



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:13 AM GMT

PDB ID : 3LAM  
Title : Crystal structure of HIV-1 reverse transcriptase in complex with N1-propyl pyrimidinedione non-nucleoside inhibitor  
Authors : Lansdon, E.B.; Mitchell, M.L.  
Deposited on : 2010-01-06  
Resolution : 2.76 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

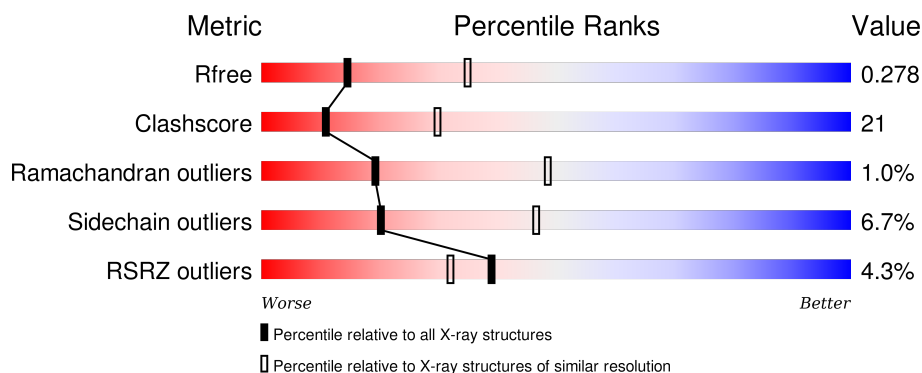
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.76 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))
$R_{free}$	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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. 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	560	<div> <div>4%</div> <div>55%</div> <div>39%</div> <div>5%</div> </div>
1	B	560	<div> <div>3%</div> <div>43%</div> <div>26%</div> <div>28%</div> </div>

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
3	SO4	A	564	-	-	-	X

## 2 Entry composition [i](#)

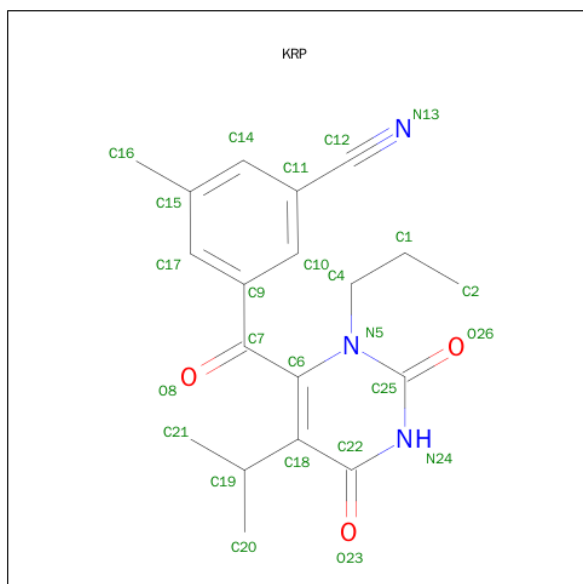
There are 4 unique types of molecules in this entry. The entry contains 7995 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HIV Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4508	2914	752	834	8			
1	B	403	Total	C	N	O	S	0	0	0
			3334	2173	550	605	6			

- Molecule 2 is 3-METHYL-5-{[5-(1-METHYLETHYL)-2,6-DIOXO-3-PROPYL-1,2,3,6-TETRAHYDROPYRIMIDIN-4-YL]CARBONYL}BENZONITRILE (three-letter code: KRP) (formula: C<sub>19</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	19	3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

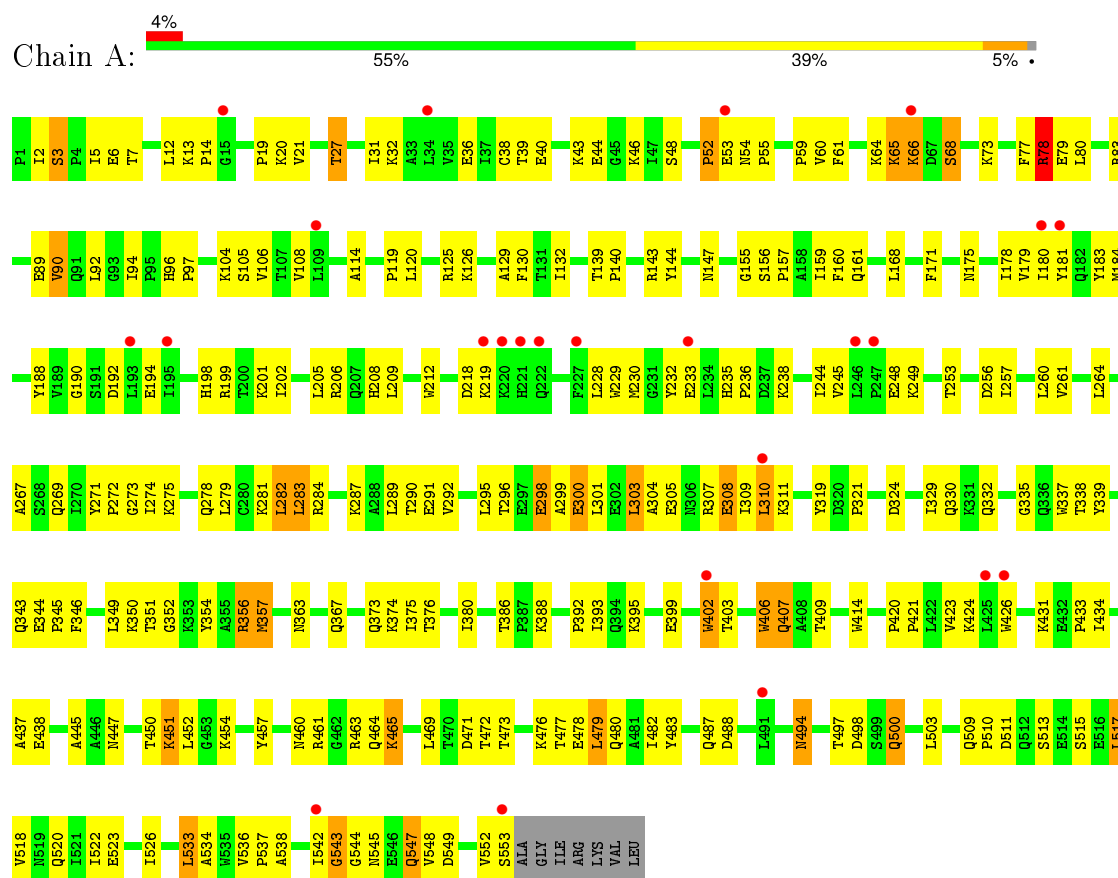
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	45	Total	O	0	0
			45	45		

