



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:49 AM UTC

PDB ID : 2Q1F / pdb_00002q1f
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

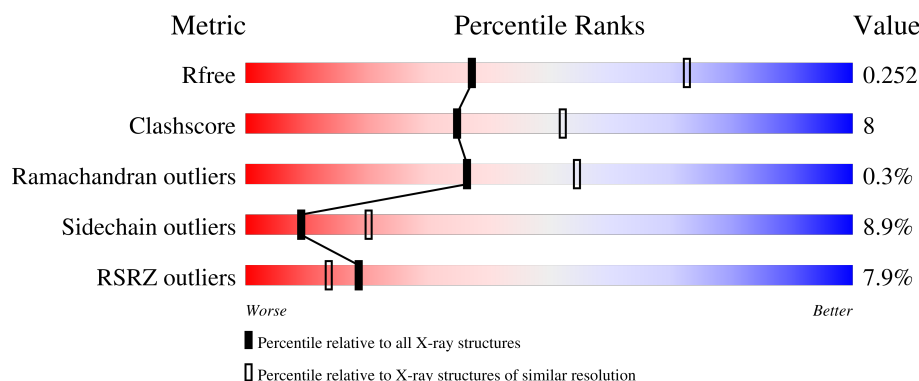
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	1022	
1	B	1022	

2 Entry composition [i](#)

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.

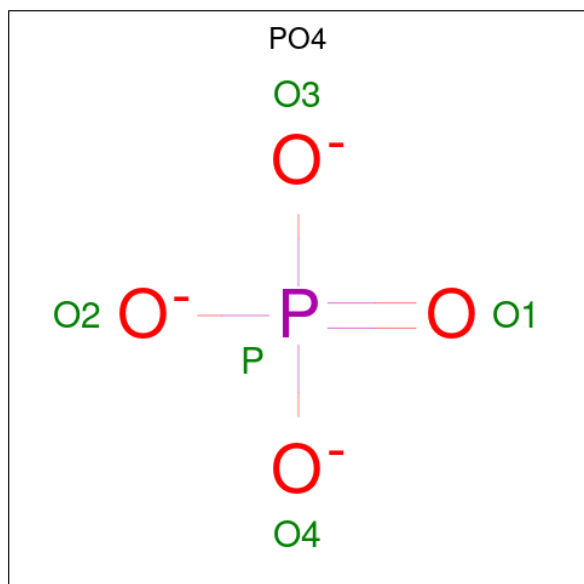
- Molecule 1 is a protein called Chondroitinase.

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 (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

