



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:35 PM GMT

PDB ID : 1XSJ  
Title : Structure of a Family 31 alpha glycosidase  
Authors : Lovering, A.L.; Lee, S.S.; Kim, Y.W.; Withers, S.G.; Strynadka, N.C.  
Deposited on : 2004-10-19  
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

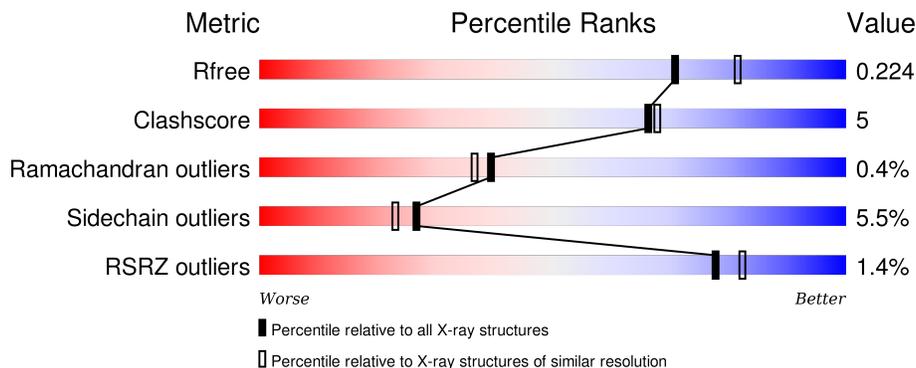
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ . 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% 13% ..
1	B	778	 2% 83% 15% ..
1	C	778	 1% 83% 13% ..
1	D	778	 1% 85% 13% ..
1	E	778	 2% 84% 12% ..

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Mol	Chain	Length	Quality of chain
1	F	778	

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
2	TRS	A	2002	-	-	-	X
2	TRS	B	2004	-	-	-	X
2	TRS	C	2005	-	-	-	X
2	TRS	C	2006	-	-	-	X
2	TRS	D	2007	-	-	-	X
2	TRS	E	2009	-	-	-	X
2	TRS	E	2010	-	-	-	X
2	TRS	E	2012	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 38890 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 Putative family 31 glucosidase yicI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	773	6226	3978	1069	1147	32	0	0	0
1	B	773	6226	3978	1069	1147	32	0	0	0
1	C	773	6226	3978	1069	1147	32	0	0	0
1	D	773	6226	3978	1069	1147	32	0	0	0
1	E	773	6226	3978	1069	1147	32	0	0	0
1	F	773	6226	3978	1069	1147	32	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

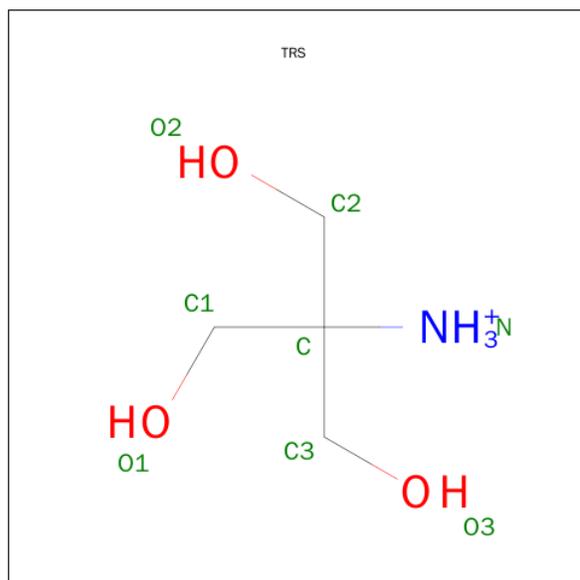
Chain	Residue	Modelled	Actual	Comment	Reference
A	773	HIS	-	EXPRESSION TAG	UNP P31434
A	774	HIS	-	EXPRESSION TAG	UNP P31434
A	775	HIS	-	EXPRESSION TAG	UNP P31434
A	776	HIS	-	EXPRESSION TAG	UNP P31434
A	777	HIS	-	EXPRESSION TAG	UNP P31434
A	778	HIS	-	EXPRESSION TAG	UNP P31434
B	773	HIS	-	EXPRESSION TAG	UNP P31434
B	774	HIS	-	EXPRESSION TAG	UNP P31434
B	775	HIS	-	EXPRESSION TAG	UNP P31434
B	776	HIS	-	EXPRESSION TAG	UNP P31434
B	777	HIS	-	EXPRESSION TAG	UNP P31434
B	778	HIS	-	EXPRESSION TAG	UNP P31434
C	773	HIS	-	EXPRESSION TAG	UNP P31434
C	774	HIS	-	EXPRESSION TAG	UNP P31434
C	775	HIS	-	EXPRESSION TAG	UNP P31434
C	776	HIS	-	EXPRESSION TAG	UNP P31434
C	777	HIS	-	EXPRESSION TAG	UNP P31434