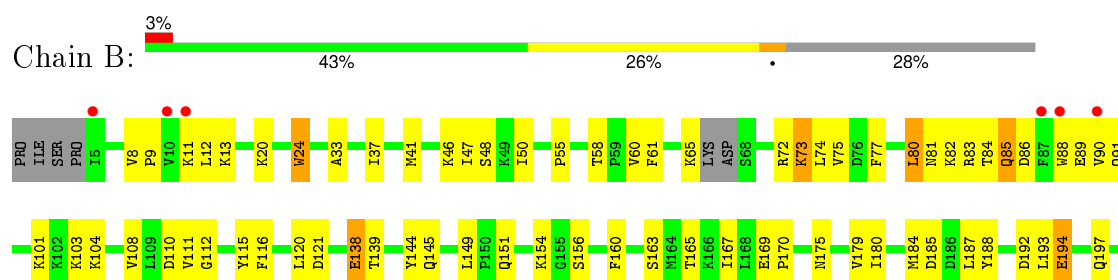
### 3 Residue-property plots

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: HIV Reverse transcriptase



#### • Molecule 1: HIV Reverse transcriptase



IIE	ALA	ARG	1270	K201
IIE	ALA	GLY	Y271	L205
GLN	ASN	ALA		
ALA	ARG	H361	1274	L209
GLN	GLU	T362	K275	
PRO	THR	H363	V276	
ASP	LYS	H364		
GLN	LEU	V365	L279	G212
SER	GLY	K366	C280	G213
GLU	LYS	K367	K281	L214
SER	ALA	L368	T282	T215
GLU	GLY	T369		THR
LEU	THR		R284	PRO
VAL	VAL	V372	G285	ASP
ASN	THR	K373	T286	LYS
GLN	ASN	K374	K287	HIS
IIE	ARG		A288	GLN
IIE	GLY	E378	L289	LYS
GLU	ARG	S379	T290	GLU
GLN	GLN			PRO
LEU	VAL	K385	L293	PRO
IIE	VAL	T386	P294	PRO
LYS	VAL	P387	L295	PHE
LYS	THR		T296	LEU
GLU	LEU	K395	E297	TRP
LYS	THR		E298	MET
VAL	ASP	E399	A299	GLY
TYR	THR	T400	E300	V232
LEU	THR	H401		E233
ALA	ASN			L234
TRP	GLN	H405	E305	H235
VAL	LYS	H406	R306	P236
PRO	THR	Q407	R307	D237
ALA	GLU		K238	K239
HIS	LEU	E413	I309	H239
LYS	GLN		L310	T240
GLY	IIE	P420	Y319	V241
IIE	IIE	P421		Q242
GLY	TYR	L422	K323	P243
GLY	LEU	H423		T244
ASN	ALA	K424	E328	
GLU	LEU	L425	I329	E248
GLN	GLN		K331	K249
VAL	VAL	Q428		D250
ASP	SER	L429	K331	S251
LYS	GLY		Q334	H252
LEU	LEU	GLU		V254
VAL	VAL	GLU	H337	H255
SER	VAL	PRO	T338	D256
ALA	ASN	IIE	Y339	I257
GLY	IIE	VAL		
IIE	VAL	GLY	E344	L260
ARG	THR	GLY	P345	V261
LYS	ASP	GLU	P346	
VAL	SER	THR	K347	L264
LEU	GLN	PHE		H265
	TYR	VAL	G352	H266
	ALA	VAL		A267
	LEU	GLY	R356	S268
	GLY	GLY	H357	H269

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.64Å 154.47Å 153.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 2.76 47.30 – 2.76	Depositor EDS
% Data completeness (in resolution range)	93.3 (29.91-2.76) 93.4 (47.30-2.76)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 2.77Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, $R_{free}$	0.231 , 0.280 0.224 , 0.278	Depositor DCC
$R_{free}$ test set	1716 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.0	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 36429 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7995	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KRP, SO4

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	0.38	0/4625	0.54	0/6284
1	B	0.39	0/3426	0.54	0/4655
All	All	0.39	0/8051	0.54	0/10939

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	PRO	Peptide
1	A	65	LYS	Peptide
1	A	66	LYS	Peptide

### 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	4508	0	4558	209	0
1	B	3334	0	3365	133	0
2	A	25	0	21	4	0
3	A	20	0	0	0	0
3	B	5	0	0	0	0
4	A	58	0	0	3	0
4	B	45	0	0	2	0
All	All	7995	0	7944	332	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 21.