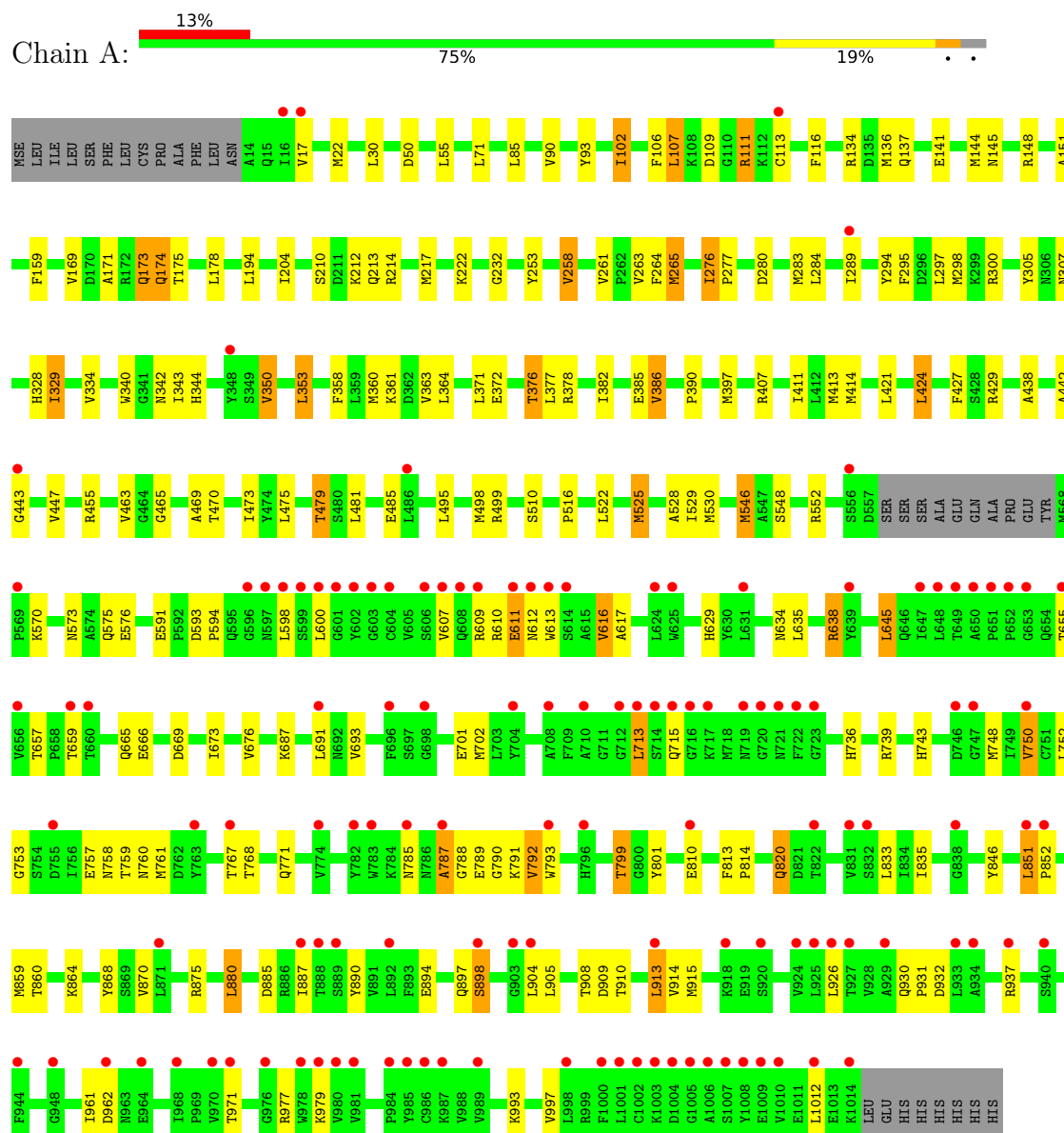
- Molecule 4 is water.

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

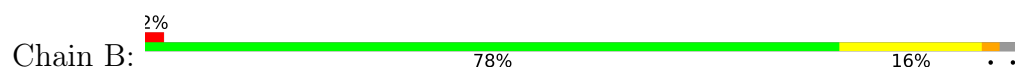
3 Residue-property plots [i](#)

