



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:41 pm GMT

PDB ID : 2P6U  
Title : Apo structure of the Hel308 superfamily 2 helicase  
Authors : Buettner, K.; Nehring, S.; Hopfner, K.P.  
Deposited on : 2007-03-19  
Resolution : 3.14 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

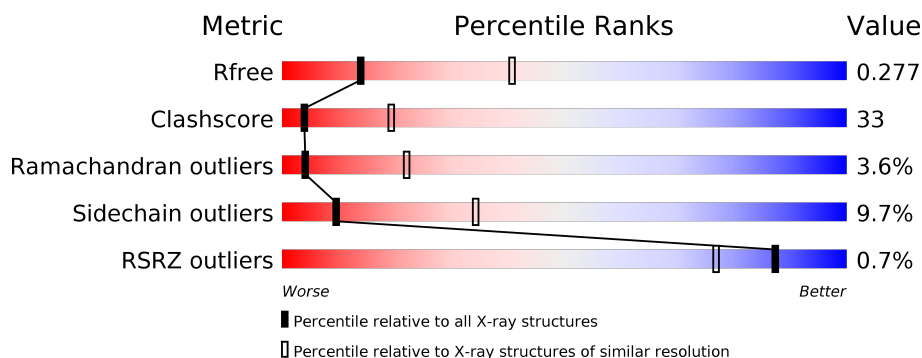
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.14 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	1234 (3.18-3.10)
Clashscore	112137	1345 (3.18-3.10)
Ramachandran outliers	110173	1301 (3.18-3.10)
Sidechain outliers	110143	1301 (3.18-3.10)
RSRZ outliers	101464	1240 (3.18-3.10)

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	702	<div> <div></div> <div>44%</div> <div>45%</div> <div>6%</div> <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
2	PO4	A	703	-	-	-	X
2	PO4	A	704	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	706	-	-	-	X
2	PO4	A	708	-	-	-	X
2	PO4	A	709	-	-	X	-
2	PO4	A	710	-	-	-	X
2	PO4	A	712	-	-	-	X

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5368 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 afuHEL308 HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	671	5318	3364	940	992	22	158	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

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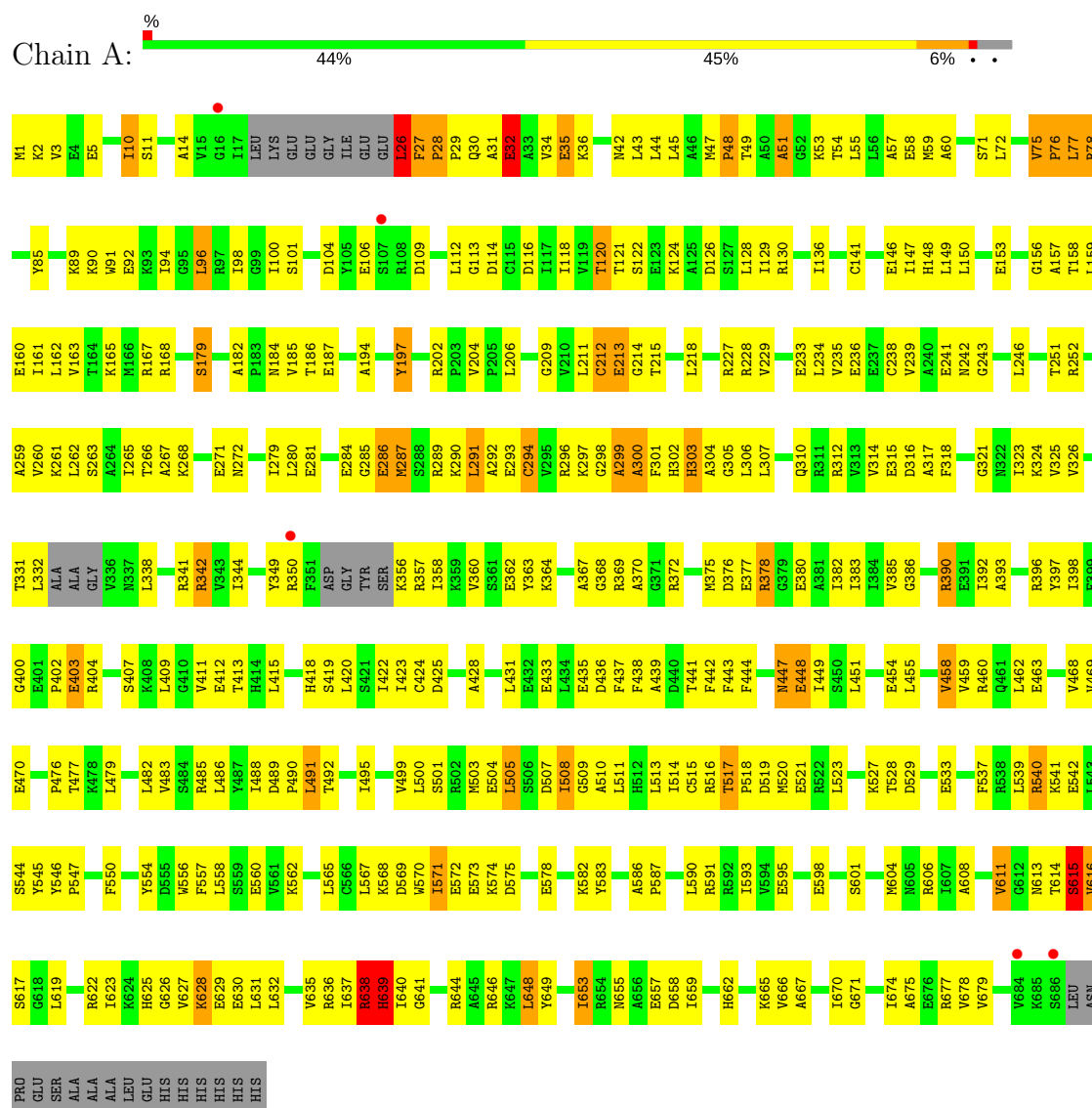
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

### 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: afuHEL308 HELICASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.15Å 136.15Å 230.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.14 19.90 – 3.14	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-3.14) 98.2 (19.90-3.14)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 3.15Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.230 , 0.276 0.234 , 0.277	Depositor DCC
$R_{free}$ test set	1082 reflections (4.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.5	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 60.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.41	0/5400	0.66	2/7271 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	638	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	A	26	LEU	CA-CB-CG	5.66	128.32	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	TYR	Sidechain

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5318	0	5420	347	0
2	A	50	0	0	15	0
All	All	5368	0	5420	347	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 33.

