	1338	365	389	9			
1	J	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			
1	K	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			
1	L	285	Total	C	N	O	S	0	0	0
			2077	1324	360	384	9			

- Molecule 2 is S,R MESO-TARTARIC ACID (CCD ID: SRT) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		
2	C	1	Total	C	O	0	0
			10	4	6		
2	D	1	Total	C	O	0	0
			10	4	6		
2	E	1	Total	C	O	0	0
			10	4	6		
2	F	1	Total	C	O	0	0
			10	4	6		
2	G	1	Total	C	O	0	0
			10	4	6		
2	H	1	Total	C	O	0	0
			10	4	6		
2	I	1	Total	C	O	0	0
			10	4	6		
2	J	1	Total	C	O	0	0
			10	4	6		
2	K	1	Total	C	O	0	0
			10	4	6		
2	L	1	Total	C	O	0	0
			10	4	6		

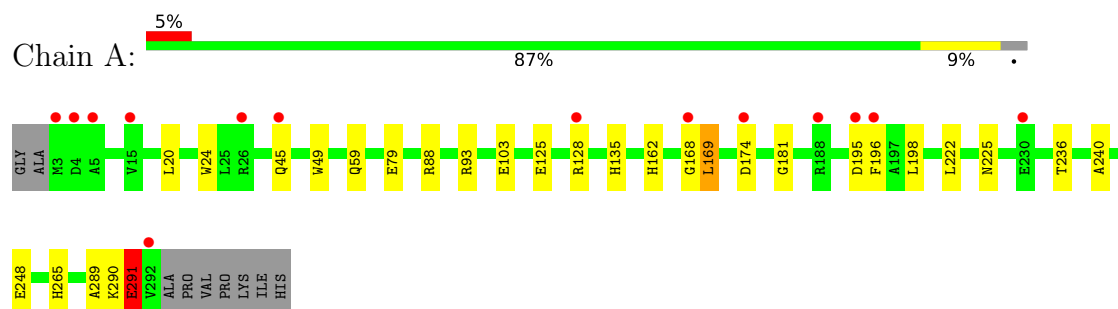
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	375	Total 375	O 375	0	0
3	B	324	Total 324	O 324	0	0
3	C	280	Total 280	O 280	0	0
3	D	292	Total 292	O 292	0	0
3	E	267	Total 267	O 267	0	0
3	F	315	Total 315	O 315	0	0
3	G	181	Total 181	O 181	0	0
3	H	127	Total 127	O 127	0	0
3	I	269	Total 269	O 269	0	0
3	J	256	Total 256	O 256	0	0
3	K	206	Total 206	O 206	0	0
3	L	148	Total 148	O 148	0	0

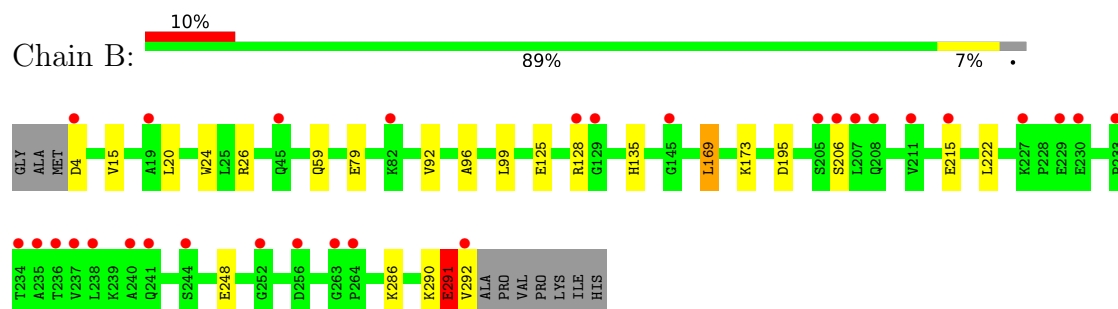
3 Residue-property plots

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

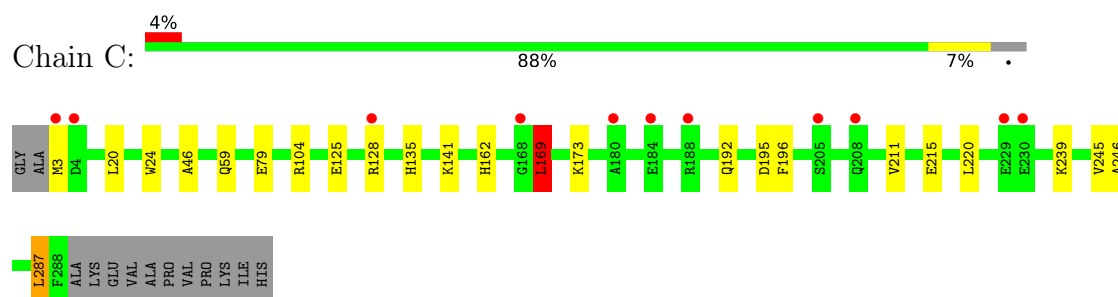
• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE



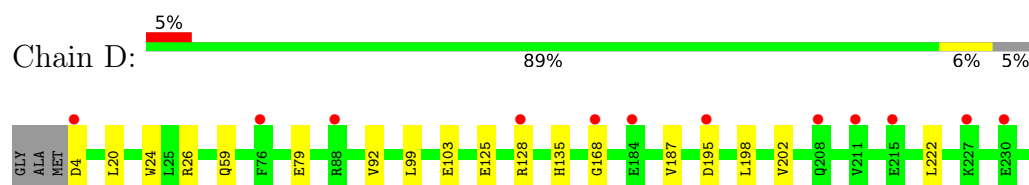
• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE



• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

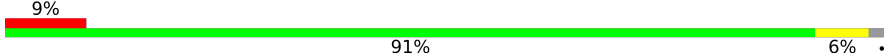


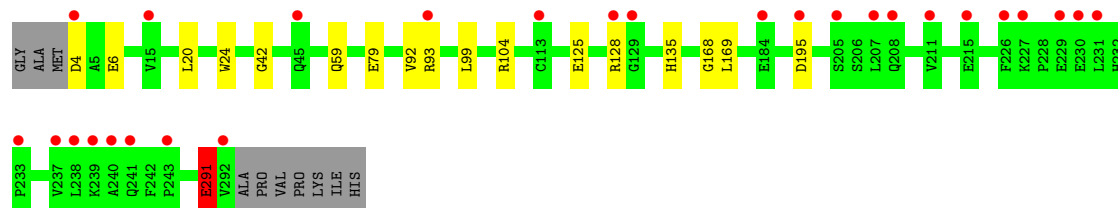
• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE



