



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:00 PM GMT

PDB ID : 2HND
Title : Crystal Structure of K101E Mutant HIV-1 Reverse Transcriptase in Complex with Nevirapine
Authors : Ren, J.; Nichols, C.E.; Stamp, A.; Chamberlain, P.P.; Stammers, D.K.
Deposited on : 2006-07-12
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

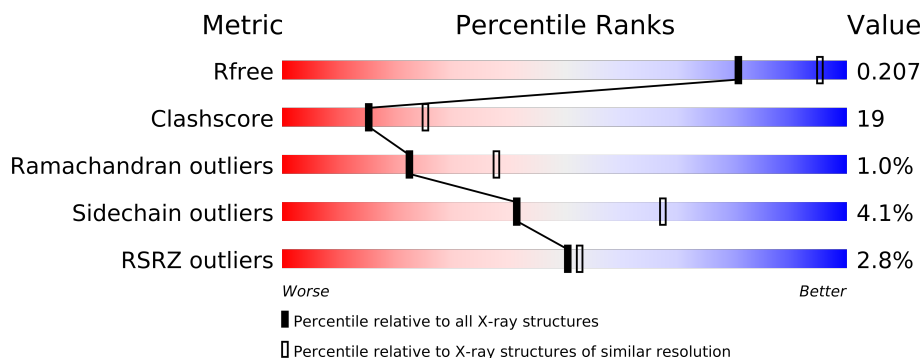
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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 ≥ 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	534	
2	B	422	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	PO4	A	1300	-	X
3	PO4	A	1302	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7681 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 Reverse transcriptase/ribonucleaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	0	0
			4295	2782	709	796	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	GLU	LYS	ENGINEERED	UNP P04585
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

- Molecule 2 is a protein called Reverse transcriptase/ribonucleaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	0	0
			3270	2131	540	593	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	101	GLU	LYS	ENGINEERED	UNP P04585

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

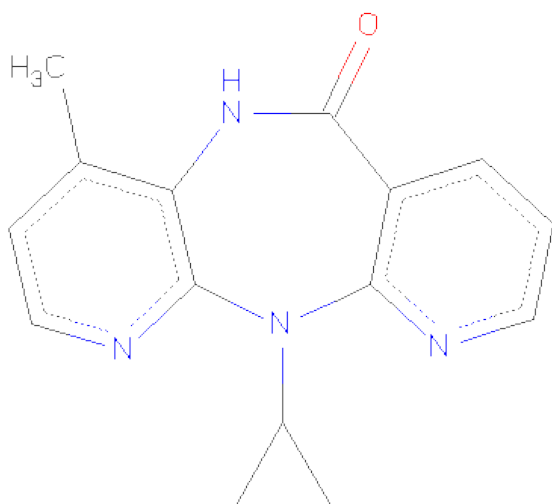


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (three-letter code: NVP) (formula: C₁₅H₁₄N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	15	4	1		

- Molecule 6 is water.

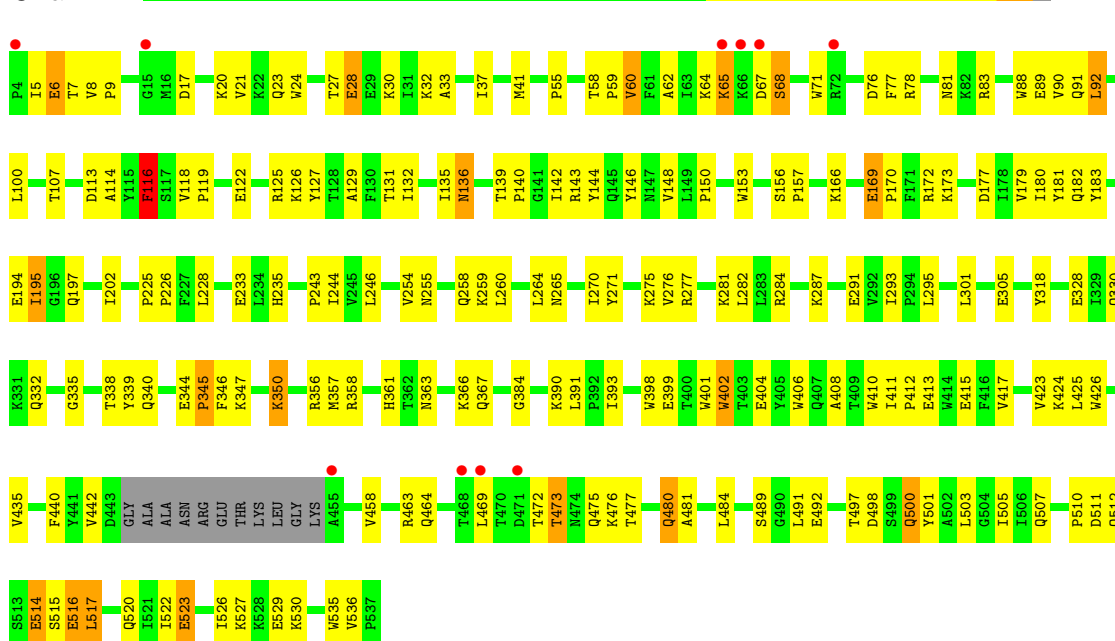
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	52	Total	O	0	0
			52	52		
6	B	28	Total	O	0	0
			28	28		