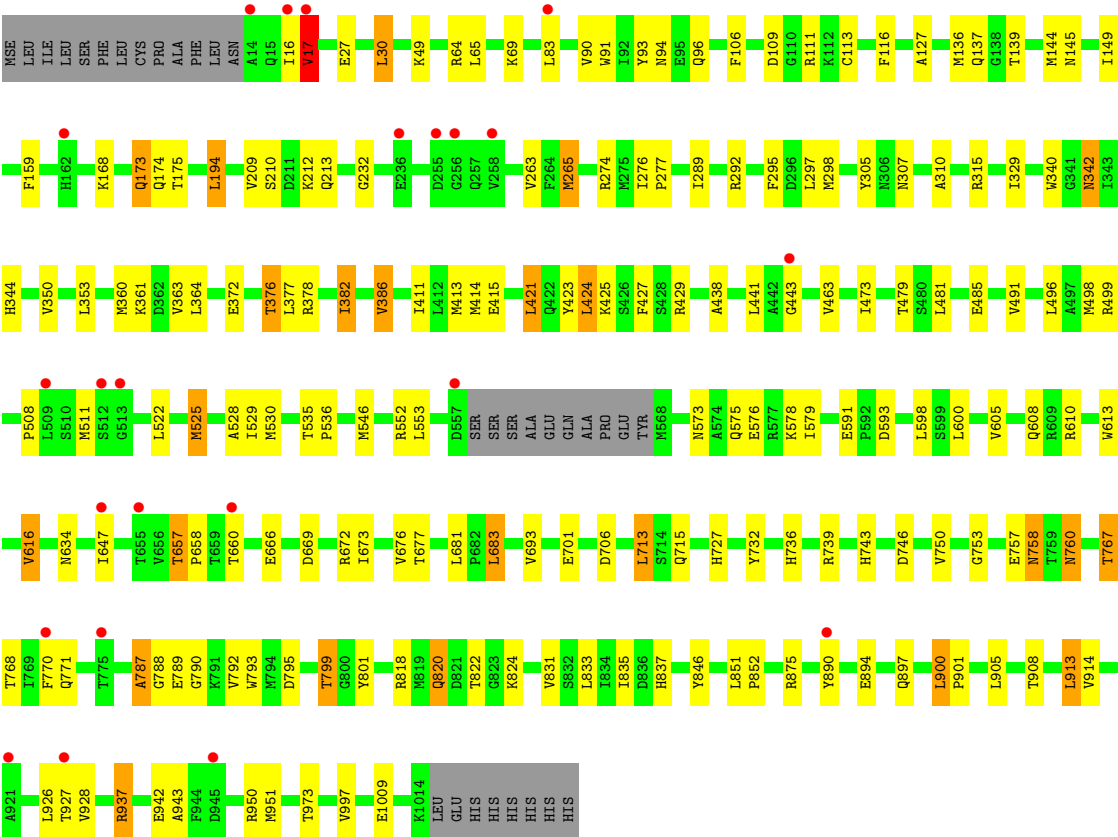
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Chondroitinase



• Molecule 1: Chondroitinase





4 Data and refinement statistics

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 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	94.8 (50.00-2.85) 94.9 (50.00-2.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.262 0.211 , 0.252	Depositor DCC
R_{free} test set	3599 reflections (4.80%)	wwPDB-VP
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 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.44	2/8072 (0.0%)	0.78	1/10852 (0.0%)
1	B	0.42	0/8072	0.77	1/10852 (0.0%)
All	All	0.43	2/16144 (0.0%)	0.77	2/21704 (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	6.88	1.38	1.25
1	A	810	GLU	CD-OE2	6.69	1.38	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	787	ALA	N-CA-C	6.31	117.83	111.07
1	A	787	ALA	N-CA-C	6.16	117.66	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7912	0	7770	127	0
1	B	7912	0	7770	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	236	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 8.