ALA
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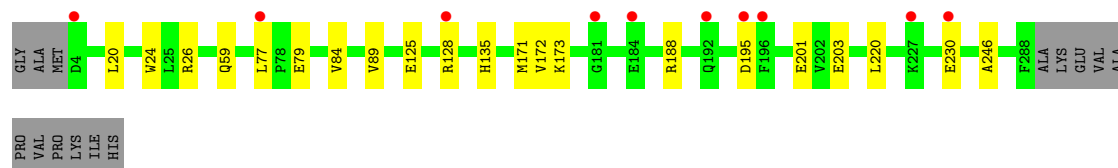
• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain E: 



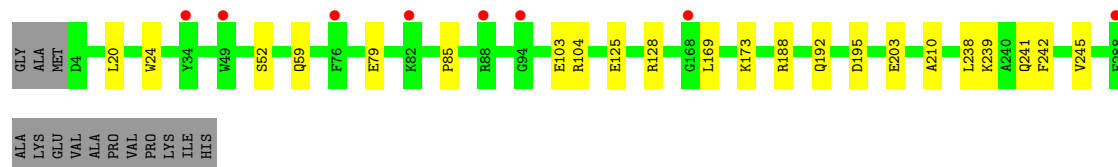
• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain F: 

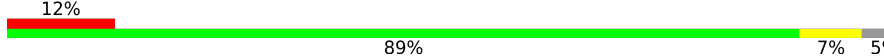


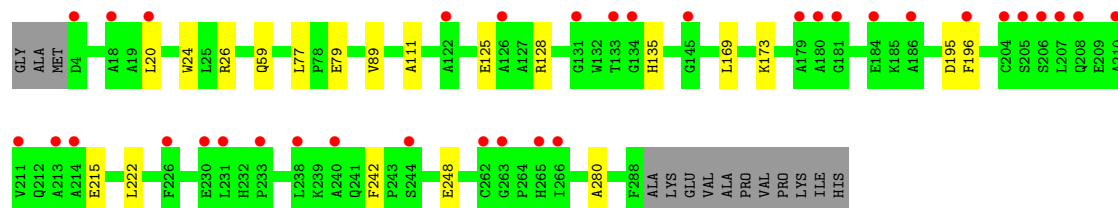
• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain G: 



• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

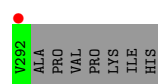
Chain H: 



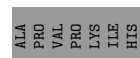
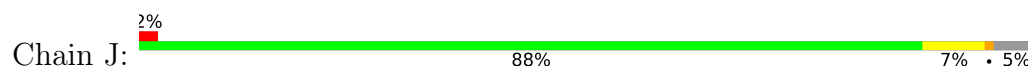
• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE

Chain I: 

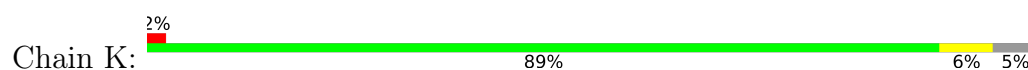




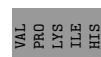
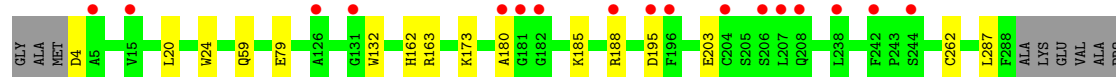
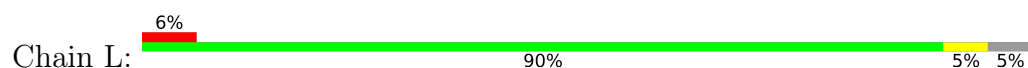
• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE



• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE



• Molecule 1: NICOTINATE-NUCLEOTIDE PYROPHOSPHORYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.92Å 179.29Å 194.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.97 – 2.00 60.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.4 (60.97-2.00) 91.3 (60.97-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.176 , 0.208 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.8	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	0.92	EDS
Total number of atoms	28196	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6514e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SRT

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	0.78	1/2152 (0.0%)	0.84	0/2933
1	B	0.69	1/2144 (0.0%)	0.80	0/2923
1	C	0.66	0/2128	0.80	1/2901 (0.0%)
1	D	0.64	0/2120	0.77	0/2891
1	E	0.66	1/2144 (0.0%)	0.80	0/2923
1	F	0.66	0/2120	0.79	0/2891
1	G	0.53	0/2120	0.76	0/2891
1	H	0.51	0/2120	0.76	0/2891
1	I	0.63	1/2144 (0.0%)	0.77	0/2923
1	J	0.62	0/2120	0.81	2/2891 (0.1%)
1	K	0.54	0/2120	0.76	0/2891
1	L	0.51	0/2120	0.74	0/2891
All	All	0.62	4/25552 (0.0%)	0.78	3/34840 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	291	GLU	C-N	-7.16	1.23	1.33
1	A	291	GLU	C-N	-6.68	1.24	1.33
1	B	291	GLU	C-N	-6.63	1.24	1.33
1	I	291	GLU	C-N	-6.42	1.24	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	45	GLN	CA-CB-CG	9.03	132.16	114.10
1	J	45	GLN	CB-CG-CD	8.77	127.51	112.60
1	C	169	LEU	N-CA-C	-5.47	99.68	108.55

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	2109	0	2128	23	3
1	B	2101	0	2119	18	0
1	C	2085	0	2104	21	0
1	D	2077	0	2095	14	0
1	E	2101	0	2119	20	0
1	F	2077	0	2095	20	0
1	G	2077	0	2095	12	0
1	H	2077	0	2095	14	0
1	I	2101	0	2119	23	3
1	J	2077	0	2095	15	0
1	K	2077	0	2095	12	0
1	L	2077	0	2095	10	0
2	A	10	0	4	1	0
2	B	10	0	4	0	0
2	C	10	0	4	2	0
2	D	10	0	4	2	0
2	E	10	0	4	0	0
2	F	10	0	4	2	0
2	G	10	0	4	1	0
2	H	10	0	4	1	0
2	I	10	0	4	0	0
2	J	10	0	4	2	0
2	K	10	0	4	0	0
2	L	10	0	4	1	0
3	A	375	0	0	12	0
3	B	324	0	0	6	0
3	C	280	0	0	7	0
3	D	292	0	0	2	0
3	E	267	0	0	10	0
3	F	315	0	0	6	0
3	G	181	0	0	2	0
3	H	127	0	0	1	0
3	I	269	0	0	8	0
3	J	256	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	206	0	0	2	0
3	L	148	0	0	5	0
All	All	28196	0	25302	190	3

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 4.

