Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:43 PM GMT

PDB ID	:	1C7T
Title	:	BETA-N-ACETYLHEXOSAMINIDASE MUTANT E540D COMPLEXED WITH DI-N ACETYL-D-GLUCOSAMINE (CHITOBIASE)
Authors	:	Prag, G.; Papanikolau, Y.; Tavlas, G.; Vorgias, C.E.; Petratos, K.; Oppenheim, A.B.
Deposited on	:	2000-03-17
Resolution	:	1.90 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:

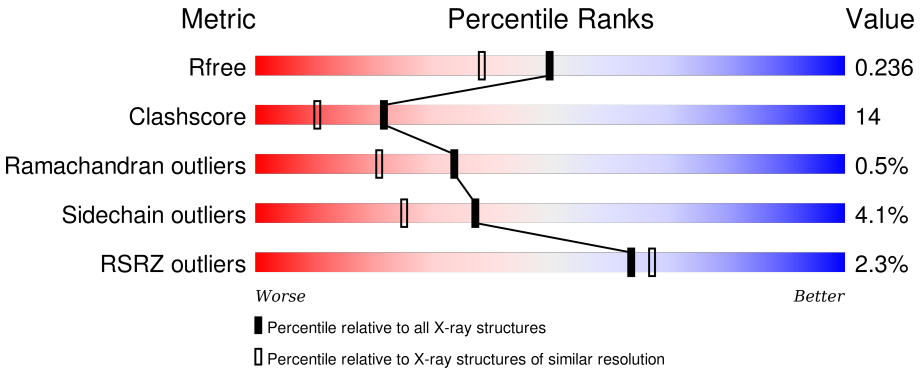
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	858	2% 72% 23%

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	2004	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7657 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.

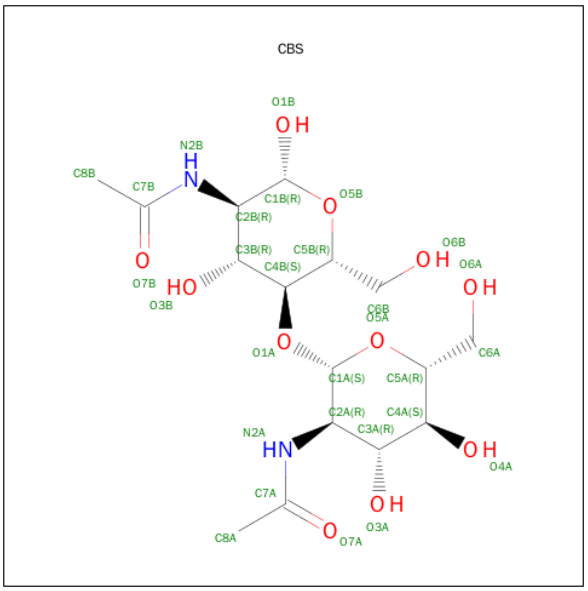
- Molecule 1 is a protein called BETA-N-ACETYLHEXOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	858	Total	C	N	O	S	0	3	0
			6776	4287	1185	1282	22			

There are 3 discrepancies between the modelled and reference sequences:

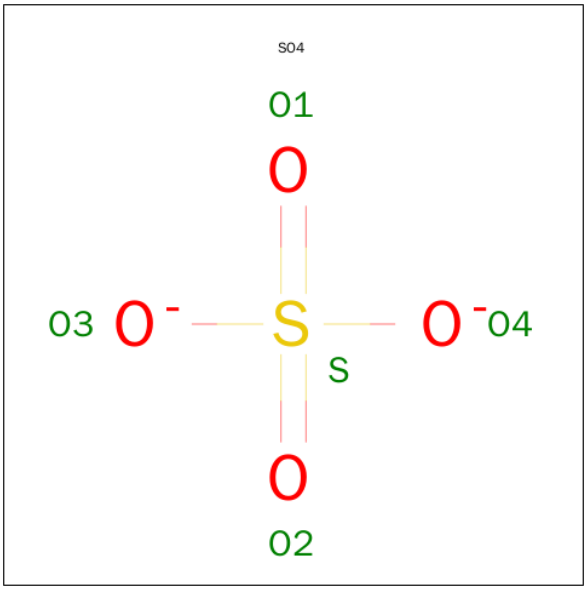
Chain	Residue	Modelled	Actual	Comment	Reference
A	484	GLN	PRO	CONFLICT	UNP Q54468
A	540	ASP	GLU	ENGINEERED	UNP Q54468
A	828	GLY	ALA	CONFLICT	UNP Q54468

- Molecule 2 is SUGAR (DI(N-ACETYL-D-GLUCOSAMINE)) (three-letter code: CBS) (formula: $C_{16}H_{28}N_2O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	16	2	11		

- 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

- Molecule 4 is water.