All (236) 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:767:THR:HG23	1:B:837:HIS:HE1	1.14	1.13
1:B:789:GLU:CB	1:B:790:GLY:HA3	1.76	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:HG3	1:A:638:ARG:HH11	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:HE2	1:B:413:MSE:HA	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:HE3	1:A:525:MSE:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:A:638:ARG:CG	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:342:ASN:C	1:B:342:ASN:HD22	2.06	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:HA	1:A:525:MSE:CE	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:232:GLY:H	1:B:307:ASN:ND2	2.01	0.58
1:B:498:MSE:HE3	1:B:522:LEU:HB2	1.84	0.58
1:A:860:THR:O	1:A:864:LYS:HG2	2.03	0.58
1:B:342:ASN:HD21	1:B:344:HIS:HD2	1.49	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: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:A:607:VAL:HG22	1:A:616:VAL:HB	1.87	0.56
1:B:30:LEU:HD13	1:B:30:LEU:H	1.71	0.56
1:B:525:MSE:HE2	1:B:528:ALA:HB3	1.87	0.56
1:A:204:ILE:HG13	1:A:429:ARG:NH2	2.21	0.56
1:B:377:LEU:HD12	1:B:413:MSE:HG3	1.88	0.56
1:B:743:HIS:HB2	1:B:750:VAL:CG1	2.36	0.55
1:B:610:ARG:HB2	1:B:613:TRP:CZ2	2.42	0.55
1:B:835:ILE:HD13	1:B:846:TYR:HB2	1.87	0.55
1:A:378:ARG:HD3	1:A:414:MSE:CE	2.36	0.55
1:A:358:PHE:CD1	1:A:413:MSE:HE3	2.42	0.55
1:B:673:ILE:O	1:B:676:VAL:HG22	2.07	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:A:386:VAL:CG2	1:A:427:PHE:HA	2.40	0.52
1:B:647:ILE:HD13	1:B:799:THR:HG21	1.91	0.52
1:A:106:PHE:CE1	1:A:136:MSE:HE1	2.45	0.51
1:A:173:GLN:HE21	1:A:173:GLN:CA	2.21	0.51
1:B:305:TYR:CG	1:B:360:MSE:HE1	2.45	0.51
1:A:342:ASN:C	1:A:342:ASN:HD22	2.16	0.51
1:B:943:ALA:HB1	1:B:951:MSE:HE3	1.91	0.51
1:A:342:ASN:HD22	1:A:343:ILE:N	2.08	0.51
1:A:516:PRO:HD2	1:A:820:GLN:NE2	2.25	0.51
1:B:113:CYS:HB2	1:B:144:MSE:CE	2.40	0.51
1:B:530:MSE:HB2	1:B:546:MSE:HG2	1.92	0.51
1:B:795:ASP:OD2	1:B:799:THR:HG23	2.10	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:530:MSE:CB	1:A:546:MSE:HG2	2.43	0.49
1:A:792:VAL:HG21	1:A:859:MSE:HB3	1.95	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: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:350:VAL:HG12	1:B:350:VAL:O	2.13	0.48
1:B:91:TRP:CE2	1:B:127:ALA:HB2	2.48	0.48
1:B:525:MSE:CE	1:B:528:ALA:HB3	2.42	0.48
1:A:214:ARG:HA	1:A:217:MSE:HE2	1.94	0.48
1:A:305:TYR:CG	1:A:360:MSE:HE1	2.48	0.48
1:A:358:PHE:HD1	1:A:413:MSE:HE3	1.77	0.48
1:B:372:GLU:O	1:B:376:THR:HG23	2.13	0.48
1:B:438:ALA:CB	1:B:443:GLY:HA3	2.43	0.48
1:B:713:LEU:HD23	1:B:913:LEU:HB3	1.96	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:759:THR:O	1:A:761:MSE:HE3	2.13	0.47
1:B:350:VAL:O	1:B:350:VAL:CG1	2.63	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:386:VAL:HG21	1:B:427:PHE:HA	1.96	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:111:ARG:NH1	1:A:141:GLU:OE2	2.48	0.46
1:A:378:ARG:CD	1:A:414:MSE:HE2	2.45	0.46
1:A:835:ILE:HD13	1:A:846:TYR:HB2	1.96	0.46
1:B:647:ILE:O	1:B:647:ILE:HD12	2.16	0.46
