Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 12:43 AM EDT

PDB ID	:	5GSL
Title	:	Glycoside hydrolase A
Authors	:	Watanabe, M.; Kamachi, S.; Mine, S.
Deposited on	:	2016-08-16
Resolution	:	2.60 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:

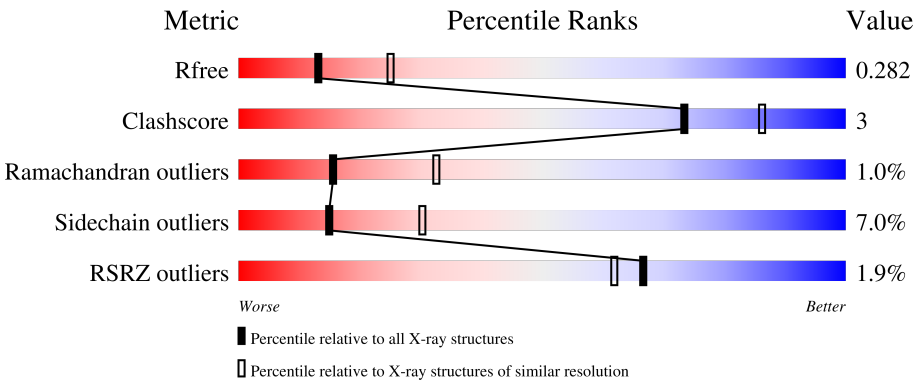
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	778	% 84% 14% ·
1	B	778	3% 84% 14% ·

2 Entry composition (i)

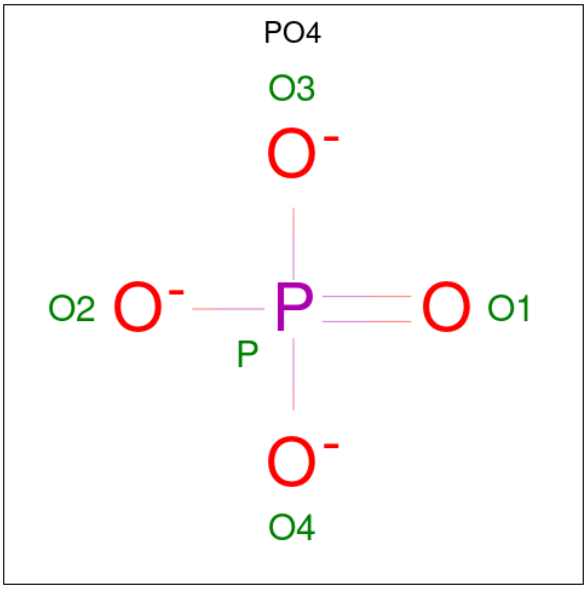
There are 3 unique types of molecules in this entry. The entry contains 13033 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 778aa long hypothetical beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	775	6442	4185	1076	1166	15	0	0	0
1	B	775	6442	4185	1076	1166	15	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0

- Molecule 3 is water.

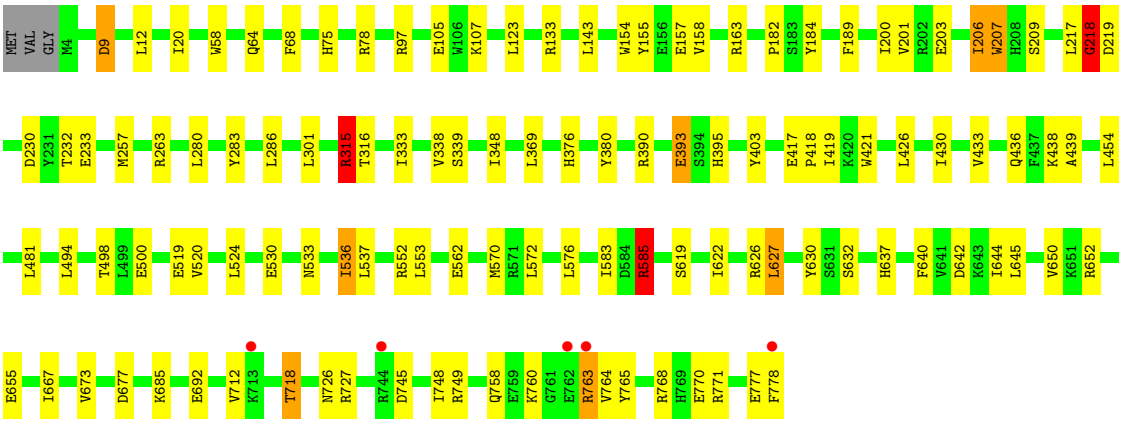
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	78	78	78	0	0
			Total	O		
3	B	56	56	56	0	0

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.

