



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:22 AM UTC

PDB ID : 6JR6 / pdb_00006jr6
Title : Flavobacterium johnsoniae GH31 dextranase, FjDex31A
Authors : Tonozuka, T.
Deposited on : 2019-04-02
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

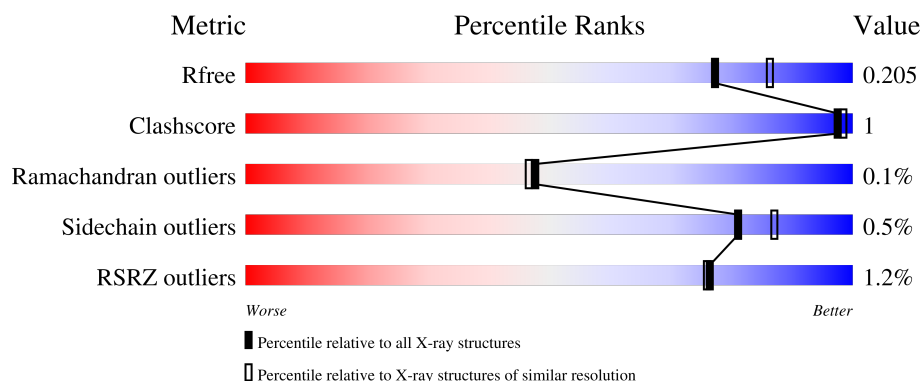
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

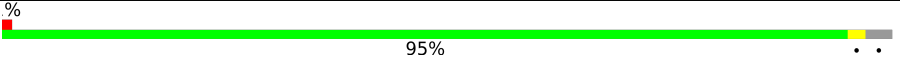
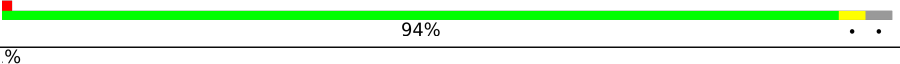
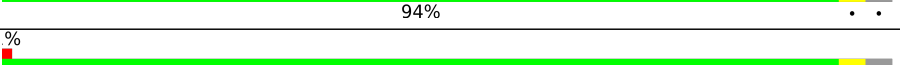
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	838	 95% . .
1	B	838	 94% . .
1	C	838	 94% . .
1	D	838	 94% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28801 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 Candidate alpha-glycosidase Glycoside hydrolase family 31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	812	Total	C	N	O	S	0	0	0
			6585	4221	1103	1230	31			
1	B	812	Total	C	N	O	S	0	0	0
			6585	4221	1103	1230	31			
1	C	812	Total	C	N	O	S	0	0	0
			6585	4221	1103	1230	31			
1	D	812	Total	C	N	O	S	0	0	0
			6585	4221	1103	1230	31			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP A5FBI1
A	0	GLY	-	expression tag	UNP A5FBI1
A	1	SER	-	expression tag	UNP A5FBI1
A	2	SER	-	expression tag	UNP A5FBI1
A	3	HIS	-	expression tag	UNP A5FBI1
A	4	HIS	-	expression tag	UNP A5FBI1
A	5	HIS	-	expression tag	UNP A5FBI1
A	6	HIS	-	expression tag	UNP A5FBI1
A	7	HIS	-	expression tag	UNP A5FBI1
A	8	HIS	-	expression tag	UNP A5FBI1
A	9	SER	-	expression tag	UNP A5FBI1
A	10	SER	-	expression tag	UNP A5FBI1
A	11	GLY	-	expression tag	UNP A5FBI1
A	12	LEU	-	expression tag	UNP A5FBI1
A	13	VAL	-	expression tag	UNP A5FBI1
A	14	PRO	-	expression tag	UNP A5FBI1
A	15	ARG	-	expression tag	UNP A5FBI1
A	16	GLY	-	expression tag	UNP A5FBI1
A	17	SER	-	expression tag	UNP A5FBI1
A	18	HIS	-	expression tag	UNP A5FBI1
A	19	MET	-	expression tag	UNP A5FBI1