All (347) 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:441:THR:HG22	1:A:443:PHE:H	1.13	1.05
1:A:674:ILE:HD12	1:A:674:ILE:H	1.27	1.00
1:A:78:ARG:HD2	1:A:78:ARG:H	1.25	1.00
1:A:307:LEU:HD11	1:A:587:PRO:HB2	1.45	0.98
1:A:631:LEU:HD11	1:A:646:ARG:NH1	1.84	0.92
1:A:252:ARG:HH11	1:A:304:ALA:HB3	1.34	0.91
1:A:674:ILE:O	1:A:678:VAL:HG23	1.71	0.90
1:A:78:ARG:CD	1:A:78:ARG:H	1.84	0.90
1:A:571:ILE:HD11	1:A:623:ILE:HA	1.53	0.90
1:A:545:TYR:HE1	1:A:547:PRO:HG3	1.35	0.90
1:A:622:ARG:CD	1:A:628:LYS:O	2.21	0.89
1:A:262:LEU:HD13	1:A:325:VAL:HG11	1.56	0.87
1:A:285:GLY:HA2	1:A:289:ARG:HH11	1.41	0.86
1:A:26:LEU:HD21	1:A:55:LEU:HD22	1.62	0.81
1:A:272:ASN:O	1:A:296:ARG:HA	1.81	0.80
1:A:279:ILE:HD12	1:A:292:ALA:HA	1.63	0.80
1:A:630:GLU:HG3	1:A:631:LEU:HD12	1.64	0.80
1:A:78:ARG:HD2	1:A:78:ARG:N	1.98	0.79
1:A:11:SER:HB3	1:A:59:MET:HE2	1.65	0.79
1:A:655:ASN:O	1:A:659:ILE:HG13	1.83	0.77
1:A:505:LEU:HD12	1:A:510:ALA:HA	1.66	0.77
1:A:504:GLU:O	1:A:504:GLU:HG3	1.83	0.77
1:A:638:ARG:HG3	2:A:709:PO4:O4	1.84	0.76
1:A:639:HIS:O	2:A:709:PO4:O4	2.02	0.76
1:A:234:LEU:CD2	1:A:342:ARG:HH11	1.98	0.76
1:A:545:TYR:CE1	1:A:547:PRO:HG3	2.18	0.75
1:A:431:LEU:O	1:A:435:GLU:HG3	1.85	0.75
1:A:571:ILE:HD11	1:A:623:ILE:CA	2.17	0.74
1:A:49:THR:HG22	1:A:51:ALA:H	1.52	0.74
1:A:571:ILE:CD1	1:A:623:ILE:HA	2.18	0.73
1:A:146:GLU:HG2	1:A:148:HIS:CE1	2.23	0.73
1:A:266:THR:HG22	1:A:324:LYS:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:HG2	1:A:148:HIS:HE1	1.52	0.73
1:A:218:LEU:HD11	1:A:380:GLU:OE1	1.88	0.73
1:A:285:GLY:HA2	1:A:289:ARG:NH1	2.03	0.72
1:A:622:ARG:HD3	1:A:628:LYS:O	1.87	0.72
1:A:529:ASP:OD1	1:A:562:LYS:NZ	2.18	0.72
1:A:482:LEU:O	1:A:486:LEU:HD13	1.90	0.71
1:A:26:LEU:HD21	1:A:55:LEU:CD2	2.21	0.71
1:A:235:VAL:HG11	1:A:262:LEU:HD22	1.72	0.70
1:A:163:VAL:O	1:A:167:ARG:HG3	1.91	0.70
1:A:298:GLY:O	1:A:323:ILE:HG23	1.92	0.70
1:A:653:ILE:HD11	1:A:665:LYS:HD3	1.74	0.69
1:A:441:THR:HG22	1:A:443:PHE:N	1.98	0.69
1:A:101:SER:HB2	1:A:112:LEU:HD11	1.74	0.68
1:A:641:GLY:HA3	2:A:704:PO4:P	2.33	0.68
1:A:57:ALA:O	1:A:60:ALA:HB3	1.94	0.68
1:A:632:LEU:O	1:A:636:ARG:HG3	1.94	0.68
1:A:622:ARG:HD2	1:A:628:LYS:O	1.94	0.67
1:A:318:PHE:CD2	1:A:326:VAL:HG23	2.29	0.67
1:A:48:PRO:HG2	1:A:49:THR:H	1.58	0.67
1:A:409:LEU:HD22	1:A:441:THR:HG21	1.76	0.66
1:A:3:VAL:HG12	1:A:34:VAL:HG12	1.77	0.66
1:A:280:LEU:HG	1:A:284:GLU:HG2	1.76	0.66
1:A:349:TYR:HE2	1:A:357:ARG:HH11	1.44	0.66
1:A:640:ILE:HA	2:A:709:PO4:P	2.35	0.66
1:A:627:VAL:HG11	1:A:635:VAL:HG11	1.78	0.66
1:A:124:LYS:O	1:A:128:LEU:HD12	1.95	0.65
1:A:106:GLU:OE2	1:A:606:ARG:NH2	2.29	0.65
