



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:24 PM GMT

PDB ID : 4I7F  
Title : HIV-1 Reverse Transcriptase in complex with a phosphonate analog of nevirapine  
Authors : Lansdon, E.B.; Parrish, J.  
Deposited on : 2012-11-30  
Resolution : 2.50 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

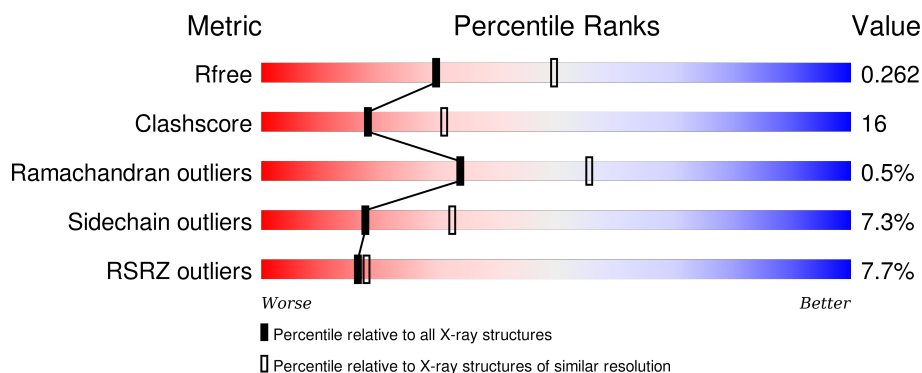
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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  $\geq 3$ , 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>5%</div> <div>60%</div> <div>34%</div> <div>• •</div> </div>
2	B	440	<div> <div>10%</div> <div>64%</div> <div>24%</div> <div>• 8%</div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7999 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.

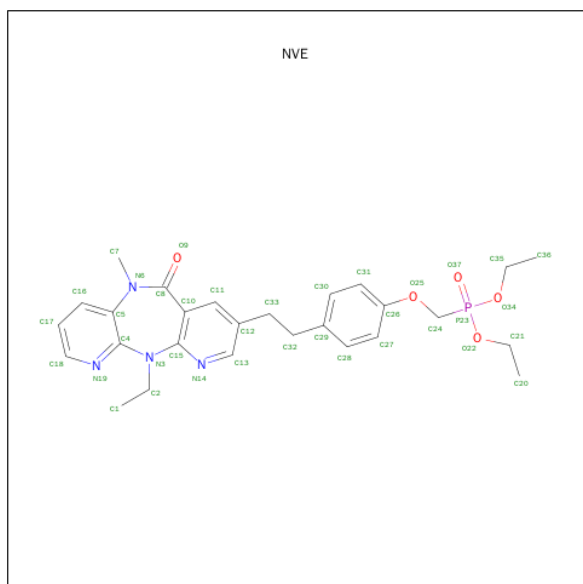
- Molecule 1 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4502	2911	751	832	8			

- Molecule 2 is a protein called Reverse transcriptase.

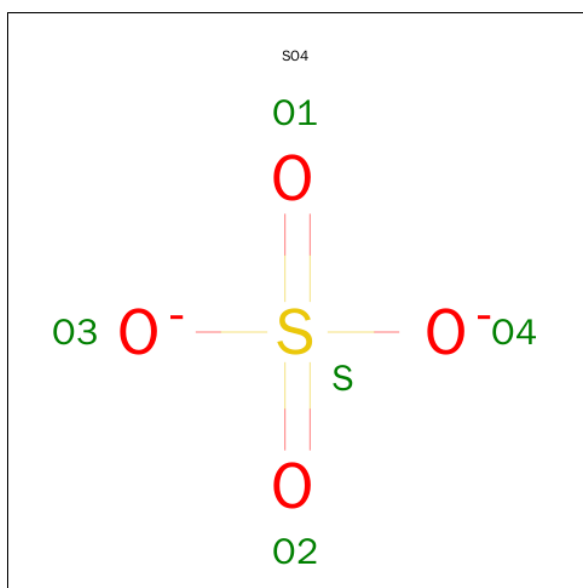
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3353	2184	553	610	6			

- Molecule 3 is DIETHYL ({4-[2-(11-ETHYL-5-METHYL-6-OXO-6,11-DIHYDRO-5H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-8-YL)ETHYL]PHENOXY}METHYL)PHOSPHONATE (three-letter code: NVE) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>4</sub>O<sub>5</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			37	27	4	5	1		