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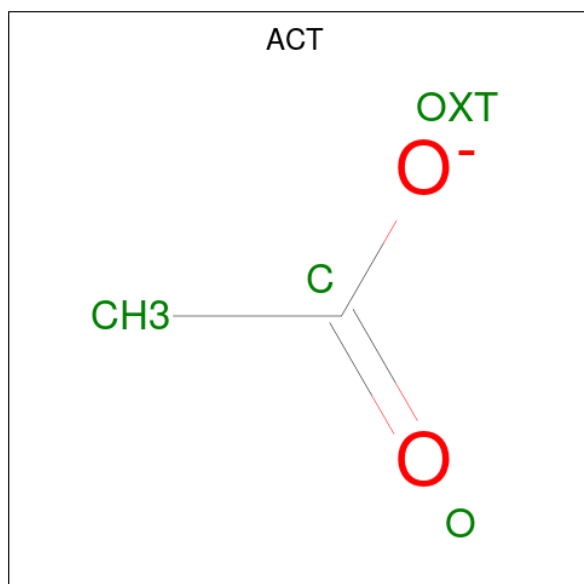
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	expression tag	UNP A5FBI1
B	-1	MET	-	expression tag	UNP A5FBI1
B	0	GLY	-	expression tag	UNP A5FBI1
B	1	SER	-	expression tag	UNP A5FBI1
B	2	SER	-	expression tag	UNP A5FBI1
B	3	HIS	-	expression tag	UNP A5FBI1
B	4	HIS	-	expression tag	UNP A5FBI1
B	5	HIS	-	expression tag	UNP A5FBI1
B	6	HIS	-	expression tag	UNP A5FBI1
B	7	HIS	-	expression tag	UNP A5FBI1
B	8	HIS	-	expression tag	UNP A5FBI1
B	9	SER	-	expression tag	UNP A5FBI1
B	10	SER	-	expression tag	UNP A5FBI1
B	11	GLY	-	expression tag	UNP A5FBI1
B	12	LEU	-	expression tag	UNP A5FBI1
B	13	VAL	-	expression tag	UNP A5FBI1
B	14	PRO	-	expression tag	UNP A5FBI1
B	15	ARG	-	expression tag	UNP A5FBI1
B	16	GLY	-	expression tag	UNP A5FBI1
B	17	SER	-	expression tag	UNP A5FBI1
B	18	HIS	-	expression tag	UNP A5FBI1
B	19	MET	-	expression tag	UNP A5FBI1
B	20	ALA	-	expression tag	UNP A5FBI1
C	-1	MET	-	expression tag	UNP A5FBI1
C	0	GLY	-	expression tag	UNP A5FBI1
C	1	SER	-	expression tag	UNP A5FBI1
C	2	SER	-	expression tag	UNP A5FBI1
C	3	HIS	-	expression tag	UNP A5FBI1
C	4	HIS	-	expression tag	UNP A5FBI1
C	5	HIS	-	expression tag	UNP A5FBI1
C	6	HIS	-	expression tag	UNP A5FBI1
C	7	HIS	-	expression tag	UNP A5FBI1
C	8	HIS	-	expression tag	UNP A5FBI1
C	9	SER	-	expression tag	UNP A5FBI1
C	10	SER	-	expression tag	UNP A5FBI1
C	11	GLY	-	expression tag	UNP A5FBI1
C	12	LEU	-	expression tag	UNP A5FBI1
C	13	VAL	-	expression tag	UNP A5FBI1
C	14	PRO	-	expression tag	UNP A5FBI1
C	15	ARG	-	expression tag	UNP A5FBI1
C	16	GLY	-	expression tag	UNP A5FBI1
C	17	SER	-	expression tag	UNP A5FBI1