All (190) 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:A:174:ASP:HB2	3:A:2248:HOH:O	1.40	1.22
1:A:196:PHE:HB2	3:C:2187:HOH:O	1.55	1.06
1:K:128:ARG:NH1	3:K:2111:HOH:O	1.83	1.05
1:A:225:ASN:HB3	3:A:2295:HOH:O	1.58	1.01
1:C:162:HIS:CE1	3:C:2187:HOH:O	2.13	0.99
1:C:162:HIS:HE1	3:C:2187:HOH:O	1.51	0.87
1:J:229:GLU:HG3	3:J:2208:HOH:O	1.76	0.84
3:A:2249:HOH:O	1:B:286:LYS:HD2	1.77	0.83
1:L:162:HIS:HE1	3:L:2092:HOH:O	1.62	0.82
1:L:162:HIS:CE1	3:L:2092:HOH:O	2.34	0.79
1:L:180:ALA:O	1:L:185:LYS:HD3	1.83	0.79
1:E:291:GLU:HA	3:E:2265:HOH:O	1.82	0.78
1:F:230:GLU:HG3	3:F:2135:HOH:O	1.86	0.74
1:C:211:VAL:O	1:C:215:GLU:HG3	1.87	0.74
1:H:196:PHE:HB2	3:L:2092:HOH:O	1.88	0.74
1:E:291:GLU:CA	3:E:2265:HOH:O	2.37	0.73
1:I:173:LYS:HE2	3:J:2118:HOH:O	1.88	0.73
1:A:196:PHE:CB	3:C:2187:HOH:O	2.24	0.71
1:I:39:SER:O	1:I:290:LYS:NZ	2.24	0.70
1:D:195:ASP:OD1	1:E:135:HIS:ND1	2.24	0.70
1:J:46:ALA:HB2	1:J:287:LEU:HD12	1.75	0.68
1:A:181:GLY:HA2	3:A:2251:HOH:O	1.96	0.66
1:A:49:TRP:CZ3	1:A:88:ARG:HB2	2.31	0.65
1:J:77:LEU:HD12	1:J:89:VAL:HG12	1.78	0.65
1:B:4:ASP:N	3:B:2002:HOH:O	2.30	0.64
1:E:93:ARG:HD2	3:E:2127:HOH:O	1.99	0.62
1:H:196:PHE:CB	3:L:2092:HOH:O	2.45	0.62
1:D:4:ASP:N	3:D:2002:HOH:O	2.33	0.60
1:E:291:GLU:CB	3:E:2265:HOH:O	2.49	0.60
1:B:96:ALA:HB2	1:B:290:LYS:HD2	1.85	0.59
1:F:26:ARG:CZ	3:F:2041:HOH:O	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:230:GLU:HG3	3:J:2209:HOH:O	2.03	0.58
1:E:4:ASP:N	3:E:2003:HOH:O	2.36	0.58
3:A:2236:HOH:O	1:C:196:PHE:HB2	2.03	0.58
1:D:135:HIS:ND1	1:E:195:ASP:OD1	2.37	0.57
1:E:291:GLU:HG3	3:E:2265:HOH:O	2.04	0.57
1:B:195:ASP:OD1	1:F:135:HIS:ND1	2.36	0.57
1:G:210:ALA:HB1	1:G:238:LEU:HD11	1.86	0.57
1:B:20:LEU:HG	1:B:24:TRP:CZ2	2.41	0.55
1:D:20:LEU:HG	1:D:24:TRP:CZ2	2.42	0.55
1:E:20:LEU:HG	1:E:24:TRP:CZ2	2.42	0.55
1:F:26:ARG:NH1	3:F:2046:HOH:O	2.38	0.55
3:B:2053:HOH:O	1:D:26:ARG:CZ	2.54	0.54
1:E:59:GLN:HG3	1:E:79:GLU:OE1	2.06	0.54
1:A:290:LYS:O	1:A:291:GLU:HB3	2.08	0.54
1:A:103:GLU:OE2	1:B:173:LYS:NZ	2.34	0.54
1:C:104:ARG:HD3	2:D:401:SRT:O2	2.08	0.54
1:C:59:GLN:HG3	1:C:79:GLU:OE1	2.07	0.54
1:B:135:HIS:HD1	1:F:195:ASP:CG	2.16	0.54
1:A:59:GLN:HG3	1:A:79:GLU:OE1	2.08	0.53
1:A:93:ARG:HD3	3:A:2173:HOH:O	2.08	0.53
2:D:401:SRT:H2	3:D:2172:HOH:O	2.08	0.53
1:G:103:GLU:OE2	1:H:173:LYS:NZ	2.42	0.53
1:H:215:GLU:HG2	3:H:2106:HOH:O	2.09	0.53
1:F:20:LEU:HG	1:F:24:TRP:CZ2	2.44	0.52
1:B:15:VAL:HB	3:B:2031:HOH:O	2.08	0.52
1:K:91:GLU:OE2	1:K:93:ARG:HD3	2.09	0.52
1:G:20:LEU:HG	1:G:24:TRP:CZ2	2.44	0.52
1:I:20:LEU:HG	1:I:24:TRP:CZ2	2.45	0.52
1:I:125:GLU:CD	3:I:2147:HOH:O	2.52	0.52
1:I:125:GLU:OE2	3:I:2147:HOH:O	2.18	0.52
1:D:59:GLN:HG3	1:D:79:GLU:OE1	2.09	0.52
1:A:45:GLN:CD	1:A:289:ALA:HB3	2.35	0.52
1:H:26:ARG:CZ	3:J:2033:HOH:O	2.59	0.51
1:C:173:LYS:HE3	2:C:401:SRT:C1	2.40	0.51
1:K:20:LEU:HG	1:K:24:TRP:CZ2	2.45	0.51
1:C:173:LYS:HE3	2:C:401:SRT:O11	2.10	0.51
1:I:128:ARG:CZ	3:I:2147:HOH:O	2.59	0.51
1:J:20:LEU:HG	1:J:24:TRP:CZ2	2.46	0.51
2:A:401:SRT:H2	3:A:2216:HOH:O	2.09	0.51
1:H:20:LEU:HG	1:H:24:TRP:CZ2	2.45	0.51
1:A:20:LEU:HG	1:A:24:TRP:CZ2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:77:LEU:HD12	1:H:89:VAL:HG22	1.93	0.51
1:A:291:GLU:HG2	3:A:2371:HOH:O	2.11	0.50
1:L:20:LEU:HG	1:L:24:TRP:CZ2	2.46	0.50
1:G:241:GLN:HG2	1:G:242:PHE:CE1	2.46	0.50
1:I:125:GLU:OE1	1:I:128:ARG:NH2	2.44	0.50
1:F:59:GLN:HG3	1:F:79:GLU:OE1	2.12	0.49
1:I:104:ARG:HD3	2:J:401:SRT:O2	2.12	0.49
1:F:77:LEU:HD12	1:F:89:VAL:HG12	1.93	0.49
1:J:59:GLN:HG3	1:J:79:GLU:OE1	2.11	0.49
1:B:59:GLN:HG3	1:B:79:GLU:OE1	2.12	0.49
1:I:128:ARG:NH2	3:I:2147:HOH:O	2.45	0.49
1:D:92:VAL:HG12	1:D:99:LEU:CD2	2.42	0.49
1:J:26:ARG:CZ	3:J:2033:HOH:O	2.59	0.49
1:J:135:HIS:ND1	1:K:195:ASP:OD1	2.46	0.49
1:K:59:GLN:HG3	1:K:79:GLU:OE1	2.13	0.49
1:C:20:LEU:HG	1:C:24:TRP:CZ2	2.47	0.48
1:B:286:LYS:HE2	3:B:2314:HOH:O	2.13	0.48
1:E:42:GLY:HA3	3:E:2265:HOH:O	2.14	0.48
1:I:104:ARG:HD2	2:J:401:SRT:O4	2.14	0.48
1:I:265:HIS:HD2	3:I:2239:HOH:O	1.95	0.47
1:I:173:LYS:NZ	1:J:103:GLU:OE2	2.45	0.47
2:G:401:SRT:H2	3:G:2106:HOH:O	2.15	0.47
1:I:59:GLN:HG3	1:I:79:GLU:OE1	2.15	0.47
