Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 05:48 AM GMT

PDB ID	:	2UVE
Title	:	STRUCTURE OF YERSINIA ENTEROCOLITICA FAMILY 28 EXOPOLY-GALACTURONASE
Authors	:	Abbott, D.W.; Boraston, A.B.
Deposited on	:	2007-03-09
Resolution	:	2.19 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

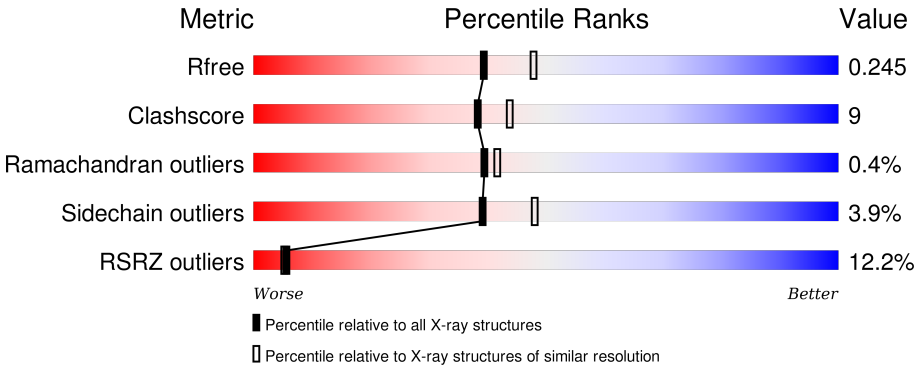
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	608	12% 75% 16% • 6%
1	B	608	11% 77% 13% • 7%

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	SO4	A	1612	-	-	-	X
3	SO4	A	1615	-	-	-	X
3	SO4	A	1616	-	-	X	X
3	SO4	A	1617	-	-	-	X
3	SO4	A	1618	-	-	-	X
3	SO4	A	1619	-	-	-	X
3	SO4	A	1620	-	-	-	X
3	SO4	B	1612	-	-	-	X
3	SO4	B	1619	-	-	X	-
4	ACT	B	1620	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9409 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.

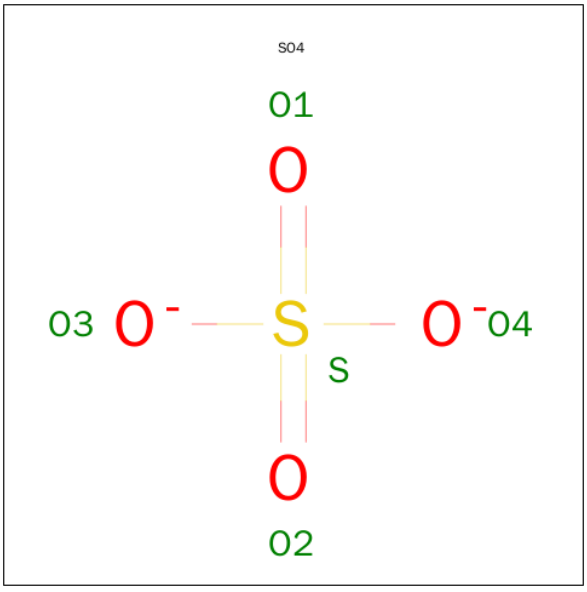
- Molecule 1 is a protein called EXOPOLYGALACTURONASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	2	0
			4439	2784	776	864	15			
1	B	566	Total	C	N	O	S	0	1	0
			4399	2764	769	851	15			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

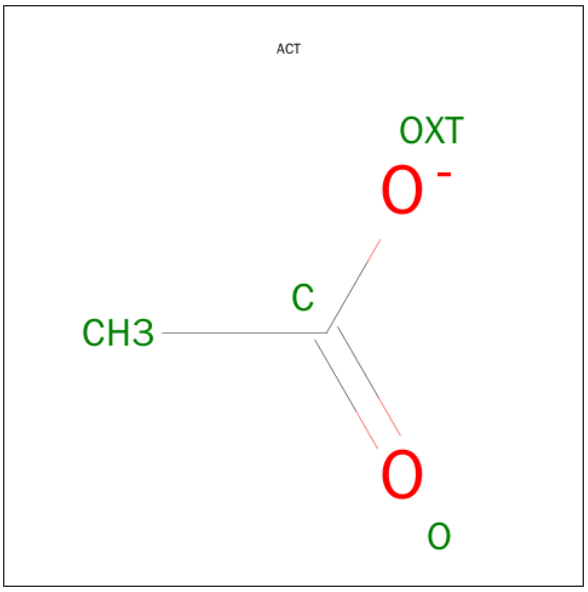
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Ni	0	0
			5	5		
2	A	4	Total	Ni	0	0
			4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

