



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:46 PM GMT

PDB ID : 2Q1F  
Title : Crystal structure of chondroitin sulfate lyase abc from bacteroides thetaio-  
taomicron wal2926  
Authors : Shaya, D.; Cygler, M.  
Deposited on : 2007-05-24  
Resolution : 2.85 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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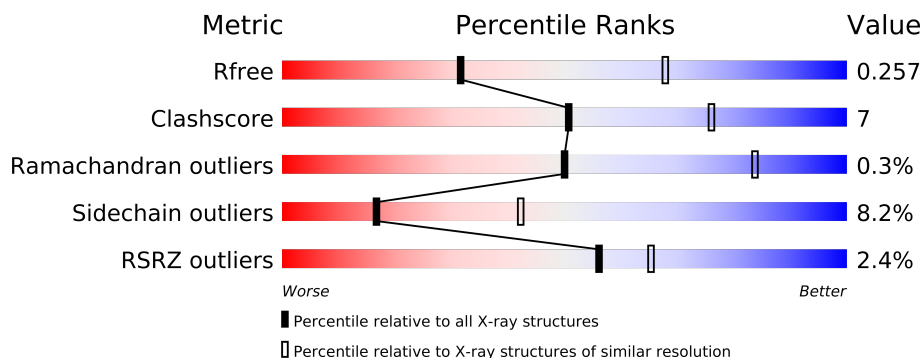
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.85 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	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)

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. 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	1022	
1	B	1022	

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	2003	-	X
3	PO4	A	2005	-	X
3	PO4	A	2006	-	X
3	PO4	A	2007	-	X
3	PO4	A	2008	-	X
3	PO4	A	2009	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	PO4	B	2004	-	X
3	PO4	B	2005	-	X
3	PO4	B	2006	-	X
3	PO4	B	2007	-	X
3	PO4	B	2008	-	X
3	PO4	B	2009	-	X
3	PO4	B	2010	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15973 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.

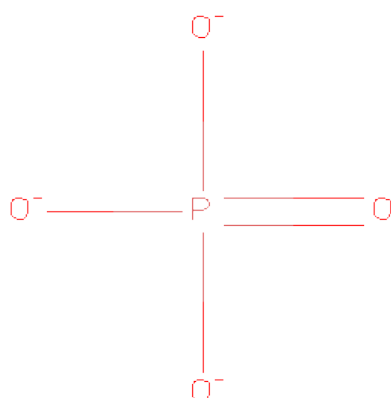
- Molecule 1 is a protein called Chondroitinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	991	Total	C	N	O	S	Se	0	0	0
			7912	5024	1371	1471	11	35			
1	B	991	Total	C	N	O	S	Se	0	0	0
			7912	5024	1371	1471	11	35			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

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



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

- Molecule 4 is water.

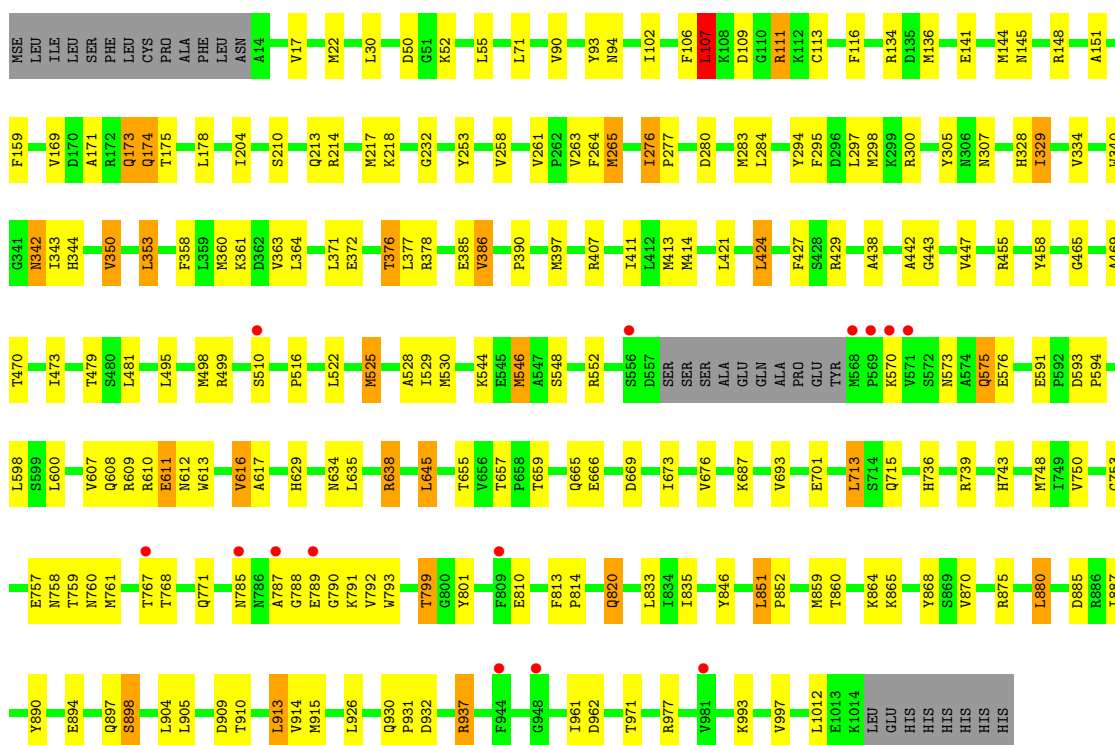
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	25	Total	O	0	0
			25	25		

