



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:10 am GMT

PDB ID : 2HNZ  
Title : Crystal Structure of E138K Mutant HIV-1 Reverse Transcriptase in Complex with PETT-2  
Authors : Ren, J.; Nichols, C.E.; Stamp, A.; Chamberlain, P.P.; Stammers, D.K.  
Deposited on : 2006-07-13  
Resolution : 3.00 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](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

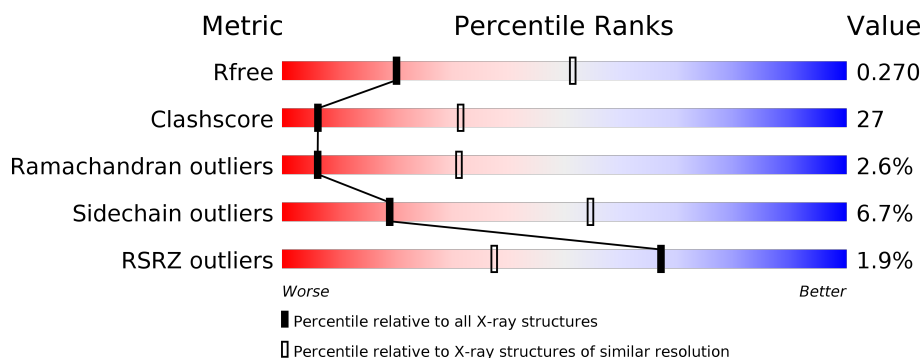
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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. 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	534	<div> <div>2%</div> <div> <div></div> <div>51%</div> <div>39%</div> <div>6%</div> <div></div> </div> </div>
2	B	422	<div> <div>%</div> <div> <div></div> <div>50%</div> <div>40%</div> <div>5%</div> <div>5%</div> </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	PO4	A	1300	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7600 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			4251	2755	703	785	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	LYS	GLU	ENGINEERED	UNP P04585
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

- Molecule 2 is a protein called Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	399	Total	C	N	O	S	0	0	0
			3316	2166	548	595	7			

There is a discrepancy between the modelled and reference sequences:

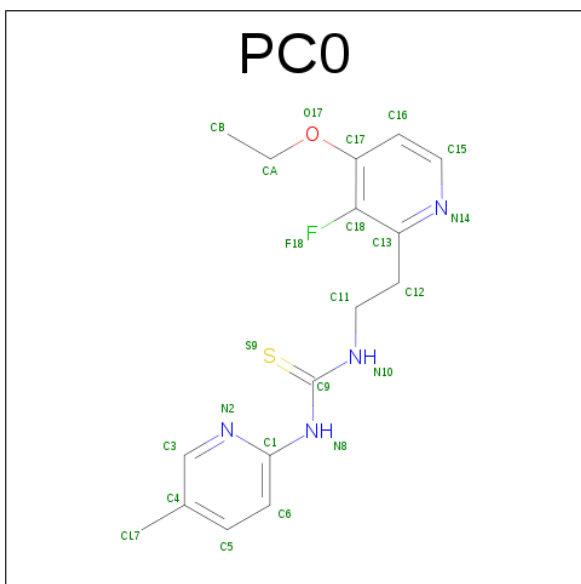
Chain	Residue	Modelled	Actual	Comment	Reference
B	138	LYS	GLU	ENGINEERED	UNP P03368

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is 1-[2-(4-ETHOXY-3-FLUOROPYRIDIN-2-YL)ETHYL]-3-(5-METHYLPYRIDIN-2-YL)THIOUREA (three-letter code: PC0) (formula: C<sub>16</sub>H<sub>19</sub>FN<sub>4</sub>OS).