1:A:287:MET:HE3	1:A:586:ALA:HB1	1.77	0.65
1:A:619:LEU:O	1:A:623:ILE:HG12	1.97	0.64
1:A:372:ARG:HH21	1:A:375:MET:HB3	1.62	0.64
1:A:441:THR:HG22	1:A:442:PHE:N	2.13	0.64
1:A:209:GLY:O	1:A:382:ILE:HA	1.97	0.64
1:A:42:ASN:HB3	1:A:194:ALA:HB2	1.80	0.64
1:A:89:LYS:O	1:A:92:GLU:HG3	1.98	0.64
1:A:447:ASN:O	1:A:449:ILE:HG13	1.99	0.62
1:A:655:ASN:HD21	1:A:657:GLU:HB3	1.63	0.62
1:A:488:ILE:HD12	1:A:492:THR:HG22	1.81	0.62
1:A:571:ILE:HG23	1:A:622:ARG:NH1	2.13	0.62
1:A:515:CYS:O	1:A:560:GLU:HG2	1.98	0.62
1:A:639:HIS:O	2:A:709:PO4:P	2.57	0.62
1:A:267:ALA:HB2	1:A:297:LYS:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:HD23	1:A:342:ARG:HH11	1.65	0.62
1:A:608:ALA:O	1:A:611:VAL:HG12	2.00	0.62
1:A:638:ARG:NH2	1:A:677:ARG:NH2	2.48	0.61
1:A:147:ILE:HG22	1:A:179:SER:HB3	1.81	0.61
1:A:571:ILE:HD11	1:A:623:ILE:N	2.15	0.61
1:A:489:ASP:O	1:A:492:THR:HB	2.01	0.61
1:A:418:HIS:O	1:A:422:ILE:HG13	2.00	0.60
1:A:500:LEU:HD13	1:A:608:ALA:HB2	1.82	0.60
1:A:360:VAL:HB	1:A:403:GLU:OE2	2.01	0.60
1:A:302:HIS:HE1	1:A:315:GLU:OE1	1.85	0.60
1:A:501:SER:CB	1:A:611:VAL:HG21	2.32	0.60
1:A:537:PHE:O	1:A:540:ARG:HG2	2.00	0.60
1:A:263:SER:HA	1:A:266:THR:OG1	2.02	0.59
1:A:291:LEU:HD11	1:A:306:LEU:HD13	1.84	0.59
1:A:94:ILE:O	1:A:94:ILE:HG22	2.02	0.59
1:A:332:LEU:HD21	1:A:338:LEU:HD12	1.84	0.59
1:A:653:ILE:CG2	1:A:659:ILE:HA	2.32	0.59
1:A:85:TYR:CE2	1:A:89:LYS:HE3	2.37	0.59
1:A:411:VAL:O	1:A:415:LEU:HG	2.02	0.59
1:A:363:TYR:CE1	1:A:383:ILE:HD11	2.38	0.59
1:A:591:ARG:HG2	1:A:591:ARG:HH21	1.67	0.59
1:A:501:SER:HB3	1:A:611:VAL:HG21	1.84	0.58
1:A:32:GLU:O	1:A:36:LYS:HG3	2.04	0.58
1:A:150:LEU:HD11	1:A:160:GLU:HG2	1.86	0.58
1:A:505:LEU:CD1	1:A:510:ALA:HA	2.33	0.58
1:A:671:GLY:O	1:A:675:ALA:HB2	2.04	0.57
1:A:463:GLU:OE1	1:A:470:GLU:HB2	2.05	0.57
1:A:511:LEU:HD13	1:A:567:LEU:HB2	1.87	0.57
1:A:469:VAL:HG13	1:A:477:THR:HG22	1.87	0.56
1:A:639:HIS:O	2:A:709:PO4:O3	2.23	0.56
1:A:505:LEU:HD12	1:A:510:ALA:CA	2.34	0.56
1:A:85:TYR:CD1	1:A:100:ILE:HB	2.39	0.56
1:A:184:ASN:HB2	1:A:187:GLU:OE2	2.04	0.56
1:A:409:LEU:CD2	1:A:441:THR:HG21	2.35	0.56
1:A:638:ARG:HG3	1:A:638:ARG:O	2.06	0.56
1:A:259:ALA:CB	1:A:301:PHE:HB3	2.36	0.56
1:A:462:LEU:HB3	1:A:468:VAL:CG2	2.35	0.56
1:A:289:ARG:HG2	1:A:289:ARG:HH21	1.71	0.56
1:A:638:ARG:HH22	1:A:677:ARG:HH22	1.52	0.56
1:A:640:ILE:HG22	1:A:644:ARG:HB2	1.87	0.56
1:A:444:PHE:CD1	1:A:448:GLU:HA	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ILE:N	1:A:98:ILE:HD12	2.22	0.55
1:A:372:ARG:HB3	1:A:376:ASP:HB2	1.89	0.55
1:A:500:LEU:HD13	1:A:608:ALA:CB	2.36	0.55
1:A:310:GLN:O	1:A:314:VAL:HG23	2.07	0.55
1:A:491:LEU:O	1:A:495:ILE:HG13	2.06	0.55