All (332) 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:337:TRP:HE1	1:A:367:GLN:NE2	1.65	0.95
1:B:282:LEU:HB3	1:B:293:ILE:HD13	1.46	0.93
1:A:472:THR:HG23	1:A:476:LYS:HB2	1.51	0.92
1:A:228:LEU:H	1:A:228:LEU:HD12	1.32	0.91
1:A:547:GLN:HE21	1:A:547:GLN:H	1.22	0.86
1:A:547:GLN:HE21	1:A:547:GLN:N	1.73	0.86
1:B:344:GLU:HB3	1:B:347:LYS:HD3	1.59	0.85
1:B:13:LYS:HE3	1:B:85:GLN:HG3	1.57	0.84
1:B:296:THR:HG22	1:B:298:GLU:H	1.44	0.83
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.61	0.81
1:B:194:GLU:HG3	1:B:197:GLN:HG3	1.61	0.81
1:A:257:ILE:O	1:A:261:VAL:HG23	1.81	0.80
1:A:278:GLN:HB3	1:A:299:ALA:HA	1.64	0.79
1:A:278:GLN:HG3	1:A:298:GLU:HB2	1.63	0.79
1:A:40:GLU:O	1:A:44:GLU:HG2	1.84	0.78
1:B:60:VAL:HG12	1:B:75:VAL:HG22	1.66	0.76
1:B:282:LEU:HB3	1:B:293:ILE:CD1	2.15	0.76
1:B:58:THR:HG23	4:B:563:HOH:O	1.84	0.76
1:B:61:PHE:CZ	1:B:74:LEU:HD23	2.22	0.75
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.21	0.74
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.23	0.74
1:B:61:PHE:CE2	1:B:74:LEU:HD23	2.23	0.73
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.71	0.72
1:A:298:GLU:H	1:A:298:GLU:CD	1.93	0.72
1:B:296:THR:O	1:B:300:GLU:HG3	1.90	0.72
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.37	0.71
1:B:276:VAL:HG12	1:B:280:CYS:SG	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ALA:O	1:A:477:THR:HG21	1.91	0.70
1:A:518:VAL:O	1:A:522:ILE:HG13	1.92	0.70
1:B:86:ASP:O	1:B:90:VAL:HG22	1.91	0.70
1:B:297:GLU:H	1:B:297:GLU:CD	1.93	0.69
1:B:279:LEU:HD23	1:B:282:LEU:HD12	1.73	0.69
1:B:20:LYS:HE2	1:B:55:PRO:HB2	1.76	0.68
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.76	0.67
1:A:450:THR:CG2	1:A:452:LEU:HB2	2.24	0.67
1:A:244:ILE:HD12	1:A:267:ALA:HB2	1.76	0.67
1:B:13:LYS:CE	1:B:85:GLN:HG3	2.25	0.66
1:B:296:THR:HG22	1:B:298:GLU:N	2.09	0.66
1:A:3:SER:OG	1:A:5:ILE:HG22	1.96	0.66
1:A:175:ASN:HD21	1:A:201:LYS:HE2	1.59	0.65
1:B:138:GLU:HG3	1:B:139:THR:HG23	1.77	0.65
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.77	0.65
1:A:472:THR:HG23	1:A:476:LYS:CB	2.26	0.64
1:A:450:THR:HG22	1:A:452:LEU:HB2	1.79	0.64
1:B:369:THR:HG21	1:B:405:TYR:HB2	1.78	0.64
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.27	0.64
1:A:228:LEU:CD1	1:A:228:LEU:H	2.07	0.64
1:B:253:THR:O	1:B:257:ILE:HG12	1.97	0.64
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.63	0.63
1:A:228:LEU:N	1:A:228:LEU:HD12	2.09	0.62
1:A:181:TYR:CZ	1:A:183:TYR:HB2	2.33	0.62
1:A:230:MET:HA	1:A:230:MET:HE2	1.80	0.62
1:A:155:GLY:O	1:A:159:ILE:HG13	1.98	0.62
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.33	0.62
1:A:354:TYR:HD1	1:A:374:LYS:HD3	1.64	0.62
1:B:194:GLU:CG	1:B:197:GLN:HG3	2.29	0.62
1:B:337:TRP:HE1	1:B:367:GLN:HE21	1.47	0.62
1:A:447:ASN:HB3	1:A:450:THR:HB	1.81	0.61
1:A:305:GLU:O	1:A:309:ILE:HG13	2.00	0.61
1:A:105:SER:O	1:A:190:GLY:HA2	2.00	0.61
1:B:252:TRP:HB3	1:B:257:ILE:HD11	1.82	0.61
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.31	0.60