1:L:59:GLN:HG3	1:L:79:GLU:OE1	2.15	0.47
1:A:125:GLU:OE1	1:A:128:ARG:NH2	2.46	0.47
1:C:3:MET:HB3	3:C:2002:HOH:O	2.15	0.47
1:I:183:VAL:O	1:I:187:VAL:HG23	2.14	0.46
1:F:171:MET:HE2	1:F:172:VAL:O	2.15	0.46
1:G:195:ASP:HB3	3:G:2139:HOH:O	2.16	0.46
1:G:59:GLN:HG3	1:G:79:GLU:OE1	2.15	0.46
1:G:188:ARG:O	1:G:192:GLN:HG3	2.15	0.46
1:E:6:GLU:HG3	3:E:2001:HOH:O	2.14	0.46
1:C:192:GLN:HG3	3:C:2209:HOH:O	2.15	0.46
1:A:195:ASP:OD1	1:C:135:HIS:ND1	2.49	0.46
1:K:4:ASP:N	3:K:2002:HOH:O	2.48	0.46
1:A:225:ASN:CG	3:A:2295:HOH:O	2.59	0.45
1:A:265:HIS:HE1	3:A:2340:HOH:O	1.98	0.45
1:C:46:ALA:HB2	1:C:287:LEU:HD12	1.97	0.45
1:L:4:ASP:HA	3:L:2001:HOH:O	2.17	0.45
1:G:125:GLU:OE1	1:G:128:ARG:NH2	2.49	0.45
1:B:222:LEU:HD13	1:B:248:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:401:SRT:H2	3:F:2173:HOH:O	2.15	0.45
1:A:168:GLY:O	1:A:198:LEU:HD22	2.16	0.45
1:E:291:GLU:CG	3:E:2265:HOH:O	2.60	0.45
1:J:192:GLN:HG3	3:J:2176:HOH:O	2.16	0.45
1:K:111:ALA:HB1	1:K:280:ALA:HB1	1.99	0.45
1:B:173:LYS:HB3	1:B:173:LYS:HE3	1.82	0.44
1:C:169:LEU:C	1:C:169:LEU:HD12	2.42	0.44
1:I:173:LYS:HB3	1:I:173:LYS:HE3	1.67	0.44
1:F:220:LEU:HG	1:F:246:ALA:HB3	1.97	0.44
1:G:173:LYS:HA	1:G:203:GLU:HB3	1.99	0.44
1:H:59:GLN:HG3	1:H:79:GLU:OE1	2.17	0.44
1:I:92:VAL:HG12	1:I:99:LEU:CD2	2.47	0.44
1:A:225:ASN:CB	3:A:2295:HOH:O	2.35	0.44
1:G:104:ARG:HH11	2:H:401:SRT:C1	2.31	0.44
1:C:141:LYS:HE2	3:C:2170:HOH:O	2.17	0.44
1:B:135:HIS:ND1	1:F:195:ASP:OD1	2.51	0.44
1:D:195:ASP:CG	1:E:135:HIS:HD1	2.26	0.44
1:J:15:VAL:HB	3:J:2020:HOH:O	2.18	0.44
1:F:171:MET:HE3	1:F:172:VAL:N	2.32	0.43
1:H:111:ALA:HB1	1:H:280:ALA:HB1	1.99	0.43
1:J:187:VAL:HG22	1:J:202:VAL:HG21	2.00	0.43
1:A:222:LEU:HD13	1:A:248:GLU:HG2	1.99	0.43
1:B:292:VAL:N	3:B:2320:HOH:O	2.51	0.43
1:F:125:GLU:OE1	1:F:128:ARG:NH2	2.51	0.43
1:H:135:HIS:ND1	1:L:195:ASP:OD1	2.51	0.43
1:K:44:SER:HB3	1:K:287:LEU:HD21	2.00	0.43
1:L:173:LYS:HA	1:L:203:GLU:HB3	2.01	0.43
1:C:169:LEU:HD12	1:C:169:LEU:O	2.19	0.43
1:F:84:VAL:HB	1:I:93:ARG:NH1	2.33	0.43
1:B:92:VAL:HG12	1:B:99:LEU:CD2	2.48	0.43
1:B:169:LEU:HD12	1:B:169:LEU:C	2.43	0.43
1:K:77:LEU:HD12	1:K:89:VAL:HG22	2.00	0.43
1:D:135:HIS:HD1	1:E:195:ASP:CG	2.27	0.43
1:G:52:SER:C	1:G:85:PRO:HG3	2.44	0.43
1:I:128:ARG:HH11	1:I:128:ARG:HG2	1.83	0.43
1:B:26:ARG:CZ	3:B:2053:HOH:O	2.66	0.43
1:H:222:LEU:HD13	1:H:248:GLU:HG2	2.01	0.43
1:E:104:ARG:HD3	2:F:401:SRT:O2	2.19	0.43
1:H:215:GLU:HG3	1:H:242:PHE:HZ	1.83	0.43
1:D:125:GLU:OE1	1:D:128:ARG:NH2	2.51	0.43
1:J:173:LYS:HA	1:J:203:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:125:GLU:OE1	1:K:128:ARG:NH2	2.52	0.42
1:C:239:LYS:HE2	1:C:245:VAL:O	2.19	0.42
1:H:125:GLU:OE1	1:H:128:ARG:NH2	2.53	0.42
1:I:174:ASP:HB2	3:I:2182:HOH:O	2.19	0.42
1:I:290:LYS:O	1:I:291:GLU:CB	2.67	0.42
1:D:187:VAL:HG22	1:D:202:VAL:HG21	2.03	0.41
1:F:173:LYS:HA	1:F:203:GLU:HB3	2.02	0.41
1:L:163:ARG:HE	2:L:401:SRT:C4	2.34	0.41
1:A:162:HIS:CE1	3:A:2236:HOH:O	2.73	0.41
1:A:169:LEU:HD12	1:A:169:LEU:C	2.45	0.41
1:E:93:ARG:NH2	3:E:2126:HOH:O	2.53	0.41
1:F:77:LEU:HG	3:I:2117:HOH:O	2.19	0.41
1:D:168:GLY:O	1:D:198:LEU:HD22	2.20	0.41
1:E:92:VAL:HG12	1:E:99:LEU:CD2	2.50	0.41
1:I:239:LYS:HE3	1:I:247:VAL:HG23	2.03	0.41
1:K:75:TRP:CE3	1:K:90:ALA:HB2	2.56	0.41
1:C:125:GLU:OE1	1:C:128:ARG:NH2	2.53	0.41
1:G:239:LYS:HE2	1:G:245:VAL:O	2.20	0.41
1:F:171:MET:HE3	1:F:172:VAL:H	1.86	0.41
1:F:171:MET:HE3	1:F:201:GLU:O	2.20	0.41
1:F:195:ASP:HB3	3:F:2232:HOH:O	2.21	0.41
1:I:222:LEU:HD13	1:I:248:GLU:HG2	2.02	0.41
1:D:222:LEU:HD13	1:D:248:GLU:HG2	2.03	0.41
1:C:220:LEU:HG	1:C:246:ALA:HB3	2.03	0.41
1:J:48:LEU:HD23	1:J:89:VAL:HG23	2.03	0.41
1:J:173:LYS:HB2	1:J:173:LYS:HE3	1.94	0.41
1:E:125:GLU:OE1	1:E:128:ARG:NH2	2.52	0.40
1:H:169:LEU:C	1:H:169:LEU:HD12	2.45	0.40
1:L:132:TRP:HB2	1:L:262:CYS:HB3	2.03	0.40
1:E:168:GLY:O	1:E:169:LEU:C	2.64	0.40
1:F:188:ARG:NH2	3:F:2219:HOH:O	2.52	0.40
1:A:135:HIS:HD1	1:C:195:ASP:CG	2.29	0.40
1:B:125:GLU:OE1	1:B:128:ARG:NH2	2.55	0.40
1:C:173:LYS:NZ	1:D:103:GLU:OE2	2.54	0.40
1:I:290:LYS:NZ	3:I:2263:HOH:O	2.43	0.40
1:K:21:VAL:HG22	1:K:65:ILE:HG13	2.03	0.40