### 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.

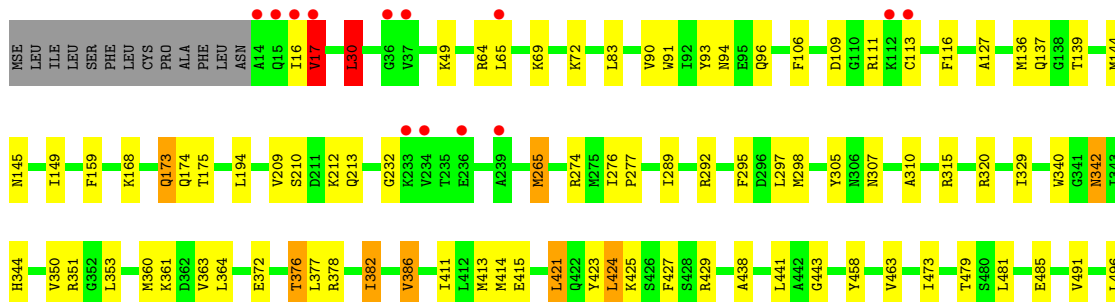
#### • Molecule 1: Chondroitinase

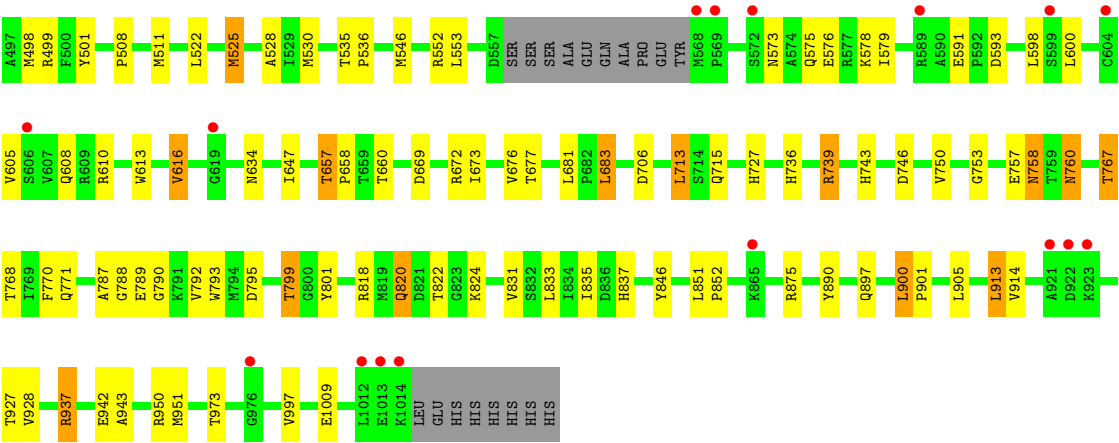
Chain A: 



#### • Molecule 1: Chondroitinase

Chain B: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.36Å 223.36Å 112.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.85 44.38 – 2.85	Depositor EDS
% Data completeness (in resolution range)	94.8 (50.00-2.85) 94.9 (44.38-2.85)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.220 , 0.262 0.218 , 0.257	Depositor DCC
$R_{free}$ test set	3599 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.6	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 48.8	EDS
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 71079 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15973	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 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: PO4, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.38	2/8072 (0.0%)	0.53	2/10852 (0.0%)
1	B	0.32	0/8072	0.52	1/10852 (0.0%)
All	All	0.35	2/16144 (0.0%)	0.53	3/21704 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	810	GLU	CD-OE1	11.60	1.38	1.25
1	A	810	GLU	CD-OE2	11.28	1.38	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	713	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	107	LEU	CA-CB-CG	5.20	127.25	115.30
1	B	30	LEU	CA-CB-CG	5.11	127.05	115.30

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	7912	0	7770	125	0
1	B	7912	0	7770	107	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	40	0	0	0	0
3	B	40	0	0	0	0
4	A	42	0	0	0	0
4	B	25	0	0	0	0
All	All	15973	0	15540	232	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 7.