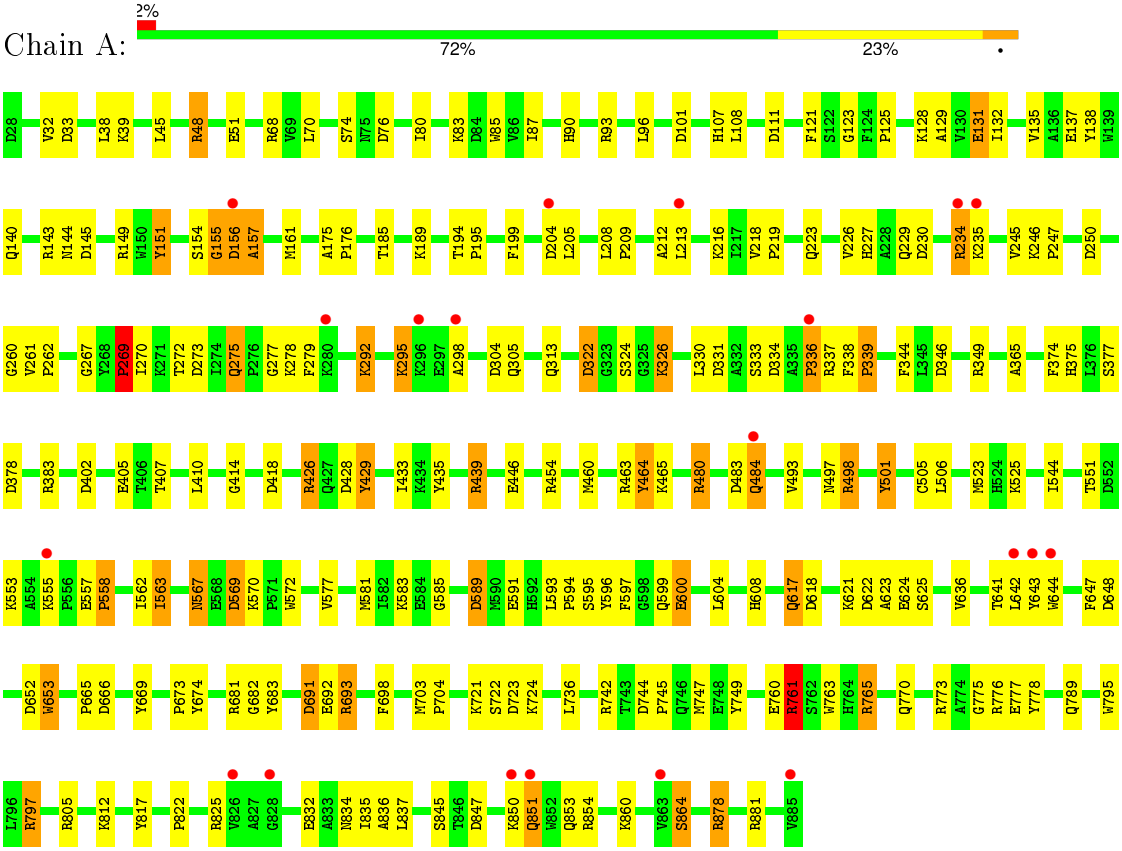
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	832	Total O 832 832	0	0

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: BETA-N-ACETYLHEXOSAMINIDASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	109.17Å 99.42Å 86.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 86.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (10.00-1.90) 96.2 (86.56-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.01 (at 1.90Å)	Xtriage
Refinement program	REFMAC, ARP	Depositor
R, R_{free}	0.191 , 0.246 0.190 , 0.236	Depositor DCC
R_{free} test set	3743 reflections (5.48%)	DCC
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 67.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 74856 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7657	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: CBS, SO4