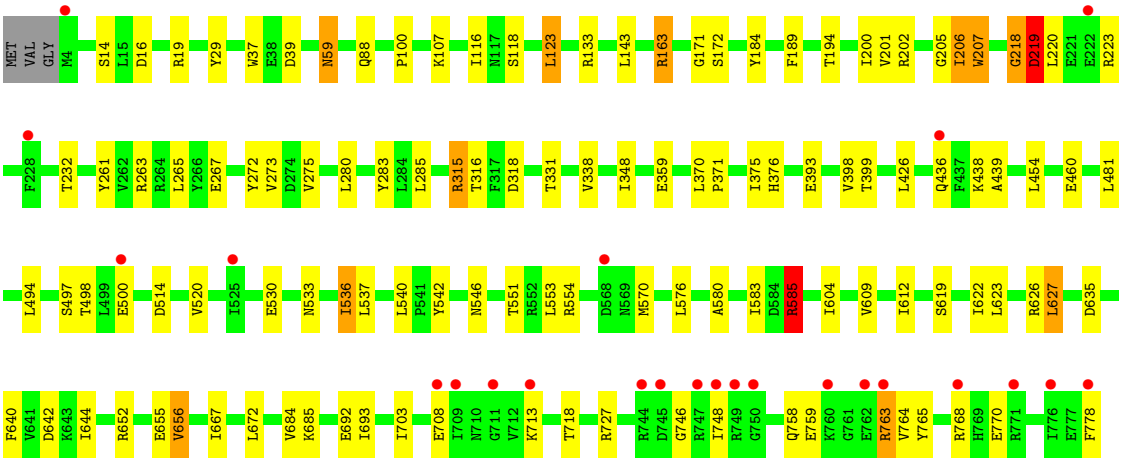
• Molecule 1: 778aa long hypothetical beta-galactosidase

Chain A:



• Molecule 1: 778aa long hypothetical beta-galactosidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	146.84Å 148.77Å 165.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.1 (30.00-2.60) 92.2 (29.95-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.217 , 0.288 0.218 , 0.282	Depositor DCC
R_{free} test set	2568 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 9.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.036 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13033	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.54	1/6624 (0.0%)	0.80	9/8986 (0.1%)
1	B	0.51	1/6624 (0.0%)	0.75	3/8986 (0.0%)
All	All	0.53	2/13248 (0.0%)	0.78	12/17972 (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	3
1	B	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	TRP	CB-CG	6.30	1.61	1.50
1	B	207	TRP	CB-CG	5.43	1.60	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	763	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	A	207	TRP	N-CA-CB	7.04	123.26	110.60
1	B	207	TRP	N-CA-CB	6.60	122.48	110.60
1	A	315	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	537	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	97	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	552	ARG	NE-CZ-NH1	5.39	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	315	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	206	ILE	C-N-CA	5.23	134.77	121.70
1	B	206	ILE	C-N-CA	5.09	134.42	121.70
1	A	585	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	585	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	ILE	Peptide
1	A	218	GLY	Peptide
1	A	536	ILE	Peptide
1	B	206	ILE	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	6442	0	6336	41	1
1	B	6442	0	6336	50	1
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	78	0	0	1	2
3	B	56	0	0	0	1
All	All	13033	0	12672	85	3