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.

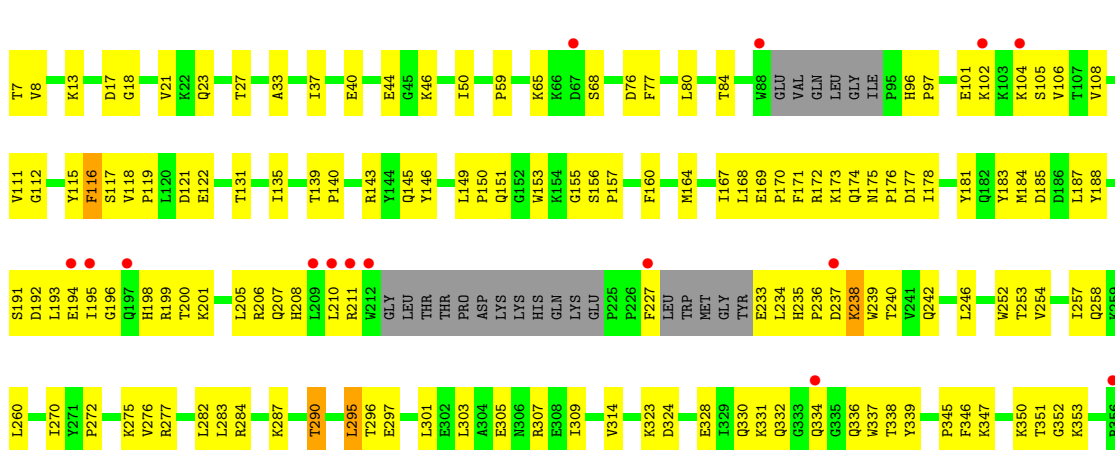
• Molecule 1: Reverse transcriptase/ribonucleaseH

Chain A:



• Molecule 2: Reverse transcriptase/ribonucleaseH

Chain B:



MET	
ARG	
GLY	
ALA	
HIS	
T362	
N363	
D364	
V365	
K366	
Q367	
L368	
T369	
E370	
A371	
V372	
Q373	
T377	
E378	
S379	
I380	
G384	
K385	
T386	
P387	
K388	
I393	
Q394	
K395	
E396	
T397	
W398	
E399	
T400	
W401	
W414	
N418	
T419	
P420	
P421	
L422	
V423	
K424	
L425	
W426	
Y427	
Q428	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	138.90Å 114.90Å 65.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 2.50 29.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.4 (29.72-2.50) 94.4 (29.72-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.269 0.195 , 0.207	Depositor DCC
R_{free} test set	1740 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.9	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 35019 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7681	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: CSD, PO4, MG, NVP

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	0.43	0/4401	0.63	0/5984
2	B	0.40	0/3363	0.63	0/4567
All	All	0.42	0/7764	0.63	0/10551

There are no bond length outliers.

There are no bond angle outliers.

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	4295	0	4324	155	0
2	B	3270	0	3291	142	0
3	A	15	0	0	0	0
4	A	1	0	0	0	0
5	A	20	0	14	1	0
6	A	52	0	0	8	0
6	B	28	0	0	0	0
All	All	7681	0	7629	286	0

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 19.