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



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		

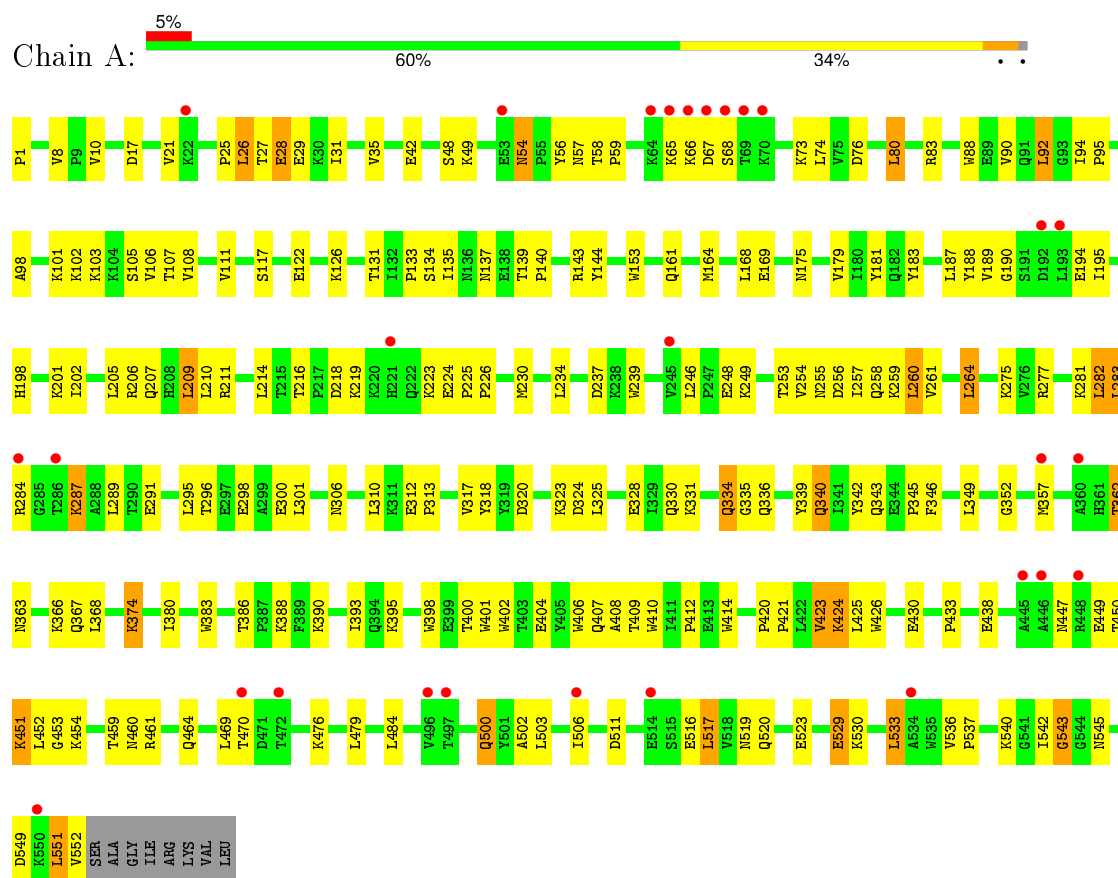
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	49	Total 49	O 49	0	0
7	B	35	Total 35	O 35	0	0

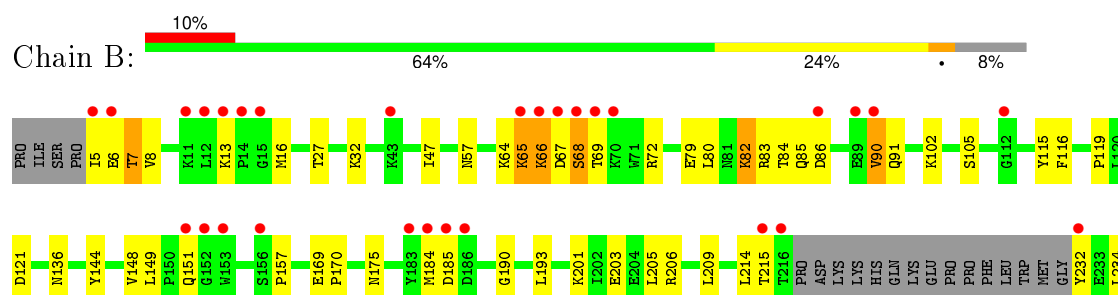
### 3 Residue-property plots

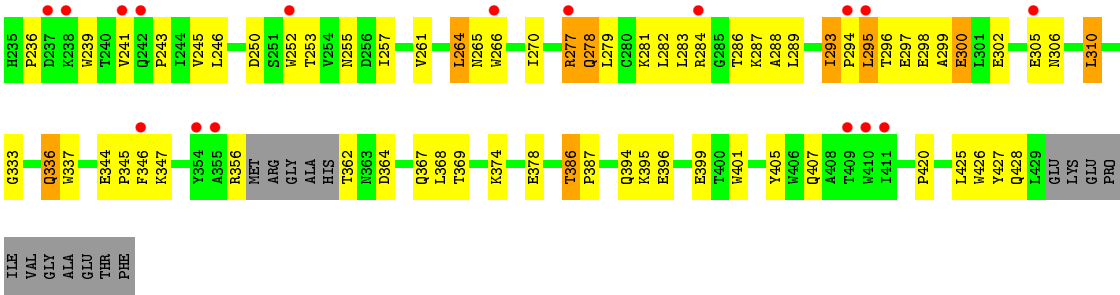
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: Reverse transcriptase