All (232) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:789:GLU:CB	1:B:790:GLY:HA3	1.76	1.13
1:B:767:THR:HG23	1:B:837:HIS:HE1	1.14	1.13
1:A:789:GLU:CB	1:A:790:GLY:HA3	1.74	1.13
1:B:789:GLU:HB3	1:B:790:GLY:CA	1.89	1.02
1:A:411:ILE:HA	1:A:414:MSE:HE3	1.36	1.02
1:A:789:GLU:HB3	1:A:790:GLY:CA	1.90	1.01
1:B:767:THR:CG2	1:B:837:HIS:HE1	1.75	0.99
1:B:767:THR:HG23	1:B:837:HIS:CE1	1.96	0.99
1:B:789:GLU:HB3	1:B:790:GLY:HA3	1.00	0.99
1:A:789:GLU:HB3	1:A:790:GLY:HA3	0.99	0.98
1:A:638:ARG:HH11	1:A:638:ARG:HG3	1.29	0.94
1:A:479:THR:HG22	1:A:481:LEU:H	1.35	0.89
1:B:479:THR:HG22	1:B:481:LEU:H	1.42	0.85
1:B:411:ILE:HA	1:B:414:MSE:HE3	1.59	0.82
1:B:413:MSE:HA	1:B:413:MSE:HE2	1.61	0.81
1:A:469:ALA:O	1:A:473:ILE:HG12	1.81	0.81
1:A:377:LEU:HD12	1:A:413:MSE:HG3	1.64	0.79
1:A:525:MSE:HE2	1:A:528:ALA:HB3	1.65	0.78
1:A:573:ASN:HD21	1:A:575:GLN:HG2	1.49	0.78
1:B:937:ARG:HG2	1:B:937:ARG:HH11	1.49	0.78
1:B:113:CYS:HB2	1:B:144:MSE:HE1	1.66	0.75
1:A:789:GLU:CB	1:A:790:GLY:CA	2.58	0.74
1:A:210:SER:H	1:A:213:GLN:HE21	1.36	0.73
1:A:525:MSE:HA	1:A:525:MSE:HE3	1.71	0.72
1:A:106:PHE:CD1	1:A:136:MSE:HE1	2.24	0.72
1:A:295:PHE:CD2	1:A:298:MSE:HE2	2.25	0.71
1:B:669:ASP:H	1:B:771:GLN:HE22	1.38	0.71
1:A:669:ASP:H	1:A:771:GLN:HE22	1.37	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:473:ILE:CD1	1:B:491:VAL:HG11	2.21	0.70
1:A:525:MSE:CE	1:A:528:ALA:HB3	2.22	0.70
1:B:378:ARG:HD3	1:B:414:MSE:HE2	1.71	0.70
1:A:173:GLN:HA	1:A:173:GLN:HE21	1.57	0.69
1:A:799:THR:HB	1:A:852:PRO:HA	1.75	0.69
1:B:93:TYR:HB3	1:B:159:PHE:HB2	1.75	0.68
1:A:342:ASN:HD21	1:A:344:HIS:HD2	1.39	0.68
1:A:743:HIS:HB2	1:A:750:VAL:HG13	1.74	0.68
1:A:573:ASN:HD22	1:A:576:GLU:H	1.42	0.67
1:B:706:ASP:OD2	1:B:727:HIS:HD2	1.78	0.67
1:B:265:MSE:HE1	1:B:344:HIS:O	1.94	0.66
1:B:116:PHE:HD2	1:B:136:MSE:HE3	1.61	0.66
1:B:210:SER:H	1:B:213:GLN:HE21	1.43	0.65
1:A:638:ARG:CG	1:A:638:ARG:HH11	2.08	0.65
1:B:789:GLU:CB	1:B:790:GLY:CA	2.61	0.65
1:A:378:ARG:HD3	1:A:414:MSE:HE2	1.79	0.64
1:B:361:LYS:HB2	1:B:413:MSE:HE1	1.79	0.64
1:B:683:LEU:HD23	1:B:818:ARG:HG3	1.78	0.64
1:A:411:ILE:HG21	1:A:424:LEU:HD13	1.81	0.63
1:B:937:ARG:HH11	1:B:937:ARG:CG	2.11	0.63
1:B:295:PHE:CD2	1:B:298:MSE:HE3	2.34	0.62
1:B:799:THR:HB	1:B:852:PRO:HA	1.81	0.62
1:A:930:GLN:HE21	1:A:932:ASP:H	1.48	0.61
1:A:93:TYR:HB3	1:A:159:PHE:HB2	1.81	0.61
1:B:106:PHE:CD1	1:B:136:MSE:HE1	2.36	0.60
1:A:913:LEU:HD22	1:A:931:PRO:HG3	1.82	0.60
1:B:295:PHE:CE2	1:B:353:LEU:HD13	2.36	0.60
1:A:358:PHE:HA	1:A:413:MSE:CE	2.31	0.60
1:B:522:LEU:HD11	1:B:553:LEU:HD22	1.84	0.60
1:A:887:ILE:HG21	1:A:915:MSE:HE3	1.84	0.59
1:A:525:MSE:CE	1:A:525:MSE:HA	2.32	0.59
1:B:414:MSE:HE1	1:B:423:TYR:CD1	2.38	0.59
1:A:265:MSE:HE1	1:A:344:HIS:O	2.03	0.59
1:B:508:PRO:HB3	1:B:616:VAL:HG11	1.84	0.59
1:B:498:MSE:HE3	1:B:522:LEU:HB2	1.84	0.58
1:B:232:GLY:H	1:B:307:ASN:ND2	2.01	0.58
1:B:342:ASN:C	1:B:342:ASN:HD22	2.06	0.58
1:A:860:THR:O	1:A:864:LYS:HG2	2.03	0.58
1:B:767:THR:CG2	1:B:837:HIS:CE1	2.67	0.58
1:B:342:ASN:HD21	1:B:344:HIS:HD2	1.49	0.58
1:B:657:THR:HG22	1:B:658:PRO:HD2	1.85	0.57
1:A:361:LYS:HB2	1:A:413:MSE:HE1	1.85	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:885:ASP:HB3	1:A:887:ILE:HD12	1.86	0.57
1:A:887:ILE:CG2	1:A:915:MSE:HE3	2.34	0.57
1:A:657:THR:HG22	1:A:659:THR:H	1.69	0.56
1:A:71:LEU:HD12	1:A:144:MSE:HG3	1.87	0.56
1:B:30:LEU:H	1:B:30:LEU:HD13	1.71	0.56
1:A:607:VAL:HG22	1:A:616:VAL:HB	1.87	0.56
1:B:525:MSE:HE2	1:B:528:ALA:HB3	1.87	0.56
1:B:377:LEU:HD12	1:B:413:MSE:HG3	1.88	0.56