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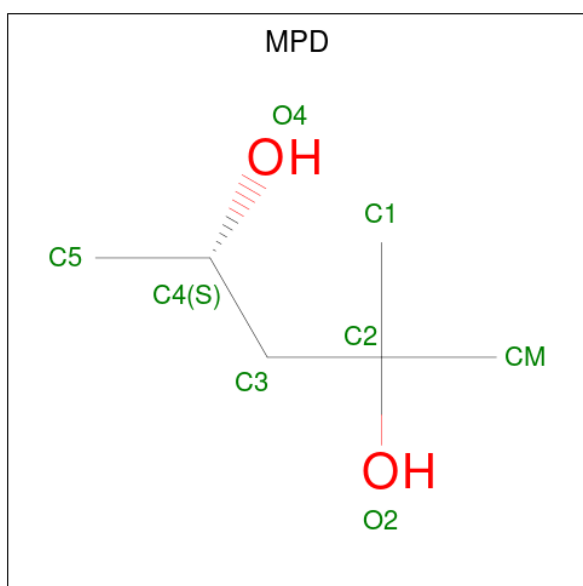
Chain	Residue	Modelled	Actual	Comment	Reference
C	18	HIS	-	expression tag	UNP A5FBI1
C	19	MET	-	expression tag	UNP A5FBI1
C	20	ALA	-	expression tag	UNP A5FBI1
D	-1	MET	-	expression tag	UNP A5FBI1
D	0	GLY	-	expression tag	UNP A5FBI1
D	1	SER	-	expression tag	UNP A5FBI1
D	2	SER	-	expression tag	UNP A5FBI1
D	3	HIS	-	expression tag	UNP A5FBI1
D	4	HIS	-	expression tag	UNP A5FBI1
D	5	HIS	-	expression tag	UNP A5FBI1
D	6	HIS	-	expression tag	UNP A5FBI1
D	7	HIS	-	expression tag	UNP A5FBI1
D	8	HIS	-	expression tag	UNP A5FBI1
D	9	SER	-	expression tag	UNP A5FBI1
D	10	SER	-	expression tag	UNP A5FBI1
D	11	GLY	-	expression tag	UNP A5FBI1
D	12	LEU	-	expression tag	UNP A5FBI1
D	13	VAL	-	expression tag	UNP A5FBI1
D	14	PRO	-	expression tag	UNP A5FBI1
D	15	ARG	-	expression tag	UNP A5FBI1
D	16	GLY	-	expression tag	UNP A5FBI1
D	17	SER	-	expression tag	UNP A5FBI1
D	18	HIS	-	expression tag	UNP A5FBI1
D	19	MET	-	expression tag	UNP A5FBI1
D	20	ALA	-	expression tag	UNP A5FBI1

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		

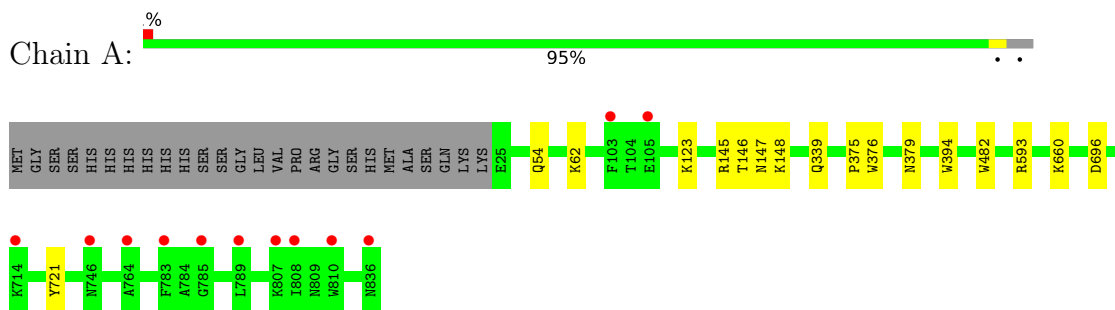
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	611	Total 611	O 611	0	0
4	B	599	Total 599	O 599	0	0
4	C	569	Total 569	O 569	0	0
4	D	602	Total 602	O 602	0	0

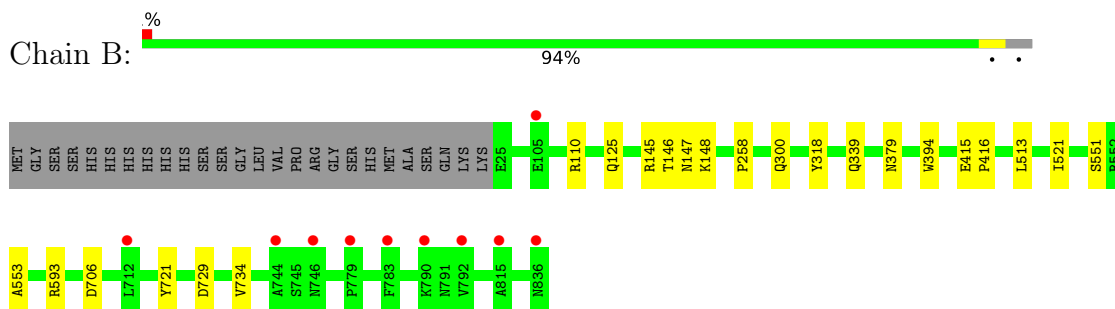
3 Residue-property plots [i](#)

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.

