Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2026 – 11:29 PM UTC

PDB ID	:	1Y7B / pdb_00001y7b
Title	:	BETA-D-XYLOSIDASE, A FAMILY 43 GLYCOSIDE HYDROLASE
Authors	:	Teplyakov, A.; Fedorov, E.; Gilliland, G.L.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-12-08
Resolution	:	1.60 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 (i) 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 (i)) were used in the production of this report:

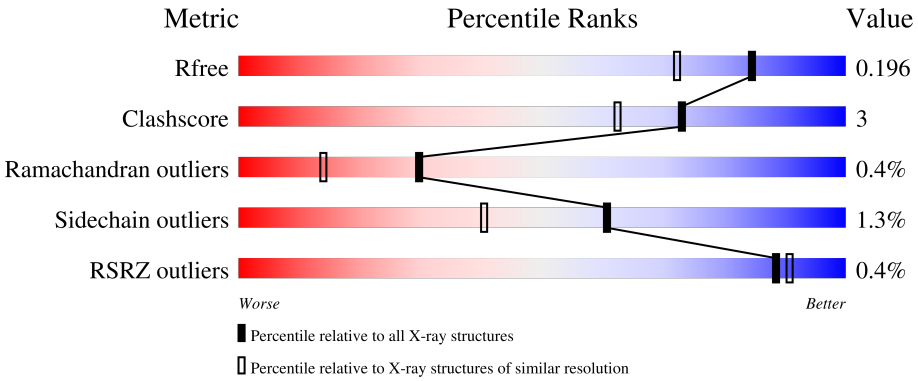
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 <=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	542	91% 8% ·
1	B	542	91% 7% ··
1	C	542	% 89% 8% ··
1	D	542	91% 6% ··

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20552 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 Beta-xylosidase, family 43 glycosyl hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4341	2783	723	821	14			
1	B	534	Total	C	N	O	S	0	0	0
			4341	2783	723	821	14			
1	C	534	Total	C	N	O	S	0	0	0
			4341	2783	723	821	14			
1	D	534	Total	C	N	O	S	0	0	0
			4341	2783	723	821	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	cloning artifact	UNP Q97DM1
A	3	LEU	-	cloning artifact	UNP Q97DM1
A	535	GLU	LEU	cloning artifact	UNP Q97DM1
A	536	GLY	-	cloning artifact	UNP Q97DM1
A	537	HIS	-	expression tag	UNP Q97DM1
A	538	HIS	-	expression tag	UNP Q97DM1
A	539	HIS	-	expression tag	UNP Q97DM1
A	540	HIS	-	expression tag	UNP Q97DM1
A	541	HIS	-	expression tag	UNP Q97DM1
A	542	HIS	-	expression tag	UNP Q97DM1
B	2	SER	-	cloning artifact	UNP Q97DM1
B	3	LEU	-	cloning artifact	UNP Q97DM1
B	535	GLU	LEU	cloning artifact	UNP Q97DM1
B	536	GLY	-	cloning artifact	UNP Q97DM1
B	537	HIS	-	expression tag	UNP Q97DM1
B	538	HIS	-	expression tag	UNP Q97DM1
B	539	HIS	-	expression tag	UNP Q97DM1
B	540	HIS	-	expression tag	UNP Q97DM1
B	541	HIS	-	expression tag	UNP Q97DM1
B	542	HIS	-	expression tag	UNP Q97DM1
C	2	SER	-	cloning artifact	UNP Q97DM1

Continued on next page...