1:B:342:ASN:C	1:B:342:ASN:ND2	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:HH22	1:A:174:GLN:HG2	1.81	0.46
1:B:413:MSE:HA	1:B:413:MSE:CE	2.39	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:A:890:TYR:HB2	1:A:914:VAL:HB	1.98	0.46
1:B:508:PRO:HG2	1:B:511:MSE:SE	2.66	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:A:552:ARG:NH1	1:A:593:ASP:OD1	2.49	0.45
1:B:525:MSE:HE3	1:B:576:GLU:HG3	1.99	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:A:276:ILE:HA	1:A:277:PRO:HD3	1.80	0.44
1:A:294:TYR:CE2	1:A:329:ILE:HG12	2.53	0.44
1:A:676:VAL:O	1:A:767:THR:HA	2.16	0.44
1:B:937:ARG:CG	1:B:937:ARG:NH1	2.75	0.44
1:A:610:ARG:HB2	1:A:613:TRP:CZ2	2.52	0.44
1:A:748:MSE:HB2	1:A:851:LEU:HD22	1.99	0.44
1:A:750:VAL:HG11	1:A:880:LEU:HD11	1.98	0.44
1:B:634:ASN:H	1:B:820:GLN:NE2	2.16	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:350:VAL:HG22	1:A:353:LEU:HD12	2.00	0.44
1:A:594:PRO:O	1:A:609:ARG:HD3	2.18	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:611:GLU:HB3	1:A:612:ASN:H	1.61	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:B:499:ARG:NH1	1:B:591:GLU:OE2	2.51	0.43
1:B:767:THR:HG21	1:B:846:TYR:CD2	2.53	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:A:30:LEU:HD21	1:A:55:LEU:HD13	2.01	0.42
1:B:411:ILE:HG21	1:B:424:LEU:HD13	2.00	0.42
1:B:65:LEU:HD22	1:B:149:ILE:HD12	2.00	0.42
1:A:977:ARG:HH21	1:A:993:LYS:HG2	1.85	0.42
1:B:758:ASN:HD22	1:B:760:ASN:H	1.68	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:638:ARG:CG	1:A:638:ARG:NH1	2.74	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:16:ILE:O	1:B:17:VAL:HG12	2.20	0.42
1:B:49:LYS:HG2	1:B:91:TRP:CG	2.55	0.42
1:A:442:ALA:HB2	1:A:962:ASP:OD2	2.20	0.42
1:A:530:MSE:HG3	1:A:546:MSE:HE3	2.00	0.42
1:A:136:MSE:HE2	1:A:136:MSE:HB3	1.99	0.42
1:A:813:PHE:HA	1:A:814:PRO:HA	1.88	0.41
1:A:385:GLU:OE1	1:A:407:ARG:NH2	2.53	0.41
1:B:168:LYS:HB2	1:B:274:ARG:HG3	2.02	0.41
1:B:552:ARG:NH1	1:B:593:ASP:OD1	2.53	0.41
1:B:914:VAL:HG22	1:B:928:VAL:HG22	2.02	0.41
1:A:937:ARG:HA	1:A:937:ARG:HD3	1.93	0.41
1:B:209:VAL:HG22	1:B:421:LEU:HD12	2.03	0.41
1:B:701:GLU:OE1	1:B:732:TYR:OH	2.35	0.41
1:B:736:HIS:HA	1:B:757:GLU:O	2.21	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:A:372:GLU:O	1:A:376:THR:HG23	2.21	0.41
1:A:617:ALA:HB2	1:A:645:LEU:HD23	2.02	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:495:LEU:HD13	1:A:546:MSE:HE3	2.03	0.41
1:A:713:LEU:C	1:A:713:LEU:HD12	2.46	0.41
1:A:897:GLN:O	1:A:898:SER:CB	2.69	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:A:767:THR:OG1	1:A:835:ILE:HB	2.21	0.40
1:B:683:LEU:HD12	1:B:683:LEU:HA	1.89	0.40
1:A:342:ASN:C	1:A:342:ASN:ND2	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LYS:HE2	1:B:578:LYS:HB3	1.97	0.40
1:B:743:HIS:HB2	1:B:750:VAL:HG12	2.03	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 [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%)	36	54
1	B	987/1022 (97%)	949 (96%)	36 (4%)	2 (0%)	43	62
All	All	1974/2044 (97%)	1898 (96%)	71 (4%)	5 (0%)	36	54

