



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 11:25 PM GMT

PDB ID : 2JBM  
Title : QPRTASE STRUCTURE FROM HUMAN  
Authors : Liu, H.; Naismith, J.H.  
Deposited on : 2006-12-08  
Resolution : 2.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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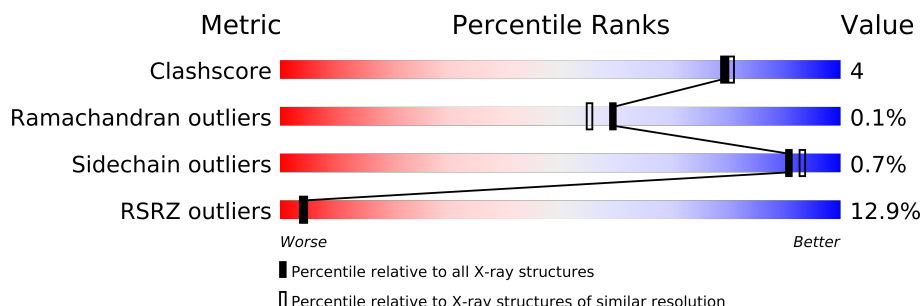
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	299	
1	B	299	
1	C	299	
1	D	299	
1	E	299	
1	F	299	
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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SRT	G	401	-	X
2	SRT	H	401	-	X
2	SRT	I	401	-	X
2	SRT	L	401	-	X

## 2 Entry composition

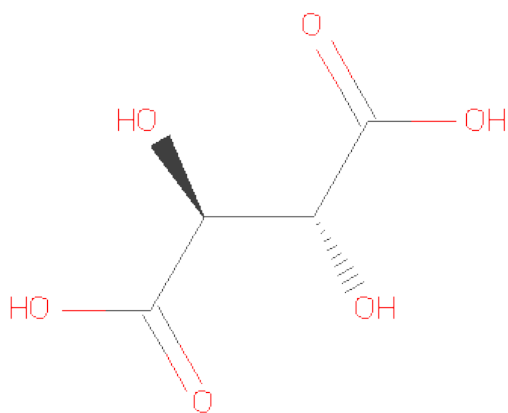
There are 3 unique types of molecules in this entry. The entry contains 28196 atoms, of which 0 are hydrogen and 0 are deuterium.

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-NUCLEOTIDEPYROPHOSPHORYLASE.

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 (three-letter code: SRT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



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.

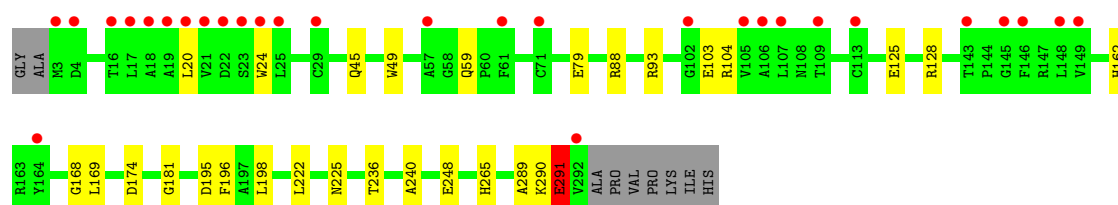
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	375	Total 375	O 375	0	0
3	B	324	Total 324	O 324	0	0
3	C	280	Total 280	O 280	0	0
3	D	292	Total 292	O 292	0	0
3	E	267	Total 267	O 267	0	0
3	F	315	Total 315	O 315	0	0
3	G	181	Total 181	O 181	0	0
3	H	127	Total 127	O 127	0	0
3	I	269	Total 269	O 269	0	0
3	J	256	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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

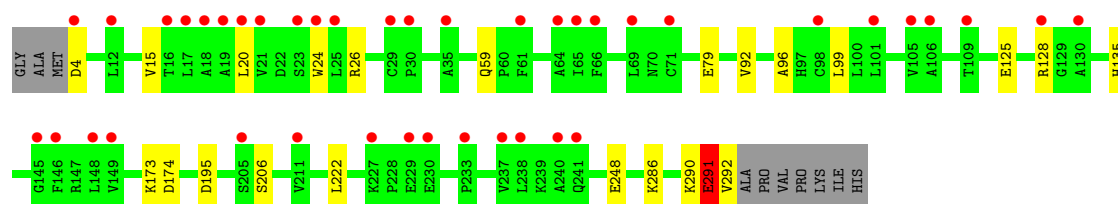
#### • Molecule 1: NICOTINATE-NUCLEOTIDEPYROPHOSPHORYLASE

Chain A: 