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	0.80	0/6959	1.48	77/9423 (0.8%)

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	2

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	878	ARG	NE-CZ-NH2	-14.16	113.22	120.30
1	A	48	ARG	NE-CZ-NH1	13.23	126.92	120.30
1	A	498	ARG	NE-CZ-NH1	12.93	126.77	120.30
1	A	681	ARG	NE-CZ-NH1	11.91	126.26	120.30
1	A	383	ARG	NE-CZ-NH1	11.01	125.81	120.30
1	A	143	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	A	622	ASP	CB-CG-OD1	10.32	127.58	118.30
1	A	426	ARG	NE-CZ-NH1	-10.21	115.19	120.30
1	A	464	TYR	CB-CG-CD2	-10.15	114.91	121.00
1	A	498	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	A	878	ARG	CD-NE-CZ	9.37	136.72	123.60
1	A	693	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	A	597	PHE	CB-CG-CD2	-8.82	114.63	120.80
1	A	48	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	A	681	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	A	349	ARG	NE-CZ-NH2	-8.69	115.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	439	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	A	681	ARG	CD-NE-CZ	8.59	135.62	123.60
1	A	76	ASP	CB-CG-OD2	-8.49	110.66	118.30
1	A	761	ARG	CD-NE-CZ	8.46	135.45	123.60
1	A	93	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	878	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	A	597	PHE	CB-CG-CD1	8.31	126.62	120.80
1	A	761	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	A	464	TYR	CB-CG-CD1	7.83	125.70	121.00
1	A	589	ASP	CB-CG-OD2	7.56	125.11	118.30
1	A	653	TRP	N-CA-C	-7.33	91.20	111.00
1	A	76	ASP	CB-CG-OD1	7.18	124.77	118.30
1	A	854	ARG	CD-NE-CZ	7.15	133.62	123.60
1	A	797	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	A	742	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	749	TYR	CB-CG-CD1	6.93	125.16	121.00
1	A	454	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	A	805	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	A	151	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	A	653	TRP	N-CA-CB	6.54	122.38	110.60
1	A	480	ARG	CD-NE-CZ	6.51	132.71	123.60
1	A	33	ASP	CB-CG-OD1	-6.50	112.45	118.30
1	A	600	GLU	OE1-CD-OE2	6.49	131.09	123.30
1	A	501	TYR	CB-CG-CD1	-6.46	117.12	121.00
1	A	339	PRO	CA-N-CD	-6.28	102.70	111.50
1	A	334	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	817	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	A	435	TYR	CB-CG-CD1	6.17	124.70	121.00
1	A	558	PRO	CA-N-CD	-6.15	102.89	111.50
1	A	825	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	A	589	ASP	OD1-CG-OD2	-6.11	111.70	123.30
1	A	825	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	426	ARG	NH1-CZ-NH2	6.00	126.00	119.40
1	A	557	GLU	CB-CA-C	5.98	122.36	110.40
1	A	693	ARG	CD-NE-CZ	5.86	131.80	123.60
1	A	269	PRO	CA-N-CD	-5.75	103.45	111.50
1	A	304	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	429	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	A	131	GLU	OE1-CD-OE2	-5.68	116.48	123.30
1	A	761	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	749	TYR	CB-CG-CD2	-5.66	117.61	121.00
1	A	881	ARG	NE-CZ-NH2	-5.60	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	435	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	A	446	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	A	418	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	623	ALA	N-CA-CB	-5.51	102.39	110.10
1	A	691	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	336	PRO	CA-N-CD	-5.50	103.80	111.50
1	A	428	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	589	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	622	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	765	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	322	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	498	ARG	CD-NE-CZ	5.24	130.94	123.60
1	A	339	PRO	CA-C-N	-5.13	105.92	117.20
1	A	463	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	33	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	653	TRP	CA-CB-CG	-5.06	104.08	113.70
1	A	563	ILE	CA-CB-CG1	5.05	120.60	111.00
1	A	101	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	742	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ILE	Mainchain
1	A	96	LEU	Mainchain

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	6776	0	6571	188	2
2	A	29	0	27	0	0
3	A	20	0	0	2	0
4	A	832	0	0	20	2
All	All	7657	0	6598	188	4

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 14.