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 (85) 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:460:GLU:HA	1:B:460:GLU:OE1	1.81	0.80
1:B:218:GLY:N	1:B:219:ASP:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:ILE:HD13	1:B:718:THR:HG23	1.70	0.71
1:B:708:GLU:OE2	1:B:713:LYS:NZ	2.23	0.70
1:B:580:ALA:HB3	1:B:583:ILE:HG13	1.74	0.69
1:B:746:GLY:O	1:B:763:ARG:NH1	2.34	0.61
1:B:285:LEU:HD21	1:B:454:LEU:HD22	1.84	0.60
1:B:273:VAL:HG13	1:B:275:VAL:HG22	1.84	0.59
1:B:640:PHE:CE2	1:B:644:ILE:HD11	2.41	0.56
1:B:718:THR:HG22	1:B:718:THR:O	2.05	0.56
1:B:280:LEU:HD13	1:B:348:ILE:HG22	1.87	0.56
1:A:642:ASP:OD1	1:A:652:ARG:NH2	2.40	0.54
1:B:580:ALA:HB3	1:B:583:ILE:CG1	2.37	0.54
1:B:223:ARG:NH1	1:B:546:ASN:OD1	2.40	0.54
1:A:280:LEU:HD13	1:A:348:ILE:HG22	1.90	0.53
1:A:640:PHE:CE2	1:A:644:ILE:HD11	2.44	0.53
1:B:672:LEU:HD12	1:B:703:ILE:CD1	2.40	0.52
1:B:604:ILE:HD12	1:B:609:VAL:HG11	1.91	0.51
1:B:494:LEU:HB3	1:B:520:VAL:CG2	2.40	0.51
1:B:280:LEU:HD13	1:B:348:ILE:CG2	2.40	0.51
1:A:494:LEU:HB3	1:A:520:VAL:CG2	2.42	0.50
1:A:585:ARG:NH2	1:B:398:VAL:HG23	2.26	0.50
1:B:261:TYR:CZ	1:B:265:LEU:HD11	2.46	0.50
1:A:105:GLU:HG3	1:A:395:HIS:HB2	1.93	0.50
1:B:642:ASP:OD1	1:B:652:ARG:NH2	2.45	0.50
1:A:418:PRO:HA	1:A:421:TRP:CD1	2.46	0.49
1:A:390:ARG:HA	1:B:585:ARG:NH1	2.28	0.49
1:A:760:LYS:HB3	1:A:764:VAL:HG22	1.95	0.48
1:A:105:GLU:HG3	1:A:395:HIS:CB	2.43	0.48
1:A:68:PHE:CZ	1:A:157:GLU:HG3	2.49	0.48
1:A:677:ASP:HB3	1:B:359:GLU:HG2	1.95	0.48
1:B:116:ILE:HG23	1:B:123:LEU:HD11	1.95	0.48
1:B:542:TYR:HA	1:B:551:THR:HG22	1.95	0.47
1:A:630:TYR:HB2	1:A:637:HIS:CE1	2.50	0.47
1:B:163:ARG:HG3	1:B:272:TYR:O	2.15	0.47
1:A:218:GLY:CA	1:A:219:ASP:HB2	2.45	0.46
1:A:315:ARG:HD3	1:A:316:THR:O	2.15	0.46
1:B:189:PHE:HA	1:B:454:LEU:HD21	1.98	0.46
1:A:12:LEU:HD22	1:A:20:ILE:O	2.15	0.46
1:A:315:ARG:NH2	1:B:318:ASP:OD2	2.36	0.46
1:B:727:ARG:HG2	1:B:778:PHE:HB2	1.97	0.45
1:A:12:LEU:HD21	1:A:433:VAL:HG11	1.99	0.45
1:B:370:LEU:HB2	1:B:371:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:THR:HG22	1:B:375:ILE:HD12	1.99	0.45
1:B:537:LEU:HD12	1:B:623:LEU:HD12	1.99	0.45
1:A:218:GLY:HA3	1:A:219:ASP:HB2	2.00	0.44
1:A:189:PHE:HA	1:A:454:LEU:HD21	1.98	0.44
1:A:632:SER:CB	1:B:399:THR:HG21	2.47	0.44
1:B:202:ARG:O	1:B:205:GLY:N	2.49	0.44
1:B:540:LEU:O	1:B:554:ARG:NH2	2.51	0.44
1:B:748:ILE:HD12	1:B:765:TYR:CG	2.53	0.44
1:A:75:HIS:HB3	1:A:78:ARG:HG3	2.00	0.43
1:B:315:ARG:NH1	1:B:316:THR:OG1	2.51	0.43
1:A:645:LEU:HG	1:A:650:VAL:CG2	2.49	0.43
1:B:263:ARG:O	1:B:267:GLU:HG2	2.18	0.43
1:A:155:TYR:HA	1:A:158:VAL:HG12	1.99	0.43
1:B:59:ASN:ND2	1:B:107:LYS:O	2.51	0.43
1:B:536:ILE:HD12	1:B:540:LEU:HD23	2.00	0.43
1:A:263:ARG:HG3	1:A:301:LEU:HD11	2.01	0.43
1:B:200:ILE:HG22	1:B:201:VAL:H	1.84	0.43
1:B:494:LEU:HB3	1:B:520:VAL:HG21	2.00	0.42
1:A:727:ARG:HG2	1:A:778:PHE:HB2	2.01	0.42
1:A:9:ASP:N	1:A:9:ASP:OD1	2.52	0.42
1:B:29:TYR:HB2	1:B:37:TRP:CZ2	2.55	0.42
1:B:656:VAL:HG12	1:B:684:VAL:HG22	2.01	0.42
1:A:481:LEU:HD23	1:A:627:LEU:HD13	2.01	0.42
1:A:417:GLU:N	1:A:418:PRO:HD2	2.34	0.42
1:A:718:THR:CG2	1:A:718:THR:O	2.68	0.41
1:B:219:ASP:O	1:B:220:LEU:HB2	2.20	0.41
1:B:693:ILE:CD1	1:B:718:THR:HG23	2.46	0.41
1:B:88:GLN:HE22	1:B:171:GLY:HA2	1.84	0.41
1:A:200:ILE:O	1:A:201:VAL:HB	2.20	0.41
1:A:430:ILE:HD12	3:A:946:HOH:O	2.19	0.41
1:A:143:LEU:HD23	1:A:257:MET:HG2	2.03	0.41
1:A:286:LEU:HB3	1:A:333:ILE:HG21	2.02	0.41
1:A:748:ILE:HD12	1:A:765:TYR:CG	2.55	0.41
1:B:533:ASN:HA	1:B:619:SER:O	2.21	0.41
1:A:58:TRP:HA	1:A:154:TRP:CZ3	2.56	0.41
1:A:533:ASN:ND2	1:A:619:SER:OG	2.48	0.41
1:A:369:LEU:HD21	1:A:673:VAL:HG21	2.03	0.41
1:A:200:ILE:HD11	1:A:257:MET:HE1	2.03	0.40
1:A:393:GLU:HG3	1:B:585:ARG:HH11	1.86	0.40
1:A:380:TYR:CE2	1:A:419:ILE:HG23	2.56	0.40
1:B:200:ILE:HG22	1:B:201:VAL:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:LEU:CD2	1:B:627:LEU:HD22	2.52	0.40