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	840/832 (101%)	758 (90%)	82 (10%)	7	16
1	B	840/832 (101%)	772 (92%)	68 (8%)	11	23
All	All	1680/1664 (101%)	1530 (91%)	150 (9%)	9	20

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MSE
1	A	50	ASP
1	A	85	LEU
1	A	90	VAL
1	A	102	ILE
1	A	107	LEU
1	A	111	ARG
1	A	137	GLN
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	194	LEU
1	A	212	LYS
1	A	222	LYS
1	A	258	VAL
1	A	265	MSE
1	A	276	ILE
1	A	289	ILE
1	A	297	LEU
1	A	300	ARG
1	A	329	ILE
1	A	340	TRP
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	382	ILE
1	A	386	VAL
1	A	421	LEU
1	A	424	LEU

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Mol	Chain	Res	Type
1	A	447	VAL
1	A	463	VAL
1	A	470	THR
1	A	475	LEU
1	A	479	THR
1	A	485	GLU
1	A	510	SER
1	A	525	MSE
1	A	529	ILE
1	A	546	MSE
1	A	548	SER
1	A	570	LYS
1	A	598	LEU
1	A	600	LEU
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	691	LEU
1	A	693	VAL
1	A	702	MSE
1	A	713	LEU
1	A	750	VAL
1	A	752	LEU
1	A	768	THR
1	A	785	ASN
1	A	791	LYS
1	A	792	VAL
1	A	799	THR
1	A	820	GLN
1	A	833	LEU
1	A	851	LEU
1	A	870	VAL
1	A	880	LEU
1	A	894	GLU
1	A	904	LEU
1	A	905	LEU
1	A	908	THR
1	A	910	THR

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Mol	Chain	Res	Type
1	A	913	LEU
1	A	926	LEU
1	A	979	LYS
1	A	997	VAL
1	A	1012	LEU
1	B	17	VAL
1	B	27	GLU
1	B	30	LEU
1	B	64	ARG
1	B	69	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	194	LEU
1	B	212	LYS
1	B	263	VAL
1	B	265	MSE
1	B	289	ILE
1	B	292	ARG
1	B	297	LEU
1	B	329	ILE
1	B	340	TRP
1	B	342	ASN
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	463	VAL
1	B	485	GLU

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Mol	Chain	Res	Type
1	B	496	LEU
1	B	525	MSE
1	B	529	ILE
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	666	GLU
1	B	681	LEU
1	B	683	LEU
1	B	693	VAL
1	B	713	LEU
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	894	GLU
1	B	897	GLN
1	B	900	LEU
1	B	905	LEU
1	B	908	THR
1	B	913	LEU
1	B	926	LEU
1	B	937	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	94	ASN
1	A	145	ASN
1	A	162	HIS
1	A	173	GLN
1	A	174	GLN
1	A	197	HIS

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Mol	Chain	Res	Type
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	488	HIS
1	A	515	HIS
1	A	573	ASN
1	A	575	GLN
1	A	586	ASN
1	A	608	GLN
1	A	633	HIS
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	897	GLN
1	A	930	GLN
1	B	40	GLN
1	B	94	ASN
1	B	98	GLN
1	B	137	GLN
1	B	145	ASN
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	401	ASN
1	B	506	ASN