#### • Molecule 2: Reverse transcriptase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.32Å 154.70Å 154.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.50) 91.3 (29.93-2.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.28 (at 2.51Å)	Xtriage
Refinement program	CNX2005	Depositor
R, $R_{free}$	0.221 , 0.267 0.215 , 0.262	Depositor DCC
$R_{free}$ test set	2411 reflections (5.66%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 48003 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7999	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NVE, CL, MG, 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	0.37	0/4619	0.52	0/6276
2	B	0.36	0/3446	0.51	0/4683
All	All	0.36	0/8065	0.52	0/10959

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	362	THR	Peptide

### 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	4502	0	4553	166	0
2	B	3353	0	3388	97	0
3	A	37	0	33	2	0
4	A	20	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	49	0	0	3	0
7	B	35	0	0	0	0
All	All	7999	0	7974	250	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 16.

All (250) 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:459:THR:HG22	1:A:461:ARG:H	0.97	1.09
1:A:131:THR:HG22	1:A:143:ARG:HD2	1.36	1.08
1:A:459:THR:HG22	1:A:461:ARG:N	1.79	0.97
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.49	0.92
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.51	0.91
1:A:275:LYS:H	1:A:306:ASN:HD21	1.20	0.89
1:A:459:THR:CG2	1:A:461:ARG:H	1.87	0.83
1:A:131:THR:CG2	1:A:143:ARG:HD2	2.13	0.79
1:A:320:ASP:H	1:A:343:GLN:HE22	1.32	0.78
2:B:333:GLY:O	2:B:336:GLN:HG3	1.83	0.78
1:A:102:LYS:HE3	1:A:237:ASP:HB3	1.67	0.75
2:B:86:ASP:O	2:B:90:VAL:HG22	1.86	0.75
1:A:194:GLU:H	1:A:194:GLU:CD	1.89	0.74
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.32	0.74
1:A:287:LYS:HD3	1:A:291:GLU:HG2	1.67	0.73
2:B:281:LYS:O	2:B:284:ARG:HG2	1.89	0.72
1:A:25:PRO:HG3	1:A:137:ASN:ND2	2.03	0.72
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.72	0.72
2:B:425:LEU:HD12	2:B:428:GLN:NE2	2.06	0.70
1:A:460:ASN:HD22	2:B:288:ALA:HB2	1.57	0.70
2:B:5:ILE:HG22	2:B:6:GLU:H	1.57	0.69
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.91	0.69
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.91	0.69
2:B:278:GLN:HB3	2:B:298:GLU:HG3	1.73	0.69
2:B:395:LYS:O	2:B:399:GLU:HG2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:GLN:HG2	2:B:396:GLU:OE2	1.93	0.69
1:A:503:LEU:HD12	1:A:533:LEU:CD1	2.23	0.68
2:B:278:GLN:HE21	2:B:278:GLN:HA	1.56	0.68
1:A:460:ASN:ND2	2:B:288:ALA:HB2	2.09	0.67
1:A:54:ASN:ND2	1:A:56:TYR:H	1.92	0.67
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.10	0.67
1:A:57:ASN:OD1	1:A:131:THR:HG23	1.95	0.66
2:B:13:LYS:HB2	2:B:16:MET:SD	2.35	0.66
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.30	0.66
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.25	0.66
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.77	0.66
1:A:25:PRO:HG3	1:A:137:ASN:HD21	1.59	0.66
2:B:306:ASN:O	2:B:310:LEU:HD22	1.96	0.65
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.31	0.65
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.46	0.64
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.79	0.63
1:A:536:VAL:HG11	1:A:542:ILE:HG21	1.81	0.63