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Chain	Residue	Modelled	Actual	Comment	Reference
C	778	HIS	-	EXPRESSION TAG	UNP P31434
D	773	HIS	-	EXPRESSION TAG	UNP P31434
D	774	HIS	-	EXPRESSION TAG	UNP P31434
D	775	HIS	-	EXPRESSION TAG	UNP P31434
D	776	HIS	-	EXPRESSION TAG	UNP P31434
D	777	HIS	-	EXPRESSION TAG	UNP P31434
D	778	HIS	-	EXPRESSION TAG	UNP P31434
E	773	HIS	-	EXPRESSION TAG	UNP P31434
E	774	HIS	-	EXPRESSION TAG	UNP P31434
E	775	HIS	-	EXPRESSION TAG	UNP P31434
E	776	HIS	-	EXPRESSION TAG	UNP P31434
E	777	HIS	-	EXPRESSION TAG	UNP P31434
E	778	HIS	-	EXPRESSION TAG	UNP P31434
F	773	HIS	-	EXPRESSION TAG	UNP P31434
F	774	HIS	-	EXPRESSION TAG	UNP P31434
F	775	HIS	-	EXPRESSION TAG	UNP P31434
F	776	HIS	-	EXPRESSION TAG	UNP P31434
F	777	HIS	-	EXPRESSION TAG	UNP P31434
F	778	HIS	-	EXPRESSION TAG	UNP P31434

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
2	A	1	8	4	1	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	E	1	Total	C	N	O	0	0
			8	4	1	3		
2	E	1	Total	C	N	O	0	0
			8	4	1	3		
2	F	1	Total	C	N	O	0	0
			8	4	1	3		
2	E	1	Total	C	N	O	0	0
			8	4	1	3		

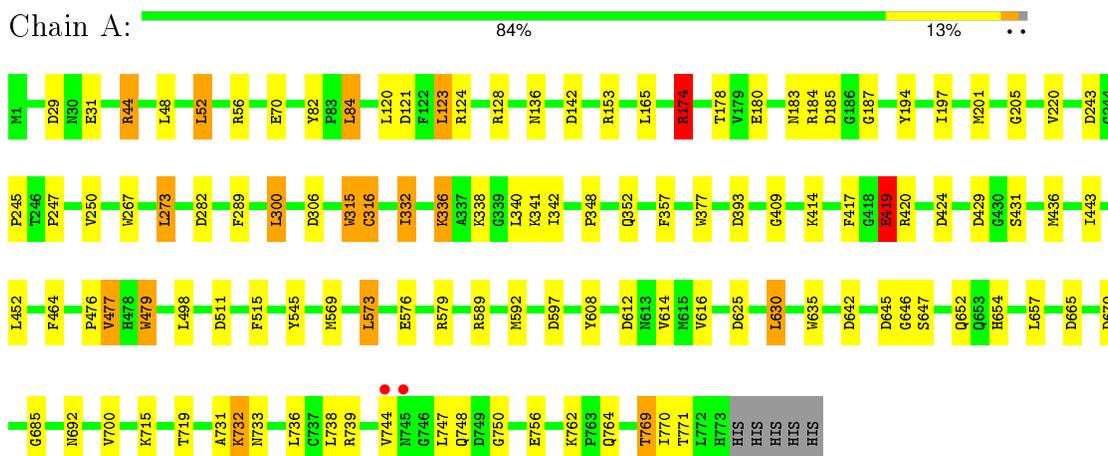
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	295	Total	O	0	0
			295	295		
3	B	208	Total	O	0	0
			208	208		
3	C	234	Total	O	0	0
			234	234		
3	D	267	Total	O	0	0
			267	267		
3	E	243	Total	O	0	0
			243	243		
3	F	191	Total	O	0	0
			191	191		