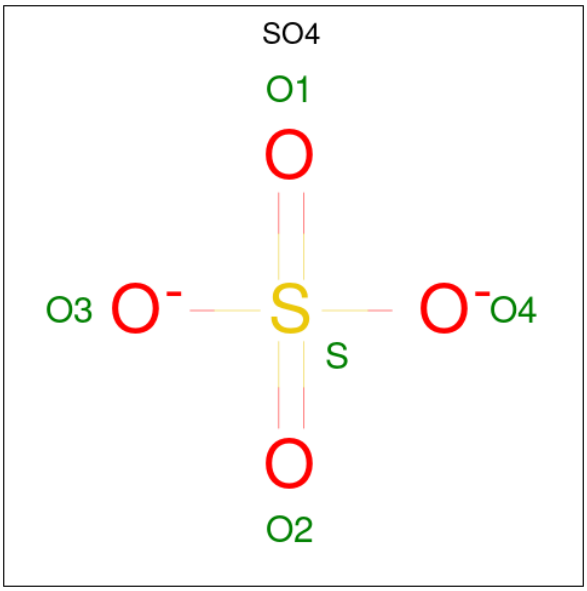
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	LEU	-	cloning artifact	UNP Q97DM1
C	535	GLU	LEU	cloning artifact	UNP Q97DM1
C	536	GLY	-	cloning artifact	UNP Q97DM1
C	537	HIS	-	expression tag	UNP Q97DM1
C	538	HIS	-	expression tag	UNP Q97DM1
C	539	HIS	-	expression tag	UNP Q97DM1
C	540	HIS	-	expression tag	UNP Q97DM1
C	541	HIS	-	expression tag	UNP Q97DM1
C	542	HIS	-	expression tag	UNP Q97DM1
D	2	SER	-	cloning artifact	UNP Q97DM1
D	3	LEU	-	cloning artifact	UNP Q97DM1
D	535	GLU	LEU	cloning artifact	UNP Q97DM1
D	536	GLY	-	cloning artifact	UNP Q97DM1
D	537	HIS	-	expression tag	UNP Q97DM1
D	538	HIS	-	expression tag	UNP Q97DM1
D	539	HIS	-	expression tag	UNP Q97DM1
D	540	HIS	-	expression tag	UNP Q97DM1
D	541	HIS	-	expression tag	UNP Q97DM1
D	542	HIS	-	expression tag	UNP Q97DM1

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

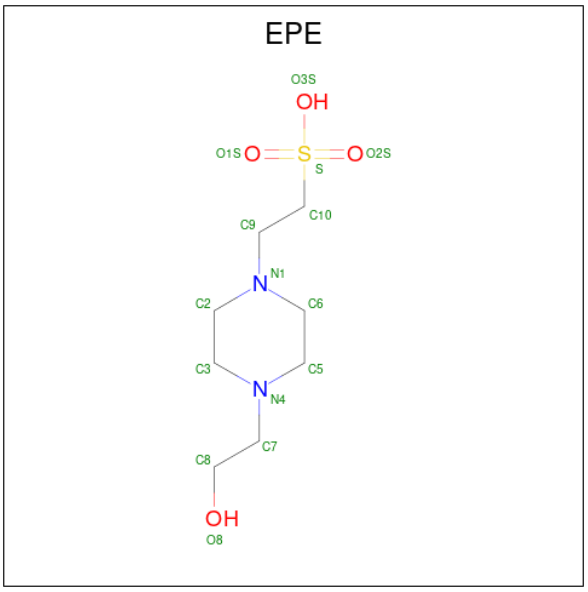
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



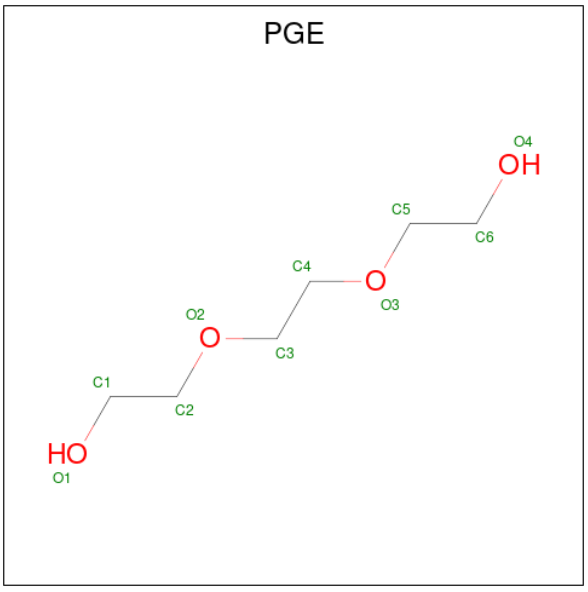
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