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.80	0.63
1:A:380:ILE:HD12	2:B:27:THR:HG22	1.80	0.63
1:A:406:TRP:HD1	1:A:407:GLN:HE21	1.47	0.63
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.14	0.62
1:A:424:LYS:HD2	1:A:426:TRP:CE2	2.34	0.62
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.64	0.62
2:B:175:ASN:HD21	2:B:201:LYS:HZ3	1.47	0.62
1:A:536:VAL:HG13	1:A:537:PRO:HD2	1.82	0.61
2:B:5:ILE:HG22	2:B:6:GLU:N	2.15	0.61
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.36	0.61
1:A:94:ILE:HD13	1:A:230:MET:CE	2.31	0.61
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.83	0.61
1:A:103:LYS:HE3	1:A:179:VAL:HG21	1.82	0.60
2:B:241:VAL:O	2:B:243:PRO:HD3	2.02	0.60
1:A:223:LYS:HD3	1:A:224:GLU:H	1.65	0.60
1:A:260:LEU:HD22	1:A:264:LEU:HD22	1.84	0.60
2:B:253:THR:O	2:B:257:ILE:HG12	2.02	0.60
1:A:27:THR:HG22	1:A:29:GLU:H	1.66	0.60
1:A:139:THR:OG1	1:A:140:PRO:HD2	2.01	0.59
2:B:344:GLU:HG2	2:B:347:LYS:HE3	1.83	0.59
1:A:94:ILE:HD13	1:A:230:MET:HE2	1.84	0.59
2:B:295:LEU:HD23	2:B:295:LEU:N	2.18	0.59
1:A:334:GLN:NE2	7:A:735:HOH:O	2.34	0.59
1:A:320:ASP:H	1:A:343:GLN:NE2	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LYS:CD	1:A:291:GLU:HG2	2.32	0.59
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.38	0.59
2:B:66:LYS:HA	2:B:407:GLN:NE2	2.17	0.58
1:A:542:ILE:O	1:A:543:GLY:O	2.22	0.58
1:A:27:THR:HG22	1:A:28:GLU:N	2.17	0.58
1:A:545:ASN:O	1:A:549:ASP:HB2	2.04	0.58
2:B:296:THR:O	2:B:300:GLU:HB2	2.04	0.57
2:B:297:GLU:HG2	2:B:298:GLU:N	2.19	0.57
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.41	0.56
1:A:42:GLU:OE1	1:A:49:LYS:HE2	2.05	0.56
1:A:296:THR:HB	1:A:298:GLU:OE2	2.04	0.56
1:A:401:TRP:HD1	1:A:402:TRP:CD1	2.24	0.56
1:A:102:LYS:HE3	1:A:237:ASP:CB	2.34	0.56
1:A:343:GLN:CG	1:A:349:LEU:HD11	2.31	0.56
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.88	0.56
1:A:209:LEU:HD23	1:A:216:THR:HG21	1.87	0.56
1:A:27:THR:CG2	1:A:28:GLU:N	2.68	0.56
1:A:210:LEU:O	1:A:210:LEU:HD12	2.05	0.56
1:A:281:LYS:HD2	1:A:284:ARG:NH2	2.21	0.55
1:A:194:GLU:N	1:A:194:GLU:CD	2.59	0.55
1:A:54:ASN:HD22	1:A:56:TYR:H	1.54	0.55
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.71	0.55
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.42	0.55
1:A:529:GLU:O	1:A:530:LYS:HG3	2.06	0.55
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.90	0.54
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.07	0.54
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.55	0.54
1:A:401:TRP:HB2	1:A:425:LEU:HD11	1.90	0.54
1:A:254:VAL:O	1:A:258:GLN:HG3	2.07	0.54
2:B:302:GLU:HA	2:B:305:GLU:OE2	2.08	0.53
1:A:368:LEU:HD22	1:A:423:VAL:HG11	1.89	0.53
1:A:253:THR:HA	1:A:291:GLU:O	2.08	0.53
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.74	0.53
1:A:542:ILE:HD11	2:B:261:VAL:HG11	1.89	0.53
1:A:28:GLU:OE1	1:A:135:ILE:HD13	2.08	0.53
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.09	0.53
1:A:17:ASP:O	1:A:83:ARG:NE	2.39	0.53
2:B:396:GLU:N	2:B:396:GLU:OE2	2.33	0.53
2:B:84:THR:O	2:B:84:THR:HG22	2.08	0.53
2:B:296:THR:HG22	2:B:297:GLU:N	2.24	0.53
1:A:459:THR:CG2	1:A:460:ASN:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASP:OD2	1:A:323:LYS:NZ	2.40	0.52
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.33	0.52
2:B:214:LEU:HG	2:B:215:THR:N	2.25	0.52