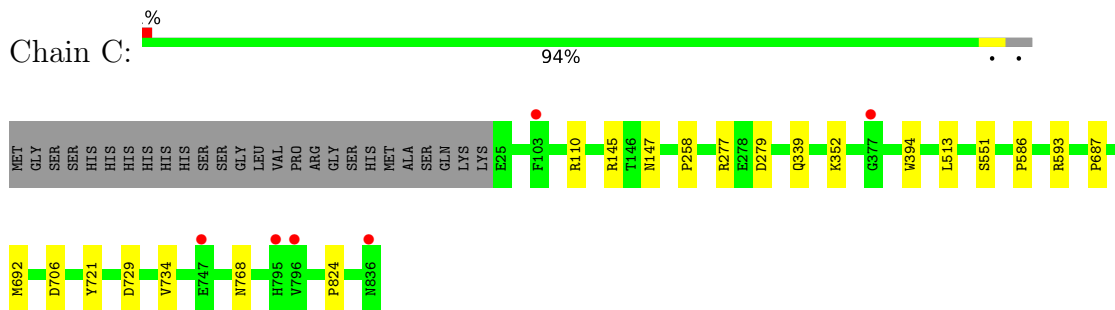
- Molecule 1: Candidate alpha-glycosidase Glycoside hydrolase family 31



- Molecule 1: Candidate alpha-glycosidase Glycoside hydrolase family 31

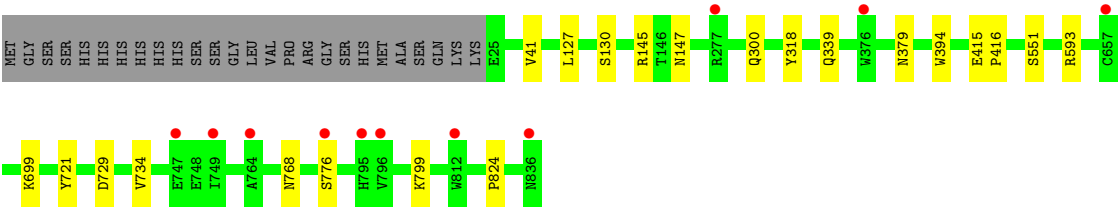


- Molecule 1: Candidate alpha-glycosidase Glycoside hydrolase family 31



- Molecule 1: Candidate alpha-glycosidase Glycoside hydrolase family 31





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	102.47Å 112.74Å 114.25Å 111.13° 92.86° 114.54°	Depositor
Resolution (Å)	48.45 – 2.00 48.45 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.3 (48.45-2.00) 90.3 (48.45-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.165 , 0.199 0.172 , 0.205	Depositor DCC
R_{free} test set	12837 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28801	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ACT, MPD

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	0.60	0/6767	0.78	0/9156
1	B	0.60	0/6767	0.78	0/9156
1	C	0.59	0/6767	0.76	0/9156
1	D	0.61	0/6767	0.78	0/9156
All	All	0.60	0/27068	0.78	0/36624

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	6585	0	6343	8	0
1	B	6585	0	6343	13	0
1	C	6585	0	6343	9	0
1	D	6585	0	6343	11	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	1	0
3	A	16	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	28	0	0
3	C	16	0	28	0	0
3	D	16	0	28	0	0
4	A	611	0	0	0	0
4	B	599	0	0	0	0
4	C	569	0	0	0	0
4	D	602	0	0	0	0
All	All	28801	0	25496	39	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 1.