All (188) 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:A:336:PRO:HD3	1:A:763:TRP:CH2	1.84	1.10
1:A:336:PRO:HD3	1:A:763:TRP:CZ2	1.94	1.02
1:A:525:LYS:HE2	4:A:2674:HOH:O	1.62	0.98
1:A:336:PRO:HG3	1:A:763:TRP:CZ3	2.00	0.96
1:A:267:GLY:O	1:A:269:PRO:HD3	1.75	0.86
1:A:567:ASN:N	1:A:567:ASN:HD22	1.73	0.85
1:A:407:THR:HG21	4:A:2318:HOH:O	1.76	0.85
1:A:273:ASP:HB3	1:A:275:GLN:NE2	1.93	0.84
1:A:234:ARG:NE	1:A:234:ARG:HA	1.92	0.83
1:A:567:ASN:H	1:A:567:ASN:HD22	1.26	0.82
1:A:234:ARG:NE	1:A:234:ARG:CA	2.41	0.82
1:A:227:HIS:NE2	1:A:331:ASP:OD2	2.14	0.80
1:A:617:GLN:HB2	1:A:636:VAL:HG21	1.64	0.79
1:A:234:ARG:CZ	1:A:234:ARG:HA	2.13	0.79
1:A:336:PRO:CD	1:A:763:TRP:CH2	2.66	0.78
1:A:326:LYS:NZ	1:A:326:LYS:HB3	1.97	0.78
1:A:864:SER:HA	4:A:2648:HOH:O	1.84	0.77
1:A:229:GLN:HB2	1:A:295:LYS:NZ	1.99	0.77
1:A:213:LEU:N	1:A:213:LEU:HD22	2.02	0.74
1:A:480:ARG:NH1	1:A:484:GLN:HG2	2.03	0.74
1:A:570:LYS:HE2	1:A:591:GLU:OE1	1.89	0.72
1:A:567:ASN:ND2	1:A:567:ASN:H	1.87	0.72
1:A:212:ALA:C	1:A:213:LEU:HD22	2.10	0.72
1:A:230:ASP:O	1:A:295:LYS:NZ	2.23	0.70
1:A:480:ARG:HH12	1:A:484:GLN:HG2	1.58	0.68
1:A:617:GLN:CB	1:A:636:VAL:HG21	2.24	0.67
1:A:595:SER:O	1:A:599:GLN:HG3	1.93	0.67
1:A:273:ASP:HB3	1:A:275:GLN:HE21	1.58	0.67
1:A:189:LYS:HE2	4:A:2583:HOH:O	1.93	0.67
1:A:270:ILE:HG12	1:A:298:ALA:HB3	1.74	0.67
1:A:878:ARG:HD3	4:A:2250:HOH:O	1.94	0.67
1:A:617:GLN:HA	1:A:636:VAL:CG2	2.25	0.67
1:A:295:LYS:HA	1:A:295:LYS:HE2	1.78	0.66
1:A:229:GLN:HB2	1:A:295:LYS:HZ2	1.60	0.66
1:A:245:VAL:HG23	1:A:305:GLN:OE1	1.96	0.65
1:A:234:ARG:NH2	1:A:261:VAL:HA	2.12	0.64
1:A:365:ALA:HB2	1:A:439:ARG:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HD21	1:A:80:ILE:HD12	1.79	0.64
1:A:229:GLN:CD	1:A:295:LYS:HE3	2.17	0.64
1:A:405:GLU:CD	1:A:410:LEU:HG	2.20	0.63
1:A:85:TRP:CZ3	1:A:87:ILE:HD12	2.34	0.62
1:A:593:LEU:N	1:A:594:PRO:CD	2.63	0.62
1:A:617:GLN:CA	1:A:636:VAL:CG2	2.77	0.62
1:A:48:ARG:HD3	1:A:185:THR:CA	2.30	0.61
1:A:832:GLU:HG3	1:A:860:LYS:HE3	1.83	0.60
1:A:617:GLN:CB	1:A:636:VAL:CG2	2.78	0.60
1:A:208:LEU:CB	1:A:213:LEU:HD21	2.31	0.60
1:A:48:ARG:HD3	1:A:185:THR:HA	1.84	0.60
1:A:497:ASN:HB3	3:A:2001:SO4:O3	2.02	0.59