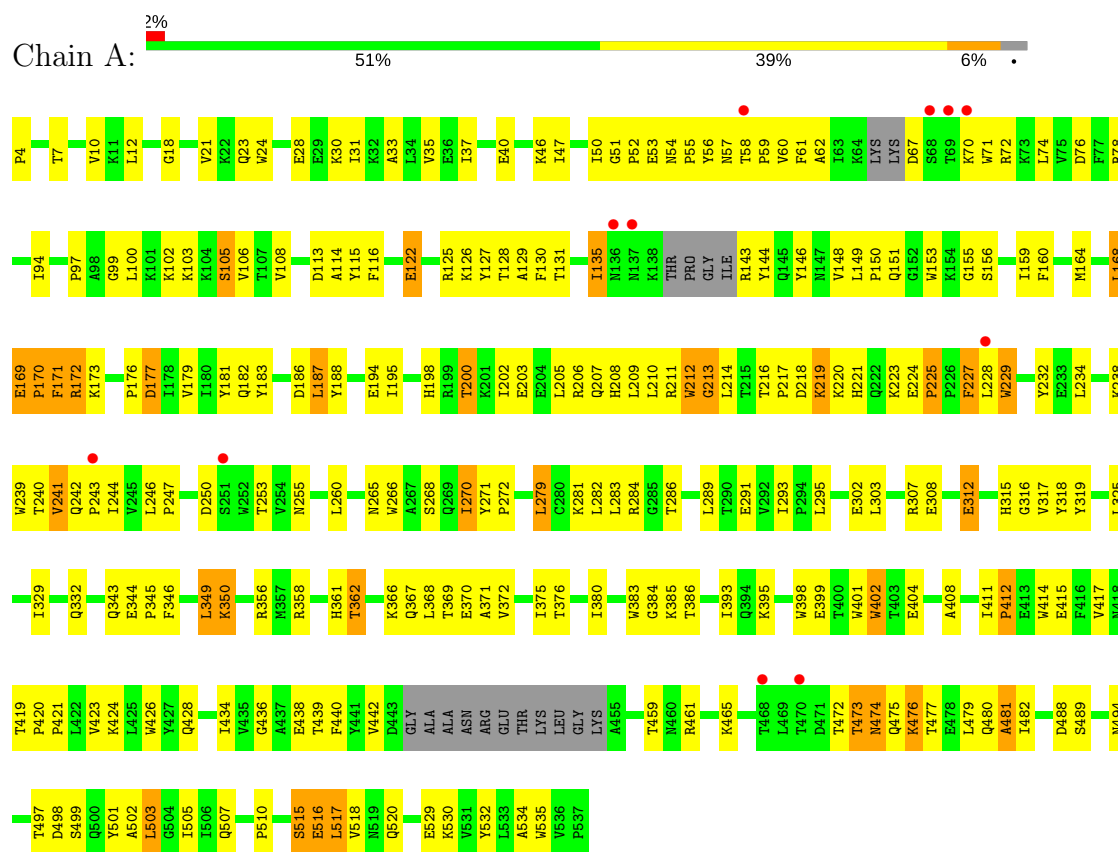


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			23	16	1	4	1	1		

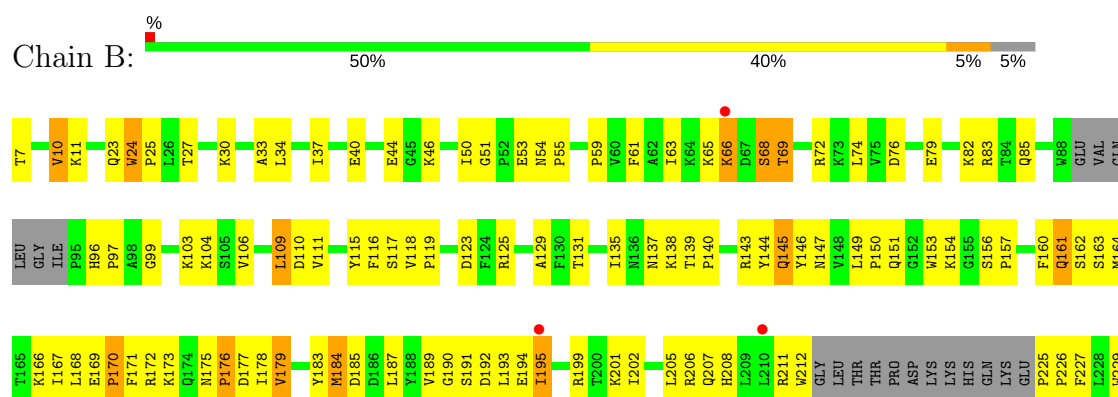
### 3 Residue-property plots

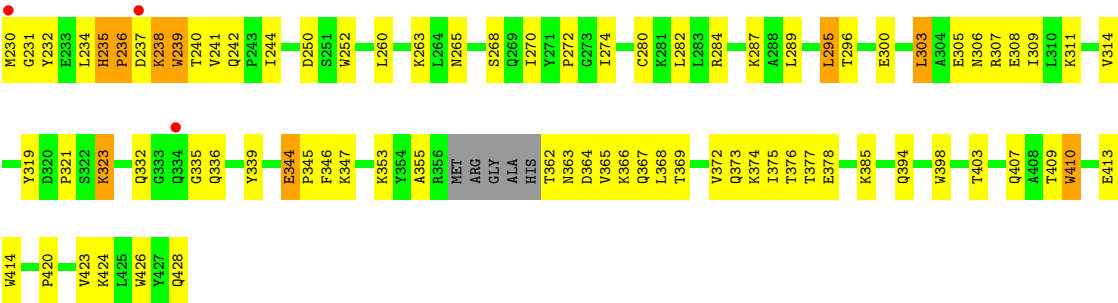
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Reverse transcriptase/ribonuclease H



#### • Molecule 2: Reverse transcriptase/ribonuclease H





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.80Å 114.90Å 65.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 3.00 19.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.1 (19.96-3.00) 88.2 (19.96-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226 , 0.277 0.212 , 0.270	Depositor DCC
$R_{free}$ test set	929 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 0.333 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: CSD, PO4, PC0

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	0.57	0/4354	0.73	0/5916
2	B	0.59	0/3413	0.76	2/4635 (0.0%)
All	All	0.58	0/7767	0.74	2/10551 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	236	PRO	N-CA-C	6.14	128.07	112.10
2	B	244	ILE	N-CA-C	-6.13	94.44	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4251	0	4282	218	0
2	B	3316	0	3348	196	0
3	A	10	0	0	4	0
4	A	23	0	19	2	0
All	All	7600	0	7649	409	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 27.