2:B:65:LYS:HD2	2:B:72:ARG:HD2	1.92	0.52
2:B:13:LYS:HD2	2:B:16:MET:SD	2.50	0.52
1:A:95:PRO:HG2	3:A:601:NVE:H12	1.91	0.51
2:B:345:PRO:O	2:B:346:PHE:HB2	2.09	0.51
1:A:452:LEU:HD12	1:A:470:THR:HA	1.93	0.51
1:A:108:VAL:HG22	1:A:188:TYR:CE2	2.46	0.51
1:A:516:GLU:HG3	1:A:520:GLN:NE2	2.25	0.51
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.92	0.51
1:A:105:SER:O	1:A:190:GLY:HA2	2.11	0.50
1:A:454:LYS:HE3	1:A:552:VAL:O	2.12	0.50
1:A:106:VAL:HA	1:A:189:VAL:O	2.11	0.50
1:A:459:THR:HG22	1:A:460:ASN:N	2.26	0.50
1:A:66:LYS:O	1:A:67:ASP:HB3	2.12	0.50
1:A:255:ASN:O	1:A:259:LYS:HG3	2.12	0.50
1:A:107:THR:CG2	3:A:601:NVE:H33	2.41	0.50
2:B:66:LYS:HA	2:B:407:GLN:HE21	1.75	0.50
1:A:402:TRP:CD2	1:A:409:THR:HG21	2.47	0.50
1:A:400:THR:O	1:A:404:GLU:HG3	2.12	0.50
1:A:295:LEU:HD12	1:A:300:GLU:OE1	2.12	0.50
1:A:287:LYS:NZ	1:A:287:LYS:HB3	2.25	0.50
1:A:134:SER:CB	1:A:139:THR:HG23	2.42	0.49
1:A:420:PRO:HA	1:A:421:PRO:C	2.33	0.49
1:A:345:PRO:HA	1:A:346:PHE:HA	1.61	0.49
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.94	0.49
1:A:223:LYS:CD	1:A:224:GLU:H	2.25	0.49
2:B:279:LEU:HD13	2:B:282:LEU:HD12	1.94	0.49
1:A:54:ASN:HD21	1:A:56:TYR:HB2	1.78	0.48
1:A:175:ASN:OD1	1:A:201:LYS:HD2	2.13	0.48
1:A:54:ASN:O	1:A:143:ARG:NH2	2.46	0.48
1:A:27:THR:O	1:A:31:ILE:HG13	2.13	0.48
1:A:1:PRO:O	1:A:117:SER:HA	2.14	0.48
1:A:363:ASN:HA	1:A:511:ASP:CG	2.33	0.48
1:A:430:GLU:OE2	1:A:530:LYS:HG2	2.13	0.48
1:A:282:LEU:HD11	1:A:296:THR:HG23	1.96	0.48
1:A:65:LYS:HG2	1:A:66:LYS:HG2	1.95	0.48
1:A:131:THR:CG2	1:A:143:ARG:HH11	2.27	0.47
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.29	0.47
2:B:286:THR:O	2:B:286:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LYS:HE2	2:B:69:THR:HA	1.96	0.47
2:B:374:LYS:O	2:B:378:GLU:HG3	2.13	0.47
1:A:48:SER:O	1:A:144:TYR:HA	2.14	0.47
1:A:500:GLN:HE22	2:B:420:PRO:HB3	1.80	0.47
1:A:8:VAL:O	1:A:10:VAL:HG23	2.15	0.47
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.97	0.47
1:A:249:LYS:HE3	1:A:256:ASP:OD2	2.15	0.47
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.50	0.47
1:A:54:ASN:HD22	1:A:54:ASN:C	2.18	0.47
1:A:80:LEU:HD13	1:A:153:TRP:CD1	2.50	0.47
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.97	0.47
2:B:296:THR:CG2	2:B:298:GLU:HG2	2.45	0.46
2:B:7:THR:HG22	2:B:7:THR:O	2.15	0.46
2:B:90:VAL:CG2	2:B:91:GLN:N	2.78	0.46
2:B:278:GLN:NE2	2:B:278:GLN:HA	2.27	0.46
1:A:95:PRO:HB3	2:B:136:ASN:O	2.16	0.46
1:A:73:LYS:HG2	1:A:74:LEU:N	2.30	0.46
1:A:323:LYS:HG3	1:A:323:LYS:HZ2	1.55	0.46
1:A:398:TRP:CE2	1:A:402:TRP:CD1	3.04	0.46
1:A:409:THR:O	2:B:364:ASP:HB2	2.16	0.46
2:B:116:PHE:HA	2:B:148:VAL:HG21	1.97	0.46
1:A:516:GLU:HG3	1:A:520:GLN:HE21	1.80	0.46
1:A:66:LYS:C	1:A:68:SER:H	2.20	0.45
1:A:194:GLU:O	1:A:195:ILE:C	2.55	0.45
1:A:205:LEU:HD13	1:A:209:LEU:HD22	1.98	0.45
1:A:380:ILE:HD11	1:A:386:THR:CG2	2.47	0.45
1:A:395:LYS:HD2	1:A:414:TRP:CZ3	2.52	0.45
2:B:65:LYS:HE2	2:B:66:LYS:H	1.82	0.45
1:A:169:GLU:O	1:A:169:GLU:OE1	2.35	0.45
2:B:175:ASN:ND2	2:B:201:LYS:HZ2	2.15	0.44
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.53	0.44
1:A:281:LYS:O	1:A:284:ARG:HG3	2.16	0.44
2:B:293:ILE:HD13	2:B:294:PRO:N	2.32	0.44
1:A:225:PRO:HA	1:A:226:PRO:C	2.38	0.44
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.81	0.44