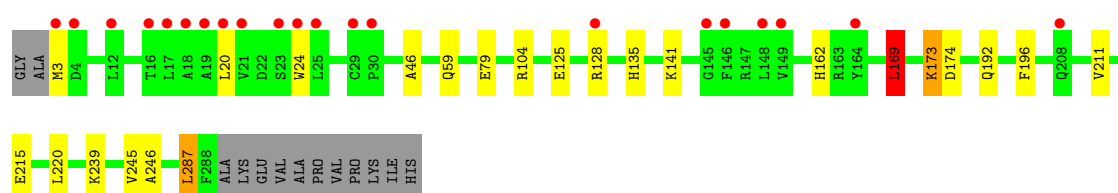
#### • Molecule 1: NICOTINATE-NUCLEOTIDEPYROPHOSPHORYLASE

Chain B: 



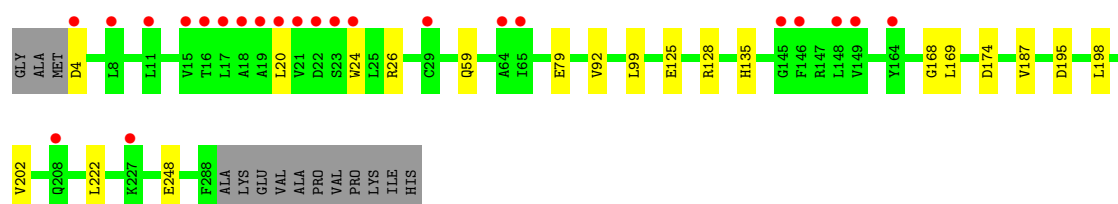
#### • Molecule 1: NICOTINATE-NUCLEOTIDEPYROPHOSPHORYLASE

Chain C: 

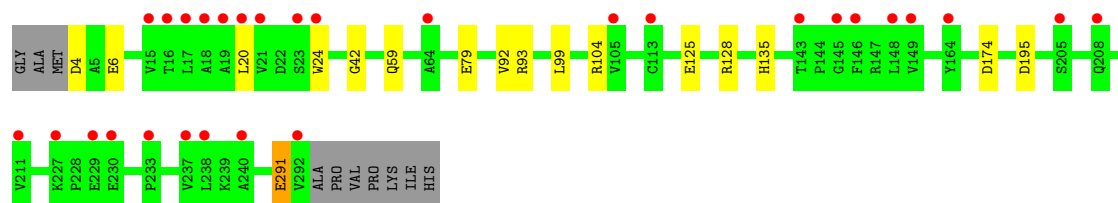


#### • Molecule 1: NICOTINATE-NUCLEOTIDEPYROPHOSPHORYLASE

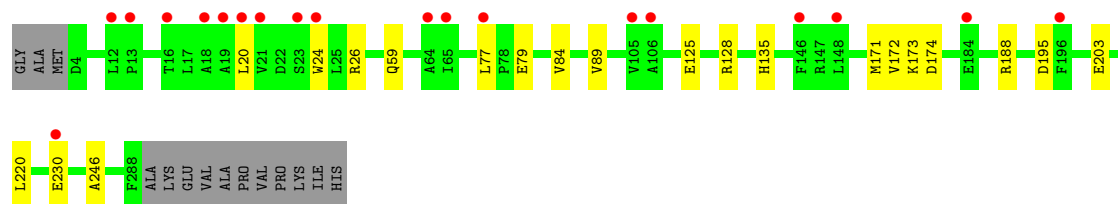
Chain D: 



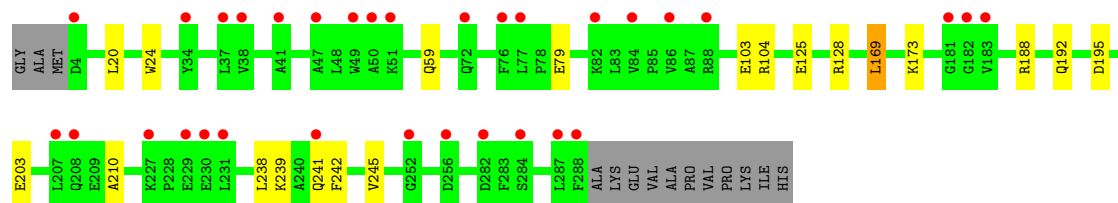
- Molecule 1: NICOTINATE-NUCLEOTIDEPYROPHOSPHORYLASE

Chain E: 