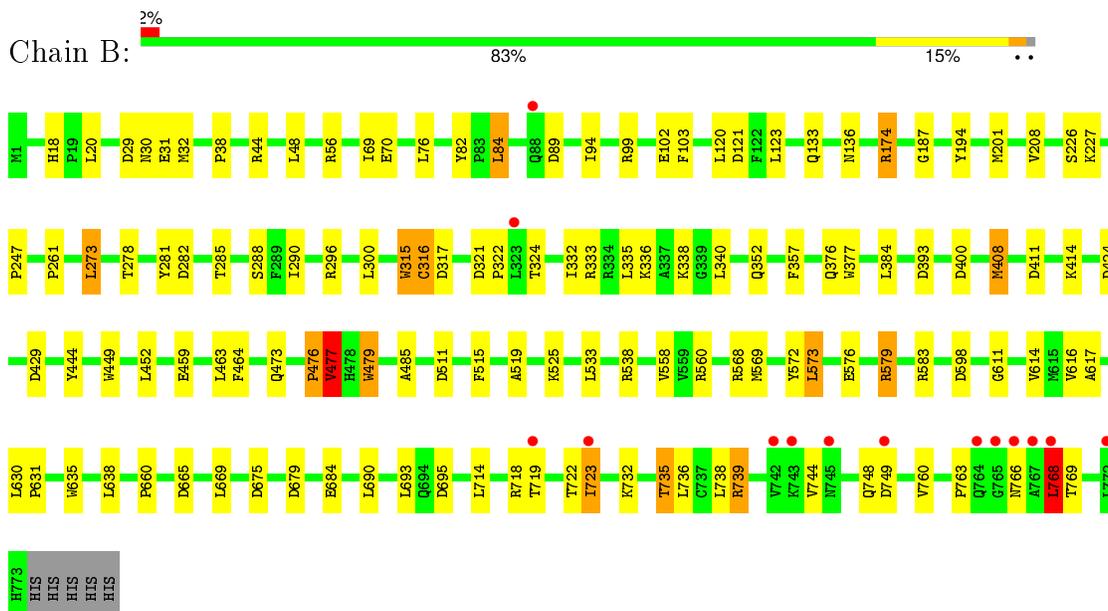
### 3 Residue-property plots

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.

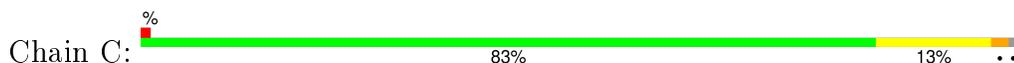
- Molecule 1: Putative family 31 glucosidase yicI



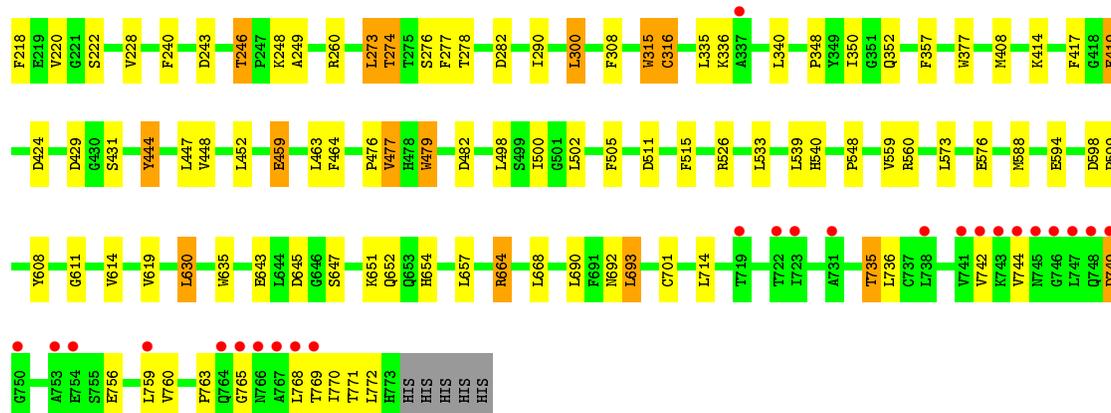
- Molecule 1: Putative family 31 glucosidase yicI



- Molecule 1: Putative family 31 glucosidase yicI







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.53Å 224.44Å 154.12Å 90.00° 101.75° 90.00°	Depositor
Resolution (Å)	29.98 – 2.10 66.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.2 (29.98-2.10) 88.8 (66.09-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.90 (at 2.00Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.180 , 0.220 0.187 , 0.224	Depositor DCC
$R_{free}$ test set	15119 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtrriage
Anisotropy	0.469	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.7	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	0 of 330993 reflections	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	38890	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: TRS