1:A:182:ALA:O	1:A:185:VAL:HG13	2.06	0.55
1:A:562:LYS:HE3	1:A:583:TYR:HD1	1.71	0.55
1:A:492:THR:OG1	1:A:518:PRO:HD2	2.07	0.55
1:A:168:ARG:NH1	1:A:437:PHE:HA	2.22	0.54
1:A:47:MET:HB3	1:A:48:PRO:HD2	1.90	0.54
1:A:653:ILE:HG21	1:A:659:ILE:HA	1.89	0.54
1:A:635:VAL:O	1:A:639:HIS:HA	2.07	0.54
1:A:317:ALA:HB3	1:A:323:ILE:HD12	1.89	0.54
1:A:393:ALA:O	1:A:398:ILE:HG13	2.08	0.54
1:A:211:LEU:HD23	1:A:211:LEU:C	2.28	0.54
1:A:235:VAL:O	1:A:239:VAL:HG23	2.08	0.54
1:A:517:THR:HG23	1:A:519:ASP:H	1.73	0.54
1:A:109:ASP:HB3	1:A:112:LEU:HD12	1.89	0.53
1:A:266:THR:CG2	1:A:324:LYS:HB2	2.38	0.53
1:A:505:LEU:HD13	1:A:509:GLY:O	2.07	0.53
1:A:637:ILE:HB	1:A:640:ILE:HD11	1.90	0.53
1:A:540:ARG:HG2	1:A:540:ARG:HH11	1.73	0.53
1:A:112:LEU:O	1:A:114:ASP:N	2.41	0.53
1:A:420:LEU:CD2	1:A:490:PRO:HB3	2.39	0.53
1:A:31:ALA:O	1:A:32:GLU:C	2.47	0.53
1:A:630:GLU:HG3	1:A:631:LEU:CD1	2.37	0.53
1:A:204:VAL:HG13	1:A:378:ARG:H	1.73	0.53
1:A:42:ASN:C	1:A:194:ALA:HB1	2.29	0.53
1:A:11:SER:HB3	1:A:59:MET:CE	2.38	0.52
1:A:420:LEU:HD22	1:A:490:PRO:HB3	1.91	0.52
1:A:479:LEU:O	1:A:483:VAL:HG23	2.08	0.52
1:A:129:ILE:HG12	1:A:136:ILE:HD13	1.91	0.52
1:A:565:LEU:O	1:A:568:LYS:HB3	2.10	0.52
1:A:540:ARG:C	1:A:542:GLU:H	2.11	0.52
1:A:505:LEU:O	1:A:615:SER:HB2	2.08	0.52
1:A:299:ALA:O	1:A:300:ALA:HB2	2.10	0.52
1:A:43:LEU:HA	1:A:194:ALA:HB1	1.92	0.52
1:A:586:ALA:HB1	1:A:587:PRO:HD2	1.90	0.52
1:A:215:THR:HA	1:A:227:ARG:O	2.09	0.52
1:A:420:LEU:HD12	1:A:424:CYS:HG	1.75	0.52
1:A:377:GLU:O	1:A:378:ARG:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:HIS:CD2	1:A:305:GLY:H	2.27	0.52
1:A:454:GLU:H	1:A:454:GLU:CD	2.14	0.52
1:A:252:ARG:NH1	1:A:304:ALA:HB3	2.16	0.51
1:A:571:ILE:HG23	1:A:622:ARG:HH12	1.74	0.51
1:A:640:ILE:HG23	2:A:709:PO4:O1	2.10	0.51
1:A:441:THR:CG2	1:A:442:PHE:N	2.74	0.51
1:A:625:HIS:HE2	2:A:710:PO4:P	2.34	0.51
1:A:377:GLU:O	1:A:378:ARG:HB2	2.11	0.51
1:A:43:LEU:HD11	1:A:45:LEU:CD2	2.40	0.51
1:A:77:LEU:HD23	1:A:77:LEU:N	2.24	0.51
1:A:147:ILE:CG2	1:A:179:SER:HB3	2.41	0.51
1:A:3:VAL:CG1	1:A:34:VAL:HG12	2.40	0.51
1:A:412:GLU:O	1:A:415:LEU:HB2	2.11	0.51
1:A:85:TYR:CE1	1:A:98:ILE:HG22	2.45	0.51
1:A:75:VAL:O	1:A:121:THR:HA	2.10	0.51
1:A:638:ARG:CG	1:A:638:ARG:O	2.59	0.51
1:A:211:LEU:HD12	1:A:234:LEU:HD11	1.93	0.51
1:A:407:SER:HB2	1:A:442:PHE:HD2	1.76	0.50
1:A:520:MET:HG3	1:A:521:GLU:O	2.11	0.50
1:A:331:THR:OG1	2:A:712:PO4:O2	2.20	0.50
1:A:396:ARG:O	1:A:400:GLY:HA3	2.11	0.50
1:A:54:THR:HG22	1:A:58:GLU:OE2	2.11	0.50
1:A:638:ARG:CG	2:A:709:PO4:O4	2.58	0.50
1:A:265:ILE:HA	1:A:268:LYS:HE2	1.93	0.50
1:A:91:TRP:HE3	1:A:94:ILE:HD12	1.77	0.50