1:A:234:ARG:HE	1:A:234:ARG:C	2.04	0.59
1:A:212:ALA:O	1:A:213:LEU:HD13	2.02	0.58
1:A:70:LEU:HD11	1:A:131:GLU:HB3	1.85	0.58
1:A:330:LEU:HD12	1:A:330:LEU:C	2.23	0.58
1:A:246:LYS:HE3	1:A:250:ASP:OD1	2.04	0.58
1:A:642:LEU:HD22	1:A:647:PHE:HB3	1.87	0.57
1:A:498:ARG:HG3	4:A:2416:HOH:O	2.04	0.57
1:A:209:PRO:O	1:A:213:LEU:HD23	2.05	0.57
1:A:199:PHE:CD1	1:A:199:PHE:C	2.78	0.57
1:A:295:LYS:CA	1:A:295:LYS:HE2	2.29	0.56
1:A:208:LEU:HB2	1:A:213:LEU:HD21	1.86	0.56
1:A:429:TYR:CE2	1:A:433:ILE:HD11	2.40	0.56
1:A:812:LYS:HE3	4:A:2500:HOH:O	2.04	0.56
1:A:326:LYS:HZ2	1:A:326:LYS:HB3	1.68	0.56
1:A:234:ARG:HH22	1:A:261:VAL:HA	1.71	0.56
1:A:589:ASP:OD1	1:A:591:GLU:HB3	2.06	0.55
1:A:213:LEU:N	1:A:213:LEU:CD2	2.70	0.55
1:A:497:ASN:OD1	1:A:498:ARG:N	2.40	0.55
1:A:648:ASP:OD1	1:A:724:LYS:HE3	2.07	0.54
1:A:643:TYR:HE1	1:A:644:TRP:CE2	2.25	0.54
1:A:773:ARG:HD2	1:A:776:ARG:NE	2.22	0.54
1:A:744:ASP:N	1:A:745:PRO:CD	2.71	0.54
1:A:229:GLN:HG3	1:A:295:LYS:CE	2.38	0.54
1:A:525:LYS:HE3	4:A:2535:HOH:O	2.06	0.54
1:A:156:ASP:O	1:A:157:ALA:C	2.45	0.53
1:A:326:LYS:HZ3	1:A:326:LYS:HB3	1.73	0.53
1:A:272:THR:O	1:A:273:ASP:OD1	2.27	0.52
1:A:83:LYS:HD3	4:A:2170:HOH:O	2.08	0.52
1:A:812:LYS:CE	4:A:2500:HOH:O	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:GLU:HB2	4:A:2715:HOH:O	2.09	0.52
1:A:465:LYS:HE3	4:A:2438:HOH:O	2.09	0.52
1:A:665:PRO:HA	1:A:669:TYR:CD1	2.44	0.52
1:A:121:PHE:CZ	1:A:123:GLY:HA2	2.45	0.52
1:A:229:GLN:HB2	1:A:295:LYS:HZ1	1.75	0.51
1:A:770:GLN:OE1	1:A:778:TYR:OH	2.18	0.51
1:A:108:LEU:HB3	4:A:2719:HOH:O	2.09	0.51
1:A:267:GLY:O	1:A:269:PRO:CD	2.54	0.51
1:A:234:ARG:HH21	1:A:262:PRO:HD2	1.75	0.51
1:A:336:PRO:CG	1:A:763:TRP:CZ3	2.84	0.51
1:A:484:GLN:NE2	4:A:2833:HOH:O	2.44	0.50
1:A:234:ARG:NH2	1:A:260:GLY:O	2.45	0.50
1:A:204:ASP:OD2	1:A:693:ARG:NH2	2.39	0.50
1:A:377:SER:O	1:A:378:ASP:HB2	2.12	0.50
1:A:292:LYS:HG3	1:A:331:ASP:OD1	2.12	0.50
1:A:234:ARG:HH21	1:A:262:PRO:CD	2.25	0.50
1:A:493:VAL:HA	1:A:544:ILE:HG21	1.93	0.50
1:A:246:LYS:HB3	1:A:247:PRO:HD3	1.93	0.49
1:A:501:TYR:CD1	1:A:501:TYR:N	2.79	0.49
1:A:209:PRO:O	1:A:213:LEU:CD2	2.60	0.49
1:A:223:GLN:HB2	1:A:333:SER:HB3	1.94	0.49