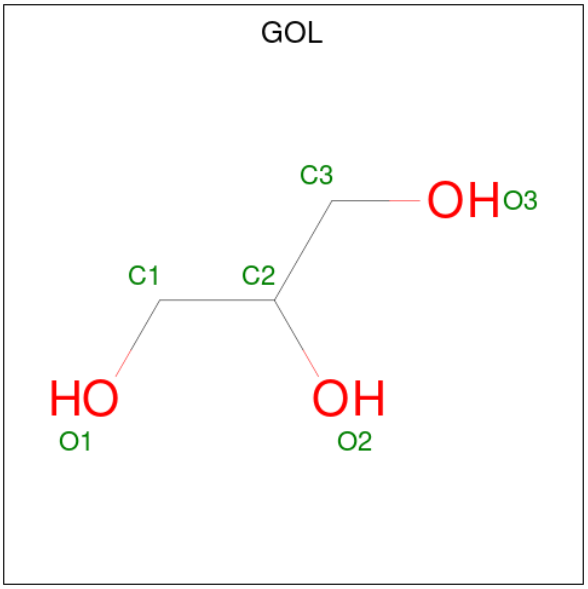
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

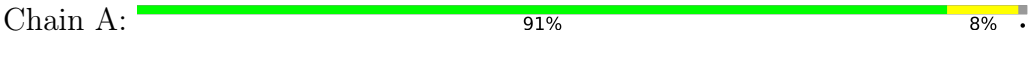
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	800	Total O 800 800	0	0
7	B	704	Total O 704 704	0	0
7	C	745	Total O 745 745	0	0
7	D	751	Total O 751 751	0	0

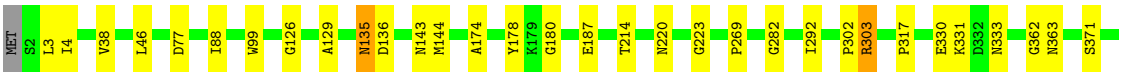
3 Residue-property plots (i)

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: Beta-xylosidase, family 43 glycosyl hydrolase

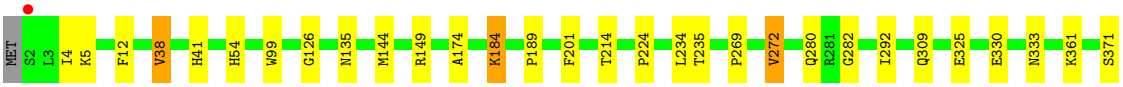
Chain A:

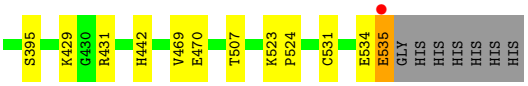




• Molecule 1: Beta-xylosidase, family 43 glycosyl hydrolase

Chain B:



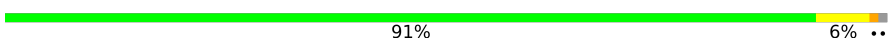


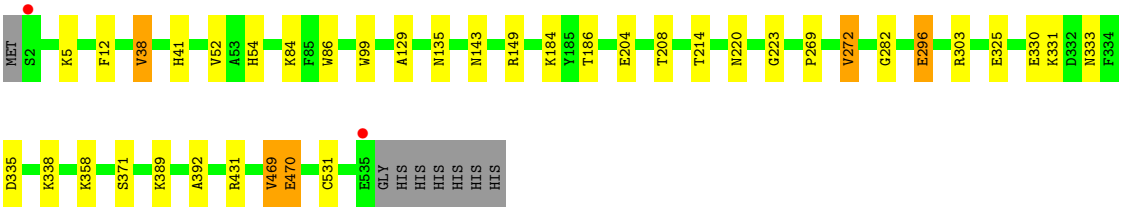
• Molecule 1: Beta-xylosidase, family 43 glycosyl hydrolase

Chain C:

• Molecule 1: Beta-xylosidase, family 43 glycosyl hydrolase

Chain D:




MET
S2
K5
F12
V38
H41
V52
A53
H54
K84
F85
W86
W99
A129
N135
N143
R149
K184
Y185
T186
E204
T208
T214
N220
G223
P269
V272
G282
E296
R303
E325
E330
K331
D332
N333
F334
D335
K338
K358
S371
K389
A392
R431
V469
E470
C531
E535
GLY
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.48Å 136.15Å 183.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.60 25.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-1.60) 93.6 (25.00-1.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.157 , 0.206 (Not available) , 0.196	Depositor DCC
R_{free} test set	5899 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	20552	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: PGE, GOL, CA, SO4, EPE

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	0.81	0/4474	0.91	0/6089
1	B	0.77	0/4474	0.91	0/6089
1	C	0.78	1/4474 (0.0%)	0.90	1/6089 (0.0%)
1	D	0.78	0/4474	0.91	2/6089 (0.0%)
All	All	0.78	1/17896 (0.0%)	0.91	3/24356 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	ILE	CA-CB	5.79	1.60	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	206	GLY	N-CA-C	-6.37	104.66	112.68
1	D	52	VAL	N-CA-C	5.53	118.94	113.53
1	D	208	THR	CB-CA-C	-5.34	107.72	114.40