1:A:259:ALA:HB2	1:A:301:PHE:HB3	1.92	0.50
1:A:317:ALA:HB1	1:A:323:ILE:HG13	1.93	0.50
1:A:31:ALA:HB1	1:A:35:GLU:OE2	2.12	0.50
1:A:291:LEU:HD12	1:A:306:LEU:HD22	1.94	0.50
1:A:42:ASN:CB	1:A:194:ALA:HB2	2.40	0.50
1:A:184:ASN:O	1:A:187:GLU:HG2	2.12	0.50
1:A:243:GLY:O	1:A:372:ARG:NE	2.40	0.50
1:A:460:ARG:O	1:A:463:GLU:HB2	2.12	0.50
1:A:214:GLY:O	1:A:228:ARG:HA	2.12	0.50
1:A:29:PRO:HG2	1:A:30:GLN:H	1.77	0.49
1:A:47:MET:HB2	1:A:53:LYS:HD3	1.94	0.49
1:A:104:ASP:O	1:A:124:LYS:NZ	2.34	0.49
1:A:94:ILE:CG2	1:A:94:ILE:O	2.59	0.49
1:A:148:HIS:C	1:A:150:LEU:H	2.14	0.49
1:A:265:ILE:O	1:A:268:LYS:HG2	2.12	0.49
1:A:262:LEU:CD1	1:A:325:VAL:HG11	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:CYS:SG	1:A:386:GLY:O	2.70	0.49
1:A:504:GLU:HB2	1:A:615:SER:OG	2.12	0.49
1:A:675:ALA:O	1:A:679:VAL:HG23	2.13	0.49
1:A:491:LEU:HD13	1:A:495:ILE:HD11	1.94	0.49
1:A:212:CYS:O	1:A:213:GLU:C	2.51	0.48
1:A:238:CYS:HB2	1:A:342:ARG:HD3	1.95	0.48
1:A:72:LEU:HD12	1:A:118:ILE:O	2.13	0.48
1:A:10:ILE:HG22	1:A:11:SER:N	2.27	0.48
1:A:393:ALA:HA	1:A:397:TYR:HD2	1.78	0.48
1:A:415:LEU:O	1:A:419:SER:OG	2.22	0.48
1:A:234:LEU:HD23	1:A:342:ARG:NH1	2.28	0.48
1:A:483:VAL:HG11	1:A:490:PRO:HA	1.96	0.48
1:A:655:ASN:OD1	1:A:658:ASP:OD1	2.31	0.48
1:A:516:ARG:HA	1:A:560:GLU:OE1	2.13	0.48
1:A:523:LEU:N	1:A:523:LEU:HD12	2.28	0.48
1:A:227:ARG:HG2	1:A:228:ARG:N	2.28	0.48
1:A:241:GLU:O	1:A:242:ASN:HB3	2.13	0.48
1:A:604:MET:CE	1:A:616:VAL:HG11	2.44	0.48
1:A:640:ILE:HA	2:A:709:PO4:O1	2.14	0.48
1:A:14:ALA:HB1	1:A:90:LYS:CG	2.44	0.48
1:A:499:VAL:O	1:A:503:MET:HG2	2.14	0.48
1:A:638:ARG:O	1:A:639:HIS:O	2.32	0.47
1:A:341:ARG:HB2	1:A:376:ASP:OD1	2.14	0.47
1:A:428:ALA:HA	1:A:433:GLU:HG3	1.95	0.47
1:A:126:ASP:HA	1:A:129:ILE:HD12	1.97	0.47
1:A:147:ILE:O	1:A:150:LEU:HB2	2.15	0.47
1:A:76:PRO:HG2	1:A:77:LEU:H	1.80	0.47
1:A:363:TYR:CZ	1:A:383:ILE:HD11	2.50	0.47
1:A:671:GLY:O	1:A:675:ALA:CB	2.61	0.47
1:A:570:TRP:CE2	1:A:626:GLY:HA3	2.49	0.47
1:A:648:LEU:O	1:A:653:ILE:O	2.33	0.47
1:A:674:ILE:H	1:A:674:ILE:CD1	2.03	0.47
1:A:523:LEU:HD11	1:A:593:ILE:HD13	1.97	0.46
1:A:43:LEU:CA	1:A:194:ALA:HB1	2.45	0.46
1:A:382:ILE:HD12	1:A:382:ILE:N	2.30	0.46
1:A:571:ILE:HG13	1:A:622:ARG:HB3	1.97	0.46
1:A:266:THR:HB	1:A:298:GLY:HA3	1.97	0.46
1:A:85:TYR:HB2	1:A:100:ILE:HD12	1.96	0.46
1:A:444:PHE:CE1	1:A:448:GLU:HA	2.51	0.46
1:A:517:THR:HG23	1:A:519:ASP:N	2.31	0.46
1:A:591:ARG:NH2	1:A:591:ARG:HG2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:GLU:HB2	1:A:649:TYR:CZ	2.51	0.46
1:A:236:GLU:HA	1:A:239:VAL:HB	1.97	0.46
1:A:2:LYS:HD2	1:A:5:GLU:HG2	1.98	0.46
1:A:631:LEU:HD11	1:A:646:ARG:CZ	2.44	0.45