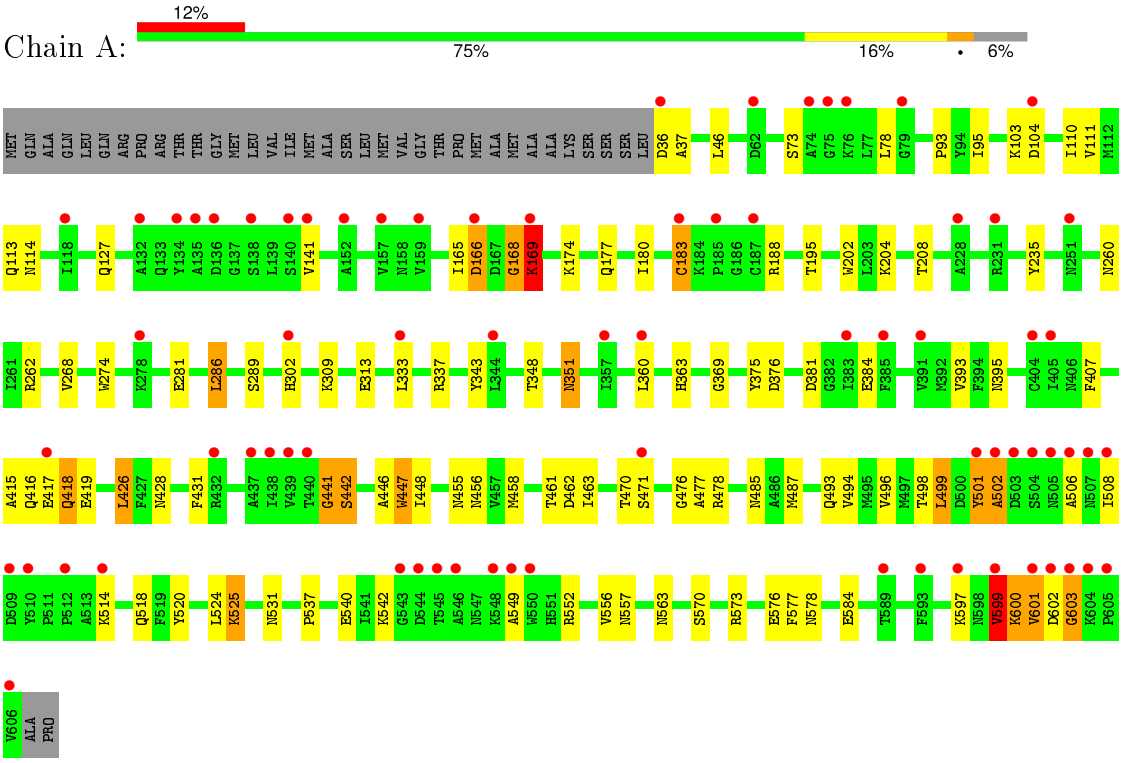
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	177	Total O 177 177	0	0
5	B	286	Total O 286 286	0	0

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.

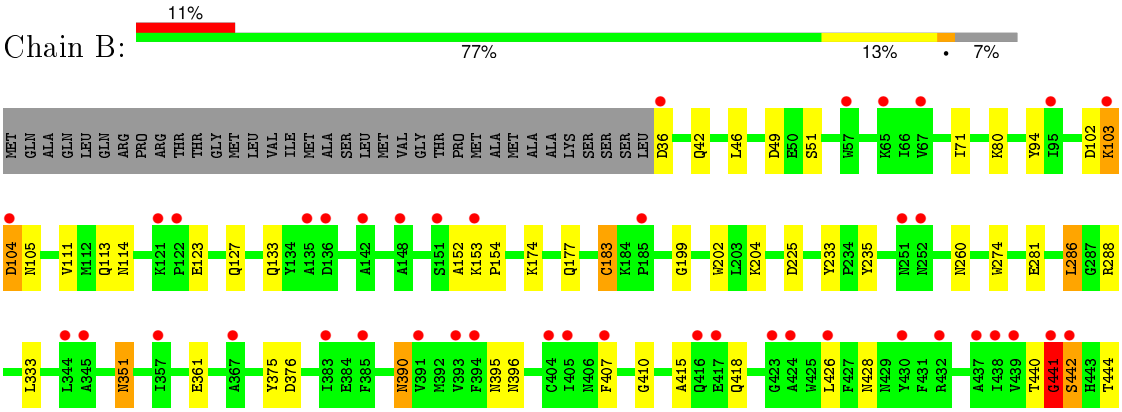
- Molecule 1: EXOPOLYGALACTURONASE

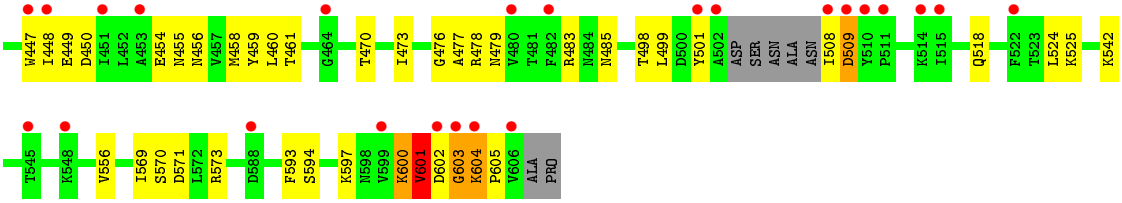
Chain A:



- Molecule 1: EXOPOLYGALACTURONASE

Chain B:




W447
I448
E449
D450
T451
L452
A453
E454
N455
N456
V457
M458
Y459
L460
T461
G464
T470
I473
G476
A477
R478
N479
V480
T481
F482
R483
N484
N485
T498
L499
D500
Y501
A502
ASP
SER
ASN
ALA
ASN
I508
D509
Y510
P511
K514
I515
Q518
F522
T523
L524
K525
K542
T545
K548
V556
I569
S570
D571
L572
R573
D588
F593
S594
K597
N598
V599
K600
V601
D602
G603
K604
P605
V606
ALA
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.95Å 78.76Å 98.19Å 90.00° 103.61° 90.00°	Depositor
Resolution (Å)	34.42 – 2.19 36.84 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.42-2.19) 99.4 (36.84-2.07)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.228 0.245 , 0.245	Depositor DCC
R_{free} test set	3467 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 80343 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9409	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: NI, SO4, ACT

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	0.85	1/4532 (0.0%)	0.82	2/6153 (0.0%)
1	B	0.94	1/4491 (0.0%)	0.86	5/6094 (0.1%)
All	All	0.90	2/9023 (0.0%)	0.84	7/12247 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	7
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	183	CYS	CB-SG	-8.56	1.67	1.82
1	A	183	CYS	CB-SG	-7.20	1.70	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	601	VAL	N-CA-C	8.21	133.16	111.00
1	B	442	SER	N-CA-CB	6.96	120.93	110.50
1	A	188	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	441	GLY	C-N-CA	6.09	136.93	121.70
1	B	49	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	603	GLY	CA-C-O	-5.21	111.22	120.60
1	A	462	ASP	CB-CG-OD1	5.16	122.94	118.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	GLY	Peptide
1	A	441	GLY	Peptide
1	A	501	TYR	Peptide
1	A	502	ALA	Peptide
1	A	599	VAL	Peptide
1	A	600	LYS	Mainchain
1	A	601	VAL	Peptide
1	A	603	GLY	Peptide
1	B	102	ASP	Peptide
1	B	440	THR	Peptide
1	B	441	GLY	Peptide
1	B	501	TYR	Peptide
1	B	600	LYS	Peptide
1	B	601	VAL	Peptide
1	B	604	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4439	0	4323	83	0
1	B	4399	0	4298	70	0
2	A	4	0	0	0	0
2	B	5	0	0	0	0
3	A	55	0	0	6	0
3	B	40	0	0	4	0
4	B	4	0	3	0	0
5	A	177	0	0	5	0
5	B	286	0	0	9	0
All	All	9409	0	8624	157	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 9.