All (286) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:356:ARG:HH21	1:A:358:ARG:HD2	1.25	0.99
1:A:92:LEU:HD12	1:A:92:LEU:H	1.25	0.99
1:A:507:GLN:HE22	2:B:421:PRO:HB3	1.29	0.94
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.32	0.91
2:B:238:LYS:HD2	2:B:238:LYS:H	1.35	0.91
2:B:270:ILE:O	2:B:272:PRO:HD3	1.73	0.89
2:B:238:LYS:HD2	2:B:238:LYS:N	1.87	0.88
1:A:67:ASP:O	1:A:68:SER:HB3	1.72	0.87
1:A:136:ASN:HD22	1:A:139:THR:HB	1.41	0.84
1:A:113:ASP:HA	1:A:116:PHE:CD2	2.13	0.83
1:A:469:LEU:HD11	1:A:480:GLN:HG3	1.61	0.82
1:A:500:GLN:H	1:A:500:GLN:NE2	1.76	0.82
2:B:295:LEU:HD12	2:B:295:LEU:N	1.94	0.82
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.62	0.81
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.63	0.80
1:A:92:LEU:HD12	1:A:92:LEU:N	1.95	0.80
2:B:112:GLY:HA3	2:B:151:GLN:HE21	1.47	0.78
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.65	0.76
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.67	0.76
1:A:136:ASN:HD22	1:A:139:THR:CB	2.00	0.75
2:B:106:VAL:HG13	2:B:234:LEU:HB2	1.69	0.75
1:A:65:LYS:HA	1:A:65:LYS:HE2	1.70	0.73
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.24	0.73
1:A:92:LEU:H	1:A:92:LEU:CD1	2.01	0.72
2:B:246:LEU:HD12	2:B:307:ARG:HG2	1.71	0.72
1:A:113:ASP:HA	1:A:116:PHE:CE2	2.25	0.71
1:A:473:THR:HG23	1:A:476:LYS:HB2	1.71	0.70
2:B:8:VAL:O	2:B:121:ASP:HB2	1.92	0.70
1:A:357:MET:CE	1:A:512:GLN:HE21	2.05	0.70
2:B:254:VAL:O	2:B:258:GLN:HG3	1.93	0.69
1:A:358:ARG:NH2	2:B:394:GLN:HG2	2.08	0.69
1:A:116:PHE:CD1	1:A:116:PHE:N	2.55	0.68
1:A:507:GLN:HE22	2:B:421:PRO:CB	2.05	0.68
2:B:206:ARG:HD2	2:B:227:PHE:CE1	2.30	0.67
2:B:295:LEU:HD12	2:B:295:LEU:H	1.58	0.67
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.75	0.67
2:B:420:PRO:HG2	2:B:423:VAL:HG12	1.78	0.66
1:A:332:GLN:HG2	1:A:332:GLN:O	1.95	0.66
2:B:238:LYS:O	2:B:240:THR:HG23	1.96	0.65
2:B:420:PRO:HG2	2:B:423:VAL:CG1	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:172:ARG:O	2:B:176:PRO:HG3	1.97	0.65
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.32	0.64
2:B:423:VAL:HG13	2:B:424:LYS:N	2.12	0.64
1:A:270:ILE:HG23	1:A:271:TYR:CD2	2.32	0.64
1:A:28:GLU:HG3	1:A:135:ILE:CG2	2.28	0.64
1:A:356:ARG:NH2	1:A:358:ARG:HD2	2.07	0.63
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.63	0.63
2:B:297:GLU:O	2:B:301:LEU:HG	1.99	0.62
1:A:469:LEU:CD1	1:A:480:GLN:HG3	2.28	0.62
1:A:356:ARG:NH2	6:A:1038:HOH:O	2.33	0.62
1:A:275:LYS:HE2	1:A:332:GLN:NE2	2.15	0.61
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.81	0.61
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.00	0.61
1:A:281:LYS:HE3	1:A:284:ARG:CZ	2.31	0.61
2:B:242:GLN:OE1	2:B:353:LYS:HE2	2.00	0.61
2:B:350:LYS:HG2	2:B:351:THR:N	2.16	0.61
2:B:365:VAL:O	2:B:369:THR:HG23	2.01	0.60