1:A:44:GLU:HB2	1:A:46:LYS:HG2	1.83	0.60
1:B:334:GLN:N	1:B:334:GLN:HE21	1.99	0.60
1:B:169:GLU:HB3	1:B:170:PRO:HD3	1.83	0.60
1:A:27:THR:O	1:A:31:ILE:HG13	2.02	0.60
1:A:494:ASN:N	1:A:494:ASN:HD22	1.99	0.59
1:B:284:ARG:O	1:B:287:LYS:HE3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:O	1:A:68:SER:HB3	2.03	0.59
1:B:101:LYS:HG2	4:B:573:HOH:O	2.02	0.58
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.86	0.58
1:A:106:VAL:HG21	2:A:561:KRP:H2B	1.86	0.57
1:A:407:GLN:HA	1:A:407:GLN:NE2	2.19	0.57
1:B:50:ILE:CG2	1:B:145:GLN:HG2	2.35	0.57
1:B:395:LYS:O	1:B:399:GLU:HG3	2.03	0.57
1:A:183:TYR:CE2	1:A:184:MET:HG3	2.39	0.57
1:B:88:TRP:CE2	1:B:154:LYS:HD2	2.40	0.57
1:A:52:PRO:HA	1:A:54:ASN:N	2.20	0.57
1:A:392:PRO:O	1:A:423:VAL:HG12	2.04	0.57
1:B:422:LEU:N	1:B:422:LEU:HD22	2.20	0.57
1:B:260:LEU:HD22	1:B:264:LEU:CD1	2.35	0.56
1:B:306:ASN:O	1:B:310:LEU:HD22	2.05	0.56
1:A:536:VAL:HG13	1:A:537:PRO:HD2	1.86	0.56
1:A:552:VAL:O	1:A:553:SER:HB3	2.04	0.56
1:A:60:VAL:HG12	1:A:61:PHE:N	2.20	0.56
1:A:295:LEU:HB2	1:A:300:GLU:OE2	2.05	0.56
1:B:319:TYR:OH	1:B:385:LYS:HE2	2.05	0.56
1:A:89:GLU:HG3	1:A:92:LEU:HD11	1.87	0.56
1:A:233:GLU:CD	1:A:235:HIS:HE2	2.08	0.56
1:A:454:LYS:HD3	1:A:553:SER:H	1.71	0.56
1:A:105:SER:HB3	1:A:198:HIS:CG	2.40	0.56
1:A:424:LYS:HD2	1:A:426:TRP:CH2	2.41	0.56
1:B:175:ASN:HD21	1:B:201:LYS:NZ	2.04	0.56
1:A:175:ASN:ND2	1:A:201:LYS:HE2	2.19	0.56
1:B:295:LEU:HD22	1:B:295:LEU:N	2.21	0.56
1:A:480:GLN:HG2	1:A:517:LEU:HD11	1.88	0.55
1:A:273:GLY:HA2	1:A:332:GLN:NE2	2.20	0.55
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.87	0.55
1:B:24:TRP:HH2	1:B:61:PHE:CE1	2.25	0.55
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.88	0.55
1:A:343:GLN:HG3	1:A:349:LEU:CD1	2.37	0.55
1:B:275:LYS:H	1:B:306:ASN:HD21	1.54	0.55
1:B:237:ASP:C	1:B:239:TRP:H	2.10	0.55
1:A:520:GLN:HA	1:A:523:GLU:HG2	1.90	0.54
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.22	0.54
1:B:81:ASN:CG	1:B:154:LYS:HG3	2.27	0.54
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.72	0.54
1:B:72:ARG:HG2	1:B:73:LYS:N	2.23	0.54
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:PRO:O	1:B:346:PHE:HB2	2.08	0.54
1:B:260:LEU:HD22	1:B:264:LEU:HD11	1.90	0.54
1:A:298:GLU:HA	1:A:301:LEU:HD12	1.90	0.53
1:A:40:GLU:HA	1:A:40:GLU:OE2	2.08	0.53
1:A:229:TRP:HB2	2:A:561:KRP:N13	2.23	0.53
1:B:11:LYS:HG2	1:B:12:LEU:O	2.08	0.53
1:B:47:ILE:HD12	1:B:144:TYR:CD1	2.44	0.53
1:A:433:PRO:HB2	1:B:290:THR:HG22	1.90	0.53
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.09	0.53
1:A:434:ILE:HB	1:A:494:ASN:HD21	1.74	0.52
1:B:257:ILE:HB	1:B:283:LEU:HD21	1.92	0.52
1:A:194:GLU:CD	1:A:194:GLU:H	2.12	0.52
1:B:241:VAL:O	1:B:243:PRO:HD3	2.09	0.52
1:B:151:GLN:HB3	1:B:185:ASP:OD2	2.10	0.52
1:B:368:LEU:O	1:B:372:VAL:HG23	2.09	0.52
1:B:149:LEU:HD13	1:B:156:SER:HA	1.92	0.52
1:B:429:LEU:HD12	1:B:429:LEU:N	2.23	0.52
1:B:213:GLY:C	1:B:214:LEU:HD12	2.30	0.52
1:A:90:VAL:HG23	1:A:161:GLN:HG2	1.92	0.52
1:A:89:GLU:HG3	1:A:92:LEU:HD21	1.92	0.52