All (157) 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:604:LYS:HB3	1:B:605:PRO:HD3	1.27	1.16
1:A:602:ASP:N	1:A:603:GLY:HA2	1.72	1.05
1:B:603:GLY:O	1:B:604:LYS:CG	2.05	1.04
1:B:604:LYS:CB	1:B:605:PRO:HD3	1.89	1.01
1:A:415:ALA:O	1:A:418:GLN:HG3	1.61	1.00
1:B:603:GLY:O	1:B:604:LYS:HG2	1.66	0.93
1:A:313:GLU:HG3	5:A:2094:HOH:O	1.67	0.91
3:A:1619:SO4:O1	5:A:2176:HOH:O	1.89	0.90
1:A:601:VAL:HG12	1:A:602:ASP:HB3	1.53	0.90
1:B:407:PHE:O	1:B:441:GLY:HA3	1.72	0.89
1:B:603:GLY:O	1:B:604:LYS:HG3	1.71	0.88
1:B:113:GLN:H	1:B:428:ASN:HD21	1.15	0.88
1:A:602:ASP:H	1:A:603:GLY:HA2	1.40	0.86
1:B:450:ASP:OD1	1:B:479:ASN:ND2	2.09	0.85
1:A:113:GLN:H	1:A:428:ASN:HD21	1.24	0.85
1:B:602:ASP:N	1:B:603:GLY:HA2	1.94	0.81
3:B:1619:SO4:S	5:B:2285:HOH:O	2.37	0.81
1:A:418:GLN:OE1	5:A:2135:HOH:O	1.99	0.80
1:A:37:ALA:HB2	1:A:141:VAL:HG23	1.63	0.80
1:B:177:GLN:HE22	1:B:202:TRP:H	1.29	0.80
1:B:600:LYS:NZ	1:B:604:LYS:HE2	1.97	0.79
1:A:599:VAL:HG23	1:A:600:LYS:H	1.48	0.79
1:A:177:GLN:HE22	1:A:202:TRP:H	1.29	0.78
1:A:531[A]:ASN:HD22	1:A:563[A]:ASN:HB3	1.49	0.76
1:B:604:LYS:HB3	1:B:605:PRO:CD	2.14	0.75
1:A:577:PHE:O	1:A:602:ASP:HB2	1.86	0.75
1:A:602:ASP:N	1:A:603:GLY:CA	2.50	0.74
1:B:415:ALA:HA	1:B:418:GLN:HE21	1.51	0.74
1:A:600:LYS:HE2	3:A:1616:SO4:O2	1.87	0.74
1:A:506:ALA:HB1	1:A:508:ILE:HG12	1.68	0.73
1:A:281:GLU:OE1	1:A:289:SER:HB2	1.90	0.72
1:B:601:VAL:HG23	1:B:602:ASP:HB3	1.71	0.72
1:A:600:LYS:HD3	3:A:1616:SO4:O2	1.90	0.71
3:B:1619:SO4:O2	5:B:2285:HOH:O	2.07	0.71
1:B:288[A]:ARG:NH1	5:B:2157:HOH:O	2.06	0.69
1:A:168:GLY:O	1:A:169:LYS:HB3	1.92	0.69
1:A:600:LYS:CE	3:A:1616:SO4:O2	2.41	0.68
1:A:456:ASN:H	1:A:485:ASN:HD22	1.40	0.67
1:A:499:LEU:HD13	1:A:549:ALA:HB1	1.77	0.67
1:B:456:ASN:H	1:B:485:ASN:HD22	1.44	0.66
1:B:274:TRP:H	1:B:351:ASN:HD21	1.42	0.66
1:B:600:LYS:HZ2	1:B:604:LYS:HE2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLN:N	1:A:428:ASN:HD21	1.94	0.66
3:B:1613:SO4:O3	5:B:2282:HOH:O	2.10	0.65
1:B:361:GLU:HG3	5:B:2190:HOH:O	1.94	0.65
1:B:183:CYS:HB2	1:B:204:LYS:HE2	1.78	0.65
1:A:363:HIS:NE2	1:A:419:GLU:OE1	2.21	0.65
1:B:600:LYS:HD3	1:B:604:LYS:HG2	1.79	0.64
1:A:601:VAL:CG1	1:A:602:ASP:HB3	2.26	0.63
1:B:604:LYS:CB	1:B:605:PRO:CD	2.71	0.62
1:B:508:ILE:N	5:B:2245:HOH:O	2.32	0.62
1:A:166:ASP:HB2	1:A:195:THR:O	1.99	0.62
1:A:602:ASP:O	1:A:602:ASP:CG	2.37	0.61