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Mol	Chain	Res	Type
1	B	573	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	786	ASN
1	B	812	ASN
1	B	815	GLN
1	B	820	GLN
1	B	837	HIS
1	B	873	GLN
1	B	930	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	2008	-	4,4,4	0.96	0	6,6,6	0.43	0
3	PO4	B	2003	-	4,4,4	0.95	0	6,6,6	0.51	0
3	PO4	A	2009	-	4,4,4	0.93	0	6,6,6	0.44	0
3	PO4	A	2006	-	4,4,4	0.94	0	6,6,6	0.43	0
3	PO4	A	2002	-	4,4,4	0.95	0	6,6,6	0.51	0
3	PO4	A	2008	-	4,4,4	0.95	0	6,6,6	0.44	0
3	PO4	B	2009	-	4,4,4	0.91	0	6,6,6	0.46	0
3	PO4	B	2010	-	4,4,4	0.93	0	6,6,6	0.51	0
3	PO4	A	2007	-	4,4,4	0.87	0	6,6,6	0.45	0
3	PO4	B	2005	-	4,4,4	0.94	0	6,6,6	0.44	0
3	PO4	B	2007	-	4,4,4	0.74	0	6,6,6	0.50	0
3	PO4	A	2003	-	4,4,4	0.96	0	6,6,6	0.46	0
3	PO4	B	2004	-	4,4,4	0.95	0	6,6,6	0.50	0
3	PO4	A	2004	-	4,4,4	0.94	0	6,6,6	0.41	0
3	PO4	B	2006	-	4,4,4	0.95	0	6,6,6	0.49	0
3	PO4	A	2005	-	4,4,4	0.96	0	6,6,6	0.49	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	956/1022 (93%)	0.89	129 (13%) 7 5	49, 59, 64, 76	0
1	B	956/1022 (93%)	0.52	23 (2%) 59 51	50, 59, 63, 76	0
All	All	1912/2044 (93%)	0.71	152 (7%) 18 14	49, 59, 64, 76	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	ILE	4.7
1	A	1007	SER	3.9
1	B	443	GLY	3.9
1	A	597	ASN	3.8
1	A	655	THR	3.8
1	A	1008	TYR	3.8
1	A	716	GLY	3.8
1	A	712	GLY	3.6
1	A	831	VAL	3.4
1	A	1009	GLU	3.3
1	A	1004	ASP	3.3
1	A	614	SER	3.2
1	A	1012	LEU	3.2
1	B	255	ASP	3.2
1	A	601	GLY	3.1
1	A	611	GLU	3.1
1	A	556	SER	3.1
1	A	720	GLY	3.1
1	A	989	VAL	3.1
1	A	604	CYS	3.0
1	A	650	ALA	3.0
1	A	609	ARG	3.0
1	A	656	VAL	2.9
1	A	838	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1005	GLY	2.9
1	A	603	GLY	2.9
1	A	348	TYR	2.9
1	A	926	LEU	2.9
1	A	1001	LEU	2.9
1	A	602	TYR	2.9
1	A	612	ASN	2.9
1	A	631	LEU	2.9
1	A	1002	CYS	2.9
1	A	903	GLY	2.8
1	A	1014	LYS	2.8
1	A	607	VAL	2.8
1	A	978	TRP	2.8
1	A	755	ASP	2.8
1	A	569	PRO	2.8
1	A	985	TYR	2.8
1	B	83	LEU	2.8
1	A	723	GLY	2.8
1	A	660	THR	2.8
1	B	258	VAL	2.7
1	A	927	THR	2.7
1	A	715	GLN	2.7
1	B	655	THR	2.7
1	A	598	LEU	2.7
1	B	647	ILE	2.7
1	A	937	ARG	2.7
1	A	596	GLY	2.7
1	A	832	SER	2.7
1	A	717	LYS	2.6
1	A	639	TYR	2.6
1	A	443	GLY	2.6
1	A	767	THR	2.6
1	A	17	VAL	2.6
1	A	851	LEU	2.6
1	B	17	VAL	2.6
1	A	968	ILE	2.6
1	A	599	SER	2.6
1	A	984	PRO	2.6
1	A	659	THR	2.6
1	A	719	ASN	2.6
1	A	934	ALA	2.6