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	0/6409	0.92	32/8711 (0.4%)
1	B	0.75	0/6409	0.89	24/8711 (0.3%)
1	C	0.76	0/6409	0.88	20/8711 (0.2%)
1	D	0.82	1/6409 (0.0%)	0.94	32/8711 (0.4%)
1	E	0.80	0/6409	0.93	27/8711 (0.3%)
1	F	0.75	0/6409	0.88	18/8711 (0.2%)
All	All	0.78	1/38454 (0.0%)	0.91	153/52266 (0.3%)

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	1
1	B	0	1
1	C	1	0
1	D	0	1
1	E	0	1
1	F	1	0
All	All	2	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	664	ARG	CB-CG	-5.12	1.38	1.52

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	739	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	D	174	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	E	476	PRO	CA-C-N	-8.36	98.80	117.20
1	C	424	ASP	CB-CG-OD2	7.90	125.41	118.30
1	C	282	ASP	CB-CG-OD2	7.89	125.40	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	316	CYS	CA
1	F	316	CYS	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	315	TRP	Peptide
1	B	315	TRP	Peptide
1	D	315	TRP	Peptide
1	E	315	TRP	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	6226	0	5934	53	0
1	B	6226	0	5934	66	0
1	C	6226	0	5934	65	0
1	D	6226	0	5934	53	0
1	E	6226	0	5934	59	0
1	F	6226	0	5934	67	0
2	A	24	0	36	3	0
2	B	16	0	24	1	0
2	C	16	0	24	2	0
2	D	8	0	12	1	0
2	E	24	0	36	0	0
2	F	8	0	12	1	0
3	A	295	0	0	2	0
3	B	208	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	234	0	0	2	0
3	D	267	0	0	4	0
3	E	243	0	0	2	0
3	F	191	0	0	1	0
All	All	38890	0	35748	358	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 5.

The worst 5 of 358 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:F:274:THR:HG22	1:F:276:SER:H	1.08	1.11
1:F:274:THR:HG21	1:F:540:HIS:ND1	1.67	1.06
1:E:668:LEU:HD21	1:E:714:LEU:HD12	1.33	1.06
1:F:32:MET:CE	1:F:94:ILE:HG23	1.99	0.92
1:F:32:MET:HE2	1:F:94:ILE:HG23	1.52	0.90

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	771/778 (99%)	742 (96%)	25 (3%)	4 (0%)	34 30
1	B	771/778 (99%)	746 (97%)	24 (3%)	1 (0%)	56 58
1	C	771/778 (99%)	745 (97%)	24 (3%)	2 (0%)	46 45
1	D	771/778 (99%)	741 (96%)	28 (4%)	2 (0%)	46 45
1	E	771/778 (99%)	738 (96%)	27 (4%)	6 (1%)	24 17
1	F	771/778 (99%)	737 (96%)	29 (4%)	5 (1%)	30 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4626/4668 (99%)	4449 (96%)	157 (3%)	20 (0%)	39 37

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	477	VAL
1	E	766	ASN
1	F	749	ASP
1	C	749	ASP
1	A	338	LYS

### 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	659/665 (99%)	627 (95%)	32 (5%)	31 28
1	B	659/665 (99%)	622 (94%)	37 (6%)	26 22
1	C	659/665 (99%)	622 (94%)	37 (6%)	26 22
1	D	659/665 (99%)	625 (95%)	34 (5%)	29 25
1	E	659/665 (99%)	624 (95%)	35 (5%)	28 25
1	F	659/665 (99%)	617 (94%)	42 (6%)	22 18
All	All	3954/3990 (99%)	3737 (94%)	217 (6%)	27 23

5 of 217 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	693	LEU
1	D	419	GLU
1	F	464	PHE
1	C	744	VAL
1	D	116	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	73	GLN
1	D	766	ASN
1	F	280	ASN
1	D	146	GLN
1	D	652	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