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	4341	0	4127	33	0
1	B	4341	0	4127	28	0
1	C	4341	0	4127	34	0
1	D	4341	0	4127	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	D	10	0	0	0	0
4	A	15	0	17	1	0
4	B	15	0	17	1	0
4	C	15	0	17	0	0
4	D	15	0	17	0	0
5	A	10	0	14	0	0
6	A	24	0	32	2	0
6	B	24	0	32	0	0
6	C	18	0	24	1	0
6	D	18	0	24	0	0
7	A	800	0	0	4	0
7	B	704	0	0	10	0
7	C	745	0	0	9	0
7	D	751	0	0	8	0
All	All	20552	0	16702	111	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 3.

All (111) 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:C:261:TYR:HB3	1:C:292:ILE:HD11	1.52	0.90
1:C:315:GLU:HG3	7:C:3300:HOH:O	1.73	0.88
1:C:442:HIS:HB2	7:C:3656:HOH:O	1.79	0.83
1:B:5:LYS:HG3	7:B:3299:HOH:O	1.81	0.81
1:A:303:ARG:HG3	1:A:303:ARG:HH11	1.51	0.75
1:D:335:ASP:HB2	7:D:3747:HOH:O	1.85	0.75
1:D:5:LYS:HG2	7:D:3707:HOH:O	1.89	0.71
1:B:442:HIS:HB2	7:B:3686:HOH:O	1.90	0.70
1:D:272:VAL:HG12	7:D:3376:HOH:O	1.90	0.70
1:C:389:LYS:HG2	1:C:535:GLU:HG3	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:LYS:HE2	7:C:3604:HOH:O	1.93	0.67
1:D:41:HIS:ND1	7:D:3341:HOH:O	2.11	0.67
1:D:269:PRO:HB3	1:D:282:GLY:HA3	1.75	0.66
1:C:449:SER:HA	7:C:3729:HOH:O	1.96	0.65
1:C:331:LYS:HE2	1:C:333:ASN:HD21	1.61	0.65
1:A:449:SER:HA	7:A:3625:HOH:O	1.97	0.65
1:B:272:VAL:HG23	7:B:3420:HOH:O	1.98	0.63
1:A:362:GLY:C	1:A:363:ASN:HD22	2.09	0.60
1:C:337:ASP:HB2	7:C:3752:HOH:O	2.01	0.59
1:C:84:LYS:HE3	1:C:86:TRP:CZ2	2.38	0.58
1:A:269:PRO:HB3	1:A:282:GLY:HA3	1.86	0.58
1:A:4:ILE:HG21	1:A:292:ILE:CG2	2.35	0.57
1:C:194:ILE:HG22	6:C:3020:GOL:H31	1.86	0.57
1:C:261:TYR:CB	1:C:292:ILE:HD11	2.33	0.57
1:C:269:PRO:HB3	1:C:282:GLY:HA3	1.87	0.57
1:C:272:VAL:HG23	7:C:3754:HOH:O	2.05	0.57
1:A:303:ARG:HH11	1:A:303:ARG:CG	2.17	0.57
1:B:361:LYS:HE3	7:B:3609:HOH:O	2.06	0.56
1:D:470:GLU:H	1:D:470:GLU:CD	2.12	0.55
1:C:361:LYS:HD3	7:C:3761:HOH:O	2.07	0.55
1:A:99:TRP:CD2	1:B:371:SER:HB2	2.42	0.55
1:D:220:ASN:ND2	1:D:223:GLY:O	2.40	0.54
1:B:269:PRO:HB3	1:B:282:GLY:HA3	1.90	0.52
1:D:296:GLU:HG3	7:D:3664:HOH:O	2.09	0.52
1:A:187:GLU:OE2	6:A:3017:GOL:H12	2.10	0.52
1:D:358:LYS:HG3	7:D:3404:HOH:O	2.10	0.52
1:A:331:LYS:HE2	1:A:333:ASN:HD21	1.76	0.51
1:C:4:ILE:HG21	1:C:292:ILE:HG23	1.94	0.50
1:A:129:ALA:HA	1:A:143:ASN:HB3	1.94	0.50
1:C:362:GLY:C	1:C:363:ASN:HD22	2.20	0.50
1:A:135:ASN:HD22	1:A:135:ASN:C	2.20	0.49
1:C:4:ILE:HG21	1:C:292:ILE:CG2	2.42	0.49
1:C:165:ASP:O	1:C:168:LYS:HD3	2.12	0.49
1:C:330:GLU:O	1:C:531:CYS:HA	2.13	0.49
1:B:126:GLY:HA3	1:B:144:MET:O	2.13	0.49
1:B:280:GLN:HB3	7:B:3543:HOH:O	2.13	0.48
1:A:302:PRO:O	1:A:303:ARG:HD3	2.14	0.48
1:B:523:LYS:HG3	1:B:524:PRO:HD2	1.96	0.47
1:A:371:SER:HB2	1:B:99:TRP:CD2	2.50	0.47
1:A:126:GLY:HA3	1:A:144:MET:O	2.14	0.47
1:B:12:PHE:CE1	1:B:507:THR:HA	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:SER:HB2	1:D:99:TRP:CD2	2.50	0.47
1:A:174:ALA:HB3	4:A:3006:EPE:H101	1.97	0.47
1:B:234:LEU:O	1:B:235:THR:HB	2.15	0.46
1:C:38:VAL:O	1:C:54:HIS:HA	2.16	0.46
1:C:389:LYS:HE3	1:C:469:VAL:HG23	1.98	0.46
1:A:99:TRP:CE3	1:B:371:SER:HB2	2.50	0.46
