Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:15 AM GMT

PDB ID	:	2Q1F
Title	:	Crystal structure of chondroitin sulfate lyase abc from bacteroides thetaiotaomicron wal2926
Authors	:	Shaya, D.; Cygler, M.
Deposited on	:	2007-05-24
Resolution	:	2.85 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

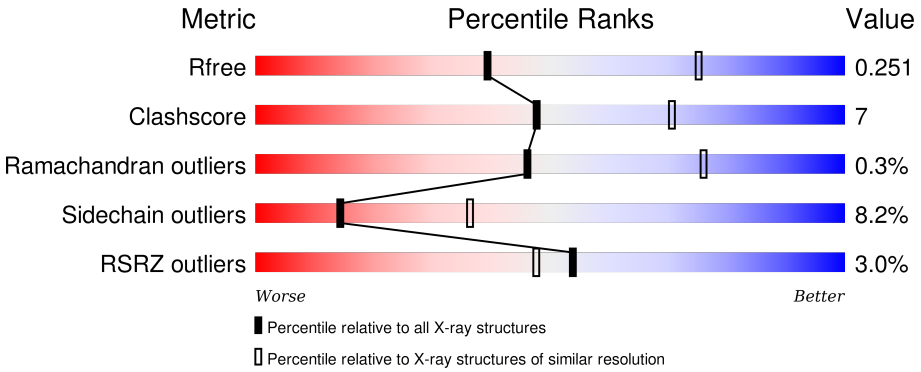
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (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 >=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 <=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	1022	2% 76% 18%
1	B	1022	4% 79% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	2002	-	-	-	X
3	PO4	A	2003	-	-	-	X
3	PO4	A	2005	-	-	-	X
3	PO4	B	2004	-	-	-	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 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.

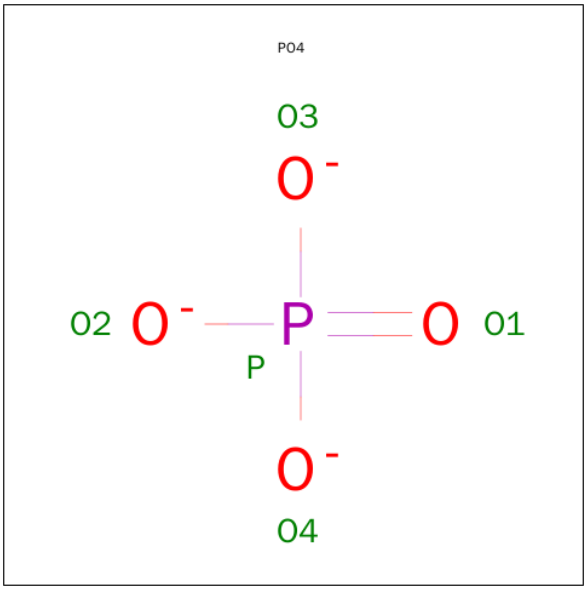
- Molecule 1 is a protein called Chondroitinase.

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_4P).



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

- Molecule 4 is water.

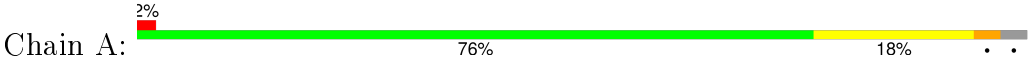
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	42	Total O 42 42	0	0
4	B	25	Total O 25 25	0	0