1:A:384:GLY:HA3	2:B:135:ILE:HD12	1.82	0.60
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.83	0.60
2:B:295:LEU:CD1	2:B:295:LEU:N	2.64	0.60
2:B:331:LYS:O	2:B:424:LYS:HE2	2.00	0.60
2:B:305:GLU:O	2:B:309:ILE:HG13	2.01	0.60
2:B:284:ARG:O	2:B:287:LYS:NZ	2.35	0.60
2:B:339:TYR:CZ	2:B:352:GLY:HA3	2.37	0.60
2:B:183:TYR:OH	2:B:386:THR:HG23	2.02	0.60
2:B:368:LEU:O	2:B:372:VAL:HG23	2.02	0.60
2:B:40:GLU:HG3	2:B:44:GLU:OE2	2.01	0.59
1:A:20:LYS:HE2	1:A:55:PRO:HB2	1.85	0.59
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.01	0.58
1:A:37:ILE:O	1:A:41:MET:HG3	2.04	0.58
1:A:497:THR:O	1:A:535:TRP:HA	2.04	0.58
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.34	0.58
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.86	0.57
2:B:195:ILE:HG22	2:B:199:ARG:HE	1.68	0.57
2:B:332:GLN:HB2	2:B:336:GLN:O	2.05	0.57
1:A:491:LEU:HD13	1:A:529:GLU:HG2	1.87	0.57
1:A:17:ASP:O	1:A:83:ARG:HD3	2.04	0.57
1:A:507:GLN:NE2	2:B:421:PRO:HB3	2.11	0.57
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.40	0.57
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.40	0.57
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.87	0.56
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:480:GLN:C	1:A:480:GLN:HE21	2.09	0.56
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.71	0.56
1:A:122:GLU:HG3	1:A:125:ARG:NH1	2.21	0.56
1:A:530:LYS:HA	6:A:1075:HOH:O	2.06	0.56
1:A:523:GLU:O	1:A:527:LYS:HG2	2.06	0.56
2:B:46:LYS:HZ3	2:B:116:PHE:HD2	1.53	0.55
2:B:149:LEU:HD13	2:B:156:SER:HA	1.89	0.55
2:B:105:SER:HB3	2:B:235:HIS:ND1	2.22	0.55
1:A:28:GLU:HG3	1:A:135:ILE:HG22	1.89	0.55
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.42	0.55
1:A:89:GLU:CD	1:A:92:LEU:HD21	2.28	0.55
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.72	0.54
1:A:500:GLN:CD	1:A:500:GLN:H	2.10	0.54
1:A:475:GLN:HB2	1:A:501:TYR:CD2	2.43	0.54
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.20	0.54
2:B:350:LYS:HG2	2:B:351:THR:H	1.73	0.54
1:A:282:LEU:HB3	1:A:293:ILE:HG21	1.90	0.54
1:A:384:GLY:CA	2:B:135:ILE:HD12	2.38	0.53
2:B:65:LYS:HB2	2:B:68:SER:HB3	1.90	0.53
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.89	0.53
1:A:254:VAL:O	1:A:258:GLN:HG3	2.09	0.53
2:B:175:ASN:ND2	2:B:201:LYS:CE	2.72	0.53
2:B:194:GLU:HG3	2:B:196:GLY:H	1.74	0.53
1:A:417:VAL:O	1:A:417:VAL:HG13	2.09	0.53
1:A:393:ILE:HB	1:A:423:VAL:CG2	2.38	0.52
2:B:169:GLU:N	2:B:170:PRO:HD2	2.25	0.52
1:A:480:GLN:HE21	1:A:480:GLN:CA	2.23	0.52
2:B:115:TYR:C	2:B:117:SER:H	2.11	0.52
2:B:233:GLU:HB3	2:B:235:HIS:CE1	2.44	0.52
2:B:423:VAL:CG1	2:B:424:LYS:N	2.71	0.52
1:A:287:LYS:HG2	1:A:291:GLU:OE2	2.10	0.52
2:B:170:PRO:HG3	2:B:208:HIS:CE1	2.45	0.51
2:B:104:LYS:HD2	2:B:192:ASP:HB3	1.93	0.51
2:B:181:TYR:HE1	2:B:183:TYR:HB2	1.74	0.51