1:A:204:ILE:HG13	1:A:429:ARG:NH2	2.21	0.56
1:B:743:HIS:HB2	1:B:750:VAL:CG1	2.36	0.55
1:B:835:ILE:HD13	1:B:846:TYR:HB2	1.87	0.55
1:B:610:ARG:HB2	1:B:613:TRP:CZ2	2.42	0.55
1:A:378:ARG:HD3	1:A:414:MSE:CE	2.36	0.55
1:B:673:ILE:O	1:B:676:VAL:HG22	2.07	0.55
1:A:358:PHE:CD1	1:A:413:MSE:HE3	2.42	0.55
1:A:386:VAL:HG21	1:A:427:PHE:HA	1.89	0.54
1:A:438:ALA:CB	1:A:443:GLY:HA3	2.38	0.54
1:A:629:HIS:HB2	1:A:701:GLU:HB3	1.88	0.54
1:A:753:GLY:HA3	1:A:846:TYR:CE2	2.43	0.54
1:A:113:CYS:HB2	1:A:144:MSE:HE1	1.89	0.53
1:B:473:ILE:HD13	1:B:491:VAL:HG11	1.89	0.53
1:A:280:ASP:H	1:A:283:MSE:HE3	1.74	0.53
1:A:909:ASP:HB2	1:A:971:THR:H	1.74	0.52
1:A:573:ASN:ND2	1:A:576:GLU:H	2.06	0.52
1:B:647:ILE:HD13	1:B:799:THR:HG21	1.91	0.52
1:A:386:VAL:CG2	1:A:427:PHE:HA	2.40	0.52
1:A:106:PHE:CE1	1:A:136:MSE:HE1	2.45	0.51
1:A:173:GLN:CA	1:A:173:GLN:HE21	2.21	0.51
1:B:305:TYR:CG	1:B:360:MSE:HE1	2.45	0.51
1:B:943:ALA:HB1	1:B:951:MSE:HE3	1.91	0.51
1:B:113:CYS:HB2	1:B:144:MSE:CE	2.40	0.51
1:A:342:ASN:HD22	1:A:343:ILE:N	2.08	0.51
1:B:795:ASP:OD2	1:B:799:THR:HG23	2.10	0.51
1:A:516:PRO:HD2	1:A:820:GLN:NE2	2.25	0.51
1:B:530:MSE:HB2	1:B:546:MSE:HG2	1.92	0.51
1:A:107:LEU:HD11	1:A:148:ARG:HH11	1.76	0.51
1:A:397:MSE:SE	1:A:465:GLY:HA3	2.61	0.51
1:B:672:ARG:HA	1:B:768:THR:HG21	1.92	0.50
1:A:295:PHE:HD2	1:A:298:MSE:HE2	1.70	0.50
1:A:897:GLN:O	1:A:898:SER:HB2	2.12	0.49
1:A:413:MSE:HA	1:A:413:MSE:HE2	1.93	0.49
1:B:525:MSE:HE1	1:B:579:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:739:ARG:NH1	1:A:875:ARG:O	2.46	0.49
1:A:498:MSE:HE3	1:A:522:LEU:HB2	1.94	0.49
1:B:753:GLY:HA3	1:B:846:TYR:CE2	2.48	0.49
1:A:295:PHE:HD2	1:A:298:MSE:CE	2.25	0.49
1:A:792:VAL:HG21	1:A:859:MSE:HB3	1.95	0.49
1:A:530:MSE:CB	1:A:546:MSE:HG2	2.43	0.49
1:A:116:PHE:HD2	1:A:136:MSE:HE3	1.77	0.49
1:A:390:PRO:HD2	1:A:429:ARG:HD3	1.95	0.49
1:B:350:VAL:HG12	1:B:350:VAL:O	2.13	0.49
1:A:295:PHE:CD2	1:A:298:MSE:CE	2.95	0.48
1:A:787:ALA:N	1:A:788:GLY:HA2	2.29	0.48
1:B:525:MSE:CE	1:B:528:ALA:HB3	2.42	0.48
1:B:91:TRP:CE2	1:B:127:ALA:HB2	2.48	0.48
1:A:358:PHE:HD1	1:A:413:MSE:HE3	1.77	0.48
1:A:305:TYR:CG	1:A:360:MSE:HE1	2.48	0.48
1:A:214:ARG:HA	1:A:217:MSE:HE2	1.94	0.48
1:B:372:GLU:O	1:B:376:THR:HG23	2.13	0.48
1:B:713:LEU:HD23	1:B:913:LEU:HB3	1.96	0.48
1:B:438:ALA:CB	1:B:443:GLY:HA3	2.43	0.48
1:B:676:VAL:O	1:B:767:THR:HA	2.14	0.48
1:A:329:ILE:HG23	1:A:334:VAL:HB	1.95	0.48
1:B:386:VAL:CG2	1:B:427:PHE:HA	2.44	0.47
1:B:421:LEU:HD22	1:B:425:LYS:HE3	1.96	0.47
1:B:535:THR:HG22	1:B:536:PRO:HD2	1.96	0.47
1:A:793:TRP:HB2	1:A:801:TYR:HB2	1.94	0.47
1:A:342:ASN:C	1:A:342:ASN:HD22	2.16	0.47
1:B:350:VAL:CG1	1:B:350:VAL:O	2.63	0.47
1:A:759:THR:O	1:A:761:MSE:HE3	2.13	0.47
1:B:386:VAL:HG21	1:B:427:PHE:HA	1.96	0.47
1:A:758:ASN:HD22	1:A:760:ASN:H	1.62	0.47
1:B:173:GLN:HA	1:B:173:GLN:HE21	1.80	0.47
1:B:573:ASN:HD21	1:B:575:GLN:HG2	1.79	0.47
1:B:787:ALA:N	1:B:788:GLY:HA2	2.30	0.46
1:A:378:ARG:CD	1:A:414:MSE:HE2	2.45	0.46
1:A:111:ARG:NH1	1:A:141:GLU:OE2	2.48	0.46
1:B:647:ILE:O	1:B:647:ILE:HD12	2.16	0.46
1:A:835:ILE:HD13	1:A:846:TYR:HB2	1.96	0.46
1:B:413:MSE:CE	1:B:413:MSE:HA	2.39	0.46
1:A:134:ARG:HH22	1:A:174:GLN:HG2	1.81	0.46
1:A:634:ASN:H	1:A:820:GLN:NE2	2.13	0.46
1:B:822:THR:HG23	1:B:824:LYS:H	1.80	0.46
1:B:927:THR:HB	1:B:1009:GLU:HB3	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:508:PRO:HG2	1:B:511:MSE:SE	2.66	0.46
1:A:890:TYR:HB2	1:A:914:VAL:HB	1.98	0.46
1:B:973:THR:HA	1:B:997:VAL:HG12	1.98	0.45
1:A:358:PHE:HA	1:A:413:MSE:HE3	1.96	0.45
1:B:342:ASN:HD21	1:B:344:HIS:CD2	2.32	0.45