All (3) 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:A:240:ALA:CB	1:I:128:ARG:NH1[4_466]	1.25	0.95
1:A:236:THR:CG2	1:I:125:GLU:OE2[4_466]	1.67	0.53
1:A:240:ALA:CA	1:I:128:ARG:NH1[4_466]	1.84	0.36

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	288/299 (96%)	284 (99%)	3 (1%)	1 (0%)	36	35
1	B	287/299 (96%)	281 (98%)	5 (2%)	1 (0%)	36	35
1	C	284/299 (95%)	281 (99%)	3 (1%)	0	100	100
1	D	283/299 (95%)	280 (99%)	3 (1%)	0	100	100
1	E	287/299 (96%)	281 (98%)	5 (2%)	1 (0%)	36	35
1	F	283/299 (95%)	281 (99%)	2 (1%)	0	100	100
1	G	283/299 (95%)	279 (99%)	4 (1%)	0	100	100
1	H	283/299 (95%)	280 (99%)	3 (1%)	0	100	100
1	I	287/299 (96%)	282 (98%)	4 (1%)	1 (0%)	36	35
1	J	283/299 (95%)	280 (99%)	3 (1%)	0	100	100
1	K	283/299 (95%)	279 (99%)	4 (1%)	0	100	100
1	L	283/299 (95%)	280 (99%)	3 (1%)	0	100	100
All	All	3414/3588 (95%)	3368 (99%)	42 (1%)	4 (0%)	48	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	GLU
1	B	291	GLU
1	E	291	GLU
1	I	291	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/219 (97%)	210 (99%)	2 (1%)	70	78
1	B	211/219 (96%)	207 (98%)	4 (2%)	50	56
1	C	210/219 (96%)	208 (99%)	2 (1%)	68	75
1	D	209/219 (95%)	209 (100%)	0	100	100
1	E	211/219 (96%)	211 (100%)	0	100	100
1	F	209/219 (95%)	209 (100%)	0	100	100
1	G	209/219 (95%)	208 (100%)	1 (0%)	81	87
1	H	209/219 (95%)	208 (100%)	1 (0%)	81	87
1	I	211/219 (96%)	209 (99%)	2 (1%)	70	78
1	J	209/219 (95%)	205 (98%)	4 (2%)	50	56
1	K	209/219 (95%)	208 (100%)	1 (0%)	81	87
1	L	209/219 (95%)	207 (99%)	2 (1%)	68	75
All	All	2518/2628 (96%)	2499 (99%)	19 (1%)	73	80

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	LEU
1	A	291	GLU
1	B	169	LEU
1	B	206	SER
1	B	215	GLU
1	B	291	GLU
1	C	169	LEU
1	C	287	LEU
1	G	169	LEU
1	H	195	ASP
1	I	184	GLU
1	I	244	SER
1	J	45	GLN
1	J	169	LEU

