Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:15 pm BST

PDB ID	:	2UVE
Title	:	Structure of Yersinia enterocolitica Family 28 Exopolygalacturonase
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
https://www.wwpdb.org/validation/2017/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:

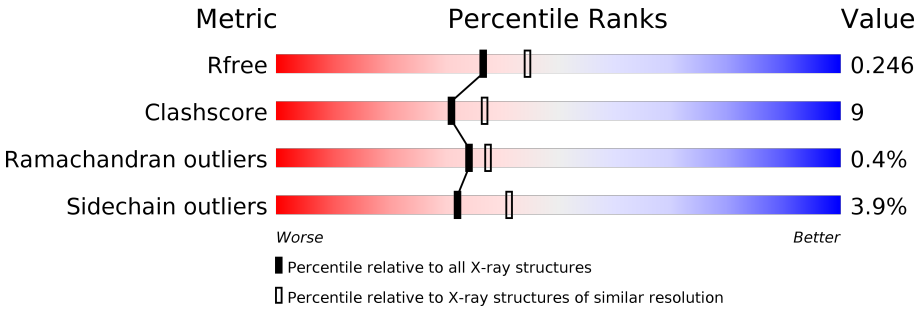
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.19 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	608	75% 16% • 6%
1	B	608	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	1616	-	-	X	-
3	SO4	B	1619	-	-	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.

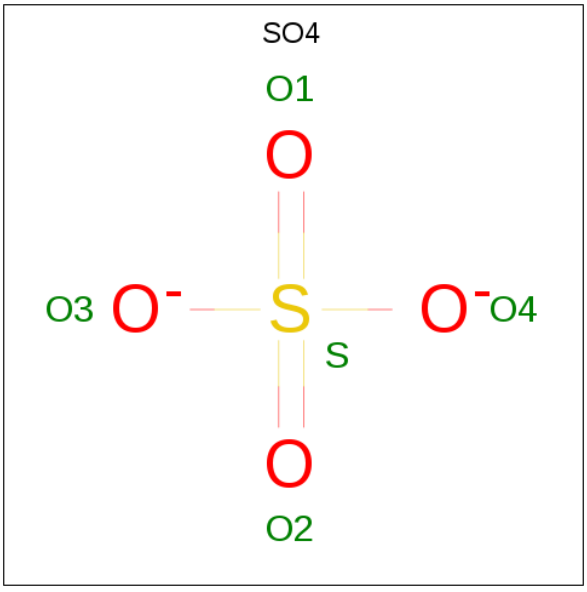
- Molecule 1 is a protein called EXOPOLYGALACTURONASE.

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).

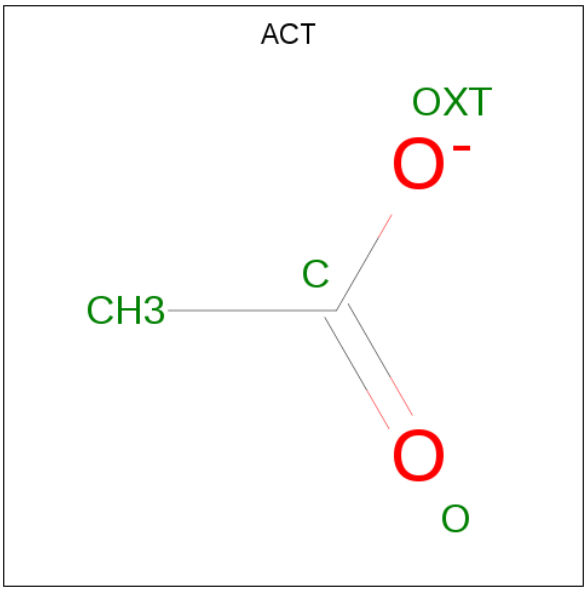
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Ni	0	0
			5	5		
2	A	4	Total	Ni	0	0
			4	4		

- 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.