1:A:578:ASN:HA	1:A:602:ASP:HB2	1.83	0.61
1:A:442:SER:CB	3:A:1621:SO4:O4	2.49	0.60
1:A:268:VAL:HG22	1:A:348:THR:HB	1.84	0.60
1:B:113:GLN:N	1:B:428:ASN:HD21	1.95	0.59
1:B:603:GLY:C	1:B:604:LYS:CG	2.70	0.58
1:A:599:VAL:HG23	1:A:600:LYS:N	2.15	0.58
1:A:600:LYS:CD	3:A:1616:SO4:O2	2.51	0.58
1:A:73:SER:HB2	1:A:78:LEU:HD11	1.87	0.57
1:A:113:GLN:H	1:A:428:ASN:ND2	1.98	0.57
1:B:603:GLY:C	1:B:604:LYS:HG3	2.24	0.57
1:B:235:TYR:OH	1:B:418:GLN:NE2	2.40	0.55
1:A:531[A]:ASN:ND2	1:A:563[A]:ASN:HB3	2.21	0.55
1:A:576:GLU:HA	1:A:600:LYS:O	2.07	0.55
1:A:501:TYR:CD2	1:A:502:ALA:HA	2.42	0.54
1:B:390:ASN:HB2	5:B:2208:HOH:O	2.07	0.54
1:A:103:LYS:O	1:A:104:ASP:HB2	2.07	0.54
1:A:302:HIS:O	1:A:309:LYS:HE3	2.08	0.54
1:B:114:ASN:HD21	1:B:395:ASN:HD21	1.57	0.53
1:A:337:ARG:HA	1:A:360:LEU:O	2.09	0.53
1:B:600:LYS:HZ3	1:B:604:LYS:HE2	1.73	0.53
1:B:274:TRP:N	1:B:351:ASN:HD21	2.07	0.52
1:A:93:PRO:HB2	1:A:286:LEU:HD21	1.92	0.52
1:A:416:GLN:C	1:A:418:GLN:H	2.13	0.52
1:A:563[A]:ASN:HA	1:A:584:GLU:O	2.09	0.52
1:A:506:ALA:HB1	1:A:508:ILE:CG1	2.40	0.52
1:A:446:ALA:O	1:A:447:TRP:HB2	2.11	0.51
1:A:183:CYS:HB2	1:A:204:LYS:HE2	1.92	0.51
1:B:602:ASP:N	1:B:603:GLY:CA	2.72	0.51
1:B:570:SER:HA	1:B:594:SER:O	2.12	0.50
1:B:454:GLU:HA	1:B:483:ARG:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:PRO:HB2	1:A:540:GLU:HB2	1.94	0.50
1:B:103:LYS:HG3	1:B:104:ASP:HA	1.93	0.50
1:B:113:GLN:H	1:B:428:ASN:ND2	1.97	0.50
1:B:470:THR:OG1	1:B:473:ILE:HG12	2.12	0.49
1:A:573:ARG:HA	1:A:597:LYS:O	2.13	0.49
1:B:390:ASN:ND2	5:B:2208:HOH:O	2.45	0.49
1:A:114:ASN:HD21	1:A:395:ASN:HD21	1.61	0.49
1:A:525:LYS:HG3	1:A:557:ASN:HB2	1.95	0.49
1:B:508:ILE:HA	1:B:509:ASP:HA	1.42	0.48
1:B:51:SER:HB3	5:B:2068:HOH:O	2.12	0.48
1:B:199:GLY:HA3	1:B:225:ASP:HB3	1.94	0.48
1:A:456:ASN:H	1:A:485:ASN:ND2	2.10	0.48
1:A:46:LEU:HD11	1:A:260:ASN:HA	1.96	0.47
1:A:578:ASN:OD1	1:A:602:ASP:HA	2.13	0.47
1:A:496:VAL:HG12	1:A:498:THR:HG23	1.96	0.47
1:A:281:GLU:OE1	1:A:289:SER:CB	2.61	0.47
1:A:407:PHE:O	1:A:441:GLY:HA3	2.13	0.47
1:A:599:VAL:CG2	1:A:600:LYS:N	2.78	0.47
1:A:499:LEU:HD12	5:A:2160:HOH:O	2.14	0.47
1:B:483:ARG:HA	1:B:525:LYS:O	2.15	0.47
1:A:274:TRP:H	1:A:351:ASN:HD21	1.62	0.47
1:A:111:VAL:H	1:A:455:ASN:ND2	2.13	0.46
1:A:487:MET:HE3	1:A:494:VAL:HG13	1.97	0.46
1:B:602:ASP:H	1:B:603:GLY:HA2	1.78	0.46
1:A:463:ILE:HA	1:A:493:GLN:O	2.15	0.46
1:A:478:ARG:HA	1:A:520:TYR:O	2.16	0.46