All (409) 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:224:GLU:HG3	1:A:225:PRO:HD2	1.22	1.14
2:B:295:LEU:HD12	2:B:295:LEU:H	1.11	1.12
2:B:227:PHE:HB3	2:B:231:GLY:HA2	1.37	1.04
1:A:28:GLU:HG3	1:A:135:ILE:HG21	1.40	1.04
1:A:23:GLN:HE22	1:A:60:VAL:H	0.91	0.90
2:B:72:ARG:HE	2:B:409:THR:HG22	1.33	0.90
1:A:224:GLU:HG3	1:A:225:PRO:CD	2.03	0.89
2:B:66:LYS:HB2	2:B:407:GLN:NE2	1.88	0.88
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.53	0.88
2:B:227:PHE:CB	2:B:231:GLY:HA2	2.05	0.85
2:B:295:LEU:HD12	2:B:295:LEU:N	1.92	0.85
2:B:82:LYS:HE2	2:B:413:GLU:OE1	1.78	0.84
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.59	0.83
1:A:23:GLN:NE2	1:A:60:VAL:H	1.75	0.83
1:A:23:GLN:HE22	1:A:60:VAL:N	1.76	0.81
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.62	0.81
2:B:295:LEU:H	2:B:295:LEU:CD1	1.93	0.81
1:A:376:THR:HG23	1:A:386:THR:HG22	1.64	0.80
2:B:362:THR:HG22	2:B:366:LYS:HD3	1.64	0.80
1:A:28:GLU:CG	1:A:135:ILE:HG21	2.11	0.79
2:B:72:ARG:HH11	2:B:72:ARG:HG3	1.48	0.78
2:B:332:GLN:HA	2:B:424:LYS:HE2	1.65	0.78
2:B:238:LYS:O	2:B:240:THR:HG23	1.84	0.78
2:B:242:GLN:HE22	2:B:353:LYS:HG3	1.46	0.78
2:B:183:TYR:CE1	2:B:184:MET:HG3	2.20	0.77
2:B:265:ASN:O	2:B:268:SER:HB3	1.85	0.77
2:B:66:LYS:HB3	2:B:66:LYS:NZ	2.00	0.76
2:B:175:ASN:HD21	2:B:201:LYS:CE	1.99	0.75
1:A:503:LEU:HD13	1:A:507:GLN:HG3	1.69	0.74
1:A:135:ILE:H	1:A:135:ILE:HD12	1.51	0.74
2:B:82:LYS:CE	2:B:413:GLU:OE1	2.36	0.73
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.53	0.73
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.23	0.72
1:A:209:LEU:O	1:A:214:LEU:HB2	1.89	0.72
2:B:365:VAL:O	2:B:369:THR:HG23	1.88	0.72
2:B:270:ILE:O	2:B:272:PRO:HD3	1.90	0.72
1:A:417:VAL:HG22	1:A:419:THR:OG1	1.90	0.72
2:B:353:LYS:NZ	2:B:428:GLN:HG3	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.73	0.71
2:B:230:MET:C	2:B:232:TYR:H	1.93	0.71
1:A:247:PRO:O	1:A:307:ARG:NH2	2.23	0.69
1:A:108:VAL:HG21	1:A:223:LYS:HB2	1.75	0.69
1:A:376:THR:HG23	1:A:386:THR:CG2	2.23	0.69
1:A:516:GLU:O	1:A:520:GLN:HG3	1.93	0.69
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.91	0.69
1:A:240:THR:OG1	1:A:241:VAL:N	2.26	0.68
2:B:238:LYS:O	2:B:240:THR:N	2.26	0.68
2:B:353:LYS:HZ1	2:B:428:GLN:HA	1.58	0.68
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.23	0.68
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.09	0.68
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.75	0.68
1:A:307:ARG:HH11	1:A:307:ARG:HG2	1.60	0.67
2:B:72:ARG:NE	2:B:409:THR:HG22	2.08	0.66
2:B:68:SER:O	2:B:69:THR:HG22	1.95	0.66
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.30	0.65
1:A:50:ILE:HD12	1:A:54:ASN:CB	2.27	0.65
2:B:353:LYS:HZ3	2:B:428:GLN:HG3	1.62	0.65
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.78	0.65
2:B:103:LYS:HG2	2:B:191:SER:N	2.12	0.64
1:A:216:THR:HB	1:A:217:PRO:HD2	1.78	0.64
2:B:242:GLN:NE2	2:B:353:LYS:HG3	2.12	0.64
1:A:343:GLN:HG3	1:A:349:LEU:CD1	2.28	0.64
2:B:44:GLU:O	2:B:46:LYS:HE3	1.97	0.64
2:B:66:LYS:HB2	2:B:407:GLN:HE22	1.63	0.63
2:B:164:MET:HA	2:B:167:ILE:HD11	1.79	0.63
1:A:319:TYR:HA	1:A:349:LEU:HD21	1.81	0.63
2:B:323:LYS:HE3	2:B:323:LYS:HA	1.79	0.63
1:A:255:ASN:HD21	1:A:289:LEU:HB3	1.61	0.63
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.29	0.63
2:B:175:ASN:ND2	2:B:201:LYS:CE	2.61	0.63
2:B:175:ASN:HD21	2:B:201:LYS:HE3	1.64	0.62
1:A:24:TRP:HZ2	1:A:61:PHE:CD2	2.16	0.62
2:B:125:ARG:HD3	2:B:147:ASN:HD22	1.65	0.62
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.34	0.62
2:B:319:TYR:OH	2:B:385:LYS:HD3	1.98	0.62
2:B:27:THR:OG1	2:B:30:LYS:HG2	1.99	0.62
2:B:23:GLN:OE1	2:B:59:PRO:HA	1.99	0.62
2:B:319:TYR:HE1	2:B:321:PRO:HG3	1.65	0.62
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:O	1:A:37:ILE:HG12	2.00	0.61