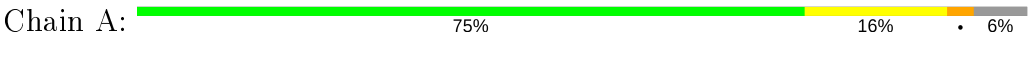
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	177	Total O 177 177	0	0
5	B	286	Total O 286 286	0	0

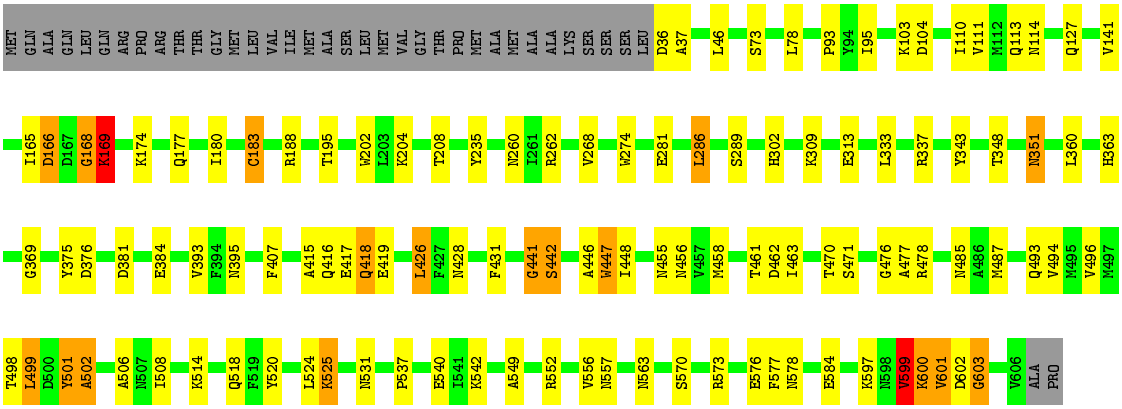
3 Residue-property plots (i)

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

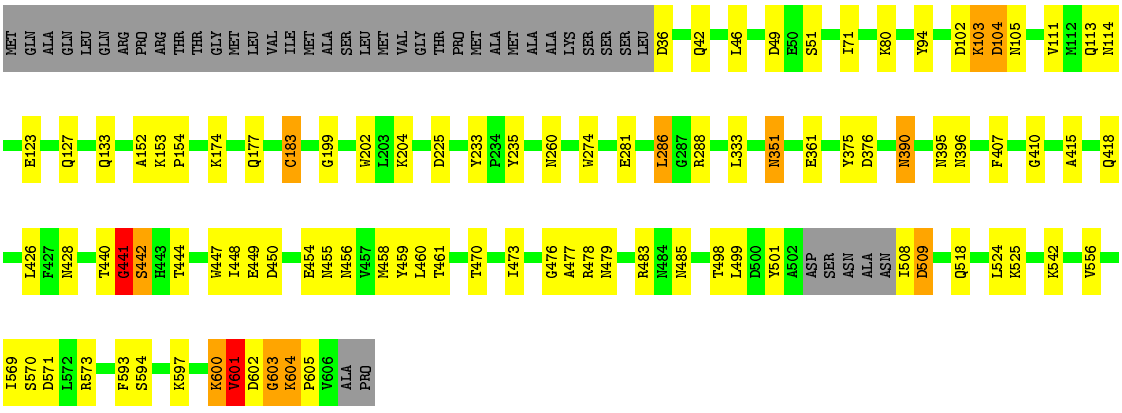
Chain A:





- Molecule 1: EXOPOLYGALACTURONASE

Chain B:



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 , 0.246	Depositor DCC
R_{free} test set	4035 reflections (5.02%)	wwPDB-VP
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
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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
3:B:1619:SO4:S	5:B:2285:HOH:O	2.37	0.81
1:B:602:ASP:N	1:B:603:GLY:HA2	1.94	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:A:113:GLN:N	1:A:428:ASN:HD21	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:LYS:HZ2	1:B:604:LYS:HE2	1.59	0.66
3:B:1613:SO4:O3	5:B:2282:HOH:O	2.10	0.65
1:B:183:CYS:HB2	1:B:204:LYS:HE2	1.78	0.65
1:B:361:GLU:HG3	5:B:2190:HOH:O	1.94	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:A:166:ASP:HB2	1:A:195:THR:O	1.99	0.62
1:B:508:ILE:N	5:B:2245:HOH:O	2.32	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:103:LYS:O	1:A:104:ASP:HB2	2.07	0.54
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: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:183:CYS:HB2	1:A:204:LYS:HE2	1.92	0.51
1:A:446:ALA:O	1:A:447:TRP:HB2	2.11	0.51
1:B:602:ASP:N	1:B:603:GLY:CA	2.72	0.51
1:B:454:GLU:HA	1:B:483:ARG:O	2.11	0.50
1:B:570:SER:HA	1:B:594:SER:O	2.12	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:A:573:ARG:HA	1:A:597:LYS:O	2.13	0.49
1:B:470:THR:OG1	1:B:473:ILE:HG12	2.12	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:496:VAL:HG12	1:A:498:THR:HG23	1.96	0.47
1:A:578:ASN:OD1	1:A:602:ASP:HA	2.13	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:A:463:ILE:HA	1:A:493:GLN:O	2.15	0.46
1:B:602:ASP:H	1:B:603:GLY:HA2	1.78	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:448:ILE:O	1:B:477:ALA:HA	2.16	0.45
1:B:524:LEU:O	1:B:556:VAL:HA	2.17	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:180:ILE:O	1:A:183:CYS:HB2	2.18	0.44
1:A:501:TYR:CG	1:A:502:ALA:HA	2.52	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:A:552:ARG:HA	1:A:573:ARG:O	2.19	0.43
1:B:444:THR:H	1:B:473:ILE:HG21	1.84	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:476:GLY:HA3	1:A:518:GLN:O	2.19	0.43
1:A:573:ARG:HD3	1:A:597:LYS:HB3	2.00	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:A:563[B]:ASN:HA	1:A:584:GLU:O	2.19	0.41
1:B:600:LYS:HZ3	1:B:604:LYS:CE	2.32	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: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:A:431:PHE:HB2	1:A:458:MET:HG3	2.02	0.40
1:A:95:ILE:HG21	1:A:110:ILE:HD11	2.04	0.40
1:A:542:LYS:HA	1:A:570:SER:HB2	2.03	0.40
1:B:476:GLY:HA3	1:B:518:GLN:O	2.21	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%)	29	31
1	B	563/608 (93%)	526 (93%)	35 (6%)	2 (0%)	34	37
All	All	1134/1216 (93%)	1052 (93%)	77 (7%)	5 (0%)	34	37

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%)	31	40
1	B	474/507 (94%)	456 (96%)	18 (4%)	33	42
All	All	953/1014 (94%)	916 (96%)	37 (4%)	32	41

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

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 (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	B	1616	-	4,4,4	0.43	0	6,6,6	0.33	0
3	SO4	A	1621	1	4,4,4	0.99	0	6,6,6	1.66	1 (16%)
3	SO4	B	1612	-	4,4,4	0.48	0	6,6,6	0.87	0
3	SO4	B	1619	-	4,4,4	0.98	0	6,6,6	1.66	1 (16%)
3	SO4	A	1617	-	4,4,4	0.47	0	6,6,6	0.87	0
3	SO4	B	1613	-	4,4,4	0.14	0	6,6,6	0.52	0
3	SO4	A	1613	-	4,4,4	0.18	0	6,6,6	0.34	0
3	SO4	A	1614	-	4,4,4	0.32	0	6,6,6	0.47	0
3	SO4	B	1614	-	4,4,4	0.23	0	6,6,6	0.31	0
4	ACT	B	1620	-	1,3,3	0.42	0	0,3,3	0.00	-
3	SO4	A	1620	-	4,4,4	0.34	0	6,6,6	0.37	0
3	SO4	A	1616	1	4,4,4	0.48	0	6,6,6	0.57	0
3	SO4	B	1617	-	4,4,4	0.38	0	6,6,6	0.66	0
3	SO4	A	1619	-	4,4,4	0.34	0	6,6,6	0.48	0
3	SO4	A	1612	-	4,4,4	0.26	0	6,6,6	0.32	0
3	SO4	A	1618	-	4,4,4	0.45	0	6,6,6	0.87	0
3	SO4	A	1615	-	4,4,4	0.67	0	6,6,6	1.14	1 (16%)
3	SO4	B	1615	-	4,4,4	0.45	0	6,6,6	0.26	0
3	SO4	B	1618	-	4,4,4	0.42	0	6,6,6	0.83	0
3	SO4	A	1611	-	4,4,4	0.33	0	6,6,6	0.49	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	1621	SO4	O4-S-O3	3.83	125.39	109.06
3	B	1619	SO4	O4-S-O3	3.82	125.36	109.06
3	A	1615	SO4	O4-S-O3	2.10	118.05	109.06

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	B	1616	SO4	1	0
3	A	1621	SO4	1	0
3	B	1619	SO4	2	0
3	B	1613	SO4	1	0
3	A	1616	SO4	4	0
3	A	1619	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.