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Mol	Chain	Res	Type
1	J	241	GLN
1	J	287	LEU
1	K	287	LEU
1	L	188	ARG
1	L	287	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	212	GLN
1	A	265	HIS
1	B	208	GLN
1	B	225	ASN
1	C	162	HIS
1	D	192	GLN
1	D	225	ASN
1	E	225	ASN
1	E	260	GLN
1	F	225	ASN
1	H	225	ASN
1	I	265	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	SRT	E	401	-	9,9,9	1.32	0	12,12,12	1.15	1 (8%)
2	SRT	I	401	-	9,9,9	1.11	0	12,12,12	2.13	3 (25%)
2	SRT	J	401	-	9,9,9	1.30	1 (11%)	12,12,12	3.36	6 (50%)
2	SRT	C	401	-	9,9,9	1.10	0	12,12,12	2.23	4 (33%)
2	SRT	L	401	-	9,9,9	1.10	0	12,12,12	1.38	2 (16%)
2	SRT	F	401	-	9,9,9	1.31	1 (11%)	12,12,12	3.27	5 (41%)
2	SRT	B	401	-	9,9,9	1.08	0	12,12,12	1.74	2 (16%)
2	SRT	H	401	-	9,9,9	1.15	0	12,12,12	1.41	1 (8%)
2	SRT	A	401	-	9,9,9	1.06	0	12,12,12	2.93	6 (50%)
2	SRT	D	401	-	9,9,9	1.09	0	12,12,12	2.82	4 (33%)
2	SRT	K	401	-	9,9,9	1.10	0	12,12,12	1.88	4 (33%)
2	SRT	G	401	-	9,9,9	1.18	0	12,12,12	1.72	3 (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
2	SRT	E	401	-	-	3/12/12/12	-
2	SRT	I	401	-	-	10/12/12/12	-
2	SRT	J	401	-	-	9/12/12/12	-
2	SRT	C	401	-	-	10/12/12/12	-
2	SRT	L	401	-	-	8/12/12/12	-
2	SRT	F	401	-	-	9/12/12/12	-
2	SRT	B	401	-	-	8/12/12/12	-
2	SRT	H	401	-	-	6/12/12/12	-
2	SRT	A	401	-	-	10/12/12/12	-
2	SRT	D	401	-	-	10/12/12/12	-
2	SRT	K	401	-	-	10/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SRT	G	401	-	-	9/12/12/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	SRT	C2-C1	-2.40	1.49	1.52
2	J	401	SRT	C3-C4	-2.39	1.49	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	SRT	O3-C3-C2	-9.16	91.52	110.17
2	F	401	SRT	O3-C3-C2	-7.62	94.66	110.17
2	D	401	SRT	O3-C3-C2	-7.03	95.85	110.17
2	A	401	SRT	O3-C3-C2	-6.58	96.77	110.17
2	C	401	SRT	O3-C3-C2	-5.64	98.68	110.17
2	I	401	SRT	O3-C3-C2	-4.85	100.29	110.17
2	F	401	SRT	O2-C2-C3	4.64	119.60	110.17
2	F	401	SRT	O11-C1-C2	-4.26	110.28	121.62
2	A	401	SRT	O11-C1-C2	-4.18	110.49	121.62
2	B	401	SRT	O3-C3-C2	-4.06	101.90	110.17
2	K	401	SRT	O3-C3-C2	-3.89	102.25	110.17
2	D	401	SRT	O11-C1-C2	-3.88	111.27	121.62
2	D	401	SRT	O1-C1-C2	3.81	123.91	113.31
2	A	401	SRT	O1-C1-C2	3.77	123.78	113.31
2	F	401	SRT	O2-C2-C1	3.72	118.64	110.69
2	J	401	SRT	O1-C1-C2	3.62	123.36	113.31
2	F	401	SRT	O1-C1-C2	3.52	123.09	113.31
2	I	401	SRT	O1-C1-C2	3.50	123.04	113.31
2	J	401	SRT	O2-C2-C1	3.30	117.75	110.69
2	A	401	SRT	O2-C2-C3	3.28	116.84	110.17
2	J	401	SRT	O11-C1-C2	-3.19	113.11	121.62
2	C	401	SRT	O1-C1-C2	3.13	122.01	113.31
2	G	401	SRT	O3-C3-C2	-2.89	104.28	110.17
2	A	401	SRT	C2-C3-C4	2.82	116.08	109.82
2	B	401	SRT	O1-C1-C2	2.79	121.07	113.31
2	G	401	SRT	O1-C1-C2	2.70	120.82	113.31
2	I	401	SRT	O11-C1-C2	-2.67	114.51	121.62
2	K	401	SRT	C2-C3-C4	2.62	115.64	109.82
2	H	401	SRT	O1-C1-C2	2.62	120.59	113.31
2	L	401	SRT	O1-C1-C2	2.62	120.59	113.31
2	J	401	SRT	O2-C2-C3	2.57	115.39	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	SRT	O11-C1-C2	-2.51	114.93	121.62
2	K	401	SRT	O1-C1-C2	2.45	120.12	113.31
2	K	401	SRT	O2-C2-C3	2.35	114.95	110.17
2	G	401	SRT	O11-C1-C2	-2.33	115.42	121.62
2	E	401	SRT	O1-C1-C2	2.32	119.76	113.31
2	L	401	SRT	C2-C3-C4	2.28	114.88	109.82
2	A	401	SRT	O2-C2-C1	2.21	115.43	110.69
2	C	401	SRT	O2-C2-C1	2.11	115.20	110.69
2	J	401	SRT	C2-C3-C4	2.11	114.49	109.82
2	D	401	SRT	O2-C2-C3	2.05	114.34	110.17