1:A:262:ARG:HG2	1:A:343:TYR:HB3	1.98	0.45
1:B:111:VAL:H	1:B:455:ASN:ND2	2.13	0.45
1:B:524:LEU:O	1:B:556:VAL:HA	2.17	0.45
1:B:448:ILE:O	1:B:477:ALA:HA	2.16	0.45
1:B:80:LYS:HE3	1:B:133:GLN:OE1	2.17	0.45
1:B:103:LYS:CG	1:B:104:ASP:HA	2.47	0.45
1:B:602:ASP:CG	1:B:602:ASP:O	2.50	0.44
1:B:498:THR:HG22	1:B:542:LYS:HD3	1.99	0.44
1:B:114:ASN:ND2	1:B:395:ASN:HD21	2.16	0.44
1:B:573:ARG:HA	1:B:597:LYS:O	2.16	0.44
1:A:501:TYR:CG	1:A:502:ALA:HA	2.52	0.44
1:A:180:ILE:O	1:A:183:CYS:HB2	2.18	0.44
1:A:524:LEU:HB3	1:A:556:VAL:HG22	1.99	0.44
1:B:459:TYR:O	1:B:460:LEU:HB2	2.17	0.44
1:B:94:TYR:CD1	1:B:286:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LYS:HA	1:B:105:ASN:H	1.82	0.43
1:B:444:THR:H	1:B:473:ILE:HG21	1.84	0.43
1:A:552:ARG:HA	1:A:573:ARG:O	2.19	0.43
1:B:42:GLN:NE2	3:B:1616:SO4:O4	2.51	0.43
1:B:600:LYS:HB3	1:B:604:LYS:HA	2.01	0.43
1:B:71:ILE:HD12	1:B:71:ILE:N	2.33	0.43
1:A:573:ARG:HD3	1:A:597:LYS:HB3	2.00	0.43
1:A:476:GLY:HA3	1:A:518:GLN:O	2.19	0.43
1:A:235:TYR:OH	1:A:418:GLN:NE2	2.53	0.42
1:A:448:ILE:O	1:A:477:ALA:HA	2.19	0.42
1:A:416:GLN:C	1:A:418:GLN:N	2.73	0.42
1:A:114:ASN:ND2	1:A:395:ASN:HD21	2.17	0.42
1:B:569:ILE:O	1:B:593:PHE:HA	2.20	0.42
1:A:114:ASN:ND2	5:A:2030:HOH:O	2.51	0.42
1:B:274:TRP:H	1:B:351:ASN:ND2	2.12	0.41
1:B:46:LEU:HD11	1:B:260:ASN:HA	2.02	0.41
1:B:449:GLU:HA	1:B:478:ARG:O	2.20	0.41
1:B:600:LYS:HZ3	1:B:604:LYS:CE	2.32	0.41
1:A:563[B]:ASN:HA	1:A:584:GLU:O	2.19	0.41
1:B:103:LYS:CB	1:B:104:ASP:HA	2.50	0.41
1:B:233:TYR:CZ	1:B:410:GLY:HA2	2.56	0.41
1:B:375:TYR:HA	1:B:376:ASP:HA	1.84	0.41
1:A:369:GLY:HA2	1:A:395:ASN:O	2.20	0.40
1:A:431:PHE:HB2	1:A:458:MET:HG3	2.02	0.40
1:A:375:TYR:HA	1:A:376:ASP:HA	1.79	0.40
1:A:381:ASP:OD2	1:A:384:GLU:OE2	2.39	0.40
1:B:476:GLY:HA3	1:B:518:GLN:O	2.21	0.40
1:A:542:LYS:HA	1:A:570:SER:HB2	2.03	0.40
1:A:95:ILE:HG21	1:A:110:ILE:HD11	2.04	0.40
1:A:208:THR:HA	1:A:262:ARG:O	2.21	0.40
1:A:393:VAL:HB	1:A:426:LEU:HD12	2.02	0.40
1:B:123:GLU:HG3	1:B:152:ALA:HA	2.04	0.40
1:B:153:LYS:HD2	1:B:154:PRO:HD2	2.02	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	571/608 (94%)	526 (92%)	42 (7%)	3 (0%)	34	35
1	B	563/608 (93%)	526 (93%)	35 (6%)	2 (0%)	39	42
All	All	1134/1216 (93%)	1052 (93%)	77 (7%)	5 (0%)	39	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	442	SER
1	A	169	LYS
1	A	417	GLU
1	B	447	TRP
1	A	447	TRP