1:A:156:ASP:C	1:A:157:ALA:O	2.49	0.49
1:A:692:GLU:HB3	1:A:795:TRP:HH2	1.78	0.49
1:A:208:LEU:HB3	1:A:213:LEU:HD21	1.95	0.49
1:A:337:ARG:HG3	1:A:338:PHE:CD2	2.48	0.49
1:A:339:PRO:HD3	4:A:2288:HOH:O	2.13	0.48
1:A:460:MET:HA	1:A:460:MET:CE	2.43	0.48
1:A:834:ASN:HB2	4:A:2514:HOH:O	2.13	0.48
1:A:234:ARG:HE	1:A:234:ARG:CA	2.23	0.48
1:A:108:LEU:HD23	1:A:108:LEU:N	2.30	0.47
1:A:39:LYS:HE3	4:A:2325:HOH:O	2.14	0.47
1:A:583:LYS:C	1:A:585:GLY:H	2.18	0.47
1:A:194:THR:HB	1:A:195:PRO:CD	2.44	0.47
1:A:722:SER:OG	1:A:724:LYS:HG3	2.14	0.47
1:A:604:LEU:O	1:A:608:HIS:HD2	1.98	0.47
1:A:674:TYR:O	1:A:691:ASP:HB3	2.15	0.47
1:A:643:TYR:HE1	1:A:644:TRP:CZ2	2.34	0.46
1:A:797:ARG:HH11	1:A:797:ARG:HD3	1.52	0.46
1:A:505:CYS:SG	1:A:581:MET:HE2	2.55	0.46
1:A:45:LEU:HD11	1:A:70:LEU:HB2	1.98	0.45
1:A:137:GLU:HG2	1:A:138:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:ND2	1:A:682:GLY:H	2.14	0.45
1:A:673:PRO:HD3	1:A:683:TYR:O	2.17	0.45
1:A:234:ARG:NE	1:A:234:ARG:C	2.67	0.45
1:A:551:THR:HG22	1:A:562:ILE:HA	1.99	0.45
1:A:723:ASP:OD1	1:A:775:GLY:HA2	2.16	0.45
1:A:32:VAL:HG23	1:A:154:SER:HB3	1.99	0.45
1:A:569:ASP:HB3	4:A:2391:HOH:O	2.16	0.45
1:A:847:ASP:OD2	1:A:851:GLN:N	2.50	0.45
1:A:641:THR:OG1	1:A:644:TRP:CE3	2.68	0.45
1:A:107:HIS:ND1	3:A:2004:SO4:O4	2.33	0.44
1:A:229:GLN:CG	1:A:295:LYS:CE	2.95	0.44
1:A:847:ASP:O	1:A:850:LYS:HG2	2.18	0.44
1:A:218:VAL:HA	1:A:219:PRO:C	2.36	0.44
1:A:156:ASP:O	1:A:157:ALA:O	2.35	0.44
1:A:596:TYR:CZ	1:A:600:GLU:HG3	2.53	0.44
1:A:74:SER:HA	1:A:129:ALA:HA	1.99	0.44
1:A:149:ARG:HG3	1:A:414:GLY:O	2.17	0.44
1:A:617:GLN:HA	1:A:636:VAL:HG23	1.98	0.44
1:A:773:ARG:HD2	1:A:776:ARG:CZ	2.48	0.44
1:A:501:TYR:HB3	1:A:572:TRP:CZ2	2.53	0.44
1:A:234:ARG:O	1:A:234:ARG:NE	2.51	0.44
1:A:205:LEU:HD21	1:A:693:ARG:HH12	1.83	0.44
1:A:68:ARG:HD3	4:A:2136:HOH:O	2.17	0.44
1:A:822:PRO:HA	1:A:835:ILE:HD12	1.98	0.44
1:A:140:GLN:HA	1:A:145:ASP:OD2	2.17	0.43
1:A:617:GLN:HG3	1:A:653:TRP:CE2	2.53	0.43
1:A:624:GLU:CD	1:A:625:SER:HB3	2.39	0.43
1:A:405:GLU:OE2	1:A:410:LEU:HG	2.18	0.43
1:A:593:LEU:HA	1:A:593:LEU:HD23	1.89	0.43
1:A:483:ASP:OD2	1:A:577:VAL:HG23	2.18	0.43