1:A:458:VAL:HG12	1:A:459:VAL:N	2.31	0.45
1:A:667:ALA:HA	1:A:675:ALA:HB2	1.97	0.45
1:A:211:LEU:HD12	1:A:234:LEU:CD1	2.46	0.45
1:A:43:LEU:HD11	1:A:45:LEU:HD21	1.99	0.45
1:A:631:LEU:HD12	1:A:631:LEU:N	2.31	0.45
1:A:463:GLU:HA	1:A:468:VAL:O	2.16	0.45
1:A:5:GLU:HA	1:A:5:GLU:OE1	2.16	0.45
1:A:14:ALA:HB1	1:A:90:LYS:HG3	1.99	0.45
1:A:307:LEU:HD23	1:A:591:ARG:HE	1.82	0.45
1:A:539:LEU:C	1:A:540:ARG:O	2.54	0.45
1:A:508:ILE:HD11	1:A:565:LEU:HD23	1.99	0.45
1:A:500:LEU:HD13	1:A:608:ALA:HA	1.99	0.45
1:A:637:ILE:C	1:A:639:HIS:N	2.70	0.45
1:A:533:GLU:HG3	1:A:554:TYR:OH	2.17	0.44
1:A:301:PHE:CE1	1:A:306:LEU:HD21	2.51	0.44
1:A:631:LEU:O	1:A:635:VAL:HG22	2.17	0.44
1:A:184:ASN:HB3	1:A:404:ARG:NH1	2.33	0.44
1:A:157:ALA:O	1:A:161:ILE:HG12	2.17	0.44
1:A:260:VAL:HG12	1:A:261:LYS:N	2.32	0.44
1:A:290:LYS:O	1:A:294:CYS:HB2	2.17	0.44
1:A:227:ARG:CG	1:A:228:ARG:N	2.80	0.44
1:A:419:SER:O	1:A:423:ILE:HG13	2.17	0.44
1:A:462:LEU:HB3	1:A:468:VAL:HG23	1.98	0.44
1:A:286:GLU:H	1:A:289:ARG:NH1	2.16	0.44
1:A:360:VAL:HB	1:A:402:PRO:HA	1.99	0.44
1:A:360:VAL:N	1:A:403:GLU:OE2	2.51	0.44
1:A:165:LYS:HG3	1:A:437:PHE:HZ	1.83	0.44
1:A:489:ASP:OD1	1:A:490:PRO:HD2	2.17	0.44
1:A:263:SER:O	1:A:267:ALA:HB2	2.17	0.44
1:A:598:GLU:O	1:A:601:SER:HB3	2.18	0.44
1:A:120:THR:OG1	1:A:121:THR:N	2.50	0.43
1:A:403:GLU:CD	1:A:403:GLU:H	2.21	0.43
1:A:500:LEU:HD13	1:A:608:ALA:CA	2.48	0.43
1:A:409:LEU:HD21	1:A:438:PHE:CD2	2.52	0.43
1:A:638:ARG:HE	2:A:709:PO4:P	2.41	0.43
1:A:106:GLU:OE1	1:A:485:ARG:HD2	2.19	0.43
1:A:263:SER:HB3	1:A:299:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ILE:HD13	1:A:382:ILE:HB	1.99	0.43
1:A:573:GLU:OE1	1:A:628:LYS:HB2	2.18	0.43
1:A:492:THR:HG1	1:A:518:PRO:HD2	1.83	0.43
1:A:503:MET:CE	1:A:544:SER:HA	2.49	0.43
1:A:129:ILE:CG1	1:A:136:ILE:HD13	2.48	0.43
1:A:364:LYS:HD3	1:A:364:LYS:HA	1.81	0.43
1:A:106:GLU:OE1	1:A:485:ARG:HB3	2.19	0.43
1:A:279:ILE:HG22	1:A:280:LEU:N	2.33	0.43
1:A:42:ASN:C	1:A:194:ALA:CB	2.87	0.43
1:A:582:LYS:HD3	1:A:583:TYR:CE2	2.54	0.43
1:A:321:GLY:O	1:A:324:LYS:HD3	2.19	0.43
1:A:96:LEU:HA	1:A:116:ASP:OD1	2.18	0.43
1:A:350:ARG:HH11	1:A:350:ARG:HG2	1.83	0.43
1:A:644:ARG:HG2	1:A:670:ILE:HG23	2.01	0.43
1:A:641:GLY:HA3	2:A:704:PO4:O2	2.19	0.43
1:A:653:ILE:HA	1:A:658:ASP:HB3	2.01	0.43
1:A:540:ARG:HG2	1:A:540:ARG:NH1	2.34	0.42
1:A:648:LEU:HD21	1:A:670:ILE:CG1	2.49	0.42
1:A:75:VAL:HG22	1:A:76:PRO:HD2	2.01	0.42
1:A:32:GLU:OE2	1:A:36:LYS:HE3	2.19	0.42
1:A:677:ARG:HH21	1:A:677:ARG:HG2	1.84	0.42
1:A:91:TRP:CE3	1:A:94:ILE:HD12	2.55	0.42
1:A:411:VAL:HG12	1:A:412:GLU:N	2.35	0.42
1:A:424:CYS:SG	1:A:476:PRO:HB3	2.59	0.42