2:B:423:VAL:HG13	2:B:424:LYS:N	2.15	0.61
1:A:37:ILE:O	1:A:40:GLU:HB3	2.00	0.61
2:B:241:VAL:HG12	2:B:242:GLN:N	2.14	0.61
1:A:28:GLU:HG3	1:A:135:ILE:CG2	2.26	0.61
1:A:399:GLU:HG3	1:A:402:TRP:HE3	1.64	0.61
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.83	0.61
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.36	0.61
2:B:229:TRP:CE3	2:B:229:TRP:HA	2.33	0.61
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.83	0.61
2:B:164:MET:SD	2:B:167:ILE:HD11	2.40	0.60
2:B:168:LEU:HD13	2:B:172:ARG:HH21	1.66	0.60
2:B:66:LYS:HD2	2:B:230:MET:HA	1.83	0.60
1:A:227:PHE:N	1:A:227:PHE:CD2	2.65	0.60
1:A:108:VAL:CG2	1:A:223:LYS:HB2	2.31	0.60
1:A:242:GLN:HB2	1:A:243:PRO:HD2	1.83	0.60
2:B:420:PRO:O	2:B:423:VAL:HG12	2.01	0.60
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.17	0.59
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.38	0.59
1:A:228:LEU:O	1:A:229:TRP:HB2	2.03	0.59
1:A:151:GLN:NE2	1:A:151:GLN:HA	2.18	0.59
1:A:125:ARG:HG2	1:A:146:TYR:O	2.03	0.58
1:A:270:ILE:O	1:A:272:PRO:HD3	2.03	0.58
1:A:220:LYS:HZ2	1:A:221:HIS:CE1	2.21	0.58
2:B:66:LYS:HB3	2:B:66:LYS:HZ3	1.68	0.58
1:A:415:GLU:O	1:A:415:GLU:HG3	2.02	0.58
1:A:198:HIS:CE1	1:A:202:ILE:HD11	2.38	0.58
2:B:235:HIS:N	2:B:236:PRO:HD3	2.15	0.58
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.19	0.58
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.39	0.58
2:B:110:ASP:HB3	2:B:226:PRO:HG2	1.84	0.58
1:A:332:GLN:HG2	1:A:332:GLN:O	2.02	0.58
2:B:208:HIS:O	2:B:211:ARG:HB3	2.04	0.58
2:B:230:MET:HB2	2:B:232:TYR:HB2	1.85	0.58
1:A:168:LEU:HD11	1:A:209:LEU:HD21	1.85	0.57
2:B:164:MET:HA	2:B:167:ILE:CD1	2.34	0.57
1:A:135:ILE:H	1:A:135:ILE:CD1	2.12	0.57
1:A:206:ARG:HH12	1:A:218:ASP:HA	1.68	0.57
2:B:175:ASN:ND2	2:B:201:LYS:HE3	2.18	0.57
2:B:66:LYS:HE3	2:B:230:MET:CA	2.33	0.57
2:B:332:GLN:HE22	2:B:424:LYS:HG3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:LYS:HZ1	2:B:428:GLN:CA	2.17	0.57
1:A:241:VAL:HG12	1:A:266:TRP:HE1	1.70	0.57
2:B:230:MET:C	2:B:232:TYR:N	2.57	0.57
1:A:401:TRP:O	1:A:404:GLU:HG2	2.04	0.57
2:B:135:ILE:O	2:B:138:LYS:HG2	2.04	0.57
1:A:108:VAL:O	1:A:108:VAL:HG23	2.05	0.57
2:B:168:LEU:CD1	2:B:172:ARG:HH21	2.18	0.57
1:A:461:ARG:NH2	3:A:1300:PO4:O2	2.35	0.56
1:A:24:TRP:HE1	1:A:61:PHE:HB3	1.71	0.56
1:A:53:GLU:O	1:A:55:PRO:HD3	2.04	0.56
1:A:207:GLN:HE21	1:A:210:LEU:HD23	1.69	0.56
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.20	0.56
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.40	0.56
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.41	0.56
1:A:475:GLN:HB2	1:A:501:TYR:CE2	2.41	0.56
2:B:161:GLN:O	2:B:164:MET:N	2.39	0.55
1:A:344:GLU:HA	1:A:344:GLU:OE1	2.07	0.55
1:A:369:THR:O	1:A:372:VAL:HB	2.06	0.55
2:B:109:LEU:HD11	2:B:227:PHE:CD1	2.41	0.55
1:A:282:LEU:HB3	1:A:293:ILE:HG21	1.89	0.55
2:B:66:LYS:HB2	2:B:407:GLN:CD	2.27	0.55
2:B:66:LYS:HE3	2:B:230:MET:HA	1.88	0.55
1:A:113:ASP:HB3	1:A:116:PHE:HB2	1.89	0.54
2:B:109:LEU:HD12	2:B:227:PHE:HA	1.89	0.54
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.37	0.54
2:B:344:GLU:CB	2:B:347:LYS:HD2	2.37	0.54
2:B:308:GLU:OE1	2:B:311:LYS:HD2	2.07	0.54
2:B:332:GLN:NE2	2:B:424:LYS:HG3	2.22	0.54
2:B:33:ALA:O	2:B:37:ILE:HG13	2.08	0.54
1:A:368:LEU:O	1:A:372:VAL:HG23	2.08	0.54
2:B:189:VAL:HG11	2:B:202:ILE:HD13	1.90	0.54
1:A:283:LEU:O	1:A:286:THR:HG23	2.08	0.54
2:B:229:TRP:HE3	2:B:229:TRP:HA	1.72	0.53
1:A:358:ARG:NH2	2:B:394:GLN:HG2	2.23	0.53
2:B:72:ARG:HH21	2:B:409:THR:CG2	2.22	0.53
1:A:255:ASN:ND2	1:A:289:LEU:HB3	2.24	0.53
1:A:399:GLU:HG3	1:A:402:TRP:CZ3	2.43	0.53
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.91	0.53
1:A:461:ARG:NH1	3:A:1300:PO4:O2	2.41	0.53
2:B:335:GLY:O	2:B:355:ALA:HA	2.09	0.52
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:HE3	1:A:116:PHE:HD1	1.74	0.52