1:D:389:LYS:HE3	1:D:389:LYS:HB2	1.72	0.46
1:B:41:HIS:ND1	7:B:3343:HOH:O	2.27	0.46
1:B:174:ALA:HB3	4:B:3005:EPE:H101	1.98	0.46
1:A:220:ASN:ND2	1:A:223:GLY:O	2.40	0.46
1:D:129:ALA:HA	1:D:143:ASN:HB3	1.98	0.45
1:C:316:ALA:HB1	1:C:317:PRO:HD2	1.99	0.45
1:A:371:SER:HB2	1:B:99:TRP:CE3	2.52	0.45
1:C:98:MET:HG3	1:C:99:TRP:CE3	2.52	0.45
1:A:3:LEU:HD12	1:A:3:LEU:O	2.17	0.45
1:C:325:GLU:HG2	7:C:3671:HOH:O	2.17	0.45
1:A:46:LEU:HD12	1:A:317:PRO:HG3	1.97	0.45
1:D:41:HIS:CE1	7:D:3341:HOH:O	2.66	0.44
1:A:330:GLU:HG3	7:A:3476:HOH:O	2.17	0.44
1:B:330:GLU:O	1:B:531:CYS:HA	2.18	0.44
1:C:43:SER:HB2	1:C:49:TRP:CD2	2.53	0.44
1:A:402:THR:HA	1:A:425:TRP:CE3	2.52	0.44
1:D:84:LYS:HE3	1:D:86:TRP:CZ2	2.53	0.44
1:C:445:MET:HE1	1:D:149:ARG:HG2	1.99	0.44
1:D:389:LYS:HE2	1:D:469:VAL:HG23	1.99	0.43
1:C:470:GLU:HG2	7:C:3502:HOH:O	2.17	0.43
1:A:429:LYS:NZ	1:A:449:SER:O	2.51	0.43
1:B:224:PRO:HD2	7:B:3520:HOH:O	2.19	0.43
1:A:77:ASP:HB3	1:A:88:ILE:HB	1.99	0.43
1:C:62:LEU:HD13	1:C:73:ILE:HD11	1.99	0.43
1:D:38:VAL:O	1:D:54:HIS:HA	2.19	0.43
1:A:445:MET:HE1	1:B:149:ARG:HG2	2.01	0.43
1:A:389:LYS:HE2	1:A:389:LYS:HB3	1.68	0.42
1:C:99:TRP:CD2	1:D:371:SER:HB2	2.54	0.42
1:D:330:GLU:O	1:D:531:CYS:HA	2.20	0.42
1:C:240:PRO:HG3	1:C:278:LEU:HD23	2.01	0.42
1:D:338:LYS:HE2	7:D:3537:HOH:O	2.18	0.42
1:A:99:TRP:CD2	1:B:371:SER:CB	3.02	0.42
1:A:303:ARG:NH2	7:A:3605:HOH:O	2.52	0.42
1:A:178:TYR:CE2	1:A:180:GLY:HA2	2.55	0.42
1:C:109:CYS:HB2	1:C:116:TRP:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ASN:HD22	1:A:136:ASP:N	2.18	0.41
1:D:392:ALA:HA	1:D:531:CYS:O	2.20	0.41
1:B:534:GLU:C	1:B:535:GLU:HG2	2.44	0.41
1:C:425:TRP:CH2	1:C:427:GLU:HA	2.56	0.41
1:A:452:ILE:HA	1:A:453:PRO:HD3	1.94	0.41
1:B:429:LYS:HE3	7:B:3630:HOH:O	2.21	0.41
1:D:186:THR:HA	1:D:204:GLU:HG2	2.02	0.41
1:B:38:VAL:O	1:B:54:HIS:HA	2.20	0.41
1:A:3:LEU:HD12	1:A:3:LEU:C	2.46	0.40
1:A:330:GLU:O	1:A:531:CYS:HA	2.21	0.40
1:B:4:ILE:HG21	1:B:292:ILE:CG2	2.50	0.40
1:B:333:ASN:ND2	7:B:3165:HOH:O	2.53	0.40
1:B:184:LYS:HE3	7:B:3089:HOH:O	2.21	0.40
1:D:303:ARG:HD3	1:D:303:ARG:HA	1.89	0.40
1:B:189:PRO:HA	1:B:201:PHE:O	2.22	0.40
6:A:3022:GOL:H11	7:A:3316:HOH:O	2.21	0.40
1:B:235:THR:O	1:B:309:GLN:HA	2.21	0.40
1:C:216:ALA:HB1	1:C:225:TYR:HB3	2.04	0.40
1:D:331:LYS:HE2	1:D:333:ASN:HD21	1.87	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	532/542 (98%)	502 (94%)	28 (5%)	2 (0%)	30	14
1	B	532/542 (98%)	509 (96%)	21 (4%)	2 (0%)	30	14
1	C	532/542 (98%)	505 (95%)	25 (5%)	2 (0%)	30	14
1	D	532/542 (98%)	504 (95%)	25 (5%)	3 (1%)	21	7
All	All	2128/2168 (98%)	2020 (95%)	99 (5%)	9 (0%)	30	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	469	VAL
1	A	469	VAL
1	C	469	VAL
1	D	469	VAL
1	D	12	PHE
1	A	38	VAL
1	B	38	VAL
1	C	38	VAL
1	D	38	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	475/482 (98%)	471 (99%)	4 (1%)	73	59
1	B	475/482 (98%)	466 (98%)	9 (2%)	50	27
1	C	475/482 (98%)	471 (99%)	4 (1%)	73	59
1	D	475/482 (98%)	467 (98%)	8 (2%)	53	30
All	All	1900/1928 (98%)	1875 (99%)	25 (1%)	61	40