All (3) 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)
3:A:901:HOH:O	3:B:951:HOH:O[6_445]	2.01	0.19
3:A:923:HOH:O	3:A:959:HOH:O[3_455]	2.08	0.12
1:A:777:GLU:OE2	1:B:263:ARG:NH2[7_454]	2.17	0.03

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	773/778 (99%)	719 (93%)	47 (6%)	7 (1%)	17	35
1	B	773/778 (99%)	707 (92%)	58 (8%)	8 (1%)	15	32
All	All	1546/1556 (99%)	1426 (92%)	105 (7%)	15 (1%)	15	32

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	ALA
1	B	439	ALA
1	A	667	ILE
1	B	59	ASN
1	B	207	TRP
1	B	667	ILE
1	A	562	GLU
1	B	219	ASP
1	B	763	ARG
1	A	207	TRP

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Mol	Chain	Res	Type
1	A	218	GLY
1	A	232	THR
1	B	218	GLY
1	A	182	PRO
1	B	100	PRO

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	690/692 (100%)	640 (93%)	50 (7%)	14	29
1	B	690/692 (100%)	644 (93%)	46 (7%)	16	33
All	All	1380/1384 (100%)	1284 (93%)	96 (7%)	15	30

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	64	GLN
1	A	107	LYS
1	A	123	LEU
1	A	133	ARG
1	A	163	ARG
1	A	184	TYR
1	A	203	GLU
1	A	209	SER
1	A	217	LEU
1	A	230	ASP
1	A	233	GLU
1	A	283	TYR
1	A	315	ARG
1	A	338	VAL
1	A	339	SER
1	A	376	HIS
1	A	393	GLU