2:B:173:LYS:O	2:B:176:PRO:HD3	2.09	0.52
2:B:242:GLN:HE22	2:B:353:LYS:CG	2.20	0.52
2:B:66:LYS:CD	2:B:230:MET:HA	2.38	0.52
2:B:195:ILE:HG22	2:B:199:ARG:HE	1.74	0.52
1:A:461:ARG:HH12	3:A:1300:PO4:P	2.32	0.52
1:A:515:SER:OG	1:A:518:VAL:HG23	2.10	0.52
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.75	0.52
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.23	0.52
1:A:345:PRO:O	1:A:346:PHE:HB2	2.09	0.51
1:A:188:TYR:N	1:A:188:TYR:CD1	2.78	0.51
1:A:135:ILE:HD12	1:A:135:ILE:N	2.21	0.51
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.93	0.51
1:A:202:ILE:O	1:A:206:ARG:HG3	2.10	0.51
1:A:234:LEU:HD13	4:A:999:PC0:HB1	1.92	0.51
1:A:57:ASN:OD1	1:A:130:PHE:HA	2.11	0.51
2:B:138:LYS:O	2:B:139:THR:HG23	2.10	0.51
2:B:241:VAL:CG1	2:B:242:GLN:N	2.74	0.51
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.92	0.50
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.11	0.50
2:B:238:LYS:HD2	2:B:238:LYS:N	2.26	0.50
2:B:344:GLU:HB3	2:B:347:LYS:HD2	1.93	0.50
1:A:58:THR:HG23	1:A:76:ASP:O	2.11	0.50
1:A:105:SER:HB2	1:A:198:HIS:CG	2.47	0.50
1:A:279:LEU:HD22	1:A:302:GLU:OE1	2.12	0.50
1:A:4:PRO:HB2	1:A:212:TRP:CD1	2.46	0.50
1:A:170:PRO:O	1:A:173:LYS:N	2.43	0.50
2:B:11:LYS:O	2:B:85:GLN:HB3	2.12	0.50
2:B:161:GLN:O	2:B:162:SER:C	2.50	0.50
1:A:164:MET:HG3	1:A:168:LEU:HD22	1.94	0.49
2:B:164:MET:HA	2:B:167:ILE:HG12	1.94	0.49
2:B:104:LYS:O	2:B:235:HIS:HA	2.12	0.49
2:B:235:HIS:H	2:B:236:PRO:HD3	1.78	0.49
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.12	0.49
1:A:207:GLN:NE2	1:A:210:LEU:HD23	2.27	0.49
1:A:51:GLY:C	1:A:53:GLU:H	2.16	0.49
2:B:163:SER:O	2:B:167:ILE:HG12	2.11	0.49
2:B:164:MET:HA	2:B:167:ILE:CG1	2.43	0.49
1:A:498:ASP:OD1	1:A:499:SER:N	2.46	0.49
1:A:148:VAL:O	1:A:150:PRO:HD3	2.13	0.49
2:B:207:GLN:OE1	2:B:207:GLN:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:PHE:CE2	2:B:178:ILE:HD11	2.47	0.49
1:A:131:THR:HG23	1:A:143:ARG:HG3	1.94	0.48
1:A:281:LYS:HE3	1:A:284:ARG:CZ	2.42	0.48
1:A:494:ASN:OD1	1:A:532:TYR:HB3	2.13	0.48
2:B:24:TRP:CD2	2:B:25:PRO:HD2	2.48	0.48
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.96	0.48
1:A:115:TYR:CD1	1:A:156:SER:HB3	2.48	0.48
1:A:438:GLU:OE1	1:A:459:THR:HG21	2.13	0.48
1:A:479:LEU:HD21	1:A:518:VAL:HG22	1.95	0.48
1:A:51:GLY:O	1:A:53:GLU:N	2.43	0.48
2:B:178:ILE:HG22	2:B:191:SER:CB	2.43	0.48
1:A:232:TYR:CD2	1:A:239:TRP:HZ3	2.32	0.48
1:A:424:LYS:NZ	1:A:426:TRP:CD2	2.82	0.48
2:B:103:LYS:HG2	2:B:190:GLY:C	2.33	0.48
2:B:314:VAL:HG13	2:B:314:VAL:O	2.13	0.48
2:B:109:LEU:HD11	2:B:227:PHE:HD1	1.79	0.48
2:B:72:ARG:HH21	2:B:409:THR:HG22	1.79	0.48
2:B:263:LYS:HE3	2:B:426:TRP:HA	1.96	0.48
1:A:94:ILE:HG13	1:A:94:ILE:O	2.13	0.48
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.49	0.47
1:A:208:HIS:CE1	1:A:212:TRP:HZ3	2.31	0.47
1:A:115:TYR:O	1:A:149:LEU:HB2	2.14	0.47
2:B:305:GLU:O	2:B:309:ILE:HG13	2.14	0.47
1:A:151:GLN:HE21	1:A:151:GLN:HA	1.77	0.47
1:A:472:THR:OG1	1:A:473:THR:N	2.47	0.47
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.49	0.47
1:A:200:THR:O	1:A:203:GLU:HB2	2.14	0.47
1:A:207:GLN:NE2	1:A:207:GLN:HA	2.29	0.47
1:A:384:GLY:HA3	2:B:135:ILE:HD12	1.96	0.47
1:A:424:LYS:NZ	1:A:426:TRP:CE3	2.83	0.47
1:A:115:TYR:N	1:A:115:TYR:CD2	2.83	0.47
1:A:370:GLU:O	1:A:371:ALA:C	2.50	0.47
2:B:168:LEU:O	2:B:172:ARG:HB2	2.15	0.47
2:B:242:GLN:HE22	2:B:353:LYS:HE3	1.80	0.47
2:B:284:ARG:O	2:B:287:LYS:HE2	2.15	0.47
2:B:96:HIS:HA	2:B:97:PRO:HD3	1.73	0.47
1:A:169:GLU:OE1	1:A:173:LYS:HE3	2.15	0.46
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.46	0.46
1:A:270:ILE:HG23	1:A:271:TYR:N	2.30	0.46
2:B:72:ARG:NH1	2:B:72:ARG:HG3	2.20	0.46
1:A:477:THR:O	1:A:480:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ASN:HD22	2:B:137:ASN:N	2.13	0.46