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	214	THR
1	A	303	ARG
1	A	470	GLU
1	B	135	ASN
1	B	184	LYS
1	B	214	THR
1	B	272	VAL
1	B	325	GLU
1	B	395	SER
1	B	431	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	470	GLU
1	B	535	GLU
1	C	135	ASN
1	C	431	ARG
1	C	470	GLU
1	C	535	GLU
1	D	135	ASN
1	D	184	LYS
1	D	214	THR
1	D	272	VAL
1	D	296	GLU
1	D	325	GLU
1	D	431	ARG
1	D	470	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	333	ASN
1	A	442	HIS
1	B	48	ASN
1	B	135	ASN
1	C	135	ASN
1	C	313	ASN
1	C	333	ASN
1	D	81	HIS
1	D	135	ASN
1	D	342	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 4 are monoatomic - leaving 25 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	$\#\|Z\| > 2$
6	GOL	A	3017	-	5,5,5	0.48	0	5,5,5	1.04	0
6	GOL	B	3021	-	5,5,5	0.23	0	5,5,5	0.65	0
3	SO4	D	3024	-	4,4,4	0.26	0	6,6,6	0.56	0
6	GOL	A	3022	-	5,5,5	0.38	0	5,5,5	0.90	0
6	GOL	D	3019	-	5,5,5	0.33	0	5,5,5	0.28	0
3	SO4	B	3026	-	4,4,4	0.30	0	6,6,6	0.38	0
3	SO4	D	3028	-	4,4,4	0.28	0	6,6,6	0.27	0
6	GOL	D	3015	-	5,5,5	0.56	0	5,5,5	1.21	0
3	SO4	B	3025	-	4,4,4	0.29	0	6,6,6	0.57	0
4	EPE	D	3007	-	15,15,15	0.95	1 (6%)	19,20,20	1.45	3 (15%)
6	GOL	C	3020	-	5,5,5	0.30	0	5,5,5	0.50	0
6	GOL	C	3014	-	5,5,5	0.54	0	5,5,5	1.25	1 (20%)
6	GOL	B	3010	-	5,5,5	0.34	0	5,5,5	1.51	1 (20%)
3	SO4	A	3027	-	4,4,4	0.32	0	6,6,6	0.35	0
6	GOL	C	3013	-	5,5,5	0.42	0	5,5,5	0.55	0
5	PGE	A	3023	-	9,9,9	0.48	0	8,8,8	0.37	0
6	GOL	A	3012	-	5,5,5	0.47	0	5,5,5	0.55	0
3	SO4	A	3029	-	4,4,4	0.20	0	6,6,6	0.21	0
6	GOL	B	3018	-	5,5,5	0.35	0	5,5,5	0.55	0
6	GOL	D	3016	-	5,5,5	0.37	0	5,5,5	0.40	0
4	EPE	B	3005	-	15,15,15	0.73	1 (6%)	19,20,20	1.36	3 (15%)
6	GOL	A	3011	-	5,5,5	0.43	0	5,5,5	1.49	1 (20%)
4	EPE	A	3006	-	15,15,15	0.91	1 (6%)	19,20,20	1.63	3 (15%)
6	GOL	B	3009	-	5,5,5	0.43	0	5,5,5	0.32	0
4	EPE	C	3008	-	15,15,15	0.80	1 (6%)	19,20,20	1.45	3 (15%)