All (39) 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:145:ARG:HE	1:B:147:ASN:HD21	1.32	0.77
1:C:145:ARG:HE	1:C:147:ASN:HD21	1.34	0.75
1:D:339:GLN:HE22	1:D:394:TRP:HE1	1.33	0.75
1:D:145:ARG:HE	1:D:147:ASN:HD21	1.33	0.74
1:B:110:ARG:HH21	1:D:379:ASN:HD21	1.35	0.74
1:B:339:GLN:HE22	1:B:394:TRP:HE1	1.36	0.74
1:A:339:GLN:HE22	1:A:394:TRP:HE1	1.41	0.69
1:C:339:GLN:HE22	1:C:394:TRP:HE1	1.46	0.63
1:A:145:ARG:HE	1:A:147:ASN:HD21	1.45	0.62
1:C:593:ARG:HD3	1:C:721:TYR:CZ	2.37	0.59
1:B:379:ASN:HD21	1:C:110:ARG:HH21	1.51	0.58
1:D:145:ARG:HE	1:D:147:ASN:ND2	2.02	0.57
1:D:768:ASN:HD22	1:D:824:PRO:HA	1.76	0.51
1:B:125:GLN:HG3	2:D:901:ACT:H1	1.92	0.50
1:D:145:ARG:NE	1:D:147:ASN:HD21	2.06	0.50
1:A:375:PRO:HB2	1:A:376:TRP:CE3	2.48	0.48
1:D:300:GLN:NE2	1:D:318:TYR:OH	2.47	0.47
1:B:145:ARG:HE	1:B:147:ASN:ND2	2.06	0.47
1:A:593:ARG:HD3	1:A:721:TYR:CZ	2.50	0.47
1:B:729:ASP:HB3	1:B:734:VAL:HB	1.97	0.47
1:B:415:GLU:N	1:B:416:PRO:HA	2.31	0.46
1:A:145:ARG:NE	1:A:147:ASN:HD21	2.13	0.46
1:C:277:ARG:NH1	1:C:279:ASP:OD1	2.49	0.45
1:B:300:GLN:NE2	1:B:318:TYR:OH	2.48	0.45
1:D:593:ARG:HD3	1:D:721:TYR:CZ	2.52	0.45
1:D:729:ASP:HB3	1:D:734:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:THR:CG2	1:A:148:LYS:HE2	2.47	0.45
1:A:145:ARG:HE	1:A:147:ASN:ND2	2.12	0.44
1:B:593:ARG:HD3	1:B:721:TYR:CZ	2.54	0.43
1:D:415:GLU:N	1:D:416:PRO:HA	2.34	0.43
1:C:258:PRO:HG3	1:C:513:LEU:HD12	2.00	0.43
1:C:729:ASP:HB3	1:C:734:VAL:HB	2.00	0.42
1:D:127:LEU:HD11	1:D:130:SER:HB2	2.00	0.42
1:C:768:ASN:HD22	1:C:824:PRO:HA	1.84	0.42
1:B:146:THR:CG2	1:B:148:LYS:HE2	2.49	0.42
1:A:54:GLN:HB3	1:A:62:LYS:HB3	2.01	0.41
1:B:521:ILE:HB	1:B:553:ALA:HA	2.02	0.41
1:C:586:PRO:HB2	1:C:687:PRO:HB2	2.02	0.41
1:B:258:PRO:HG3	1:B:513:LEU:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	810/838 (97%)	786 (97%)	24 (3%)	0	100	100
1	B	810/838 (97%)	790 (98%)	19 (2%)	1 (0%)	48	46
1	C	810/838 (97%)	787 (97%)	22 (3%)	1 (0%)	48	46
1	D	810/838 (97%)	786 (97%)	23 (3%)	1 (0%)	48	46
All	All	3240/3352 (97%)	3149 (97%)	88 (3%)	3 (0%)	48	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	551	SER
1	C	551	SER

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Mol	Chain	Res	Type
1	D	551	SER

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	703/725 (97%)	698 (99%)	5 (1%)	76	82
1	B	703/725 (97%)	702 (100%)	1 (0%)	88	92
1	C	703/725 (97%)	700 (100%)	3 (0%)	84	89
1	D	703/725 (97%)	699 (99%)	4 (1%)	78	85
All	All	2812/2900 (97%)	2799 (100%)	13 (0%)	81	87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	LYS
1	A	379	ASN
1	A	482	TRP
1	A	660	LYS
1	A	696	ASP
1	B	706	ASP
1	C	352	LYS
1	C	692	MET
1	C	706	ASP
1	D	41	VAL
1	D	699	LYS
1	D	776	SER
1	D	799	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	125	GLN

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Mol	Chain	Res	Type
1	A	147	ASN
1	A	250	ASN
1	A	300	GLN
1	A	339	GLN
1	A	379	ASN
1	A	501	ASN
1	A	768	ASN
1	A	791	ASN
1	B	112	ASN
1	B	125	GLN
1	B	147	ASN
1	B	250	ASN
1	B	300	GLN
1	B	339	GLN
1	B	379	ASN
1	B	428	ASN
1	C	112	ASN
1	C	117	GLN
1	C	125	GLN
1	C	139	ASN
1	C	147	ASN
1	C	250	ASN
1	C	300	GLN
1	C	339	GLN
1	C	379	ASN
1	C	637	GLN
1	C	655	ASN
1	C	768	ASN
1	C	791	ASN
1	C	800	ASN
1	D	47	ASN
1	D	112	ASN
1	D	117	GLN
1	D	125	GLN
1	D	147	ASN
1	D	222	ASN
1	D	250	ASN
1	D	300	GLN
1	D	316	ASN
1	D	339	GLN
1	D	379	ASN
1	D	768	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](#)