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	479/507 (94%)	460 (96%)	19 (4%)	38	47
1	B	474/507 (94%)	456 (96%)	18 (4%)	40	49
All	All	953/1014 (94%)	916 (96%)	37 (4%)	39	48

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP

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Mol	Chain	Res	Type
1	A	127	GLN
1	A	165	ILE
1	A	166	ASP
1	A	169	LYS
1	A	174	LYS
1	A	286	LEU
1	A	333	LEU
1	A	351	ASN
1	A	418	GLN
1	A	426	LEU
1	A	442	SER
1	A	461	THR
1	A	470	THR
1	A	471	SER
1	A	499	LEU
1	A	514	LYS
1	A	525	LYS
1	A	599	VAL
1	B	36	ASP
1	B	103	LYS
1	B	104	ASP
1	B	127	GLN
1	B	174	LYS
1	B	281	GLU
1	B	286	LEU
1	B	333	LEU
1	B	351	ASN
1	B	390	ASN
1	B	396	ASN
1	B	426	LEU
1	B	458	MET
1	B	461	THR
1	B	499	LEU
1	B	509	ASP
1	B	571	ASP
1	B	601	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	127	GLN

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Mol	Chain	Res	Type
1	A	177	GLN
1	A	178	GLN
1	A	324	ASN
1	A	351	ASN
1	A	387	ASN
1	A	390	ASN
1	A	418	GLN
1	A	428	ASN
1	A	455	ASN
1	A	485	ASN
1	A	592	HIS
1	B	101	ASN
1	B	114	ASN
1	B	127	GLN
1	B	177	GLN
1	B	178	GLN
1	B	351	ASN
1	B	387	ASN
1	B	390	ASN
1	B	418	GLN
1	B	428	ASN
1	B	455	ASN
1	B	485	ASN
1	B	518	GLN
1	B	531	ASN
1	B	563	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 9 are monoatomic - leaving 20 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	SO4	A	1611	-	4,4,4	0.32	0	6,6,6	0.77	0
3	SO4	A	1612	-	4,4,4	0.20	0	6,6,6	0.20	0
3	SO4	A	1613	-	4,4,4	0.20	0	6,6,6	0.20	0
3	SO4	A	1614	-	4,4,4	0.44	0	6,6,6	0.52	0
3	SO4	A	1615	-	4,4,4	1.38	0	6,6,6	1.19	1 (16%)
3	SO4	A	1616	1	4,4,4	0.60	0	6,6,6	0.34	0
3	SO4	A	1617	-	4,4,4	0.59	0	6,6,6	0.93	0
3	SO4	A	1618	-	4,4,4	0.71	0	6,6,6	0.95	0
3	SO4	A	1619	-	4,4,4	0.52	0	6,6,6	0.46	0
3	SO4	A	1620	-	4,4,4	0.50	0	6,6,6	0.22	0
3	SO4	A	1621	1	4,4,4	1.48	0	6,6,6	1.71	1 (16%)
3	SO4	B	1612	-	4,4,4	0.62	0	6,6,6	0.58	0
3	SO4	B	1613	-	4,4,4	0.15	0	6,6,6	0.43	0
3	SO4	B	1614	-	4,4,4	0.16	0	6,6,6	0.40	0
3	SO4	B	1615	-	4,4,4	0.51	0	6,6,6	0.18	0
3	SO4	B	1616	-	4,4,4	0.53	0	6,6,6	0.23	0
3	SO4	B	1617	-	4,4,4	0.46	0	6,6,6	0.49	0
3	SO4	B	1618	-	4,4,4	0.64	0	6,6,6	0.68	0
3	SO4	B	1619	-	4,4,4	1.47	0	6,6,6	1.71	1 (16%)
4	ACT	B	1620	-	1,3,3	0.45	0	0,3,3	0.00	-