2:B:266:TRP:CH2	2:B:427:TYR:OH	2.71	0.44
1:A:464:GLN:OE1	1:A:551:LEU:HD11	2.18	0.44
1:A:224:GLU:HA	1:A:225:PRO:HD3	1.84	0.44
1:A:298:GLU:OE2	1:A:298:GLU:N	2.32	0.44
1:A:449:GLU:O	1:A:451:LYS:HE2	2.17	0.44
1:A:453:GLY:O	1:A:469:LEU:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:O	1:A:94:ILE:HG13	2.17	0.43
2:B:7:THR:CG2	2:B:121:ASP:HA	2.47	0.43
2:B:296:THR:CG2	2:B:297:GLU:N	2.82	0.43
1:A:336:GLN:NE2	7:A:725:HOH:O	2.50	0.43
2:B:293:ILE:HA	2:B:294:PRO:HD3	1.76	0.43
2:B:270:ILE:HG12	2:B:346:PHE:O	2.18	0.43
1:A:374:LYS:HE3	1:A:374:LYS:HB3	1.78	0.43
1:A:479:LEU:HB3	1:A:517:LEU:HD13	2.00	0.43
2:B:5:ILE:HB	2:B:119:PRO:HD2	2.00	0.43
2:B:82:LYS:HE2	2:B:82:LYS:HB2	1.66	0.43
1:A:542:ILE:HG22	1:A:543:GLY:N	2.34	0.43
2:B:206:ARG:NH2	2:B:215:THR:O	2.52	0.42
2:B:243:PRO:O	2:B:245:VAL:HG13	2.20	0.42
2:B:67:ASP:O	2:B:68:SER:HB2	2.19	0.42
1:A:198:HIS:O	1:A:202:ILE:HG12	2.19	0.42
2:B:289:LEU:HD12	2:B:289:LEU:HA	1.85	0.42
1:A:502:ALA:O	1:A:506:ILE:HG12	2.18	0.42
2:B:266:TRP:HZ3	2:B:427:TYR:HH	1.65	0.42
1:A:26:LEU:HD22	1:A:133:PRO:HG3	2.02	0.42
1:A:283:LEU:HD12	1:A:283:LEU:HA	1.81	0.42
1:A:98:ALA:HB1	1:A:349:LEU:HB3	2.01	0.42
2:B:296:THR:HG22	2:B:298:GLU:H	1.84	0.42
2:B:214:LEU:HG	2:B:215:THR:H	1.85	0.42
1:A:65:LYS:HZ2	1:A:66:LYS:HG2	1.85	0.42
2:B:386:THR:HA	2:B:387:PRO:HD3	1.82	0.42
2:B:116:PHE:CD1	2:B:116:PHE:N	2.87	0.42
1:A:331:LYS:HB3	1:A:421:PRO:HG2	2.01	0.42
2:B:293:ILE:HD13	2:B:294:PRO:O	2.20	0.42
1:A:317:VAL:CG1	1:A:318:TYR:N	2.82	0.42
1:A:424:LYS:HD2	1:A:426:TRP:CZ2	2.54	0.42
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.18	0.42
2:B:232:TYR:N	2:B:232:TYR:CD2	2.88	0.42
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.55	0.41
2:B:32:LYS:HD3	2:B:32:LYS:HA	1.72	0.41
1:A:234:LEU:HD23	1:A:239:TRP:HB2	2.02	0.41
1:A:540:LYS:HE2	2:B:265:ASN:OD1	2.20	0.41
2:B:266:TRP:CD1	2:B:426:TRP:CZ3	3.08	0.41
1:A:88:TRP:CZ2	1:A:92:LEU:HD21	2.55	0.41
2:B:105:SER:O	2:B:190:GLY:HA2	2.20	0.41
2:B:298:GLU:CG	2:B:299:ALA:N	2.84	0.41
2:B:157:PRO:HG3	2:B:184:MET:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:THR:HG22	1:A:366:LYS:HD2	2.02	0.41
1:A:94:ILE:CD1	1:A:230:MET:HE2	2.50	0.41
2:B:293:ILE:C	2:B:293:ILE:HD13	2.41	0.41
2:B:252:TRP:HB3	2:B:257:ILE:HD11	2.01	0.41
1:A:209:LEU:HA	1:A:209:LEU:HD12	1.90	0.41
1:A:88:TRP:CZ3	2:B:57:ASN:HB2	2.54	0.41
2:B:246:LEU:HD11	2:B:264:LEU:HD11	2.01	0.41
2:B:13:LYS:CE	2:B:85:GLN:HB3	2.51	0.41
1:A:260:LEU:HD22	1:A:264:LEU:CD2	2.50	0.41
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.93	0.41
1:A:31:ILE:O	1:A:35:VAL:HG23	2.21	0.41
1:A:211:ARG:NH2	7:A:734:HOH:O	2.54	0.41
1:A:519:ASN:O	1:A:523:GLU:HG2	2.21	0.41
2:B:277:ARG:O	2:B:281:LYS:HG3	2.21	0.41
1:A:433:PRO:CG	2:B:255:ASN:ND2	2.84	0.41
1:A:257:ILE:O	1:A:261:VAL:HG23	2.21	0.40
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.21	0.40
2:B:283:LEU:O	2:B:284:ARG:C	2.60	0.40
2:B:203:GLU:HA	2:B:203:GLU:OE2	2.22	0.40
1:A:246:LEU:HD11	1:A:310:LEU:HD12	2.04	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	550/560 (98%)	528 (96%)	19 (4%)	3 (0%)	34	55
2	B	399/440 (91%)	377 (94%)	20 (5%)	2 (0%)	34	55
All	All	949/1000 (95%)	905 (95%)	39 (4%)	5 (0%)	34	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	543	GLY
2	B	66	LYS
2	B	68	SER
1	A	90	VAL
1	A	410	TRP