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Mol	Chain	Res	Type
1	A	403	TYR
1	A	426	LEU
1	A	436	GLN
1	A	438	LYS
1	A	498	THR
1	A	500	GLU
1	A	519	GLU
1	A	524	LEU
1	A	530	GLU
1	A	536	ILE
1	A	553	LEU
1	A	570	MET
1	A	572	LEU
1	A	576	LEU
1	A	583	ILE
1	A	585	ARG
1	A	622	ILE
1	A	626	ARG
1	A	627	LEU
1	A	655	GLU
1	A	685	LYS
1	A	692	GLU
1	A	712	VAL
1	A	718	THR
1	A	726	ASN
1	A	745	ASP
1	A	749	ARG
1	A	758	GLN
1	A	763	ARG
1	A	768	ARG
1	A	770	GLU
1	A	771	ARG
1	B	14	SER
1	B	16	ASP
1	B	19	ARG
1	B	39	ASP
1	B	118	SER
1	B	123	LEU
1	B	133	ARG
1	B	143	LEU
1	B	163	ARG
1	B	172	SER

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Mol	Chain	Res	Type
1	B	184	TYR
1	B	194	THR
1	B	219	ASP
1	B	232	THR
1	B	283	TYR
1	B	315	ARG
1	B	338	VAL
1	B	376	HIS
1	B	393	GLU
1	B	426	LEU
1	B	436	GLN
1	B	438	LYS
1	B	497	SER
1	B	498	THR
1	B	500	GLU
1	B	514	ASP
1	B	530	GLU
1	B	536	ILE
1	B	553	LEU
1	B	570	MET
1	B	576	LEU
1	B	585	ARG
1	B	612	ILE
1	B	622	ILE
1	B	626	ARG
1	B	627	LEU
1	B	635	ASP
1	B	655	GLU
1	B	656	VAL
1	B	685	LYS
1	B	692	GLU
1	B	758	GLN
1	B	759	GLU
1	B	764	VAL
1	B	768	ARG
1	B	770	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	415	HIS
1	A	436	GLN

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Mol	Chain	Res	Type
1	A	533	ASN
1	A	726	ASN
1	B	77	GLN
1	B	204	ASN
1	B	415	HIS
1	B	429	ASN
1	B	436	GLN
1	B	533	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	PO4	A	801	-	4,4,4	1.09	0	6,6,6	0.47	0
2	PO4	A	802	-	4,4,4	0.75	0	6,6,6	0.96	0
2	PO4	B	801	-	4,4,4	0.90	0	6,6,6	0.67	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	775/778 (99%)	-0.43	5 (0%)	89	88	17, 33, 55, 86	15 (1%)
1	B	775/778 (99%)	-0.12	24 (3%)	49	42	20, 46, 78, 129	15 (1%)
All	All	1550/1556 (99%)	-0.27	29 (1%)	66	62	17, 39, 71, 129	30 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	745	ASP	4.8
1	B	762	GLU	4.7
1	A	744	ARG	3.9
1	B	749	ARG	3.9
1	B	713	LYS	3.7
1	B	763	ARG	3.7
1	B	744	ARG	3.7
1	B	4	MET	3.6
1	B	760	LYS	3.6
1	B	708	GLU	3.2
1	B	709	ILE	3.0
1	B	748	ILE	3.0
1	B	711	GLY	3.0
1	A	762	GLU	2.6
1	B	222	GLU	2.6
1	B	750	GLY	2.5
1	B	778	PHE	2.5
1	B	228	PHE	2.4
1	B	776	ILE	2.4
1	B	747	ARG	2.2
1	B	436	GLN	2.1
1	B	525	ILE	2.1
1	B	500	GLU	2.1
1	B	768	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	771	ARG	2.1
1	A	778	PHE	2.1
1	A	763	ARG	2.0
1	A	713	LYS	2.0
1	B	568	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	A	802	5/5	0.93	0.13	65,69,74,74	0
2	PO4	B	801	5/5	0.93	0.15	57,58,63,67	0
2	PO4	A	801	5/5	0.97	0.17	57,63,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.