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	SRT	O11-C1-C2-O2
2	A	401	SRT	O2-C2-C3-O3
2	B	401	SRT	O2-C2-C3-O3
2	C	401	SRT	O1-C1-C2-O2
2	C	401	SRT	O2-C2-C3-O3
2	D	401	SRT	O11-C1-C2-O2
2	D	401	SRT	O2-C2-C3-O3
2	F	401	SRT	O11-C1-C2-O2
2	G	401	SRT	O11-C1-C2-O2
2	H	401	SRT	O1-C1-C2-O2
2	H	401	SRT	O11-C1-C2-O2
2	I	401	SRT	O2-C2-C3-O3
2	J	401	SRT	O11-C1-C2-O2
2	J	401	SRT	O2-C2-C3-O3
2	K	401	SRT	O2-C2-C3-O3
2	L	401	SRT	C1-C2-C3-O3
2	L	401	SRT	O2-C2-C3-O3
2	B	401	SRT	C1-C2-C3-O3
2	C	401	SRT	C1-C2-C3-O3
2	D	401	SRT	C1-C2-C3-O3
2	I	401	SRT	C1-C2-C3-O3
2	K	401	SRT	C1-C2-C3-O3
2	F	401	SRT	O2-C2-C3-O3
2	H	401	SRT	O2-C2-C3-O3
2	L	401	SRT	C1-C2-C3-C4
2	A	401	SRT	O1-C1-C2-O2
2	B	401	SRT	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	401	SRT	O11-C1-C2-O2
2	C	401	SRT	O11-C1-C2-O2
2	D	401	SRT	O1-C1-C2-O2
2	E	401	SRT	O1-C1-C2-O2
2	E	401	SRT	O11-C1-C2-O2
2	F	401	SRT	O1-C1-C2-O2
2	G	401	SRT	O1-C1-C2-O2
2	I	401	SRT	O1-C1-C2-O2
2	I	401	SRT	O11-C1-C2-O2
2	J	401	SRT	O1-C1-C2-O2
2	K	401	SRT	O1-C1-C2-O2
2	K	401	SRT	O11-C1-C2-O2
2	L	401	SRT	O1-C1-C2-O2
2	L	401	SRT	O11-C1-C2-O2
2	A	401	SRT	O1-C1-C2-C3
2	C	401	SRT	O1-C1-C2-C3
2	D	401	SRT	O1-C1-C2-C3
2	F	401	SRT	O1-C1-C2-C3
2	G	401	SRT	O1-C1-C2-C3
2	G	401	SRT	O11-C1-C2-C3
2	J	401	SRT	O1-C1-C2-C3
2	K	401	SRT	O1-C1-C2-C3
2	A	401	SRT	C1-C2-C3-O3
2	F	401	SRT	C1-C2-C3-O3
2	J	401	SRT	C1-C2-C3-O3
2	G	401	SRT	O2-C2-C3-O3
2	K	401	SRT	C1-C2-C3-C4
2	A	401	SRT	O2-C2-C3-C4
2	C	401	SRT	O2-C2-C3-C4
2	F	401	SRT	O2-C2-C3-C4
2	I	401	SRT	O2-C2-C3-C4
2	K	401	SRT	O2-C2-C3-C4
2	L	401	SRT	O2-C2-C3-C4
2	G	401	SRT	O3-C3-C4-O4
2	A	401	SRT	O11-C1-C2-C3
2	D	401	SRT	O11-C1-C2-C3
2	B	401	SRT	O2-C2-C3-C4
2	D	401	SRT	O2-C2-C3-C4
2	J	401	SRT	O2-C2-C3-C4
2	G	401	SRT	O3-C3-C4-O41
2	H	401	SRT	C1-C2-C3-O3
2	C	401	SRT	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	I	401	SRT	O1-C1-C2-C3
2	J	401	SRT	O11-C1-C2-C3
2	K	401	SRT	O11-C1-C2-C3
2	B	401	SRT	O1-C1-C2-C3
2	C	401	SRT	C1-C2-C3-C4
2	B	401	SRT	O11-C1-C2-C3
2	H	401	SRT	O2-C2-C3-C4
2	F	401	SRT	O11-C1-C2-C3
2	I	401	SRT	O11-C1-C2-C3
2	G	401	SRT	C1-C2-C3-O3
2	B	401	SRT	C1-C2-C3-C4
2	I	401	SRT	C1-C2-C3-C4
2	G	401	SRT	O2-C2-C3-C4
2	A	401	SRT	C1-C2-C3-C4
2	L	401	SRT	O1-C1-C2-C3
2	I	401	SRT	C2-C3-C4-O4
2	A	401	SRT	C2-C3-C4-O4
2	C	401	SRT	C2-C3-C4-O4
2	C	401	SRT	C2-C3-C4-O41
2	E	401	SRT	O2-C2-C3-O3
2	K	401	SRT	C2-C3-C4-O4
2	I	401	SRT	C2-C3-C4-O41
2	H	401	SRT	C1-C2-C3-C4
2	A	401	SRT	C2-C3-C4-O41
2	D	401	SRT	C2-C3-C4-O41
2	K	401	SRT	C2-C3-C4-O41
2	L	401	SRT	O11-C1-C2-C3
2	D	401	SRT	C1-C2-C3-C4
2	D	401	SRT	C2-C3-C4-O4
2	F	401	SRT	C1-C2-C3-C4
2	J	401	SRT	C2-C3-C4-O41
2	F	401	SRT	C2-C3-C4-O41
2	J	401	SRT	C2-C3-C4-O4