### 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	494/500 (99%)	455 (92%)	39 (8%)	15	28
2	B	370/400 (92%)	346 (94%)	24 (6%)	21	39
All	All	864/900 (96%)	801 (93%)	63 (7%)	17	32

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	28	GLU
1	A	54	ASN
1	A	58	THR
1	A	80	LEU
1	A	92	LEU
1	A	101	LYS
1	A	122	GLU
1	A	126	LYS
1	A	161	GLN
1	A	168	LEU
1	A	187	LEU
1	A	207	GLN
1	A	209	LEU
1	A	214	LEU
1	A	219	LYS
1	A	248	GLU
1	A	260	LEU
1	A	264	LEU

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Mol	Chain	Res	Type
1	A	282	LEU
1	A	283	LEU
1	A	287	LYS
1	A	301	LEU
1	A	324	ASP
1	A	334	GLN
1	A	340	GLN
1	A	357	MET
1	A	362	THR
1	A	374	LYS
1	A	388	LYS
1	A	423	VAL
1	A	424	LYS
1	A	451	LYS
1	A	476	LYS
1	A	500	GLN
1	A	517	LEU
1	A	529	GLU
1	A	533	LEU
1	A	551	LEU
2	B	7	THR
2	B	8	VAL
2	B	65	LYS
2	B	80	LEU
2	B	82	LYS
2	B	90	VAL
2	B	102	LYS
2	B	193	LEU
2	B	205	LEU
2	B	209	LEU
2	B	234	LEU
2	B	250	ASP
2	B	264	LEU
2	B	277	ARG
2	B	278	GLN
2	B	287	LYS
2	B	293	ILE
2	B	295	LEU
2	B	300	GLU
2	B	310	LEU
2	B	336	GLN
2	B	356	ARG