1:B:793:TRP:HB2	1:B:801:TYR:HB2	1.99	0.45
1:B:525:MSE:HE3	1:B:576:GLU:HG3	1.99	0.45
1:A:552:ARG:NH1	1:A:593:ASP:OD1	2.49	0.45
1:A:638:ARG:HG3	1:A:638:ARG:NH1	2.09	0.45
1:B:511:MSE:HE3	1:B:605:VAL:HG21	1.99	0.45
1:B:310:ALA:HA	1:B:315:ARG:HD3	1.98	0.45
1:A:748:MSE:HE1	1:A:868:TYR:HB3	1.99	0.45
1:A:455:ARG:CZ	1:A:961:ILE:HD12	2.47	0.44
1:B:937:ARG:NH1	1:B:937:ARG:CG	2.75	0.44
1:A:676:VAL:O	1:A:767:THR:HA	2.16	0.44
1:A:294:TYR:CE2	1:A:329:ILE:HG12	2.53	0.44
1:A:276:ILE:HA	1:A:277:PRO:HD3	1.80	0.44
1:A:750:VAL:HG11	1:A:880:LEU:HD11	1.98	0.44
1:A:748:MSE:HB2	1:A:851:LEU:HD22	1.99	0.44
1:B:634:ASN:H	1:B:820:GLN:NE2	2.16	0.44
1:A:610:ARG:HB2	1:A:613:TRP:CZ2	2.52	0.44
1:B:276:ILE:HA	1:B:277:PRO:HD3	1.89	0.44
1:B:113:CYS:HB3	1:B:139:THR:O	2.17	0.44
1:A:594:PRO:O	1:A:609:ARG:HD3	2.18	0.44
1:A:350:VAL:HG22	1:A:353:LEU:HD12	2.00	0.44
1:A:736:HIS:HA	1:A:757:GLU:O	2.18	0.44
1:A:635:LEU:HD22	1:A:687:LYS:HE3	1.99	0.44
1:A:499:ARG:NH1	1:A:591:GLU:OE2	2.51	0.43
1:A:102:ILE:HD13	1:A:151:ALA:HA	2.00	0.43
1:B:770:PHE:HE1	1:B:831:VAL:HG12	1.82	0.43
1:B:890:TYR:HB2	1:B:914:VAL:HB	2.00	0.43
1:A:673:ILE:O	1:A:676:VAL:HG22	2.18	0.43
1:B:942:GLU:HG2	1:B:950:ARG:HG2	2.00	0.43
1:A:611:GLU:HB3	1:A:612:ASN:H	1.61	0.43
1:B:767:THR:HG21	1:B:846:TYR:CD2	2.53	0.43
1:B:499:ARG:NH1	1:B:591:GLU:OE2	2.51	0.43
1:A:261:VAL:O	1:A:328:HIS:HE1	2.00	0.43
1:B:411:ILE:HG21	1:B:424:LEU:HD13	2.00	0.42
1:A:30:LEU:HD21	1:A:55:LEU:HD13	2.01	0.42
1:B:65:LEU:HD22	1:B:149:ILE:HD12	2.00	0.42
1:B:758:ASN:HD22	1:B:760:ASN:H	1.68	0.42
1:A:977:ARG:HH21	1:A:993:LYS:HG2	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:638:ARG:CG	1:A:638:ARG:NH1	2.74	0.42
1:A:171:ALA:HA	1:A:174:GLN:OE1	2.19	0.42
1:A:264:PHE:HB2	1:A:284:LEU:HD13	2.01	0.42
1:A:232:GLY:H	1:A:307:ASN:ND2	2.18	0.42
1:B:900:LEU:HA	1:B:901:PRO:HD3	1.94	0.42
1:B:49:LYS:HG2	1:B:91:TRP:CG	2.55	0.42
1:B:16:ILE:O	1:B:17:VAL:HG12	2.20	0.42
1:A:530:MSE:HG3	1:A:546:MSE:HE3	2.00	0.42
1:A:442:ALA:HB2	1:A:962:ASP:OD2	2.20	0.42
1:A:136:MSE:HB3	1:A:136:MSE:HE2	1.99	0.42
1:A:813:PHE:HA	1:A:814:PRO:HA	1.88	0.41
1:B:914:VAL:HG22	1:B:928:VAL:HG22	2.02	0.41
1:B:552:ARG:NH1	1:B:593:ASP:OD1	2.53	0.41
1:B:168:LYS:HB2	1:B:274:ARG:HG3	2.02	0.41
1:A:385:GLU:OE1	1:A:407:ARG:NH2	2.53	0.41
1:B:209:VAL:HG22	1:B:421:LEU:HD12	2.03	0.41
1:B:736:HIS:HA	1:B:757:GLU:O	2.21	0.41
1:A:937:ARG:HD3	1:A:937:ARG:HA	1.93	0.41
1:A:263:VAL:HG21	1:A:294:TYR:CD1	2.55	0.41
1:B:194:LEU:HD22	1:B:382:ILE:HG12	2.03	0.41
1:A:111:ARG:H	1:A:111:ARG:HG3	1.64	0.41
1:B:677:THR:HG23	1:B:767:THR:HG22	2.03	0.41
1:B:736:HIS:HA	1:B:758:ASN:HB3	2.03	0.41
1:B:739:ARG:NH1	1:B:875:ARG:O	2.54	0.41
1:A:617:ALA:HB2	1:A:645:LEU:HD23	2.02	0.41
1:A:372:GLU:O	1:A:376:THR:HG23	2.21	0.41
1:A:897:GLN:O	1:A:898:SER:CB	2.69	0.41
1:A:495:LEU:HD13	1:A:546:MSE:HE3	2.03	0.41
1:A:253:TYR:CE2	1:A:258:VAL:HG22	2.56	0.40
1:A:210:SER:H	1:A:213:GLN:NE2	2.10	0.40
1:B:683:LEU:HA	1:B:683:LEU:HD12	1.89	0.40
1:A:767:THR:OG1	1:A:835:ILE:HB	2.21	0.40
1:B:743:HIS:HB2	1:B:750:VAL:HG12	2.03	0.40
1:B:578:LYS:HB3	1:B:578:LYS:HE2	1.97	0.40
1:A:715:GLN:OE1	1:A:915:MSE:HE2	2.21	0.40
1:B:715:GLN:HG3	1:B:927:THR:HG21	2.03	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	987/1022 (97%)	949 (96%)	35 (4%)	3 (0%)	50	84
1	B	987/1022 (97%)	949 (96%)	36 (4%)	2 (0%)	56	88
All	All	1974/2044 (97%)	1898 (96%)	71 (4%)	5 (0%)	50	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	898	SER
1	A	109	ASP
1	B	109	ASP
1	B	17	VAL
1	A	17	VAL