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	401	SRT	2	0
2	C	401	SRT	2	0
2	L	401	SRT	1	0
2	F	401	SRT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	401	SRT	1	0
2	A	401	SRT	1	0
2	D	401	SRT	2	0
2	G	401	SRT	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	290/299 (96%)	0.53	14 (4%)	35 34	2, 7, 13, 31	0
1	B	289/299 (96%)	0.76	30 (10%)	11 10	2, 7, 13, 21	0
1	C	286/299 (95%)	0.36	11 (3%)	44 43	2, 7, 13, 28	0
1	D	285/299 (95%)	0.36	14 (4%)	35 34	2, 7, 12, 21	0
1	E	289/299 (96%)	0.63	27 (9%)	14 13	2, 7, 13, 25	0
1	F	285/299 (95%)	0.33	10 (3%)	47 46	2, 7, 12, 21	0
1	G	285/299 (95%)	0.54	8 (2%)	55 54	2, 7, 12, 21	0
1	H	285/299 (95%)	0.95	35 (12%)	8 7	2, 7, 12, 21	0
1	I	289/299 (96%)	0.34	12 (4%)	40 39	2, 7, 13, 25	0
1	J	285/299 (95%)	0.28	7 (2%)	58 58	2, 7, 12, 21	0
1	K	285/299 (95%)	0.32	5 (1%)	67 67	2, 7, 12, 21	0
1	L	285/299 (95%)	0.73	17 (5%)	27 26	2, 7, 12, 21	0
All	All	3438/3588 (95%)	0.51	190 (5%)	30 29	2, 7, 13, 31	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	VAL	15.6
1	E	292	VAL	12.3
1	I	292	VAL	9.4
1	B	229	GLU	6.3
1	A	3	MET	6.2
1	A	4	ASP	6.1
1	B	4	ASP	6.0
1	C	3	MET	5.9
1	E	229	GLU	5.7
1	B	205	SER	5.2
1	E	230	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	230	GLU	4.7
1	B	233	PRO	4.6
1	I	256	ASP	4.4
1	F	184	GLU	4.3
1	I	128	ARG	4.2
1	B	211	VAL	4.0
1	E	4	ASP	4.0
1	E	184	GLU	3.9
1	K	128	ARG	3.9
1	B	238	LEU	3.8
1	I	4	ASP	3.8
1	I	125	GLU	3.8
1	F	196	PHE	3.8
1	H	180	ALA	3.7
1	D	4	ASP	3.7
1	B	215	GLU	3.7
1	H	213	ALA	3.7
1	C	128	ARG	3.7
1	B	237	VAL	3.7
1	B	241	GLN	3.6
1	F	230	GLU	3.5
1	H	211	VAL	3.5
1	H	4	ASP	3.5
1	J	131	GLY	3.4
1	E	15	VAL	3.4
1	C	4	ASP	3.4
1	F	77	LEU	3.4
1	B	292	VAL	3.4
1	B	128	ARG	3.4
1	E	208	GLN	3.4
1	B	227	LYS	3.4
1	A	128	ARG	3.3
1	J	4	ASP	3.3
1	F	192	GLN	3.3
1	B	263	GLY	3.2
1	E	233	PRO	3.2
1	B	236	THR	3.2
1	G	49	TRP	3.2
1	F	4	ASP	3.2
1	A	188	ARG	3.2
1	A	195	ASP	3.1
1	B	256	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	229	GLU	3.1
1	H	262	CYS	3.1
1	C	208	GLN	3.1
1	B	240	ALA	3.0
1	E	211	VAL	3.0
1	E	226	PHE	3.0
1	A	45	GLN	3.0
1	H	122	ALA	3.0
1	D	128	ARG	3.0
1	D	208	GLN	3.0
1	C	205	SER	3.0
1	E	93	ARG	2.9
1	A	5	ALA	2.9
1	B	252	GLY	2.9
1	E	205	SER	2.9
1	H	181	GLY	2.9
1	L	188	ARG	2.8
1	L	208	GLN	2.8
1	F	195	ASP	2.8
1	H	207	LEU	2.8
1	A	196	PHE	2.8
1	B	207	LEU	2.8
1	F	128	ARG	2.8
1	H	196	PHE	2.8
1	H	20	LEU	2.8
1	E	45	GLN	2.7
1	B	206	SER	2.7
1	F	227	LYS	2.7
1	A	15	VAL	2.7
1	E	241	GLN	2.7
1	I	230	GLU	2.7
1	E	227	LYS	2.7
1	J	184	GLU	2.7
1	L	180	ALA	2.6
1	D	211	VAL	2.6
1	A	168	GLY	2.6
1	C	229	GLU	2.6
1	D	215	GLU	2.6
1	D	230	GLU	2.6
1	H	126	ALA	2.6
1	G	76	PHE	2.6
1	H	231	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	208	GLN	2.6
1	J	241	GLN	2.6
1	C	230	GLU	2.6
1	H	186	ALA	2.6
1	H	263	GLY	2.5
1	B	129	GLY	2.5
1	H	134	GLY	2.5
1	L	15	VAL	2.5
1	L	181	GLY	2.5
1	C	188	ARG	2.5
1	E	215	GLU	2.5
1	H	265	HIS	2.5
1	L	131	GLY	2.5
1	D	256	ASP	2.4
1	H	206	SER	2.4
1	J	128	ARG	2.4
1	H	266	ILE	2.4
1	L	206	SER	2.4
1	C	168	GLY	2.4
1	B	208	GLN	2.4
1	I	291	GLU	2.4
1	H	131	GLY	2.4
1	H	145	GLY	2.4
1	I	45	GLN	2.4
1	H	244	SER	2.4
1	H	204	CYS	2.4
1	L	195	ASP	2.3
1	L	196	PHE	2.3
1	B	244	SER	2.3
1	H	210	ALA	2.3
1	D	184	GLU	2.3
1	E	240	ALA	2.3
1	E	195	ASP	2.3
1	L	238	LEU	2.3
1	H	184	GLU	2.3
1	B	234	THR	2.3
1	J	236	THR	2.3
1	C	180	ALA	2.3
1	D	168	GLY	2.3
1	G	94	GLY	2.3
1	L	182	GLY	2.3
1	E	237	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	88	ARG	2.2
1	H	230	GLU	2.2
1	I	208	GLN	2.2
1	K	205	SER	2.2
1	B	264	PRO	2.2
1	D	195	ASP	2.2
1	J	230	GLU	2.2
1	G	34	TYR	2.2
1	D	76	PHE	2.2
1	D	288	PHE	2.2
1	G	288	PHE	2.2
1	C	184	GLU	2.2
1	F	181	GLY	2.2
1	K	215	GLU	2.2
1	I	192	GLN	2.2
1	E	231	LEU	2.2
1	E	238	LEU	2.2
1	A	174	ASP	2.2
1	B	45	GLN	2.1
1	G	88	ARG	2.1
1	K	211	VAL	2.1
1	H	179	ALA	2.1
1	H	214	ALA	2.1
1	A	230	GLU	2.1
1	H	226	PHE	2.1
1	L	242	PHE	2.1
1	D	227	LYS	2.1
1	B	235	ALA	2.1
1	L	5	ALA	2.1
1	H	205	SER	2.1
1	E	243	PRO	2.1
1	K	181	GLY	2.1
1	B	82	LYS	2.1
1	E	239	LYS	2.1
1	E	207	LEU	2.0
1	H	238	LEU	2.0
1	L	207	LEU	2.0
1	E	113	CYS	2.0
1	L	204	CYS	2.0
1	H	133	THR	2.0
1	G	82	LYS	2.0
1	B	145	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	196	PHE	2.0
1	L	244	SER	2.0
1	B	19	ALA	2.0
1	H	18	ALA	2.0
1	H	240	ALA	2.0
1	L	126	ALA	2.0
1	A	26	ARG	2.0
1	E	128	ARG	2.0
1	H	233	PRO	2.0
1	E	129	GLY	2.0
1	G	168	GLY	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(Å ²)	Q<0.9
2	SRT	H	401	10/10	0.77	0.20	16,18,21,22	0
2	SRT	L	401	10/10	0.80	0.18	19,22,25,25	0
2	SRT	I	401	10/10	0.81	0.14	16,22,26,27	0
2	SRT	E	401	10/10	0.83	0.13	10,16,19,24	0
2	SRT	K	401	10/10	0.84	0.10	12,16,17,17	0
2	SRT	B	401	10/10	0.84	0.12	16,20,24,24	0
2	SRT	F	401	10/10	0.85	0.10	8,15,18,18	0
2	SRT	G	401	10/10	0.85	0.11	19,22,23,25	0
2	SRT	D	401	10/10	0.85	0.10	16,20,20,21	0
2	SRT	A	401	10/10	0.86	0.13	15,19,22,22	0
2	SRT	C	401	10/10	0.88	0.10	16,19,23,24	0
2	SRT	J	401	10/10	0.90	0.08	7,11,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.