1:B:65:LYS:C	1:B:407:GLN:HE21	2.13	0.52
1:B:242:GLN:HB2	1:B:352:GLY:HA2	1.90	0.52
1:A:289:LEU:HD12	1:A:290:THR:N	2.25	0.51
1:B:361:HIS:C	1:B:363:ASN:H	2.13	0.51
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.92	0.51
1:B:24:TRP:CH2	1:B:61:PHE:CD1	2.98	0.51
1:A:407:GLN:HA	1:A:407:GLN:HE21	1.76	0.51
1:B:331:LYS:O	1:B:424:LYS:HE3	2.09	0.51
1:A:39:THR:O	1:A:43:LYS:HG2	2.10	0.51
1:B:395:LYS:HG2	1:B:399:GLU:OE1	2.10	0.51
1:A:324:ASP:OD1	1:A:388:LYS:HE2	2.08	0.51
1:A:64:LYS:O	1:A:66:LYS:HA	2.11	0.51
1:A:273:GLY:C	1:A:332:GLN:HE22	2.14	0.51
1:B:37:ILE:O	1:B:41:MET:HG2	2.10	0.51
1:B:344:GLU:CB	1:B:347:LYS:HD3	2.37	0.51
1:B:88:TRP:CZ2	1:B:154:LYS:HD2	2.46	0.51
1:B:112:GLY:HA3	1:B:151:GLN:HE21	1.75	0.50
1:A:168:LEU:HD22	1:A:180:ILE:HD13	1.93	0.50
1:A:171:PHE:CE2	1:A:205:LEU:HD23	2.46	0.50
1:A:473:THR:H	1:A:476:LYS:HD2	1.75	0.50
1:A:433:PRO:CG	1:B:255:ASN:ND2	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:O	1:A:380:ILE:HG12	2.11	0.50
1:B:271:TYR:O	1:B:274:ILE:HG12	2.11	0.50
1:A:500:GLN:OE1	1:B:422:LEU:HD23	2.11	0.50
1:B:61:PHE:CD1	1:B:61:PHE:N	2.79	0.50
1:A:5:ILE:HG12	1:A:6:GLU:O	2.11	0.50
1:A:308:GLU:O	1:A:311:LYS:HB2	2.12	0.50
1:B:425:LEU:O	1:B:428:GLN:HG2	2.12	0.50
1:A:356:ARG:HG3	1:A:357:MET:H	1.76	0.50
1:A:494:ASN:HB3	1:B:289:LEU:HD12	1.93	0.50
1:B:379:SER:OG	1:B:387:PRO:HD3	2.12	0.49
1:A:450:THR:HG21	1:A:452:LEU:HB2	1.94	0.49
1:A:271:TYR:HB3	1:A:274:ILE:HD11	1.95	0.49
1:B:115:TYR:HB3	1:B:149:LEU:HB2	1.94	0.49
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.94	0.49
1:B:346:PHE:HD1	1:B:346:PHE:N	2.11	0.49
1:B:328:GLU:O	1:B:339:TYR:HA	2.12	0.49
1:B:33:ALA:O	1:B:37:ILE:HG13	2.13	0.48
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.27	0.48
1:A:420:PRO:HA	1:A:421:PRO:C	2.33	0.48
1:B:346:PHE:CD1	1:B:346:PHE:N	2.81	0.48
1:B:154:LYS:HG2	1:B:184:MET:SD	2.53	0.48
1:A:500:GLN:HE22	1:B:421:PRO:HD2	1.79	0.48
1:A:460:ASN:ND2	1:B:288:ALA:HB2	2.28	0.48
1:B:330:GLN:NE2	1:B:338:THR:OG1	2.44	0.48
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.54	0.48
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.94	0.48
1:A:544:GLY:HA3	1:B:286:THR:HG22	1.96	0.48
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.95	0.48
1:A:296:THR:HB	1:A:298:GLU:OE1	2.13	0.48
1:A:183:TYR:CD2	1:A:184:MET:HG3	2.49	0.48
1:A:108:VAL:HG12	1:A:188:TYR:HD2	1.79	0.48
1:B:305:GLU:O	1:B:309:ILE:HG13	2.13	0.48
1:B:24:TRP:CZ3	1:B:61:PHE:CD1	3.02	0.48
1:A:89:GLU:OE2	1:A:89:GLU:HA	2.13	0.48
1:B:163:SER:O	1:B:167:ILE:HG13	2.13	0.48
1:A:406:TRP:HE3	1:A:407:GLN:NE2	2.12	0.47
1:B:193:LEU:CD1	1:B:201:LYS:HG3	2.44	0.47
1:A:175:ASN:HD21	1:A:201:LYS:CE	2.25	0.47
1:B:194:GLU:H	1:B:197:GLN:HE21	1.61	0.47
1:B:252:TRP:HB3	1:B:257:ILE:CD1	2.44	0.47
1:A:54:ASN:O	1:A:143:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:TYR:O	1:A:487:GLN:HG3	2.15	0.47
1:A:48:SER:O	1:A:144:TYR:HA	2.15	0.47
1:A:438:GLU:HG3	1:A:461:ARG:HD2	1.97	0.47
1:A:545:ASN:O	1:A:549:ASP:HB2	2.14	0.47