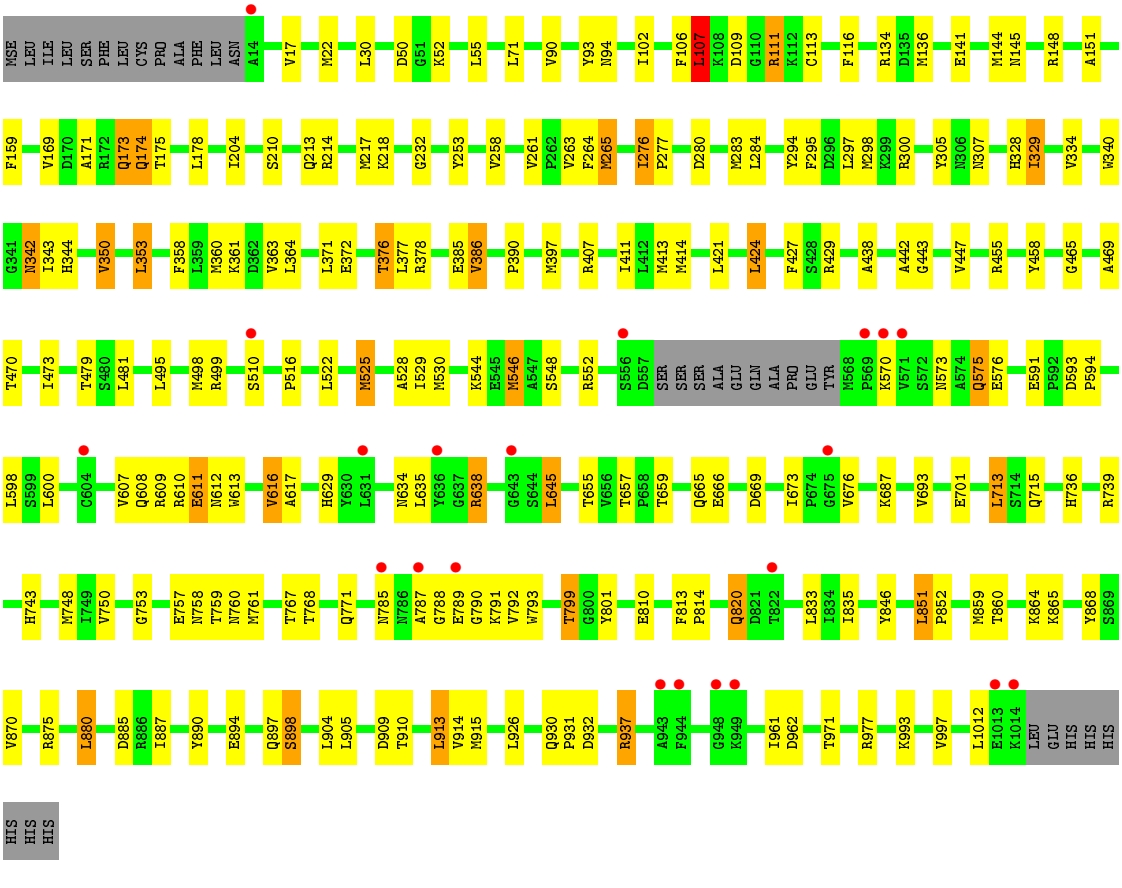
3 Residue-property plots (i)

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

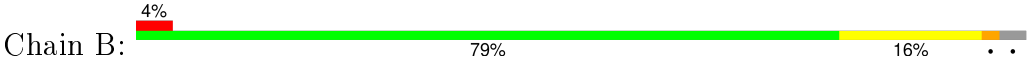
Chain A:

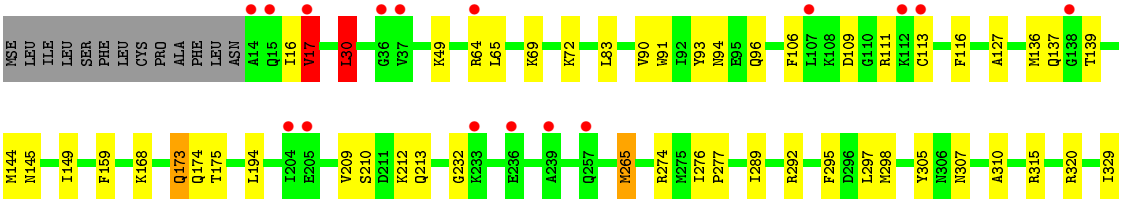


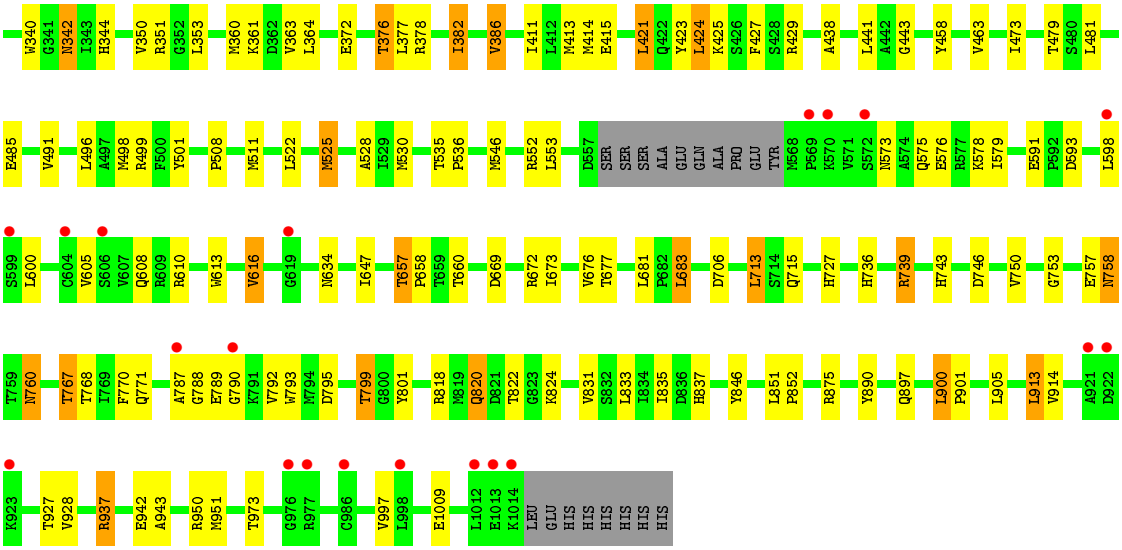


- Molecule 1: Chondroitinase

Chain B:






W340 G341 N342 I343 H344 V350 R351 G352 L353 M360 K361 D362 V363 L364 E372 T376 L377 R378 I382 V386 I411 L412 M413 M414 E415 L421 Q422 Y423 L424 K425 S426 F427 S428 R429 A438 L441 A442 G443 Y458 V463 I473 T479 S480 L481
E485 V491 L496 A497 M498 R499 F500 Y501 P508 M511 L522 M525 A528 I529 M530 T535 P536 M546 R552 L553 D557 SER SER SER ALA GLU GLN ALA PRO GLU TYR M568 P569 K570 V571 S572 N573 A574 Q575 E576 R577 K578 I579 E591 P592 D593 L598
S599 L600 C604 V605 S606 V607 Q608 R609 R610 W613 V616 G619 M634 I647 T657 P658 T659 T660 D669 R672 I673 V676 T677 L681 P682 L683 D706 L713 S714 Q715 H727 H736 R739 H743 D746 V750 G753 E757 N758
T759 M760 T767 T768 T769 F770 Q771 A787 G788 E789 G790 K791 V792 W793 M794 D795 T799 G800 Y801 R818 M819 Q820 D821 T822 Q823 K824 V831 S832 L833 I834 I835 D836 H837 Y846 L851 P852 R875 Y890 Q897 L900 P901 L905 I913 V914 A921 D922
K923 T927 V928 R937 E942 A943 R950 M951 T973 G976 R977 C986 V997 L998 E1009 L1012 E1013 K1014 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.75 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.262 0.211 , 0.251	Depositor DCC
R_{free} test set	3594 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	65.6	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 60.0	EDS
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 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(^{o})	Ideal(^{o})
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 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	7912	0	7770	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 7.

All (232) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:GLN:HG3	1:B:927:THR:HG21	2.03	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	987/1022 (97%)	949 (96%)	35 (4%)	3 (0%)	46 76
1	B	987/1022 (97%)	949 (96%)	36 (4%)	2 (0%)	52 82
All	All	1974/2044 (97%)	1898 (96%)	71 (4%)	5 (0%)	46 76

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 (i)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	840/832 (101%)	768 (91%)	72 (9%)	13 34
1	B	840/832 (101%)	775 (92%)	65 (8%)	16 39
All	All	1680/1664 (101%)	1543 (92%)	137 (8%)	14 36

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	B	837	HIS
1	B	873	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