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Mol	Chain	Res	Type
2	B	368	LEU
2	B	386	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	137	ASN
1	A	207	GLN
1	A	258	GLN
1	A	306	ASN
1	A	336	GLN
1	A	340	GLN
1	A	343	GLN
1	A	373	GLN
1	A	407	GLN
1	A	475	GLN
1	A	500	GLN
1	A	520	GLN
2	B	147	ASN
2	B	161	GLN
2	B	175	ASN
2	B	182	GLN
2	B	242	GLN
2	B	258	GLN
2	B	278	GLN
2	B	334	GLN
2	B	336	GLN
2	B	348	ASN
2	B	367	GLN
2	B	407	GLN
2	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	NVE	A	601	-	32,40,40	2.74	19 (59%)	35,56,56	2.25	11 (31%)
4	SO4	A	602	-	4,4,4	0.22	0	6,6,6	0.12	0
4	SO4	A	603	-	4,4,4	0.26	0	6,6,6	0.20	0
4	SO4	A	604	-	4,4,4	0.24	0	6,6,6	0.10	0
4	SO4	A	605	-	4,4,4	0.23	0	6,6,6	0.08	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
3	NVE	A	601	-	-	0/19/21/21	0/3/4/4
4	SO4	A	602	-	-	0/0/0/0	0/0/0/0
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0
4	SO4	A	604	-	-	0/0/0/0	0/0/0/0
4	SO4	A	605	-	-	0/0/0/0	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NVE	C27-C28	2.02	1.42	1.38
3	A	601	NVE	C7-N6	2.08	1.51	1.47
3	A	601	NVE	C17-C18	2.15	1.44	1.37
3	A	601	NVE	C16-C5	2.30	1.45	1.41
3	A	601	NVE	C17-C16	2.48	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NVE	C13-N14	2.66	1.36	1.31
3	A	601	NVE	P23-O34	2.85	1.64	1.57
3	A	601	NVE	C27-C26	3.06	1.44	1.38
3	A	601	NVE	C4-N19	3.06	1.40	1.35
3	A	601	NVE	C33-C12	3.19	1.60	1.51
3	A	601	NVE	C31-C30	3.52	1.45	1.38
3	A	601	NVE	C30-C29	3.54	1.46	1.38
3	A	601	NVE	C18-N19	3.63	1.39	1.32
3	A	601	NVE	C11-C12	3.88	1.46	1.37
3	A	601	NVE	C15-N14	3.88	1.41	1.35
3	A	601	NVE	P23-O22	3.89	1.66	1.57
3	A	601	NVE	C28-C29	4.36	1.48	1.38
3	A	601	NVE	C10-C15	5.25	1.45	1.40
3	A	601	NVE	C31-C26	5.29	1.49	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NVE	C33-C12-C13	-4.58	114.08	121.85
3	A	601	NVE	C10-C15-N14	-3.99	118.78	123.53
3	A	601	NVE	C12-C13-N14	-2.97	118.78	123.82
3	A	601	NVE	C17-C18-N19	-2.59	119.88	123.94
3	A	601	NVE	P23-O34-C35	-2.55	113.18	122.21
3	A	601	NVE	O34-P23-C24	2.28	112.36	104.22
3	A	601	NVE	C11-C12-C13	2.77	119.50	116.58
3	A	601	NVE	C33-C12-C11	3.16	126.42	120.78
3	A	601	NVE	C1-C2-N3	3.26	118.67	111.70
3	A	601	NVE	C18-N19-C4	5.08	123.24	116.93
3	A	601	NVE	C13-N14-C15	6.03	124.85	116.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NVE	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	552/560 (98%)	0.30	28 (5%)	32 36	34, 59, 89, 113	0
2	B	405/440 (92%)	0.44	46 (11%)	7 6	35, 58, 101, 117	0
All	All	957/1000 (95%)	0.36	74 (7%)	16 18	34, 59, 96, 117	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	67	ASP	6.8
2	B	66	LYS	6.4
2	B	70	LYS	5.7
2	B	14	PRO	5.7
2	B	68	SER	5.5
1	A	70	LYS	5.1
1	A	65	LYS	4.6
2	B	69	THR	4.5
2	B	409	THR	4.4
1	A	67	ASP	4.4
2	B	90	VAL	4.3
2	B	232	TYR	4.1
2	B	284	ARG	4.0
2	B	65	LYS	4.0
2	B	216	THR	3.9
1	A	66	LYS	3.6
1	A	357	MET	3.6
1	A	69	THR	3.5
1	A	445	ALA	3.4
1	A	286	THR	3.3
2	B	183	TYR	3.2
1	A	446	ALA	3.2
2	B	305	GLU	3.2
2	B	277	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	13	LYS	3.1
2	B	411	ILE	3.1
2	B	184	MET	3.1
2	B	242	GLN	3.1
1	A	284	ARG	2.9
2	B	252	TRP	2.9
2	B	410	TRP	2.9
1	A	68	SER	2.8
1	A	53	GLU	2.7
1	A	497	THR	2.6
2	B	43	LYS	2.6
1	A	448	ARG	2.5
2	B	215	THR	2.4
2	B	355	ALA	2.4
2	B	15	GLY	2.4
2	B	185	ASP	2.4
2	B	153	TRP	2.3
2	B	238	LYS	2.3
2	B	6	GLU	2.3
2	B	12	LEU	2.3
1	A	360	ALA	2.3
2	B	156	SER	2.3
1	A	534	ALA	2.3
2	B	5	ILE	2.3
2	B	152	GLY	2.3
2	B	266	TRP	2.3
1	A	221	HIS	2.2
2	B	295	LEU	2.2
2	B	346	PHE	2.2
2	B	294	PRO	2.2
1	A	193	LEU	2.2
2	B	354	TYR	2.2
2	B	89	GLU	2.2
1	A	470	THR	2.2
1	A	192	ASP	2.2
2	B	86	ASP	2.1
1	A	22	LYS	2.1
1	A	64	LYS	2.1
2	B	237	ASP	2.1
1	A	245	VAL	2.1
2	B	186	ASP	2.1
2	B	241	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	506	ILE	2.1
2	B	112	GLY	2.1
2	B	11	LYS	2.1
2	B	151	GLN	2.1
1	A	514	GLU	2.1
1	A	496	VAL	2.0
1	A	472	THR	2.0
1	A	550	LYS	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	NVE	A	601	37/37	0.94	0.19	0.48	37,45,67,68	0
4	SO4	A	602	5/5	0.92	0.15	-0.11	94,96,96,96	0
4	SO4	A	603	5/5	0.95	0.12	-0.62	75,78,79,79	0
4	SO4	A	605	5/5	0.92	0.13	-0.87	119,119,119,120	0
6	CL	A	607	1/1	0.88	0.25	-	94,94,94,94	0
4	SO4	A	604	5/5	0.91	0.17	-	119,119,119,120	0
6	CL	B	501	1/1	0.82	0.14	-	68,68,68,68	0
5	MG	A	606	1/1	0.92	0.24	-	77,77,77,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.