1:A:698:PHE:O	1:A:761:ARG:HD2	2.19	0.43
1:A:426:ARG:HG3	1:A:523:MET:HG2	2.00	0.43
1:A:591:GLU:OE1	1:A:591:GLU:HA	2.19	0.43
1:A:151:TYR:HA	1:A:161:MET:HA	2.01	0.43
1:A:402:ASP:OD2	1:A:407:THR:HG22	2.18	0.43
1:A:212:ALA:HB3	1:A:213:LEU:HD22	2.00	0.43
1:A:339:PRO:HG3	4:A:2434:HOH:O	2.18	0.43
1:A:736:LEU:CD2	1:A:747:MET:HG3	2.49	0.42
1:A:497:ASN:CG	1:A:498:ARG:H	2.16	0.42
1:A:229:GLN:CG	1:A:295:LYS:HE3	2.49	0.42
1:A:484:GLN:CA	1:A:484:GLN:HE21	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ASP:HB2	1:A:506:LEU:HD21	2.01	0.42
1:A:48:ARG:HD2	1:A:51:GLU:OE1	2.19	0.42
1:A:123:GLY:O	1:A:125:PRO:HD3	2.19	0.42
1:A:154:SER:O	1:A:155:GLY:C	2.58	0.42
1:A:219:PRO:HB3	1:A:760:GLU:HA	2.02	0.42
1:A:703:MET:N	1:A:704:PRO:CD	2.82	0.42
1:A:346:ASP:HA	1:A:375:HIS:HB3	2.00	0.42
1:A:847:ASP:CG	1:A:851:GLN:H	2.23	0.42
1:A:68:ARG:HG2	1:A:135:VAL:HG22	2.02	0.42
1:A:90:HIS:HA	1:A:111:ASP:O	2.20	0.41
1:A:175:ALA:HA	1:A:176:PRO:HD3	1.87	0.41
1:A:245:VAL:CG2	1:A:305:GLN:HE22	2.33	0.41
1:A:845:SER:OG	1:A:847:ASP:OD1	2.38	0.41
1:A:617:GLN:HG3	1:A:653:TRP:CZ2	2.56	0.41
1:A:832:GLU:HG3	1:A:860:LYS:CE	2.50	0.41
1:A:204:ASP:CG	1:A:693:ARG:HH22	2.22	0.41
1:A:583:LYS:C	1:A:585:GLY:N	2.74	0.41
1:A:322:ASP:OD1	1:A:324:SER:HB3	2.21	0.41
1:A:618:ASP:N	1:A:618:ASP:OD1	2.54	0.41
1:A:277:GLY:C	1:A:279:PHE:N	2.75	0.41
1:A:836:ALA:O	1:A:837:LEU:HD23	2.20	0.41
1:A:563:ILE:HG21	1:A:563:ILE:HD13	1.70	0.41
1:A:483:ASP:C	1:A:483:ASP:OD1	2.60	0.40
1:A:593:LEU:HB2	1:A:594:PRO:HD3	2.03	0.40
1:A:721:LYS:HB3	1:A:777:GLU:HG3	2.03	0.40
1:A:464:TYR:C	1:A:464:TYR:CD2	2.94	0.40
1:A:505:CYS:SG	1:A:581:MET:CE	3.09	0.40
1:A:847:ASP:OD2	1:A:850:LYS:HB2	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2137:HOH:O	4:A:2137:HOH:O[2_565]	1.59	0.61
1:A:776:ARG:NH2	1:A:851:GLN:NE2[4_556]	1.76	0.44
1:A:776:ARG:NH2	1:A:851:GLN:CD[4_556]	1.83	0.37
4:A:2740:HOH:O	4:A:2740:HOH:O[2_565]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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	859/858 (100%)	824 (96%)	31 (4%)	4 (0%)	34 21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	ASP
1	A	155	GLY
1	A	157	ALA
1	A	652	ASP