1:A:451:LEU:O	1:A:455:LEU:HB2	2.19	0.42
1:A:569:ASP:HB3	1:A:574:LYS:HD3	2.00	0.42
1:A:575:ASP:HB3	1:A:578:GLU:HB2	2.02	0.42
1:A:317:ALA:HB3	1:A:323:ILE:CD1	2.50	0.42
1:A:356:LYS:HG2	1:A:357:ARG:N	2.34	0.42
1:A:514:ILE:O	1:A:517:THR:HB	2.19	0.42
1:A:45:LEU:HD23	1:A:197:TYR:HB3	2.01	0.41
1:A:495:ILE:HG13	1:A:495:ILE:H	1.69	0.41
1:A:662:HIS:O	1:A:666:VAL:HG23	2.20	0.41
1:A:146:GLU:O	1:A:149:LEU:HB2	2.20	0.41
1:A:383:ILE:HG22	1:A:385:VAL:HG22	2.02	0.41
1:A:407:SER:HB2	1:A:442:PHE:CD2	2.54	0.41
1:A:436:ASP:O	1:A:439:ALA:HB3	2.21	0.41
1:A:267:ALA:CB	1:A:297:LYS:HB3	2.50	0.41
1:A:554:TYR:O	1:A:558:LEU:HG	2.20	0.41
1:A:627:VAL:HG11	1:A:635:VAL:CG1	2.49	0.41
1:A:130:ARG:HA	1:A:425:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ARG:O	1:A:541:LYS:CB	2.69	0.41
1:A:614:THR:O	1:A:616:VAL:N	2.53	0.41
1:A:623:ILE:HG12	1:A:623:ILE:H	1.75	0.41
1:A:638:ARG:NH1	2:A:705:PO4:O4	2.54	0.41
1:A:572:GLU:HA	1:A:572:GLU:OE1	2.19	0.41
1:A:614:THR:C	1:A:616:VAL:H	2.23	0.41
1:A:27:PHE:HB2	1:A:28:PRO:HD2	2.01	0.41
1:A:495:ILE:HG22	1:A:513:LEU:HD11	2.03	0.41
1:A:575:ASP:O	1:A:578:GLU:HB2	2.21	0.41
1:A:504:GLU:HA	1:A:613:ASN:HD21	1.85	0.41
1:A:159:LEU:HA	1:A:159:LEU:HD23	1.85	0.41
1:A:358:ILE:CG2	1:A:362:GLU:HB2	2.50	0.41
1:A:279:ILE:CD1	1:A:292:ALA:HA	2.42	0.41
1:A:613:ASN:OD1	1:A:615:SER:OG	2.34	0.41
1:A:638:ARG:HH22	1:A:677:ARG:NH2	2.10	0.41
1:A:242:ASN:O	1:A:242:ASN:CG	2.58	0.41
1:A:42:ASN:O	1:A:194:ALA:HB1	2.21	0.41
1:A:98:ILE:CD1	1:A:98:ILE:N	2.84	0.41
1:A:286:GLU:O	1:A:289:ARG:HB3	2.21	0.41
1:A:367:ALA:C	1:A:369:ARG:H	2.25	0.41
1:A:557:PHE:O	1:A:560:GLU:HB2	2.22	0.41
1:A:206:LEU:HD13	1:A:370:ALA:HB3	2.03	0.40
1:A:280:LEU:HD13	1:A:292:ALA:HB2	2.03	0.40
1:A:641:GLY:HA3	2:A:704:PO4:O1	2.20	0.40
1:A:591:ARG:O	1:A:595:GLU:HB2	2.21	0.40
1:A:546:TYR:HA	1:A:547:PRO:HD3	1.79	0.40
1:A:71:SER:HA	1:A:141:CYS:O	2.21	0.40
1:A:383:ILE:HG22	1:A:385:VAL:CG2	2.52	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	663/702 (94%)	551 (83%)	88 (13%)	24 (4%)	4	22

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	PRO
1	A	51	ALA
1	A	113	GLY
1	A	286	GLU
1	A	629	GLU
1	A	48	PRO
1	A	213	GLU
1	A	299	ALA
1	A	378	ARG
1	A	413	THR
1	A	639	HIS
1	A	300	ALA
1	A	368	GLY
1	A	390	ARG
1	A	507	ASP
1	A	615	SER
1	A	617	SER
1	A	32	GLU
1	A	156	GLY
1	A	448	GLU
1	A	281	GLU
1	A	540	ARG
1	A	458	VAL
1	A	76	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	568/591 (96%)	513 (90%)	55 (10%)	9	34

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	ILE
1	A	26	LEU
1	A	27	PHE
1	A	32	GLU
1	A	35	GLU
1	A	44	LEU
1	A	75	VAL
1	A	77	LEU
1	A	78	ARG