### 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	840/832 (101%)	768 (91%)	72 (9%)	15	39
1	B	840/832 (101%)	775 (92%)	65 (8%)	18	46
All	All	1680/1664 (101%)	1543 (92%)	137 (8%)	17	42

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MSE
1	A	50	ASP
1	A	52	LYS
1	A	90	VAL

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Mol	Chain	Res	Type
1	A	94	ASN
1	A	107	LEU
1	A	111	ARG
1	A	145	ASN
1	A	169	VAL
1	A	173	GLN
1	A	174	GLN
1	A	175	THR
1	A	178	LEU
1	A	218	LYS
1	A	265	MSE
1	A	276	ILE
1	A	297	LEU
1	A	300	ARG
1	A	329	ILE
1	A	340	TRP
1	A	342	ASN
1	A	350	VAL
1	A	353	LEU
1	A	363	VAL
1	A	364	LEU
1	A	371	LEU
1	A	376	THR
1	A	386	VAL
1	A	421	LEU
1	A	424	LEU
1	A	447	VAL
1	A	458	TYR
1	A	470	THR
1	A	510	SER
1	A	525	MSE
1	A	529	ILE
1	A	544	LYS
1	A	546	MSE
1	A	548	SER
1	A	570	LYS
1	A	575	GLN
1	A	598	LEU
1	A	600	LEU
1	A	608	GLN
1	A	611	GLU
1	A	616	VAL