2:B:211:ARG:HH11	2:B:211:ARG:HG3	1.75	0.51
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.46	0.51
1:A:516:GLU:O	1:A:520:GLN:HG3	2.11	0.51
2:B:295:LEU:H	2:B:295:LEU:CD1	2.23	0.51
1:A:89:GLU:OE2	1:A:92:LEU:HD11	2.11	0.51
2:B:112:GLY:CA	2:B:151:GLN:HE21	2.22	0.51
1:A:472:THR:OG1	1:A:477:THR:HG23	2.12	0.50
2:B:233:GLU:N	2:B:233:GLU:OE2	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.12	0.50
1:A:125:ARG:HG2	1:A:146:TYR:O	2.12	0.50
2:B:235:HIS:N	2:B:236:PRO:HD3	2.27	0.50
1:A:23:GLN:HE22	1:A:60:VAL:H	1.59	0.49
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.93	0.49
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.48	0.49
1:A:401:TRP:O	1:A:404:GLU:HG2	2.12	0.49
1:A:361:HIS:HB2	6:A:1033:HOH:O	2.11	0.49
2:B:178:ILE:HG13	2:B:178:ILE:O	2.12	0.49
1:A:65:LYS:HA	1:A:65:LYS:CE	2.42	0.49
2:B:174:GLN:C	2:B:176:PRO:HD3	2.33	0.49
2:B:422:LEU:HB3	2:B:426:TRP:CH2	2.48	0.49
1:A:23:GLN:HE22	1:A:60:VAL:HG12	1.77	0.49
2:B:257:ILE:O	2:B:260:LEU:HB3	2.13	0.48
2:B:324:ASP:OD1	2:B:388:LYS:HE3	2.13	0.48
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.95	0.48
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.96	0.48
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.94	0.48
1:A:344:GLU:OE2	1:A:345:PRO:HD2	2.14	0.48
2:B:328:GLU:O	2:B:339:TYR:HA	2.14	0.48
1:A:172:ARG:NH1	1:A:180:ILE:O	2.46	0.48
1:A:90:VAL:HG23	6:A:1069:HOH:O	2.12	0.48
1:A:345:PRO:O	1:A:346:PHE:HB2	2.14	0.48
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.14	0.48
2:B:104:LYS:O	2:B:235:HIS:HA	2.14	0.47
2:B:33:ALA:O	2:B:37:ILE:HG13	2.14	0.47
2:B:13:LYS:HG3	2:B:84:THR:O	2.13	0.47
2:B:239:TRP:CZ2	2:B:378:GLU:HG2	2.50	0.47
1:A:522:ILE:O	1:A:526:ILE:HG13	2.14	0.47
2:B:164:MET:HA	2:B:167:ILE:HD11	1.96	0.47
1:A:475:GLN:HB2	1:A:501:TYR:CE2	2.49	0.47
2:B:395:LYS:O	2:B:399:GLU:HG2	2.15	0.47
2:B:164:MET:SD	2:B:167:ILE:HD11	2.54	0.47
1:A:366:LYS:NZ	1:A:366:LYS:HB3	2.30	0.47
1:A:424:LYS:NZ	1:A:426:TRP:CD2	2.82	0.47
2:B:345:PRO:O	2:B:347:LYS:HG3	2.13	0.47
2:B:77:PHE:CD2	2:B:80:LEU:HD23	2.50	0.47
1:A:301:LEU:O	1:A:305:GLU:HG3	2.15	0.47
1:A:514:GLU:HG3	1:A:515:SER:H	1.80	0.47
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.97	0.46
1:A:89:GLU:OE2	1:A:92:LEU:HD21	2.15	0.46
2:B:198:HIS:C	2:B:200:THR:N	2.69	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:340:GLN:NE2	6:A:1021:HOH:O	2.47	0.46
2:B:237:ASP:HB3	2:B:238:LYS:CE	2.45	0.46
2:B:377:THR:HG22	2:B:378:GLU:N	2.29	0.46
1:A:492:GLU:OE2	1:A:530:LYS:HD2	2.14	0.46
1:A:391:LEU:C	1:A:417:VAL:HG12	2.35	0.46
2:B:17:ASP:CG	2:B:18:GLY:H	2.19	0.46
2:B:101:GLU:O	2:B:236:PRO:HB2	2.15	0.46
1:A:23:GLN:HE22	1:A:60:VAL:CG1	2.29	0.46
2:B:346:PHE:CD2	2:B:346:PHE:N	2.84	0.46
2:B:181:TYR:CE1	2:B:183:TYR:HB2	2.51	0.46