2:B:40:GLU:O	2:B:44:GLU:HG3	2.16	0.46
1:A:31:ILE:O	1:A:35:VAL:HG23	2.16	0.46
2:B:50:ILE:CG2	2:B:145:GLN:HB3	2.46	0.46
2:B:118:VAL:HG11	2:B:149:LEU:HD11	1.98	0.46
1:A:479:LEU:CD2	1:A:518:VAL:HG22	2.45	0.46
2:B:229:TRP:HH2	2:B:373:GLN:OE1	1.98	0.46
2:B:166:LYS:C	2:B:166:LYS:HD3	2.36	0.46
1:A:436:GLY:HA2	3:A:1301:PO4:O1	2.16	0.46
1:A:473:THR:HG23	1:A:476:LYS:HB2	1.97	0.46
1:A:102:LYS:O	1:A:103:LYS:HG2	2.16	0.46
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.17	0.45
1:A:128:THR:HB	1:A:146:TYR:HD2	1.81	0.45
1:A:265:ASN:O	1:A:268:SER:OG	2.31	0.45
1:A:481:ALA:O	1:A:482:ILE:C	2.54	0.45
1:A:151:GLN:CA	1:A:151:GLN:HE21	2.28	0.45
1:A:232:TYR:CE2	1:A:239:TRP:HZ3	2.34	0.45
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.17	0.45
2:B:420:PRO:HG2	2:B:423:VAL:HG12	1.97	0.45
2:B:65:LYS:NZ	2:B:72:ARG:HB2	2.31	0.45
1:A:164:MET:CE	1:A:214:LEU:HD13	2.47	0.45
1:A:72:ARG:HG2	1:A:72:ARG:HH11	1.82	0.45
2:B:274:ILE:HG23	2:B:306:ASN:OD1	2.17	0.45
1:A:170:PRO:O	1:A:172:ARG:N	2.49	0.45
1:A:108:VAL:HG12	1:A:188:TYR:CD2	2.52	0.45
1:A:476:LYS:HG2	1:A:517:LEU:HD12	1.98	0.45
1:A:46:LYS:HE3	1:A:116:PHE:CD1	2.51	0.45
2:B:332:GLN:HB2	2:B:336:GLN:O	2.17	0.45
1:A:198:HIS:HE2	1:A:202:ILE:HD11	1.80	0.45
1:A:219:LYS:HD3	1:A:219:LYS:O	2.17	0.45
2:B:135:ILE:HB	2:B:138:LYS:HE2	1.98	0.45
1:A:411:ILE:O	1:A:412:PRO:O	2.35	0.45
1:A:168:LEU:O	1:A:169:GLU:C	2.55	0.45
1:A:186:ASP:HB2	1:A:188:TYR:HE1	1.82	0.45
1:A:317:VAL:HG22	1:A:318:TYR:N	2.32	0.45
2:B:175:ASN:C	2:B:177:ASP:H	2.20	0.44
1:A:420:PRO:HA	1:A:421:PRO:C	2.36	0.44
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.51	0.44
1:A:227:PHE:N	1:A:227:PHE:HD2	2.12	0.44
1:A:106:VAL:HG12	1:A:227:PHE:HZ	1.82	0.44
1:A:497:THR:O	1:A:535:TRP:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:PHE:HD1	2:B:164:MET:HB2	1.82	0.44
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.63	0.44
1:A:393:ILE:CG1	1:A:423:VAL:HG23	2.48	0.44
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.98	0.44
2:B:423:VAL:CG1	2:B:424:LYS:N	2.79	0.44
1:A:129:ALA:HA	1:A:144:TYR:O	2.18	0.44
2:B:103:LYS:HE2	2:B:179:VAL:HG12	2.00	0.44
2:B:160:PHE:O	2:B:161:GLN:C	2.56	0.44
2:B:206:ARG:NH1	2:B:227:PHE:CE2	2.86	0.44
2:B:238:LYS:O	2:B:239:TRP:C	2.57	0.44
1:A:30:LYS:HD3	1:A:62:ALA:HB3	2.00	0.43
1:A:428:GLN:HE21	1:A:428:GLN:HB3	1.64	0.43
1:A:473:THR:O	1:A:474:ASN:C	2.56	0.43
2:B:362:THR:OG1	2:B:367:GLN:NE2	2.40	0.43
1:A:170:PRO:C	1:A:172:ARG:N	2.69	0.43
1:A:312:GLU:H	1:A:312:GLU:HG3	1.55	0.43
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.33	0.43
2:B:154:LYS:HA	2:B:184:MET:HE1	2.00	0.43
2:B:368:LEU:O	2:B:372:VAL:HG23	2.19	0.43
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.54	0.43
2:B:167:ILE:HA	2:B:212:TRP:CZ3	2.53	0.43
2:B:167:ILE:O	2:B:212:TRP:HZ3	2.01	0.43
1:A:482:ILE:CD1	1:A:502:ALA:HB1	2.49	0.43
1:A:10:VAL:HG11	1:A:153:TRP:CH2	2.53	0.43
1:A:171:PHE:CD2	1:A:171:PHE:O	2.72	0.43
1:A:465:LYS:HE3	1:A:465:LYS:HB2	1.82	0.43
2:B:189:VAL:HG11	2:B:202:ILE:CD1	2.48	0.43
2:B:344:GLU:HB2	2:B:347:LYS:HD2	2.01	0.43
1:A:169:GLU:N	1:A:170:PRO:HD2	2.34	0.43
2:B:116:PHE:N	2:B:116:PHE:HD1	2.17	0.43
2:B:175:ASN:N	2:B:176:PRO:HD3	2.34	0.43
1:A:56:TYR:O	1:A:143:ARG:NH2	2.50	0.42
1:A:151:GLN:CA	1:A:151:GLN:NE2	2.81	0.42
1:A:177:ASP:N	1:A:177:ASP:OD2	2.46	0.42
1:A:228:LEU:HD22	1:A:242:GLN:HB3	2.00	0.42
1:A:238:LYS:HD2	1:A:315:HIS:CD2	2.54	0.42
1:A:350:LYS:HB2	1:A:350:LYS:HE2	1.83	0.42
2:B:44:GLU:O	2:B:46:LYS:CE	2.65	0.42
1:A:218:ASP:OD1	1:A:221:HIS:ND1	2.49	0.42
1:A:380:ILE:O	1:A:384:GLY:HA2	2.19	0.42
2:B:234:LEU:O	2:B:235:HIS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:VAL:C	2:B:242:GLN:CG	2.87	0.42
2:B:34:LEU:HA	2:B:34:LEU:HD23	1.89	0.42