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Mol	Chain	Res	Type
1	A	638	ARG
1	A	645	LEU
1	A	655	THR
1	A	665	GLN
1	A	666	GLU
1	A	693	VAL
1	A	713	LEU
1	A	768	THR
1	A	785	ASN
1	A	791	LYS
1	A	799	THR
1	A	820	GLN
1	A	833	LEU
1	A	851	LEU
1	A	865	LYS
1	A	870	VAL
1	A	880	LEU
1	A	894	GLU
1	A	904	LEU
1	A	905	LEU
1	A	910	THR
1	A	913	LEU
1	A	926	LEU
1	A	937	ARG
1	A	997	VAL
1	A	1012	LEU
1	B	17	VAL
1	B	30	LEU
1	B	64	ARG
1	B	69	LYS
1	B	72	LYS
1	B	83	LEU
1	B	90	VAL
1	B	94	ASN
1	B	96	GLN
1	B	111	ARG
1	B	137	GLN
1	B	145	ASN
1	B	173	GLN
1	B	174	GLN
1	B	175	THR
1	B	212	LYS

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Mol	Chain	Res	Type
1	B	265	MSE
1	B	289	ILE
1	B	292	ARG
1	B	297	LEU
1	B	320	ARG
1	B	329	ILE
1	B	340	TRP
1	B	342	ASN
1	B	351	ARG
1	B	363	VAL
1	B	364	LEU
1	B	376	THR
1	B	382	ILE
1	B	386	VAL
1	B	415	GLU
1	B	421	LEU
1	B	424	LEU
1	B	429	ARG
1	B	441	LEU
1	B	458	TYR
1	B	463	VAL
1	B	485	GLU
1	B	496	LEU
1	B	501	TYR
1	B	525	MSE
1	B	598	LEU
1	B	600	LEU
1	B	608	GLN
1	B	616	VAL
1	B	657	THR
1	B	660	THR
1	B	681	LEU
1	B	683	LEU
1	B	713	LEU
1	B	739	ARG
1	B	746	ASP
1	B	758	ASN
1	B	760	ASN
1	B	767	THR
1	B	792	VAL
1	B	799	THR
1	B	820	GLN

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Mol	Chain	Res	Type
1	B	833	LEU
1	B	851	LEU
1	B	897	GLN
1	B	900	LEU
1	B	905	LEU
1	B	913	LEU
1	B	937	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	145	ASN
1	A	162	HIS
1	A	173	GLN
1	A	197	HIS
1	A	213	GLN
1	A	257	GLN
1	A	307	ASN
1	A	328	HIS
1	A	332	GLN
1	A	342	ASN
1	A	393	ASN
1	A	403	GLN
1	A	573	ASN
1	A	575	GLN
1	A	597	ASN
1	A	608	GLN
1	A	642	HIS
1	A	733	ASN
1	A	736	HIS
1	A	758	ASN
1	A	771	GLN
1	A	785	ASN
1	A	812	ASN
1	A	815	GLN
1	A	820	GLN
1	A	837	HIS
1	A	873	GLN
1	A	930	GLN
1	A	995	GLN
1	B	15	GLN