5.3.2 Protein sidechains

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	709/706 (100%)	680 (96%)	29 (4%)	37 25

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LYS
1	A	216	LYS
1	A	226	VAL
1	A	234	ARG
1	A	235	LYS
1	A	269	PRO
1	A	275	GLN

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Mol	Chain	Res	Type
1	A	278	LYS
1	A	292	LYS
1	A	295	LYS
1	A	313	GLN
1	A	326	LYS
1	A	344	PHE
1	A	374	PHE
1	A	484	GLN
1	A	553	LYS
1	A	555	LYS
1	A	558	PRO
1	A	567	ASN
1	A	569	ASP
1	A	617	GLN
1	A	621	LYS
1	A	666	ASP
1	A	761	ARG
1	A	765	ARG
1	A	789	GLN
1	A	851	GLN
1	A	853	GLN
1	A	864	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	A	484	GLN
1	A	510	GLN
1	A	567	ASN
1	A	716	ASN
1	A	784	HIS
1	A	853	GLN

5.3.3 RNA

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)

5 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	CBS	A	1001	-	30,30,30	1.50	6 (20%)	36,43,43	1.91	8 (22%)
3	SO4	A	2001	-	4,4,4	1.02	0	6,6,6	0.37	0
3	SO4	A	2002	-	4,4,4	0.88	0	6,6,6	0.32	0
3	SO4	A	2003	-	4,4,4	0.91	0	6,6,6	0.35	0
3	SO4	A	2004	-	4,4,4	1.02	0	6,6,6	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CBS	A	1001	-	-	0/16/56/56	0/2/2/2
3	SO4	A	2001	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2002	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2003	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2004	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	CBS	O1B-C1B	-4.84	1.22	1.39
2	A	1001	CBS	O7A-C7A	-2.76	1.16	1.23
2	A	1001	CBS	O7B-C7B	-2.43	1.17	1.23
2	A	1001	CBS	C1A-C2A	-2.27	1.49	1.53
2	A	1001	CBS	C2B-N2B	2.17	1.49	1.45
2	A	1001	CBS	C2A-N2A	2.20	1.49	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	CBS	O1B-C1B-O5B	-4.01	99.29	110.25
2	A	1001	CBS	O1A-C1A-O5A	-3.43	101.99	110.68
2	A	1001	CBS	C3A-C4A-C5A	-2.45	105.93	110.20
2	A	1001	CBS	C1A-C2A-N2A	2.22	115.18	111.01
2	A	1001	CBS	O7A-C7A-C8A	2.83	127.25	122.06
2	A	1001	CBS	C1A-O5A-C5A	3.29	120.14	113.75
2	A	1001	CBS	O5A-C1A-C2A	4.21	119.94	110.78
2	A	1001	CBS	C1A-O1A-C4B	5.10	131.32	118.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	SO4	1	0
3	A	2004	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

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	858/858 (100%)	0.05	20 (2%) 64 67	14, 24, 44, 62	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	644	TRP	9.7
1	A	642	LEU	4.7
1	A	156	ASP	4.1
1	A	484	GLN	3.9
1	A	863	VAL	3.6
1	A	234	ARG	3.5
1	A	851	GLN	3.3
1	A	336	PRO	3.1
1	A	235	LYS	3.1
1	A	885	VAL	3.0
1	A	213	LEU	2.6
1	A	298	ALA	2.5
1	A	643	TYR	2.4
1	A	850	LYS	2.3
1	A	555	LYS	2.3
1	A	828	GLY	2.1
1	A	296	LYS	2.1
1	A	280	LYS	2.1
1	A	826	VAL	2.1
1	A	204	ASP	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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	A	2004	5/5	0.86	0.18	2.97	67,68,68,69	0
2	CBS	A	1001	29/29	0.93	0.11	1.12	20,24,29,32	0
3	SO4	A	2001	5/5	0.98	0.06	-2.00	21,23,24,26	0
3	SO4	A	2003	5/5	0.91	0.11	-	53,54,54,54	0
3	SO4	A	2002	5/5	0.97	0.13	-	41,43,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.