2:B:253:THR:O	2:B:257:ILE:HG13	2.16	0.46
2:B:106:VAL:CG1	2:B:234:LEU:HB2	2.44	0.45
1:A:363:ASN:HA	1:A:511:ASP:CG	2.35	0.45
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.98	0.45
2:B:168:LEU:O	2:B:172:ARG:HB2	2.15	0.45
2:B:164:MET:HA	2:B:167:ILE:CD1	2.46	0.45
1:A:181:TYR:HE1	1:A:183:TYR:HB2	1.79	0.45
1:A:58:THR:HG21	1:A:77:PHE:CD2	2.51	0.45
2:B:369:THR:O	2:B:373:GLN:HG3	2.16	0.45
1:A:78:ARG:O	1:A:81:ASN:HB2	2.16	0.45
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.51	0.45
1:A:413:GLU:HA	6:A:1042:HOH:O	2.17	0.45
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.86	0.45
1:A:350:LYS:HB2	1:A:350:LYS:HE2	1.68	0.45
1:A:131:THR:OG1	1:A:143:ARG:HG2	2.17	0.45
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.52	0.45
1:A:139:THR:HA	1:A:140:PRO:HD3	1.87	0.45
1:A:64:LYS:HG3	1:A:71:TRP:CZ3	2.51	0.45
1:A:150:PRO:HG2	1:A:153:TRP:HB2	1.99	0.44
1:A:179:VAL:HG12	5:A:999:NVP:HCB2	1.99	0.44
1:A:132:ILE:HB	1:A:142:ILE:HG13	1.99	0.44
1:A:277:ARG:O	1:A:281:LYS:HG3	2.17	0.44
1:A:291:GLU:HG2	1:A:293:ILE:HD12	2.00	0.44
1:A:129:ALA:HA	1:A:144:TYR:O	2.18	0.44
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.53	0.44
2:B:175:ASN:ND2	2:B:201:LYS:HE3	2.33	0.44
2:B:175:ASN:HD21	2:B:201:LYS:HE3	1.82	0.44
1:A:357:MET:HE2	1:A:512:GLN:NE2	2.33	0.43
1:A:357:MET:HE2	1:A:512:GLN:HE21	1.81	0.43
2:B:175:ASN:N	2:B:176:PRO:HD3	2.33	0.43
1:A:33:ALA:O	1:A:37:ILE:HG12	2.18	0.43
2:B:156:SER:N	2:B:157:PRO:HD2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:366:LYS:HG2	2:B:370:GLU:OE1	2.18	0.43
1:A:225:PRO:HA	1:A:226:PRO:C	2.39	0.43
1:A:28:GLU:O	1:A:32:LYS:HG3	2.18	0.43
1:A:344:GLU:HB3	1:A:347:LYS:HE3	2.01	0.43
2:B:380:ILE:O	2:B:384:GLY:N	2.51	0.43
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.54	0.43
2:B:115:TYR:O	2:B:117:SER:N	2.47	0.43
1:A:27:THR:OG1	1:A:30:LYS:HG3	2.19	0.43
2:B:118:VAL:HA	2:B:119:PRO:HD3	1.88	0.43
2:B:46:LYS:HE2	2:B:116:PHE:HB3	2.01	0.43
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.67	0.43
1:A:59:PRO:HG2	1:A:76:ASP:HB3	2.01	0.43
1:A:148:VAL:O	1:A:150:PRO:HD3	2.19	0.43
2:B:96:HIS:HA	2:B:97:PRO:HD3	1.86	0.43
1:A:264:LEU:HD13	1:A:276:VAL:HG12	2.01	0.43
1:A:358:ARG:HH22	2:B:394:GLN:HG2	1.81	0.43
2:B:153:TRP:CH2	2:B:155:GLY:HA3	2.54	0.43
2:B:275:LYS:HD3	2:B:277:ARG:NH1	2.34	0.42
2:B:211:ARG:NH1	2:B:211:ARG:HG3	2.34	0.42
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.55	0.42
1:A:8:VAL:HA	1:A:9:PRO:HD3	1.78	0.42
1:A:202:ILE:HG21	6:A:1071:HOH:O	2.18	0.42
1:A:505:ILE:O	1:A:510:PRO:HD3	2.19	0.42
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.18	0.42
2:B:175:ASN:C	2:B:177:ASP:H	2.22	0.42
2:B:350:LYS:HE3	2:B:378:GLU:OE1	2.20	0.42
1:A:107:THR:HB	1:A:202:ILE:HD11	2.01	0.42
6:A:1039:HOH:O	2:B:27:THR:HB	2.19	0.42