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Mol	Chain	Res	Type
1	B	29	GLN
1	B	94	ASN
1	B	98	GLN
1	B	145	ASN
1	B	162	HIS
1	B	173	GLN
1	B	213	GLN
1	B	257	GLN
1	B	307	ASN
1	B	328	HIS
1	B	332	GLN
1	B	342	ASN
1	B	393	ASN
1	B	403	GLN
1	B	573	ASN
1	B	586	ASN
1	B	597	ASN
1	B	608	GLN
1	B	633	HIS
1	B	727	HIS
1	B	733	ASN
1	B	736	HIS
1	B	758	ASN
1	B	760	ASN
1	B	771	GLN
1	B	812	ASN
1	B	815	GLN
1	B	820	GLN
1	B	837	HIS
1	B	873	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	2002	-	4,4,4	0.29	0	6,6,6	0.31	0
3	PO4	A	2003	-	4,4,4	0.29	0	6,6,6	0.31	0
3	PO4	A	2004	-	4,4,4	0.28	0	6,6,6	0.31	0
3	PO4	A	2005	-	4,4,4	0.30	0	6,6,6	0.31	0
3	PO4	A	2006	-	4,4,4	0.27	0	6,6,6	0.31	0
3	PO4	A	2007	-	4,4,4	0.18	0	6,6,6	0.31	0
3	PO4	A	2008	-	4,4,4	0.29	0	6,6,6	0.31	0
3	PO4	A	2009	-	4,4,4	0.27	0	6,6,6	0.31	0
3	PO4	B	2003	-	4,4,4	0.29	0	6,6,6	0.31	0
3	PO4	B	2004	-	4,4,4	0.30	0	6,6,6	0.31	0
3	PO4	B	2005	-	4,4,4	0.28	0	6,6,6	0.31	0
3	PO4	B	2006	-	4,4,4	0.28	0	6,6,6	0.31	0
3	PO4	B	2007	-	4,4,4	0.14	0	6,6,6	0.31	0
3	PO4	B	2008	-	4,4,4	0.29	0	6,6,6	0.31	0
3	PO4	B	2009	-	4,4,4	0.25	0	6,6,6	0.31	0
3	PO4	B	2010	-	4,4,4	0.28	0	6,6,6	0.31	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	PO4	A	2002	-	-	0/0/0/0	0/0/0/0
3	PO4	A	2003	-	-	0/0/0/0	0/0/0/0
3	PO4	A	2004	-	-	0/0/0/0	0/0/0/0
3	PO4	A	2005	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	2006	-	-	0/0/0/0	0/0/0/0
3	PO4	A	2007	-	-	0/0/0/0	0/0/0/0
3	PO4	A	2008	-	-	0/0/0/0	0/0/0/0
3	PO4	A	2009	-	-	0/0/0/0	0/0/0/0
3	PO4	B	2003	-	-	0/0/0/0	0/0/0/0
3	PO4	B	2004	-	-	0/0/0/0	0/0/0/0
3	PO4	B	2005	-	-	0/0/0/0	0/0/0/0
3	PO4	B	2006	-	-	0/0/0/0	0/0/0/0
3	PO4	B	2007	-	-	0/0/0/0	0/0/0/0
3	PO4	B	2008	-	-	0/0/0/0	0/0/0/0
3	PO4	B	2009	-	-	0/0/0/0	0/0/0/0
3	PO4	B	2010	-	-	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.

## 5.7 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	991/1022 (96%)	-0.06	14 (1%)	72 80	49, 59, 65, 86	0
1	B	991/1022 (96%)	0.06	29 (2%)	49 59	50, 59, 64, 85	0
All	All	1982/2044 (96%)	0.00	43 (2%)	56 67	49, 59, 65, 86	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	569	PRO	5.3
1	B	15	GLN	4.7
1	A	568	MSE	4.4
1	A	571	VAL	4.1
1	A	785	ASN	4.0
1	B	14	ALA	3.8
1	A	556	SER	3.7
1	B	568	MSE	3.5
1	A	570	LYS	3.5
1	A	787	ALA	3.3
1	B	569	PRO	3.3
1	B	36	GLY	3.2
1	B	37	VAL	3.2
1	B	113	CYS	3.1
1	B	606	SER	3.1
1	B	921	ALA	3.0
1	B	233	LYS	2.9
1	B	922	ASP	2.8
1	B	17	VAL	2.7
1	B	923	LYS	2.7
1	B	1013	GLU	2.6
1	B	239	ALA	2.6
1	B	236	GLU	2.5
1	A	948	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	572	SER	2.4
1	B	65	LEU	2.4
1	A	510	SER	2.4
1	B	1014	LYS	2.4
1	B	16	ILE	2.3
1	A	944	PHE	2.2
1	B	112	LYS	2.2
1	B	619	GLY	2.2
1	A	809	PHE	2.1
1	B	599	SER	2.1
1	A	767	THR	2.1
1	B	976	GLY	2.1
1	B	589	ARG	2.1
1	A	789	GLU	2.1
1	A	981	VAL	2.0
1	B	1012	LEU	2.0
1	B	604	CYS	2.0
1	B	234	VAL	2.0
1	B	865	LYS	2.0

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

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

## 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PO4	B	2010	5/5	0.35	23.49	70,70,70,70	0
3	PO4	B	2009	5/5	0.45	18.47	72,72,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	B	2007	5/5	0.35	15.04	92,92,93,93	0
3	PO4	B	2006	5/5	0.32	14.25	73,73,74,74	0
3	PO4	A	2003	5/5	0.37	8.65	75,75,75,75	0
3	PO4	B	2008	5/5	0.28	8.59	74,75,75,76	0
3	PO4	A	2009	5/5	0.37	8.46	92,92,93,93	0
3	PO4	A	2007	5/5	0.45	7.34	78,78,78,79	0
3	PO4	A	2005	5/5	0.42	5.06	78,78,78,79	0
3	PO4	B	2005	5/5	0.40	4.25	61,61,61,61	0
3	PO4	A	2006	5/5	0.24	4.00	86,86,86,86	0
3	PO4	B	2004	5/5	0.37	3.49	69,70,70,70	0
3	PO4	A	2008	5/5	0.33	2.37	94,94,95,95	0
2	CA	A	2001	1/1	0.19	1.27	54,54,54,54	0
3	PO4	A	2004	5/5	0.24	1.23	41,43,43,43	0
3	PO4	B	2003	5/5	0.17	0.78	57,57,57,58	0
3	PO4	A	2002	5/5	0.18	0.72	46,47,47,47	0
2	CA	B	2002	1/1	0.09	-1.89	69,69,69,69	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.