1:A:542:ILE:HG23	1:B:283:LEU:CD1	2.45	0.47
1:B:24:TRP:CH2	1:B:61:PHE:CE1	3.02	0.47
1:B:374:LYS:HE3	1:B:378:GLU:OE2	2.15	0.47
1:A:139:THR:HB	1:A:140:PRO:HD2	1.97	0.47
1:A:73:LYS:HB3	1:A:73:LYS:HZ2	1.80	0.46
1:A:77:PHE:O	1:A:78:ARG:C	2.53	0.46
1:B:257:ILE:HG23	1:B:279:LEU:HD22	1.97	0.46
1:B:12:LEU:HD23	1:B:84:THR:HG22	1.97	0.46
1:A:181:TYR:HH	1:A:183:TYR:HB2	1.81	0.46
1:A:354:TYR:CD1	1:A:374:LYS:HD3	2.47	0.46
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.51	0.46
1:A:199:ARG:HA	1:A:202:ILE:HB	1.96	0.46
1:A:402:TRP:C	1:A:402:TRP:CD1	2.89	0.46
1:A:278:GLN:CG	1:A:298:GLU:HB2	2.41	0.46
1:B:305:GLU:O	1:B:308:GLU:HB3	2.15	0.46
1:A:431:LYS:NZ	1:A:431:LYS:HB2	2.31	0.46
1:A:542:ILE:O	1:A:543:GLY:O	2.34	0.46
1:A:345:PRO:HA	1:A:346:PHE:HA	1.54	0.46
1:B:77:PHE:CE1	1:B:80:LEU:HD12	2.51	0.45
1:B:254:VAL:HG13	1:B:283:LEU:HD22	1.98	0.45
1:A:230:MET:HG3	1:A:230:MET:O	2.17	0.45
1:A:168:LEU:HD22	1:A:180:ILE:CD1	2.47	0.45
1:A:271:TYR:O	1:A:274:ILE:HG12	2.15	0.45
1:A:278:GLN:HG3	1:A:298:GLU:C	2.36	0.45
1:B:46:LYS:HZ3	1:B:116:PHE:HD2	1.64	0.45
1:A:230:MET:HE2	1:A:230:MET:CA	2.47	0.45
1:B:363:ASN:HB3	1:B:366:LYS:HB3	1.99	0.45
1:A:104:LYS:HD2	1:A:192:ASP:O	2.17	0.45
1:A:278:GLN:HB3	1:A:299:ALA:CA	2.42	0.45
1:B:420:PRO:HA	1:B:421:PRO:HD3	1.77	0.45
1:B:72:ARG:HG2	1:B:73:LYS:H	1.81	0.45
1:A:156:SER:N	1:A:157:PRO:HD2	2.31	0.45
1:B:101:LYS:O	1:B:236:PRO:HB2	2.17	0.45
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.47	0.44
1:A:281:LYS:HD2	1:A:284:ARG:CZ	2.47	0.44
1:A:463:ARG:NH2	1:A:488:ASP:O	2.48	0.44
1:A:32:LYS:O	1:A:36:GLU:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:CD	1:A:194:GLU:N	2.71	0.44
1:A:208:HIS:O	1:A:212:TRP:HD1	2.00	0.44
1:B:120:LEU:O	1:B:121:ASP:C	2.55	0.44
1:B:82:LYS:HE3	1:B:413:GLU:OE1	2.17	0.44
1:B:236:PRO:O	1:B:239:TRP:HB2	2.18	0.44
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.99	0.44
1:A:19:PRO:O	1:A:20:LYS:HG3	2.18	0.44
1:B:250:ASP:OD2	1:B:250:ASP:N	2.51	0.44
1:A:464:GLN:O	1:A:465:LYS:HB2	2.16	0.44
1:A:393:ILE:O	1:A:393:ILE:HG23	2.17	0.44
1:A:53:GLU:O	1:A:55:PRO:HD3	2.17	0.44
1:B:160:PHE:CD2	1:B:160:PHE:O	2.71	0.44
1:A:319:TYR:O	1:A:321:PRO:HD3	2.17	0.44
1:B:77:PHE:CD1	1:B:80:LEU:HD12	2.53	0.43
1:A:509:GLN:N	1:A:510:PRO:HD3	2.33	0.43
1:B:257:ILE:HG23	1:B:279:LEU:CD2	2.48	0.43
1:A:129:ALA:HA	1:A:144:TYR:O	2.17	0.43
1:B:187:LEU:HA	1:B:187:LEU:HD12	1.85	0.43
1:B:108:VAL:HG22	1:B:188:TYR:CD2	2.53	0.43
1:A:283:LEU:HA	1:A:283:LEU:HD12	1.59	0.43
1:A:282:LEU:HD11	1:A:296:THR:HG23	1.99	0.43
1:B:110:ASP:OD1	1:B:110:ASP:C	2.56	0.43
1:A:233:GLU:HG2	1:A:235:HIS:NE2	2.33	0.43
1:A:60:VAL:HG12	1:A:61:PHE:H	1.83	0.43
1:A:275:LYS:HE3	1:A:332:GLN:HG2	2.00	0.43
1:A:66:LYS:HE3	1:A:66:LYS:HB2	1.74	0.43
1:A:399:GLU:O	1:A:403:THR:HG23	2.19	0.43
1:A:233:GLU:CG	1:A:235:HIS:HE2	2.31	0.43
1:A:356:ARG:HG3	1:A:357:MET:N	2.33	0.43
1:A:52:PRO:HA	1:A:54:ASN:H	1.83	0.43
1:A:513:SER:C	1:A:515:SER:H	2.21	0.43
1:B:260:LEU:HD13	1:B:279:LEU:CD1	2.48	0.43