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
6	GOL	A	3017	-	-	2/4/4/4	-
6	GOL	B	3021	-	-	0/4/4/4	-
6	GOL	A	3022	-	-	2/4/4/4	-
6	GOL	D	3019	-	-	1/4/4/4	-
6	GOL	D	3015	-	-	0/4/4/4	-
4	EPE	D	3007	-	-	1/9/19/19	0/1/1/1
6	GOL	C	3020	-	-	0/4/4/4	-
6	GOL	C	3014	-	-	0/4/4/4	-
6	GOL	B	3010	-	-	0/4/4/4	-
6	GOL	C	3013	-	-	0/4/4/4	-
5	PGE	A	3023	-	-	0/7/7/7	-
6	GOL	A	3012	-	-	0/4/4/4	-
6	GOL	B	3018	-	-	4/4/4/4	-
6	GOL	D	3016	-	-	0/4/4/4	-
4	EPE	B	3005	-	-	1/9/19/19	0/1/1/1
6	GOL	A	3011	-	-	0/4/4/4	-
4	EPE	A	3006	-	-	1/9/19/19	0/1/1/1
6	GOL	B	3009	-	-	0/4/4/4	-
4	EPE	C	3008	-	-	0/9/19/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3007	EPE	C10-S	3.18	1.82	1.77
4	A	3006	EPE	C10-S	2.77	1.81	1.77
4	B	3005	EPE	C10-S	2.19	1.80	1.77
4	C	3008	EPE	C10-S	2.13	1.80	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3006	EPE	C5-N4-C3	4.58	118.70	108.84
4	C	3008	EPE	C5-N4-C3	3.63	116.67	108.84
4	D	3007	EPE	C5-N4-C3	3.36	116.07	108.84
6	B	3010	GOL	C3-C2-C1	-3.09	100.46	111.80
4	B	3005	EPE	C5-N4-C3	3.02	115.34	108.84
4	D	3007	EPE	C6-C5-N4	2.81	116.32	110.65
4	A	3006	EPE	C2-C3-N4	2.76	116.21	110.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	3008	EPE	C2-C3-N4	2.68	116.06	110.65
4	C	3008	EPE	C9-N1-C2	-2.49	104.61	111.24
6	A	3011	GOL	C3-C2-C1	-2.30	103.34	111.80
4	B	3005	EPE	C2-C3-N4	2.24	115.17	110.65
4	D	3007	EPE	C6-N1-C2	2.19	113.56	108.84
6	C	3014	GOL	C3-C2-C1	-2.13	103.97	111.80
4	A	3006	EPE	C7-N4-C3	2.06	116.74	111.24
4	B	3005	EPE	C9-N1-C6	-2.02	105.84	111.24