1	A	96	LEU
1	A	120	THR
1	A	122	SER
1	A	153	GLU
1	A	158	THR
1	A	162	LEU
1	A	179	SER
1	A	186	THR
1	A	202	ARG
1	A	212	CYS
1	A	229	VAL
1	A	233	GLU
1	A	246	LEU
1	A	251	THR
1	A	271	GLU
1	A	287	MET
1	A	291	LEU
1	A	293	GLU
1	A	294	CYS
1	A	303	HIS
1	A	312	ARG
1	A	316	ASP
1	A	342	ARG
1	A	390	ARG
1	A	392	ILE
1	A	403	GLU
1	A	447	ASN
1	A	491	LEU
1	A	505	LEU
1	A	508	ILE
1	A	517	THR
1	A	527	LYS
1	A	528	THR

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Mol	Chain	Res	Type
1	A	550	PHE
1	A	556	TRP
1	A	571	ILE
1	A	590	LEU
1	A	611	VAL
1	A	615	SER
1	A	616	VAL
1	A	628	LYS
1	A	638	ARG
1	A	639	HIS
1	A	648	LEU
1	A	653	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	283	ASN
1	A	302	HIS
1	A	303	HIS
1	A	310	GLN
1	A	322	ASN
1	A	464	ASN
1	A	497	HIS
1	A	512	HIS
1	A	650	ASN
1	A	655	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PO4	A	703	-	4,4,4	1.35	0	6,6,6	0.39	0
2	PO4	A	704	-	4,4,4	1.24	0	6,6,6	0.39	0
2	PO4	A	705	-	4,4,4	1.31	0	6,6,6	0.39	0
2	PO4	A	706	-	4,4,4	1.34	0	6,6,6	0.39	0
2	PO4	A	707	-	4,4,4	1.29	0	6,6,6	0.40	0
2	PO4	A	708	-	4,4,4	1.31	0	6,6,6	0.39	0
2	PO4	A	709	-	4,4,4	1.38	0	6,6,6	0.40	0
2	PO4	A	710	-	4,4,4	1.29	0	6,6,6	0.40	0
2	PO4	A	711	-	4,4,4	1.31	0	6,6,6	0.38	0
2	PO4	A	712	-	4,4,4	1.36	0	6,6,6	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	703	-	-	0/0/0/0	0/0/0/0
2	PO4	A	704	-	-	0/0/0/0	0/0/0/0
2	PO4	A	705	-	-	0/0/0/0	0/0/0/0
2	PO4	A	706	-	-	0/0/0/0	0/0/0/0
2	PO4	A	707	-	-	0/0/0/0	0/0/0/0
2	PO4	A	708	-	-	0/0/0/0	0/0/0/0
2	PO4	A	709	-	-	0/0/0/0	0/0/0/0
2	PO4	A	710	-	-	0/0/0/0	0/0/0/0
2	PO4	A	711	-	-	0/0/0/0	0/0/0/0
2	PO4	A	712	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	704	PO4	3	0
2	A	705	PO4	1	0
2	A	709	PO4	9	0
2	A	710	PO4	1	0
2	A	712	PO4	1	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	671/702 (95%)	-0.46	5 (0%) 87 77	21, 55, 96, 121	39 (5%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	ARG	2.7
1	A	107	SER	2.4
1	A	684	VAL	2.2
1	A	686	SER	2.2
1	A	16	GLY	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
2	PO4	A	710	5/5	0.86	0.51	7.74	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	A	706	5/5	0.84	0.40	5.70	135,135,135,136	0
2	PO4	A	712	5/5	0.73	0.34	4.46	112,112,113,113	0
2	PO4	A	708	5/5	0.84	0.41	4.39	125,125,125,125	0
2	PO4	A	703	5/5	0.91	0.34	3.53	128,128,128,128	0
2	PO4	A	711	5/5	0.88	0.27	1.65	92,94,94,94	0
2	PO4	A	709	5/5	0.90	0.24	-0.10	93,94,96,96	0
2	PO4	A	704	5/5	0.93	0.16	-1.11	106,106,106,106	0
2	PO4	A	707	5/5	0.61	0.69	-	162,162,162,163	0
2	PO4	A	705	5/5	0.88	0.47	-	127,127,127,128	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.