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	SO4	A	1611	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1612	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1613	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1614	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1615	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1616	1	-	0/0/0/0	0/0/0/0
3	SO4	A	1617	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1618	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1619	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1620	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1621	1	-	0/0/0/0	0/0/0/0
3	SO4	B	1612	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1613	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1614	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1615	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1616	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1617	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1618	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1619	-	-	0/0/0/0	0/0/0/0
4	ACT	B	1620	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1615	SO4	O4-S-O3	2.23	118.05	108.98
3	B	1619	SO4	O4-S-O3	4.03	125.36	108.98
3	A	1621	SO4	O4-S-O3	4.04	125.39	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1616	SO4	4	0
3	A	1619	SO4	1	0
3	A	1621	SO4	1	0
3	B	1613	SO4	1	0
3	B	1616	SO4	1	0
3	B	1619	SO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	571/608 (93%)	1.01	73 (12%)	5 4	4, 26, 45, 79	2 (0%)
1	B	566/608 (93%)	1.02	66 (11%)	6 6	3, 19, 33, 57	1 (0%)
All	All	1137/1216 (93%)	1.01	139 (12%)	5 5	3, 22, 41, 79	3 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	SER	10.4
1	B	508	ILE	9.4
1	A	508	ILE	7.6
1	A	505	ASN	7.4
1	A	503	ASP	6.6
1	A	502	ALA	6.0
1	A	506	ALA	5.7
1	A	507	ASN	5.5
1	A	231	ARG	5.3
1	A	501	TYR	5.1
1	B	432	ARG	4.8
1	A	549	ALA	4.7
1	A	606	VAL	4.7
1	A	141	VAL	4.5
1	A	605	PRO	4.5
1	A	509	ASP	4.4
1	A	75	GLY	4.4
1	A	438	ILE	4.1
1	A	432	ARG	3.9
1	B	603	GLY	3.8
1	A	135	ALA	3.7
1	B	438	ILE	3.5
1	B	502	ALA	3.4
1	A	604	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	169	LYS	3.3
1	A	157	VAL	3.2
1	A	548	LYS	3.2
1	A	550	TRP	3.2
1	B	405	ILE	3.2
1	B	416	GLN	3.2
1	A	602	ASP	3.1
1	A	251	ASN	3.1
1	B	602	ASP	3.1
1	B	393	VAL	3.1
1	B	509	ASP	3.0
1	B	426	LEU	3.0
1	B	36	ASP	3.0
1	A	383	ILE	3.0
1	A	134	TYR	3.0
1	A	278	LYS	3.0
1	B	510	TYR	3.0
1	B	423	GLY	3.0
1	B	391	VAL	2.9
1	B	453	ALA	2.9
1	B	135	ALA	2.9
1	B	367	ALA	2.9
1	B	451	ILE	2.9
1	A	514	LYS	2.9
1	B	604	LYS	2.9
1	A	74	ALA	2.9
1	A	152	ALA	2.9
1	B	441	GLY	2.8
1	B	383	ILE	2.8
1	B	515	ILE	2.8
1	B	136	ASP	2.8
1	B	439	VAL	2.8
1	A	546	ALA	2.8
1	B	430	TYR	2.7
1	B	514	LYS	2.7
1	B	357	ILE	2.7
1	A	118	ILE	2.7
1	A	439	VAL	2.7
1	A	138	SER	2.7
1	B	501	TYR	2.7
1	A	593	PHE	2.7
1	A	405	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	440	THR	2.7
1	B	65	LYS	2.7
1	B	252	ASN	2.6
1	A	36	ASP	2.6
1	A	601	VAL	2.6
1	B	148	ALA	2.6
1	B	606	VAL	2.6
1	B	522	PHE	2.5
1	B	121	LYS	2.5
1	B	251	ASN	2.5
1	B	344	LEU	2.5
1	B	104	ASP	2.5
1	A	136	ASP	2.5
1	B	424	ALA	2.5
1	B	545	THR	2.5
1	A	76	LYS	2.4
1	B	417	GLU	2.4
1	A	132	ALA	2.4
1	A	187	CYS	2.4
1	B	511	PRO	2.4
1	B	385	PHE	2.4
1	A	166	ASP	2.4
1	B	122	PRO	2.4
1	B	447	TRP	2.4
1	A	228	ALA	2.3
1	B	437	ALA	2.3
1	A	417	GLU	2.3
1	B	153	LYS	2.3
1	A	603	GLY	2.3
1	A	302	HIS	2.3
1	B	394	PHE	2.3
1	A	183	CYS	2.3
1	B	151	SER	2.3
1	A	391	VAL	2.3
1	B	448	ILE	2.3
1	A	437	ALA	2.3
1	A	471	SER	2.2
1	A	512	PRO	2.2
1	A	545	THR	2.2
1	A	357	ILE	2.2
1	A	404	CYS	2.2
1	B	57	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	185	PRO	2.2
1	A	360	LEU	2.2
1	A	385	PHE	2.2
1	B	548	LYS	2.2
1	A	140	SER	2.2
1	B	67	VAL	2.2
1	B	588	ASP	2.2
1	B	95	ILE	2.2
1	B	599	VAL	2.2
1	A	333	LEU	2.1
1	A	62	ASP	2.1
1	A	344	LEU	2.1
1	B	482	PHE	2.1
1	B	142	ALA	2.1
1	B	103	LYS	2.1
1	B	407	PHE	2.1
1	A	589	THR	2.1
1	A	104	ASP	2.1
1	B	464	GLY	2.1
1	A	599	VAL	2.1
1	B	185	PRO	2.1
1	A	510	TYR	2.1
1	A	159	VAL	2.1
1	A	544	ASP	2.1
1	B	345	ALA	2.0
1	A	597	LYS	2.0
1	B	480	VAL	2.0
1	B	404	CYS	2.0
1	B	442	SER	2.0
1	A	79	GLY	2.0
1	A	543	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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	SO4	A	1616	5/5	0.81	0.55	10.45	50,51,53,54	0
3	SO4	A	1620	5/5	0.87	0.34	9.76	43,46,50,50	0
3	SO4	A	1617	5/5	0.90	0.34	9.06	47,48,49,49	0
3	SO4	A	1615	5/5	0.87	0.32	8.88	45,45,49,52	0
3	SO4	A	1612	5/5	0.80	0.28	8.58	74,75,76,77	0
3	SO4	A	1618	5/5	0.84	0.48	3.82	52,55,57,57	0
3	SO4	B	1612	5/5	0.87	0.31	3.33	33,46,46,46	0
4	ACT	B	1620	4/4	0.87	0.28	3.18	20,20,20,20	0
3	SO4	A	1619	5/5	0.91	0.24	2.49	46,47,47,49	0
3	SO4	B	1613	5/5	0.86	0.20	1.70	58,60,60,62	0
3	SO4	A	1611	5/5	0.90	0.25	0.22	50,50,55,55	0
2	NI	B	1608	1/1	0.93	0.08	-2.84	29,29,29,29	0
2	NI	A	1607	1/1	0.95	0.07	-3.46	33,33,33,33	0
2	NI	B	1610	1/1	0.93	0.07	-7.39	35,35,35,35	0
3	SO4	A	1621	5/5	0.83	0.32	-	20,20,20,20	0
2	NI	A	1610	1/1	0.89	0.15	-	93,93,93,93	0
2	NI	A	1608	1/1	0.93	0.13	-	41,41,41,41	0
3	SO4	B	1615	5/5	0.76	0.45	-	49,53,53,56	0
2	NI	B	1609	1/1	0.93	0.14	-	38,38,38,38	0
2	NI	B	1607	1/1	0.98	0.07	-	30,30,30,30	0
3	SO4	B	1616	5/5	0.81	0.50	-	55,57,60,60	0
3	SO4	B	1617	5/5	0.89	0.30	-	51,53,54,56	0
2	NI	A	1609	1/1	0.82	0.08	-	92,92,92,92	0
3	SO4	A	1613	5/5	0.86	0.26	-	62,63,64,64	0
3	SO4	A	1614	5/5	0.90	0.18	-	38,38,41,41	0
3	SO4	B	1618	5/5	0.84	0.31	-	43,49,51,53	0
3	SO4	B	1619	5/5	0.82	0.34	-	20,20,20,20	0
2	NI	B	1611	1/1	0.49	0.08	-	136,136,136,136	0
3	SO4	B	1614	5/5	0.87	0.30	-	51,52,54,55	0

6.5 Other polymers

There are no such residues in this entry.