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3006	EPE	C8-C7-N4-C3
6	A	3017	GOL	O1-C1-C2-C3
6	B	3018	GOL	O1-C1-C2-C3
6	B	3018	GOL	C1-C2-C3-O3
6	A	3022	GOL	O1-C1-C2-C3
6	A	3017	GOL	O1-C1-C2-O2
6	B	3018	GOL	O1-C1-C2-O2
6	B	3018	GOL	O2-C2-C3-O3
6	D	3019	GOL	C1-C2-C3-O3
6	A	3022	GOL	O1-C1-C2-O2
4	B	3005	EPE	C9-C10-S-O1S
4	D	3007	EPE	C8-C7-N4-C3

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	3017	GOL	1	0
6	A	3022	GOL	1	0
6	C	3020	GOL	1	0
4	B	3005	EPE	1	0
4	A	3006	EPE	1	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	534/542 (98%)	-0.62	1 (0%)	91	92	13, 18, 35, 70	0
1	B	534/542 (98%)	-0.47	2 (0%)	88	91	14, 20, 38, 75	0
1	C	534/542 (98%)	-0.53	4 (0%)	84	87	13, 19, 37, 72	0
1	D	534/542 (98%)	-0.54	2 (0%)	88	91	14, 19, 38, 77	0
All	All	2136/2168 (98%)	-0.54	9 (0%)	88	91	13, 19, 37, 77	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	SER	3.6
1	C	272	VAL	3.0
1	D	535	GLU	2.7
1	A	388	PHE	2.5
1	C	292	ILE	2.4
1	C	535	GLU	2.3
1	C	388	PHE	2.2
1	D	2	SER	2.1
1	B	535	GLU	2.0

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

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

6.3 Carbohydrates

There are no 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, 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	B-factors(Å^2)	Q<0.9
6	GOL	B	3018	6/6	0.83	0.17	32,38,53,69	0
6	GOL	A	3017	6/6	0.87	0.21	29,47,48,107	0
6	GOL	C	3020	6/6	0.87	0.13	37,48,57,63	0
3	SO4	D	3024	5/5	0.90	0.11	32,32,65,85	0
6	GOL	D	3019	6/6	0.90	0.14	31,33,48,86	0
3	SO4	B	3025	5/5	0.91	0.09	29,30,50,58	0
3	SO4	A	3029	5/5	0.92	0.09	29,47,50,75	0
3	SO4	A	3027	5/5	0.93	0.09	32,36,43,54	0
3	SO4	D	3028	5/5	0.93	0.09	29,38,61,62	0
4	EPE	A	3006	15/15	0.94	0.09	18,24,46,73	0
6	GOL	B	3021	6/6	0.94	0.09	25,32,36,39	0
4	EPE	B	3005	15/15	0.94	0.08	18,25,51,68	0
3	SO4	B	3026	5/5	0.94	0.09	28,34,51,56	0
5	PGE	A	3023	10/10	0.95	0.08	25,32,40,46	0
4	EPE	C	3008	15/15	0.95	0.08	20,23,49,52	0
4	EPE	D	3007	15/15	0.95	0.07	19,27,38,40	0
6	GOL	A	3022	6/6	0.96	0.08	21,32,36,52	0
6	GOL	B	3010	6/6	0.96	0.07	18,18,23,29	0
6	GOL	A	3011	6/6	0.97	0.07	14,21,25,35	0
6	GOL	D	3015	6/6	0.97	0.06	15,20,23,24	0
6	GOL	C	3014	6/6	0.97	0.06	14,20,23,26	0
6	GOL	D	3016	6/6	0.98	0.04	15,16,17,19	0
6	GOL	A	3012	6/6	0.99	0.04	14,17,18,19	0
6	GOL	C	3013	6/6	0.99	0.04	14,17,19,22	0
2	CA	A	3001	1/1	0.99	0.18	27,27,27,27	0
2	CA	B	3002	1/1	0.99	0.11	26,26,26,26	0
6	GOL	B	3009	6/6	0.99	0.04	13,17,21,22	0
2	CA	C	3003	1/1	0.99	0.20	27,27,27,27	0
2	CA	D	3004	1/1	0.99	0.18	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.