1:A:5:ILE:HG13	1:A:6:GLU:N	2.33	0.42
2:B:206:ARG:HD2	2:B:227:PHE:HE1	1.80	0.42
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.54	0.42
1:A:500:GLN:CD	1:A:500:GLN:N	2.73	0.42
1:A:410:TRP:CE3	1:A:410:TRP:HA	2.55	0.42
1:A:169:GLU:HA	1:A:169:GLU:OE1	2.19	0.42
2:B:183:TYR:CE1	2:B:184:MET:HG3	2.54	0.42
1:A:255:ASN:O	1:A:259:LYS:HG3	2.19	0.42
1:A:473:THR:HG23	1:A:476:LYS:CB	2.44	0.42
2:B:160:PHE:CD1	2:B:160:PHE:O	2.73	0.42
1:A:328:GLU:O	1:A:339:TYR:HA	2.20	0.42
1:A:126:LYS:HE3	1:A:127:TYR:OH	2.19	0.41
2:B:211:ARG:HG2	2:B:211:ARG:O	2.20	0.41
2:B:323:LYS:HD3	2:B:323:LYS:HA	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:228:LEU:HD23	1:A:233:GLU:HA	2.02	0.41
1:A:282:LEU:HD11	1:A:295:LEU:CD2	2.50	0.41
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.55	0.41
2:B:205:LEU:C	2:B:207:GLN:N	2.74	0.41
1:A:390:LYS:HD3	1:A:415:GLU:CG	2.50	0.41
1:A:90:VAL:O	1:A:91:GLN:C	2.59	0.41
2:B:276:VAL:O	2:B:277:ARG:C	2.58	0.41
1:A:100:LEU:O	1:A:318:TYR:HB3	2.19	0.41
1:A:330:GLN:HB2	1:A:338:THR:OG1	2.20	0.41
1:A:480:GLN:CA	1:A:480:GLN:NE2	2.82	0.41
2:B:195:ILE:CG2	2:B:199:ARG:HE	2.34	0.41
1:A:401:TRP:HB2	1:A:425:LEU:HD11	2.03	0.41
1:A:107:THR:HB	1:A:202:ILE:CD1	2.51	0.41
1:A:275:LYS:HE2	1:A:332:GLN:HE21	1.84	0.41
1:A:143:ARG:NH1	1:A:143:ARG:HG2	2.34	0.41
2:B:191:SER:HB2	2:B:193:LEU:HD13	2.02	0.41
2:B:393:ILE:HD11	2:B:397:THR:CG2	2.51	0.41
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.20	0.41
2:B:101:GLU:HG2	2:B:102:LYS:N	2.36	0.41
2:B:173:LYS:O	2:B:176:PRO:HD3	2.21	0.41
1:A:194:GLU:HB2	1:A:197:GLN:OE1	2.21	0.41
1:A:463:ARG:CG	1:A:464:GLN:N	2.84	0.41
1:A:500:GLN:O	1:A:503:LEU:HB3	2.21	0.41
1:A:402:TRP:CD1	1:A:402:TRP:C	2.95	0.41
2:B:257:ILE:HB	2:B:283:LEU:HD21	2.02	0.41
1:A:265:ASN:N	1:A:265:ASN:HD22	2.18	0.41
2:B:198:HIS:O	2:B:200:THR:N	2.54	0.40
1:A:166:LYS:O	1:A:169:GLU:HB2	2.20	0.40
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.56	0.40
2:B:139:THR:HB	2:B:140:PRO:HD2	2.03	0.40
1:A:170:PRO:O	1:A:173:LYS:N	2.55	0.40
2:B:198:HIS:C	2:B:200:THR:H	2.24	0.40
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.22	0.40
1:A:194:GLU:O	1:A:195:ILE:C	2.60	0.40
1:A:177:ASP:N	1:A:177:ASP:OD2	2.50	0.40
1:A:498:ASP:HA	1:A:536:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/534 (97%)	482 (93%)	29 (6%)	7 (1%)	16	27
2	B	384/422 (91%)	347 (90%)	35 (9%)	2 (0%)	38	60
All	All	902/956 (94%)	829 (92%)	64 (7%)	9 (1%)	22	38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	SER
1	A	114	ALA
1	A	116	PHE
2	B	116	PHE
1	A	195	ILE
1	A	412	PRO
1	A	345	PRO
2	B	421	PRO
1	A	243	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	472/479 (98%)	449 (95%)	23 (5%)	35	59
2	B	361/384 (94%)	350 (97%)	11 (3%)	53	80
All	All	833/863 (96%)	799 (96%)	34 (4%)	41	67