1:B:167:ILE:HG12	1:B:212:TRP:CD2	2.54	0.43
1:A:253:THR:HA	1:A:292:VAL:HA	2.00	0.43
1:B:104:LYS:HG3	1:B:192:ASP:OD1	2.19	0.43
1:A:542:ILE:HD11	1:B:261:VAL:HG11	2.00	0.43
1:B:429:LEU:H	1:B:429:LEU:HD12	1.84	0.43
1:A:171:PHE:CD2	1:A:205:LEU:HD23	2.54	0.43
1:B:425:LEU:HD12	1:B:428:GLN:NE2	2.33	0.43
1:A:330:GLN:NE2	1:A:338:THR:HG23	2.34	0.43
1:B:244:ILE:HB	1:B:310:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LYS:HD3	1:B:72:ARG:HH11	1.84	0.42
1:A:7:THR:HG22	1:A:119:PRO:HB2	2.01	0.42
1:A:386:THR:HG22	4:A:571:HOH:O	2.18	0.42
1:A:479:LEU:HD12	1:A:479:LEU:HA	1.77	0.42
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.55	0.42
1:A:260:LEU:HD23	1:A:279:LEU:HD22	2.01	0.42
1:B:72:ARG:NH2	1:B:151:GLN:HE22	2.17	0.42
1:B:108:VAL:HG22	1:B:188:TYR:CE2	2.55	0.42
1:A:478:GLU:O	1:A:482:ILE:HG13	2.20	0.42
1:B:65:LYS:C	1:B:407:GLN:HB2	2.39	0.42
1:A:457:TYR:HA	1:A:548:VAL:HG21	2.00	0.42
1:A:269:GLN:HA	1:A:351:THR:O	2.19	0.42
1:B:180:ILE:HA	1:B:188:TYR:O	2.20	0.42
1:A:329:ILE:HD11	1:A:375:ILE:HD12	2.02	0.42
1:A:175:ASN:ND2	1:A:201:LYS:CE	2.82	0.41
1:A:233:GLU:HG2	1:A:235:HIS:CD2	2.55	0.41
1:B:425:LEU:CD1	1:B:428:GLN:NE2	2.83	0.41
1:A:245:VAL:HG13	1:A:245:VAL:O	2.20	0.41
1:A:310:LEU:HA	1:A:310:LEU:HD12	1.92	0.41
1:B:400:THR:HB	1:B:401:TRP:CD1	2.56	0.41
1:A:301:LEU:O	1:A:304:ALA:HB3	2.19	0.41
1:B:88:TRP:CD1	1:B:154:LYS:HB2	2.56	0.41
1:A:350:LYS:HB2	1:A:350:LYS:HE2	1.85	0.41
1:A:13:LYS:HB3	1:A:14:PRO:HD2	2.02	0.41
1:A:547:GLN:NE2	1:A:547:GLN:H	2.03	0.41
1:A:409:THR:O	1:B:364:ASP:HB2	2.20	0.41
1:A:249:LYS:HE2	1:A:256:ASP:OD1	2.21	0.41
1:A:303:LEU:O	1:A:307:ARG:HB2	2.19	0.41
1:A:208:HIS:O	1:A:208:HIS:HD2	2.04	0.41
1:A:406:TRP:CE3	1:A:407:GLN:NE2	2.89	0.41
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.91	0.41
1:A:426:TRP:HB3	1:A:526:ILE:CD1	2.50	0.41
1:A:73:LYS:HB3	1:A:73:LYS:NZ	2.35	0.41
1:A:542:ILE:O	1:A:543:GLY:C	2.58	0.41
1:A:233:GLU:HG2	1:A:235:HIS:HE2	1.86	0.41
1:A:552:VAL:O	1:A:552:VAL:HG23	2.21	0.41
1:A:77:PHE:O	1:A:79:GLU:N	2.54	0.41
1:B:46:LYS:NZ	1:B:116:PHE:HD2	2.19	0.41
1:B:8:VAL:HA	1:B:9:PRO:HD3	1.95	0.41
1:A:125:ARG:NH1	1:A:147:ASN:HB3	2.35	0.41
1:B:103:LYS:HE3	1:B:179:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG12	1:A:188:TYR:CD2	2.56	0.41
1:A:235:HIS:O	2:A:561:KRP:H1	2.21	0.40
1:B:103:LYS:HD3	1:B:103:LYS:HA	1.91	0.40
1:A:287:LYS:NZ	1:A:291:GLU:HG2	2.36	0.40
1:A:12:LEU:HB3	1:A:83:ARG:O	2.21	0.40
1:A:534:ALA:HA	4:A:609:HOH:O	2.21	0.40
1:A:2:ILE:O	1:A:3:SER:C	2.59	0.40
1:B:72:ARG:HH21	1:B:151:GLN:HE22	1.70	0.40
1:B:111:VAL:HG11	1:B:187:LEU:HD22	2.02	0.40
1:A:437:ALA:O	4:A:577:HOH:O	2.22	0.40
1:A:175:ASN:HD22	1:A:178:ILE:HD12	1.86	0.40
1:A:494:ASN:ND2	1:A:494:ASN:N	2.66	0.40
1:A:407:GLN:CA	1:A:407:GLN:HE21	2.33	0.40
1:A:219:LYS:HB3	1:A:219:LYS:HE3	1.87	0.40
1:A:179:VAL:HG23	2:A:561:KRP:H21A	2.03	0.40
1:A:536:VAL:HG13	1:A:537:PRO:CD	2.51	0.40
1:A:171:PHE:CZ	1:A:205:LEU:HD23	2.55	0.40
1:B:268:SER:HA	1:B:274:ILE:HG13	2.03	0.40