1	A	979	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	987	LYS	2.6
1	A	948	GLY	2.6
1	A	976	GLY	2.6
1	A	1006	ALA	2.6
1	A	782	TYR	2.5
1	A	981	VAL	2.5
1	A	653	GLY	2.5
1	B	512	SER	2.5
1	A	1010	VAL	2.5
1	A	625	TRP	2.5
1	A	986	CYS	2.4
1	A	962	ASP	2.4
1	A	774	VAL	2.4
1	A	787	ALA	2.4
1	A	698	GLY	2.4
1	A	980	VAL	2.4
1	A	929	ALA	2.4
1	A	648	LEU	2.4
1	A	871	LEU	2.4
1	A	904	LEU	2.4
1	A	913	LEU	2.4
1	A	925	LEU	2.4
1	A	647	ILE	2.4
1	A	651	PRO	2.4
1	B	557	ASP	2.3
1	A	486	LEU	2.3
1	A	763	TYR	2.3
1	A	810	GLU	2.3
1	A	714	SER	2.3
1	A	793	TRP	2.3
1	A	746	ASP	2.3
1	A	944	PHE	2.3
1	A	691	LEU	2.3
1	A	713	LEU	2.3
1	A	998	LEU	2.3
1	A	652	PRO	2.2
1	A	822	THR	2.2
1	A	852	PRO	2.2
1	B	775	THR	2.2
1	B	509	LEU	2.2
1	A	113	CYS	2.2
1	A	613	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	889	SER	2.2
1	B	256	GLY	2.2
1	A	708	ALA	2.2
1	A	964	GLU	2.2
1	A	924	VAL	2.2
1	A	606	SER	2.2
1	B	770	PHE	2.2
1	A	624	LEU	2.2
1	A	710	ALA	2.2
1	A	747	GLY	2.2
1	A	918	LYS	2.2
1	A	920	SER	2.2
1	A	608	GLN	2.1
1	A	970	VAL	2.1
1	A	600	LEU	2.1
1	A	696	PHE	2.1
1	A	898	SER	2.1
1	B	14	ALA	2.1
1	A	892	LEU	2.1
1	A	796	HIS	2.1
1	A	750	VAL	2.1
1	A	722	PHE	2.1
1	A	888	THR	2.1
1	A	16	ILE	2.1
1	A	933	LEU	2.1
1	A	971	THR	2.1
1	B	945	ASP	2.1
1	A	289	ILE	2.1
1	B	162	HIS	2.0
1	A	721	ASN	2.0
1	A	785	ASN	2.0
1	A	887	ILE	2.0
1	B	660	THR	2.0
1	B	921	ALA	2.0
1	B	236	GLU	2.0
1	A	1003	LYS	2.0
1	A	940	SER	2.0
1	A	1000	PHE	2.0
1	B	513	GLY	2.0
1	A	649	THR	2.0
1	B	927	THR	2.0
1	A	783	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	704	TYR	2.0
1	B	890	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	B	2007	5/5	0.63	0.23	92,92,93,93	0
3	PO4	A	2003	5/5	0.68	0.31	75,75,75,75	0
3	PO4	A	2005	5/5	0.72	0.37	78,78,78,79	0
3	PO4	B	2010	5/5	0.73	0.27	70,70,70,70	0
3	PO4	A	2009	5/5	0.75	0.28	92,92,93,93	0
3	PO4	A	2008	5/5	0.78	0.26	94,94,95,95	0
3	PO4	A	2007	5/5	0.78	0.35	78,78,78,79	0
3	PO4	B	2004	5/5	0.79	0.29	69,70,70,70	0
3	PO4	A	2006	5/5	0.80	0.29	86,86,86,86	0
3	PO4	B	2006	5/5	0.82	0.27	73,73,74,74	0
3	PO4	B	2008	5/5	0.83	0.26	74,75,75,76	0
3	PO4	B	2009	5/5	0.85	0.33	72,72,73,73	0
3	PO4	B	2005	5/5	0.86	0.29	61,61,61,61	0
3	PO4	B	2003	5/5	0.90	0.23	57,57,57,58	0
3	PO4	A	2004	5/5	0.91	0.27	41,43,43,43	0
2	CA	B	2002	1/1	0.93	0.16	69,69,69,69	0
3	PO4	A	2002	5/5	0.94	0.24	46,47,47,47	0
2	CA	A	2001	1/1	0.99	0.06	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.