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	0.47	0	6,6,6	0.27	0
3	PO4	A	2003	-	4,4,4	0.47	0	6,6,6	0.27	0
3	PO4	A	2004	-	4,4,4	0.46	0	6,6,6	0.27	0
3	PO4	A	2005	-	4,4,4	0.48	0	6,6,6	0.27	0
3	PO4	A	2006	-	4,4,4	0.44	0	6,6,6	0.27	0
3	PO4	A	2007	-	4,4,4	0.34	0	6,6,6	0.27	0
3	PO4	A	2008	-	4,4,4	0.46	0	6,6,6	0.27	0
3	PO4	A	2009	-	4,4,4	0.45	0	6,6,6	0.27	0
3	PO4	B	2003	-	4,4,4	0.47	0	6,6,6	0.27	0
3	PO4	B	2004	-	4,4,4	0.47	0	6,6,6	0.27	0
3	PO4	B	2005	-	4,4,4	0.46	0	6,6,6	0.27	0
3	PO4	B	2006	-	4,4,4	0.46	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PO4	B	2007	-	4,4,4	0.28	0	6,6,6	0.27	0
3	PO4	B	2008	-	4,4,4	0.47	0	6,6,6	0.27	0
3	PO4	B	2009	-	4,4,4	0.42	0	6,6,6	0.27	0
3	PO4	B	2010	-	4,4,4	0.45	0	6,6,6	0.27	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
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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	956/1022 (93%)	0.18	21 (2%) 65 61	49, 59, 64, 76	0
1	B	956/1022 (93%)	0.26	36 (3%) 44 37	50, 59, 63, 76	0
All	All	1912/2044 (93%)	0.22	57 (2%) 54 47	49, 59, 64, 76	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	569	PRO	5.0
1	B	15	GLN	4.6
1	A	785	ASN	4.2
1	B	113	CYS	4.1
1	A	571	VAL	3.9
1	A	556	SER	3.8
1	B	606	SER	3.6
1	B	572	SER	3.5
1	A	570	LYS	3.3
1	A	510	SER	3.3
1	B	1013	GLU	3.3
1	B	923	LYS	3.2
1	B	1012	LEU	3.1
1	B	138	GLY	3.1
1	B	37	VAL	3.1
1	B	604	CYS	3.1
1	B	922	ASP	3.0
1	B	599	SER	3.0
1	B	112	LYS	3.0
1	B	569	PRO	3.0
1	A	631	LEU	2.8
1	A	948	GLY	2.8
1	A	604	CYS	2.8
1	B	976	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	236	GLU	2.8
1	B	36	GLY	2.8
1	B	14	ALA	2.7
1	B	17	VAL	2.7
1	A	675	GLY	2.7
1	B	64	ARG	2.6
1	A	822	THR	2.6
1	A	643	GLY	2.5
1	B	239	ALA	2.5
1	B	107	LEU	2.5
1	B	1014	LYS	2.5
1	B	921	ALA	2.4
1	B	619	GLY	2.4
1	A	1014	LYS	2.4
1	B	986	CYS	2.4
1	B	787	ALA	2.3
1	A	789	GLU	2.2
1	A	949	LYS	2.2
1	B	790	GLY	2.2
1	B	233	LYS	2.2
1	B	977	ARG	2.2
1	A	943	ALA	2.2
1	B	998	LEU	2.1
1	A	1013	GLU	2.1
1	A	787	ALA	2.1
1	B	598	LEU	2.1
1	A	14	ALA	2.1
1	B	204	ILE	2.1
1	B	205	GLU	2.0
1	B	257	GLN	2.0
1	A	944	PHE	2.0
1	B	570	LYS	2.0
1	A	636	TYR	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^{th} 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^2)	Q<0.9
3	PO4	A	2003	5/5	0.87	0.43	18.19	75,75,75,75	0
3	PO4	B	2010	5/5	0.77	0.47	17.92	70,70,70,70	0
3	PO4	A	2005	5/5	0.86	0.50	6.47	78,78,78,79	0
3	PO4	B	2004	5/5	0.86	0.47	5.25	69,70,70,70	0
3	PO4	A	2002	5/5	0.95	0.26	3.57	46,47,47,47	0
2	CA	B	2002	1/1	0.46	0.15	-1.00	69,69,69,69	0
2	CA	A	2001	1/1	0.96	0.06	-4.34	54,54,54,54	0
3	PO4	B	2003	5/5	0.96	0.26	-	57,57,57,58	0
3	PO4	A	2004	5/5	0.93	0.35	-	41,43,43,43	0
3	PO4	A	2006	5/5	0.85	0.33	-	86,86,86,86	0
3	PO4	B	2009	5/5	0.78	0.58	-	72,72,73,73	0
3	PO4	B	2006	5/5	0.88	0.40	-	73,73,74,74	0
3	PO4	B	2007	5/5	0.77	0.38	-	92,92,93,93	0
3	PO4	A	2007	5/5	0.80	0.47	-	78,78,78,79	0
3	PO4	B	2008	5/5	0.91	0.34	-	74,75,75,76	0
3	PO4	A	2008	5/5	0.87	0.39	-	94,94,95,95	0
3	PO4	B	2005	5/5	0.89	0.44	-	61,61,61,61	0
3	PO4	A	2009	5/5	0.81	0.42	-	92,92,93,93	0

6.5 Other polymers (i)

There are no such residues in this entry.