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	THR
1	A	24	TRP
1	A	28	GLU
1	A	60	VAL
1	A	65	LYS
1	A	92	LEU
1	A	116	PHE
1	A	136	ASN
1	A	169	GLU
1	A	182	GLN
1	A	244	ILE
1	A	350	LYS
1	A	402	TRP
1	A	458	VAL
1	A	473	THR
1	A	480	GLN
1	A	484	LEU
1	A	500	GLN
1	A	514	GLU
1	A	516	GLU
1	A	517	LEU
1	A	523	GLU
2	B	122	GLU
2	B	171	PHE
2	B	210	LEU
2	B	238	LYS
2	B	290	THR
2	B	295	LEU
2	B	303	LEU
2	B	314	VAL
2	B	334	GLN
2	B	377	THR
2	B	414	TRP

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

Mol	Chain	Res	Type
1	A	23	GLN
1	A	136	ASN
1	A	222	GLN
1	A	265	ASN
1	A	278	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	332	GLN
1	A	336	GLN
1	A	428	GLN
1	A	475	GLN
1	A	480	GLN
1	A	500	GLN
1	A	507	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	182	GLN
2	B	278	GLN
2	B	348	ASN
2	B	407	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	7,7,8	7.21	2 (28%)	6,8,10	3.86	5 (83%)

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	-	0/3/6/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	O-C	18.81	1.24	1.11
1	A	280	CSD	CA-C	2.71	1.53	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD2-SG-CB	5.59	119.93	97.42
1	A	280	CSD	OD2-SG-OD1	5.10	117.85	109.39
1	A	280	CSD	CA-CB-SG	4.49	117.22	110.82
1	A	280	CSD	C-CA-N	-2.52	111.31	113.83
1	A	280	CSD	OD1-SG-CB	-2.37	98.98	105.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	0.86	0	6,6,6	0.31	0
3	PO4	A	1301	-	4,4,4	0.84	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	1302	-	4,4,4	0.83	0	6,6,6	0.31	0
5	NVP	A	999	-	18,23,23	1.10	0	19,34,34	1.61	3 (15%)

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
3	PO4	A	1302	-	-	0/0/0/0	0/0/0/0
5	NVP	A	999	-	-	0/0/6/6	0/0/4/4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	999	NVP	C5-C6-C7	4.10	119.48	116.82
5	A	999	NVP	C6-C7-C2	-2.93	118.66	122.58
5	A	999	NVP	C13-N14-C15	2.01	119.46	116.70

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	523/534 (97%)	-0.25	10 (1%) 64 66	28, 54, 100, 147	0
2	B	394/422 (93%)	0.02	16 (4%) 35 36	29, 59, 113, 131	0
All	All	917/956 (95%)	-0.13	26 (2%) 50 53	28, 56, 107, 147	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	4.5
2	B	88	TRP	4.0
2	B	212	TRP	3.8
1	A	468	THR	3.6
2	B	356	ARG	3.6
1	A	66	LYS	3.5
2	B	211	ARG	3.4
1	A	469	LEU	3.4
2	B	195	ILE	3.4
1	A	471	ASP	3.4
2	B	362	THR	2.9
1	A	455	ALA	2.8
2	B	209	LEU	2.8
2	B	194	GLU	2.7
2	B	197	GLN	2.7
2	B	227	PHE	2.6
1	A	4	PRO	2.6
1	A	15	GLY	2.5
2	B	67	ASP	2.4
2	B	102	LYS	2.4
2	B	237	ASP	2.4
1	A	65	LYS	2.3
2	B	210	LEU	2.1
2	B	104	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	72	ARG	2.1
2	B	334	GLN	2.0

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CSD	A	280	8/9	0.13	-0.09	43,49,78,85	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	A	1302	5/5	0.32	12.35	146,149,150,150	0
3	PO4	A	1300	5/5	0.16	3.80	129,132,140,141	0
3	PO4	A	1301	5/5	0.15	1.34	123,126,130,131	0
5	NVP	A	999	20/20	0.12	0.50	23,37,47,49	0
4	MG	A	1303	1/1	0.09	-1.43	53,53,53,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.