There are no symmetry-related clashes.

## 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	551/560 (98%)	497 (90%)	48 (9%)	6 (1%)	17	46
1	B	395/560 (70%)	367 (93%)	25 (6%)	3 (1%)	24	55
All	All	946/1120 (84%)	864 (91%)	73 (8%)	9 (1%)	19	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	27	THR
1	A	543	GLY
1	A	68	SER
1	B	238	LYS
1	B	362	THR
1	A	465	LYS
1	A	3	SER
1	B	242	GLN

### 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	495/500 (99%)	464 (94%)	31 (6%)	22	50
1	B	367/500 (73%)	340 (93%)	27 (7%)	17	40
All	All	862/1000 (86%)	804 (93%)	58 (7%)	20	46

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	90	VAL
1	A	94	ILE
1	A	120	LEU
1	A	126	LYS
1	A	209	LEU
1	A	238	LYS
1	A	248	GLU
1	A	264	LEU
1	A	282	LEU
1	A	283	LEU
1	A	298	GLU
1	A	300	GLU
1	A	303	LEU
1	A	308	GLU

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Mol	Chain	Res	Type
1	A	310	LEU
1	A	344	GLU
1	A	356	ARG
1	A	357	MET
1	A	373	GLN
1	A	402	TRP
1	A	406	TRP
1	A	407	GLN
1	A	451	LYS
1	A	479	LEU
1	A	494	ASN
1	A	497	THR
1	A	500	GLN
1	A	517	LEU
1	A	533	LEU
1	A	547	GLN
1	B	24	TRP
1	B	48	SER
1	B	73	LYS
1	B	80	LEU
1	B	83	ARG
1	B	85	GLN
1	B	89	GLU
1	B	91	GLN
1	B	138	GLU
1	B	165	THR
1	B	194	GLU
1	B	205	LEU
1	B	209	LEU
1	B	234	LEU
1	B	248	GLU
1	B	250	ASP
1	B	260	LEU
1	B	279	LEU
1	B	287	LYS
1	B	310	LEU
1	B	323	LYS
1	B	330	GLN
1	B	334	GLN
1	B	344	GLU
1	B	356	ARG
1	B	368	LEU

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Mol	Chain	Res	Type
1	B	429	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	161	GLN
1	A	175	ASN
1	A	208	HIS
1	A	221	HIS
1	A	258	GLN
1	A	330	GLN
1	A	332	GLN
1	A	340	GLN
1	A	348	ASN
1	A	367	GLN
1	A	407	GLN
1	A	428	GLN
1	A	500	GLN
1	A	547	GLN
1	B	151	GLN
1	B	174	GLN
1	B	175	ASN
1	B	197	GLN
1	B	255	ASN
1	B	258	GLN
1	B	306	ASN
1	B	330	GLN
1	B	334	GLN
1	B	336	GLN
1	B	340	GLN
1	B	348	ASN
1	B	367	GLN
1	B	407	GLN
1	B	418	ASN
1	B	428	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	KRP	A	561	-	22,26,26	2.95	10 (45%)	24,37,37	2.75	5 (20%)
3	SO4	A	562	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	A	563	-	4,4,4	0.28	0	6,6,6	0.16	0
3	SO4	A	564	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	A	565	-	4,4,4	0.21	0	6,6,6	0.12	0
3	SO4	B	561	-	4,4,4	0.38	0	6,6,6	0.09	0

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	KRP	A	561	-	-	0/17/17/17	0/2/2/2
3	SO4	A	562	-	-	0/0/0/0	0/0/0/0
3	SO4	A	563	-	-	0/0/0/0	0/0/0/0
3	SO4	A	564	-	-	0/0/0/0	0/0/0/0
3	SO4	A	565	-	-	0/0/0/0	0/0/0/0
3	SO4	B	561	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	561	KRP	C14-C11	2.61	1.44	1.39
2	A	561	KRP	C14-C15	2.84	1.43	1.38
2	A	561	KRP	C4-N5	2.91	1.58	1.47
2	A	561	KRP	C10-C11	3.53	1.46	1.39
2	A	561	KRP	C9-C7	3.59	1.55	1.49
2	A	561	KRP	C6-C7	3.78	1.56	1.50
2	A	561	KRP	C17-C15	3.80	1.45	1.38
2	A	561	KRP	C10-C9	4.72	1.46	1.39
2	A	561	KRP	C17-C9	6.04	1.48	1.39
2	A	561	KRP	C6-N5	6.05	1.48	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	561	KRP	O8-C7-C6	-3.22	116.51	120.21
2	A	561	KRP	C18-C22-N24	-3.18	120.10	125.18
2	A	561	KRP	C6-C18-C19	2.53	125.13	122.34
2	A	561	KRP	C9-C7-C6	4.04	124.19	119.53
2	A	561	KRP	C22-N24-C25	11.24	124.97	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	561	KRP	4	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, 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	553/560 (98%)	0.49	24 (4%)	39	32	38, 70, 103, 121	0
1	B	403/560 (71%)	0.44	17 (4%)	40	33	35, 63, 104, 122	0
All	All	956/1120 (85%)	0.47	41 (4%)	39	32	35, 68, 104, 122	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	GLN	5.8
1	A	193	LEU	4.8
1	B	266	TRP	4.0
1	A	181	TYR	3.8
1	B	87	PHE	3.7
1	B	252	TRP	3.5
1	A	66	LYS	3.5
1	A	542	ILE	3.5
1	A	246	LEU	3.3
1	B	5	ILE	3.2
1	B	90	VAL	3.2
1	A	195	ILE	3.1
1	A	219	LYS	3.0
1	B	11	LYS	3.0
1	A	221	HIS	2.9
1	A	15	GLY	2.9
1	B	284	ARG	2.8
1	A	402	TRP	2.8
1	B	10	VAL	2.7
1	B	88	TRP	2.7
1	A	425	LEU	2.7
1	A	109	LEU	2.7
1	B	346	PHE	2.7
1	A	34	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	227	PHE	2.4
1	B	309	ILE	2.4
1	A	180	ILE	2.4
1	B	270	ILE	2.3
1	B	293	ILE	2.3
1	A	220	LYS	2.3
1	A	310	LEU	2.2
1	A	426	TRP	2.2
1	A	491	LEU	2.2
1	B	279	LEU	2.2
1	B	251	SER	2.2
1	B	260	LEU	2.1
1	A	553	SER	2.1
1	B	271	TYR	2.1
1	A	247	PRO	2.1
1	A	233	GLU	2.0
1	A	53	GLU	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	564	5/5	0.84	0.32	3.46	165,165,165,166	0
2	KRP	A	561	25/25	0.93	0.34	1.25	73,76,79,80	0
3	SO4	A	565	5/5	0.83	0.26	0.70	132,134,134,134	0
3	SO4	A	562	5/5	0.94	0.16	0.16	83,85,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	563	5/5	0.92	0.16	-0.58	91,91,94,96	0
3	SO4	B	561	5/5	0.93	0.16	-	107,107,107,108	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.