12 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	TRS	A	2001	-	7,7,7	1.21	1 (14%)	9,9,9	0.94	0
2	TRS	A	2002	-	7,7,7	1.11	1 (14%)	9,9,9	1.95	3 (33%)
2	TRS	A	2008	-	7,7,7	1.37	1 (14%)	9,9,9	2.28	3 (33%)
2	TRS	B	2003	-	7,7,7	1.00	0	9,9,9	2.07	4 (44%)
2	TRS	B	2004	-	7,7,7	0.92	1 (14%)	9,9,9	1.26	2 (22%)
2	TRS	C	2005	-	7,7,7	1.21	1 (14%)	9,9,9	1.04	0
2	TRS	C	2006	-	7,7,7	1.14	1 (14%)	9,9,9	1.49	2 (22%)
2	TRS	D	2007	-	7,7,7	0.73	0	9,9,9	1.17	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TRS	E	2009	-	7,7,7	1.21	1 (14%)	9,9,9	1.36	1 (11%)
2	TRS	E	2010	-	7,7,7	0.89	1 (14%)	9,9,9	1.22	0
2	TRS	E	2012	-	7,7,7	1.14	1 (14%)	9,9,9	1.18	1 (11%)
2	TRS	F	2011	-	7,7,7	1.16	1 (14%)	9,9,9	0.99	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	TRS	A	2001	-	-	0/9/9/9	0/0/0/0
2	TRS	A	2002	-	-	0/9/9/9	0/0/0/0
2	TRS	A	2008	-	-	0/9/9/9	0/0/0/0
2	TRS	B	2003	-	-	0/9/9/9	0/0/0/0
2	TRS	B	2004	-	-	0/9/9/9	0/0/0/0
2	TRS	C	2005	-	-	0/9/9/9	0/0/0/0
2	TRS	C	2006	-	-	0/9/9/9	0/0/0/0
2	TRS	D	2007	-	-	0/9/9/9	0/0/0/0
2	TRS	E	2009	-	-	0/9/9/9	0/0/0/0
2	TRS	E	2010	-	-	0/9/9/9	0/0/0/0
2	TRS	E	2012	-	-	0/9/9/9	0/0/0/0
2	TRS	F	2011	-	-	0/9/9/9	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2008	TRS	C-N	-3.28	1.45	1.50
2	C	2005	TRS	C-N	-3.04	1.46	1.50
2	A	2001	TRS	C-N	-2.91	1.46	1.50
2	F	2011	TRS	C-N	-2.82	1.46	1.50
2	E	2012	TRS	C-N	-2.79	1.46	1.50

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2008	TRS	C3-C-N	-3.72	101.31	108.09
2	C	2006	TRS	C3-C-N	-3.65	101.44	108.09
2	A	2008	TRS	O2-C2-C	-3.37	104.37	111.18
2	B	2003	TRS	O2-C2-C	-2.92	105.27	111.18
2	E	2009	TRS	O2-C2-C	-2.89	105.34	111.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	TRS	1	0
2	A	2002	TRS	1	0
2	A	2008	TRS	1	0
2	B	2003	TRS	1	0
2	C	2005	TRS	1	0
2	C	2006	TRS	1	0
2	D	2007	TRS	1	0
2	F	2011	TRS	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	773/778 (99%)	-0.44	2 (0%) 94 95	9, 18, 33, 43	0
1	B	773/778 (99%)	-0.43	14 (1%) 71 76	12, 22, 48, 65	0
1	C	773/778 (99%)	-0.44	7 (0%) 85 88	11, 20, 41, 61	0
1	D	773/778 (99%)	-0.57	4 (0%) 91 93	9, 17, 32, 46	0
1	E	773/778 (99%)	-0.43	12 (1%) 74 79	9, 19, 45, 71	0
1	F	773/778 (99%)	-0.22	25 (3%) 51 60	11, 23, 53, 71	0
All	All	4638/4668 (99%)	-0.42	64 (1%) 78 82	9, 20, 42, 71	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	765	GLY	7.7
1	F	719	THR	5.2
1	B	765	GLY	5.0
1	F	766	ASN	5.0
1	E	765	GLY	4.8

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	TRS	E	2012	8/8	0.94	0.12	5.00	26,27,30,30	0
2	TRS	E	2010	8/8	0.93	0.10	4.48	23,23,26,27	0
2	TRS	C	2006	8/8	0.88	0.12	4.01	29,31,32,33	0
2	TRS	C	2005	8/8	0.94	0.11	3.21	20,21,23,26	0
2	TRS	B	2004	8/8	0.92	0.10	3.05	26,26,28,28	0
2	TRS	A	2002	8/8	0.92	0.11	2.81	28,29,29,32	0
2	TRS	D	2007	8/8	0.96	0.10	2.65	14,16,17,22	0
2	TRS	E	2009	8/8	0.95	0.09	2.54	13,14,16,21	0
2	TRS	A	2008	8/8	0.95	0.10	1.98	25,26,26,27	0
2	TRS	B	2003	8/8	0.95	0.09	1.73	18,18,19,24	0
2	TRS	A	2001	8/8	0.95	0.11	1.57	13,15,16,22	0
2	TRS	F	2011	8/8	0.96	0.10	1.19	18,21,22,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.