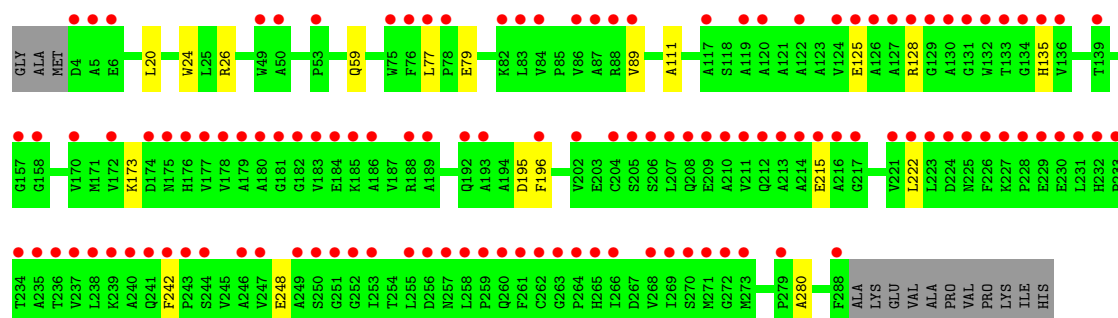
- Molecule 1: NICOTINATE-NUCLEOTIDEPYROPHOSPHORYLASE

Chain F: 

- Molecule 1: NICOTINATE-NUCLEOTIDEPYROPHOSPHORYLASE

Chain G: 

- Molecule 1: NICOTINATE-NUCLEOTIDEPYROPHOSPHORYLASE

Chain H: 

- Molecule 1: NICOTINATE-NUCLEOTIDEPYROPHOSPHORYLASE

Chain I: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.92Å 179.29Å 194.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.97 – 2.00 60.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.4 (60.97-2.00) 86.1 (60.98-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.208 0.247 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 16.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 261330 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	28196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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	0.65	0/2152	0.67	2/2933 (0.1%)
1	B	0.57	0/2144	0.64	1/2923 (0.0%)
1	C	0.54	0/2128	0.61	2/2901 (0.1%)
1	D	0.51	0/2120	0.60	1/2891 (0.0%)
1	E	0.54	0/2144	0.63	1/2923 (0.0%)
1	F	0.54	0/2120	0.62	1/2891 (0.0%)
1	G	0.43	0/2120	0.55	1/2891 (0.0%)
1	H	0.40	0/2120	0.52	0/2891
1	I	0.52	0/2144	0.60	1/2923 (0.0%)
1	J	0.50	0/2120	0.62	2/2891 (0.1%)
1	K	0.44	0/2120	0.53	0/2891
1	L	0.42	0/2120	0.53	0/2891
All	All	0.51	0/25552	0.60	12/34840 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	45	GLN	CA-CB-CG	8.53	132.16	113.40
1	B	174	ASP	CB-CG-OD1	7.39	124.95	118.30
1	D	174	ASP	CB-CG-OD1	6.92	124.53	118.30
1	I	174	ASP	CB-CG-OD1	6.82	124.43	118.30
1	E	174	ASP	CB-CG-OD1	6.38	124.04	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2109	0	2128	20	3
1	B	2101	0	2119	18	0
1	C	2085	0	2104	18	0
1	D	2077	0	2095	11	0
1	E	2101	0	2119	17	0
1	F	2077	0	2095	18	0
1	G	2077	0	2095	11	0
1	H	2077	0	2095	13	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	11	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
3	K	206	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	148	0	0	5	0
All	All	28196	0	25302	178	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 178 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	Distance(Å)	Clash(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

### 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	288/299 (96%)	284 (99%)	3 (1%)	1 (0%)	50	44
1	B	287/299 (96%)	281 (98%)	5 (2%)	1 (0%)	50	44
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%)	50	44
1	F	283/299 (95%)	281 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	50	44
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%)	59	55

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%)	87	90
1	B	211/219 (96%)	209 (99%)	2 (1%)	87	90
1	C	210/219 (96%)	207 (99%)	3 (1%)	78	81
1	D	209/219 (95%)	208 (100%)	1 (0%)	94	96
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%)	94	96
1	H	209/219 (95%)	208 (100%)	1 (0%)	94	96
1	I	211/219 (96%)	209 (99%)	2 (1%)	87	90
1	J	209/219 (95%)	207 (99%)	2 (1%)	85	88
1	K	209/219 (95%)	208 (100%)	1 (0%)	94	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	209/219 (95%)	207 (99%)	2 (1%)	85	88
All	All	2518/2628 (96%)	2501 (99%)	17 (1%)	91	93

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	169	LEU
1	G	169	LEU
1	J	241	GLN
1	C	287	LEU
1	K	287	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	265	HIS
1	J	265	HIS
1	I	265	HIS
1	C	162	HIS
1	I	276	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	401	-	9,9,9	1.02	0	12,12,12	2.75	6 (50%)
2	SRT	B	401	-	9,9,9	0.97	0	12,12,12	1.62	2 (16%)
2	SRT	C	401	-	9,9,9	1.02	0	12,12,12	2.10	4 (33%)
2	SRT	D	401	-	9,9,9	1.09	0	12,12,12	2.66	4 (33%)
2	SRT	E	401	-	9,9,9	1.28	1 (11%)	12,12,12	1.02	1 (8%)
2	SRT	F	401	-	9,9,9	1.33	1 (11%)	12,12,12	3.13	5 (41%)
2	SRT	G	401	-	9,9,9	1.12	1 (11%)	12,12,12	1.57	2 (16%)
2	SRT	H	401	-	9,9,9	1.07	0	12,12,12	1.27	1 (8%)
2	SRT	I	401	-	9,9,9	1.00	0	12,12,12	1.99	3 (25%)
2	SRT	J	401	-	9,9,9	1.33	1 (11%)	12,12,12	3.22	5 (41%)
2	SRT	K	401	-	9,9,9	1.01	0	12,12,12	1.72	4 (33%)
2	SRT	L	401	-	9,9,9	1.00	0	12,12,12	1.21	1 (8%)