1:A:315:HIS:ND1	1:A:315:HIS:N	2.65	0.42
1:A:505:ILE:O	1:A:510:PRO:HD3	2.19	0.42
2:B:116:PHE:CD1	2:B:116:PHE:N	2.86	0.42
2:B:339:TYR:CD1	2:B:375:ILE:HD11	2.53	0.42
2:B:353:LYS:HZ1	2:B:428:GLN:HG3	1.80	0.42
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.85	0.42
1:A:480:GLN:HG2	1:A:517:LEU:HD11	2.02	0.42
2:B:61:PHE:CD2	2:B:403:THR:HG21	2.55	0.42
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.54	0.42
2:B:115:TYR:CE1	2:B:156:SER:HB3	2.54	0.42
2:B:195:ILE:HD11	2:B:235:HIS:HE1	1.85	0.42
1:A:208:HIS:NE2	1:A:212:TRP:HZ3	2.17	0.42
1:A:253:THR:HA	1:A:291:GLU:O	2.19	0.42
1:A:498:ASP:O	1:A:535:TRP:NE1	2.52	0.42
2:B:10:VAL:HG21	2:B:153:TRP:HH2	1.85	0.42
2:B:11:LYS:HB3	2:B:11:LYS:HE2	1.71	0.42
2:B:160:PHE:CD1	2:B:164:MET:HB2	2.54	0.42
2:B:241:VAL:CG1	2:B:242:GLN:H	2.33	0.42
1:A:473:THR:HG23	1:A:476:LYS:CB	2.49	0.42
1:A:497:THR:HG22	1:A:534:ALA:O	2.20	0.42
2:B:208:HIS:O	2:B:211:ARG:CB	2.68	0.42
2:B:229:TRP:O	2:B:230:MET:HB2	2.19	0.42
2:B:97:PRO:C	2:B:99:GLY:N	2.72	0.42
1:A:241:VAL:HG12	1:A:266:TRP:NE1	2.34	0.42
2:B:104:LYS:HG3	2:B:192:ASP:OD1	2.20	0.41
2:B:270:ILE:HG12	2:B:346:PHE:HB3	2.02	0.41
2:B:345:PRO:O	2:B:347:LYS:N	2.50	0.41
2:B:66:LYS:CE	2:B:230:MET:H	2.33	0.41
1:A:179:VAL:CG1	4:A:999:PCO:H112	2.51	0.41
1:A:212:TRP:O	1:A:214:LEU:N	2.52	0.41
1:A:308:GLU:HA	1:A:308:GLU:OE1	2.20	0.41
2:B:194:GLU:OE2	2:B:195:ILE:N	2.53	0.41
2:B:295:LEU:HD22	2:B:300:GLU:OE1	2.19	0.41
1:A:207:GLN:O	1:A:210:LEU:HB3	2.20	0.41
1:A:473:THR:O	1:A:476:LYS:N	2.51	0.41
1:A:61:PHE:CE1	1:A:74:LEU:HD23	2.56	0.41
2:B:129:ALA:HA	2:B:144:TYR:O	2.20	0.41
2:B:363:ASN:O	2:B:364:ASP:C	2.59	0.41
2:B:79:GLU:O	2:B:83:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:PRO:C	2:B:347:LYS:H	2.23	0.41
2:B:169:GLU:N	2:B:170:PRO:HD2	2.36	0.41
2:B:314:VAL:CG1	2:B:314:VAL:O	2.68	0.41
1:A:210:LEU:O	1:A:213:GLY:N	2.54	0.41
2:B:54:ASN:C	2:B:54:ASN:OD1	2.58	0.41
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.55	0.41
2:B:242:GLN:NE2	2:B:353:LYS:HE3	2.36	0.41
2:B:303:LEU:HD13	2:B:307:ARG:NH1	2.35	0.41
1:A:115:TYR:N	1:A:115:TYR:HD2	2.18	0.41
1:A:434:ILE:HD13	1:A:530:LYS:HB3	2.03	0.41
2:B:238:LYS:CD	2:B:238:LYS:N	2.83	0.41
2:B:225:PRO:HA	2:B:226:PRO:HD2	1.94	0.41
2:B:239:TRP:CD1	2:B:239:TRP:N	2.85	0.41
2:B:374:LYS:O	2:B:378:GLU:HG3	2.20	0.41
1:A:155:GLY:O	1:A:159:ILE:HD12	2.20	0.41
1:A:361:HIS:O	1:A:362:THR:HG23	2.21	0.41
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.56	0.41
1:A:70:LYS:HG2	1:A:71:TRP:H	1.85	0.41
2:B:51:GLY:HA3	2:B:53:GLU:OE1	2.21	0.41
2:B:66:LYS:HE3	2:B:230:MET:N	2.35	0.41
1:A:97:PRO:HA	1:A:100:LEU:HG	2.01	0.40
1:A:227:PHE:H	1:A:227:PHE:HD2	1.69	0.40
1:A:503:LEU:HD13	1:A:507:GLN:CG	2.46	0.40
2:B:376:THR:O	2:B:377:THR:C	2.60	0.40
2:B:353:LYS:NZ	2:B:428:GLN:HA	2.32	0.40
1:A:173:LYS:O	1:A:176:PRO:HD3	2.21	0.40
1:A:325:LEU:HD11	1:A:383:TRP:CG	2.56	0.40
2:B:156:SER:N	2:B:157:PRO:HD2	2.36	0.40
2:B:66:LYS:CE	2:B:230:MET:HA	2.49	0.40
1:A:207:GLN:O	1:A:211:ARG:HG3	2.21	0.40
1:A:71:TRP:N	1:A:71:TRP:CD1	2.90	0.40
1:A:97:PRO:C	1:A:99:GLY:N	2.75	0.40
1:A:210:LEU:C	1:A:212:TRP:N	2.74	0.40
1:A:279:LEU:O	1:A:282:LEU:HD12	2.22	0.40
1:A:366:LYS:HB3	1:A:366:LYS:NZ	2.37	0.40
1:A:488:ASP:N	1:A:488:ASP:OD2	2.54	0.40
2:B:187:LEU:HA	2:B:187:LEU:HD12	1.90	0.40
1:A:498:ASP:OD1	1:A:498:ASP:C	2.60	0.40
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.57	0.40
1:A:515:SER:HG	1:A:518:VAL:H	1.67	0.40
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:LYS:HE2	2:B:428:GLN:HB2	2.03	0.40
2:B:97:PRO:C	2:B:99:GLY:H	2.24	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	508/534 (95%)	457 (90%)	37 (7%)	14 (3%)	6	29
2	B	391/422 (93%)	350 (90%)	32 (8%)	9 (2%)	7	35
All	All	899/956 (94%)	807 (90%)	69 (8%)	23 (3%)	6	31

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	PRO
1	A	18	GLY
1	A	195	ILE
1	A	213	GLY
1	A	229	TRP
2	B	239	TRP
1	A	171	PHE
1	A	219	LYS
2	B	140	PRO
2	B	193	LEU
1	A	52	PRO
1	A	170	PRO
1	A	402	TRP
1	A	474	ASN
2	B	161	GLN
1	A	481	ALA

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Mol	Chain	Res	Type
2	B	170	PRO
2	B	195	ILE
2	B	68	SER
1	A	270	ILE
2	B	235	HIS
1	A	225	PRO
2	B	176	PRO

### 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	467/479 (98%)	434 (93%)	33 (7%)	17	52
2	B	365/384 (95%)	342 (94%)	23 (6%)	21	57
All	All	832/863 (96%)	776 (93%)	56 (7%)	19	54

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	67	ASP
1	A	105	SER
1	A	122	GLU
1	A	135	ILE
1	A	168	LEU
1	A	169	GLU
1	A	172	ARG
1	A	177	ASP
1	A	182	GLN
1	A	187	LEU
1	A	194	GLU
1	A	200	THR
1	A	212	TRP
1	A	227	PHE
1	A	241	VAL

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Mol	Chain	Res	Type
1	A	244	ILE
1	A	250	ASP
1	A	279	LEU
1	A	295	LEU
1	A	303	LEU
1	A	312	GLU
1	A	349	LEU
1	A	350	LYS
1	A	362	THR
1	A	367	GLN
1	A	473	THR
1	A	476	LYS
1	A	503	LEU
1	A	515	SER
1	A	516	GLU
1	A	517	LEU
1	A	529	GLU
2	B	10	VAL
2	B	24	TRP
2	B	55	PRO
2	B	66	LYS
2	B	69	THR
2	B	106	VAL
2	B	109	LEU
2	B	117	SER
2	B	123	ASP
2	B	145	GLN
2	B	179	VAL
2	B	184	MET
2	B	205	LEU
2	B	237	ASP
2	B	238	LYS
2	B	250	ASP
2	B	280	CYS
2	B	295	LEU
2	B	303	LEU
2	B	323	LYS
2	B	344	GLU
2	B	410	TRP
2	B	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	151	GLN
1	A	207	GLN
1	A	222	GLN
1	A	255	ASN
1	A	265	ASN
1	A	278	GLN
1	A	336	GLN
1	A	428	GLN
1	A	475	GLN
1	A	509	GLN
1	A	512	GLN
1	A	520	GLN
2	B	147	ASN
2	B	151	GLN
2	B	175	ASN
2	B	235	HIS
2	B	242	GLN
2	B	332	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	CSD	A	280	1	4,7,8	1.64	1 (25%)	2,8,10	2.02	1 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	280	1	-	0/2/6/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	CA-C	3.00	1.54	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	O-C-CA	-2.48	118.17	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PO4	A	1300	-	4,4,4	1.34	0	6,6,6	0.41	0
3	PO4	A	1301	-	4,4,4	1.39	0	6,6,6	0.40	0
4	PC0	A	999	-	23,24,24	2.11	7 (30%)	28,31,31	1.75	6 (21%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	1300	-	-	0/0/0/0	0/0/0/0
3	PO4	A	1301	-	-	0/0/0/0	0/0/0/0
4	PC0	A	999	-	-	0/13/13/13	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	PC0	C1-N8	-2.42	1.35	1.40
4	A	999	PC0	C1-N2	2.01	1.38	1.34
4	A	999	PC0	C3-N2	2.12	1.39	1.34
4	A	999	PC0	C9-S9	2.33	1.73	1.68
4	A	999	PC0	C17-C18	2.66	1.42	1.39
4	A	999	PC0	C13-N14	5.03	1.39	1.34
4	A	999	PC0	CL7-C4	5.87	1.72	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	PC0	C4-C3-N2	-3.86	120.27	124.80
4	A	999	PC0	C16-C15-N14	-3.76	119.58	123.92
4	A	999	PC0	C11-N10-C9	-2.17	120.81	124.62
4	A	999	PC0	N8-C1-N2	2.40	122.45	115.05
4	A	999	PC0	C15-N14-C13	2.91	121.81	117.66
4	A	999	PC0	C3-N2-C1	3.12	121.15	117.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1300	PO4	3	0
3	A	1301	PO4	1	0
4	A	999	PC0	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	516/534 (96%)	-0.35	11 (2%) 64 34	20, 59, 102, 148	0
2	B	399/422 (94%)	-0.44	6 (1%) 74 47	20, 58, 113, 130	0
All	All	915/956 (95%)	-0.39	17 (1%) 67 37	20, 59, 108, 148	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	SER	3.9
2	B	66	LYS	3.4
1	A	468	THR	3.2
1	A	69	THR	3.0
1	A	228	LEU	2.9
1	A	136	ASN	2.9
1	A	470	THR	2.8
2	B	334	GLN	2.7
1	A	137	ASN	2.6
2	B	195	ILE	2.4
2	B	210	LEU	2.3
1	A	251	SER	2.3
1	A	243	PRO	2.3
1	A	70	LYS	2.2
2	B	237	ASP	2.1
1	A	58	THR	2.0
2	B	230	MET	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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( $\text{\AA}^2$ )	Q<0.9
1	CSD	A	280	8/9	0.96	0.14	-	43,48,61,65	0

### 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( $\text{\AA}^2$ )	Q<0.9
3	PO4	A	1300	5/5	0.78	0.26	0.99	119,122,123,123	0
3	PO4	A	1301	5/5	0.93	0.21	0.79	102,103,108,111	0
4	PC0	A	999	23/23	0.93	0.16	-0.10	36,48,56,65	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.