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	A	401	-	-	0/12/12/12	0/0/0/0
2	SRT	B	401	-	-	0/12/12/12	0/0/0/0
2	SRT	C	401	-	-	0/12/12/12	0/0/0/0
2	SRT	D	401	-	-	0/12/12/12	0/0/0/0
2	SRT	E	401	-	-	0/12/12/12	0/0/0/0
2	SRT	F	401	-	-	0/12/12/12	0/0/0/0
2	SRT	G	401	-	-	0/12/12/12	0/0/0/0
2	SRT	H	401	-	-	0/12/12/12	0/0/0/0
2	SRT	I	401	-	-	0/12/12/12	0/0/0/0
2	SRT	J	401	-	-	0/12/12/12	0/0/0/0
2	SRT	K	401	-	-	0/12/12/12	0/0/0/0
2	SRT	L	401	-	-	0/12/12/12	0/0/0/0

All (4) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	SRT	C2-C1	-2.65	1.49	1.52
2	J	401	SRT	C3-C4	-2.64	1.49	1.52
2	E	401	SRT	C2-C1	-2.18	1.49	1.52
2	G	401	SRT	C2-C1	-2.05	1.50	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	SRT	O3-C3-C2	-9.01	91.52	110.19
2	F	401	SRT	O3-C3-C2	-7.50	94.66	110.19
2	D	401	SRT	O3-C3-C2	-6.92	95.85	110.19
2	A	401	SRT	O3-C3-C2	-6.48	96.77	110.19
2	C	401	SRT	O3-C3-C2	-5.56	98.68	110.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	290/299 (96%)	0.91	29 (10%) 8 7	2, 7, 13, 31	0
1	B	289/299 (96%)	0.83	41 (14%) 3 3	2, 7, 13, 21	0
1	C	286/299 (95%)	0.52	21 (7%) 15 14	2, 7, 13, 28	0
1	D	285/299 (95%)	0.54	23 (8%) 12 11	2, 7, 12, 21	0
1	E	289/299 (96%)	0.68	29 (10%) 8 7	2, 7, 13, 25	0
1	F	285/299 (95%)	0.55	19 (6%) 17 17	2, 7, 12, 21	0
1	G	285/299 (95%)	0.71	32 (11%) 6 6	2, 7, 12, 21	0
1	H	285/299 (95%)	1.83	123 (43%) 1 1	2, 7, 12, 21	0
1	I	289/299 (96%)	0.30	7 (2%) 56 56	2, 7, 13, 25	0
1	J	285/299 (95%)	0.45	13 (4%) 31 30	2, 7, 12, 21	0
1	K	285/299 (95%)	0.40	19 (6%) 17 17	2, 7, 12, 21	0
1	L	285/299 (95%)	1.28	88 (30%) 1 1	2, 7, 12, 21	0
All	All	3438/3588 (95%)	0.75	444 (12%) 4 4	2, 7, 13, 31	0

The worst 5 of 444 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	292	VAL	12.4
1	A	292	VAL	12.1
1	H	231	LEU	8.0
1	H	207	LEU	7.5
1	H	134	GLY	7.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SRT	H	401	10/10	0.37	3.69	16,18,21,22	0
2	SRT	G	401	10/10	0.17	3.65	19,22,23,25	0
2	SRT	L	401	10/10	0.23	2.43	19,22,25,25	0
2	SRT	I	401	10/10	0.19	2.06	16,22,26,27	0
2	SRT	K	401	10/10	0.15	1.21	12,16,17,17	0
2	SRT	E	401	10/10	0.18	0.99	10,16,19,24	0
2	SRT	B	401	10/10	0.18	0.41	16,20,24,24	0
2	SRT	A	401	10/10	0.19	0.30	15,19,22,22	0
2	SRT	J	401	10/10	0.12	-0.21	7,11,13,13	0
2	SRT	D	401	10/10	0.14	-0.51	16,20,20,21	0
2	SRT	C	401	10/10	0.14	-0.51	16,19,23,24	0
2	SRT	F	401	10/10	0.14	-0.60	8,15,18,18	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.