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	$\# Z > 2$
3	MPD	C	902	-	7,7,7	0.22	0	9,10,10	0.42	0
3	MPD	D	903	-	7,7,7	0.28	0	9,10,10	0.44	0
2	ACT	B	901	-	3,3,3	0.78	0	3,3,3	0.89	0
3	MPD	A	902	-	7,7,7	0.28	0	9,10,10	0.29	0
3	MPD	D	902	-	7,7,7	0.34	0	9,10,10	0.33	0
3	MPD	C	903	-	7,7,7	0.34	0	9,10,10	0.41	0
2	ACT	C	901	-	3,3,3	0.91	0	3,3,3	0.80	0
3	MPD	B	902	-	7,7,7	0.34	0	9,10,10	0.31	0
3	MPD	B	903	-	7,7,7	0.31	0	9,10,10	0.50	0
3	MPD	A	903	-	7,7,7	0.26	0	9,10,10	0.25	0
2	ACT	A	901	-	3,3,3	0.77	0	3,3,3	0.86	0
2	ACT	D	901	-	3,3,3	0.83	0	3,3,3	0.73	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
3	MPD	C	902	-	-	0/5/5/5	-
3	MPD	D	903	-	-	5/5/5/5	-
3	MPD	A	902	-	-	0/5/5/5	-
3	MPD	D	902	-	-	0/5/5/5	-
3	MPD	C	903	-	-	3/5/5/5	-
3	MPD	B	902	-	-	0/5/5/5	-
3	MPD	B	903	-	-	0/5/5/5	-
3	MPD	A	903	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	903	MPD	C2-C3-C4-O4
3	D	903	MPD	C2-C3-C4-C5
3	C	903	MPD	CM-C2-C3-C4
3	D	903	MPD	C1-C2-C3-C4
3	C	903	MPD	O2-C2-C3-C4
3	D	903	MPD	O2-C2-C3-C4
3	C	903	MPD	C1-C2-C3-C4
3	D	903	MPD	CM-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	901	ACT	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, 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	812/838 (96%)	-0.26	12 (1%) 72 71	17, 26, 52, 82	0
1	B	812/838 (96%)	-0.14	10 (1%) 76 76	17, 27, 61, 96	0
1	C	812/838 (96%)	-0.16	6 (0%) 84 84	19, 28, 51, 91	0
1	D	812/838 (96%)	-0.20	11 (1%) 73 73	17, 26, 52, 87	0
All	All	3248/3352 (96%)	-0.19	39 (1%) 76 76	17, 27, 54, 96	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	712	LEU	4.7
1	A	103	PHE	3.8
1	A	764	ALA	3.8
1	B	746	ASN	3.4
1	D	836	ASN	3.1
1	B	815	ALA	3.1
1	A	714	LYS	3.0
1	C	377	GLY	2.9
1	C	747	GLU	2.9
1	D	747	GLU	2.9
1	C	836	ASN	2.8
1	A	808	ILE	2.8
1	A	836	ASN	2.8
1	C	103	PHE	2.7
1	B	779	PRO	2.6
1	D	812	TRP	2.6
1	A	810	TRP	2.5
1	A	783	PHE	2.5
1	C	796	VAL	2.4
1	A	105	GLU	2.4
1	B	783	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	795	HIS	2.4
1	B	790	LYS	2.3
1	B	744	ALA	2.3
1	D	764	ALA	2.3
1	D	776	SER	2.3
1	D	277	ARG	2.3
1	D	376	TRP	2.2
1	B	836	ASN	2.2
1	D	749	ILE	2.2
1	A	789	LEU	2.2
1	A	807	LYS	2.1
1	A	746	ASN	2.1
1	B	105	GLU	2.1
1	A	785	GLY	2.1
1	D	657	CYS	2.0
1	B	792	VAL	2.0
1	D	796	VAL	2.0
1	C	795	HIS	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 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, 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
3	MPD	C	903	8/8	0.70	0.28	72,78,81,87	0
3	MPD	D	903	8/8	0.74	0.28	71,77,81,83	0
3	MPD	B	903	8/8	0.75	0.29	71,77,78,79	0
3	MPD	D	902	8/8	0.84	0.18	49,50,53,53	0
2	ACT	A	901	4/4	0.84	0.20	39,41,41,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MPD	A	903	8/8	0.86	0.14	48,50,52,54	0
2	ACT	B	901	4/4	0.88	0.18	41,42,43,45	0
3	MPD	C	902	8/8	0.89	0.17	55,56,57,59	0
2	ACT	D	901	4/4	0.89	0.16	38,41,44,44	0
3	MPD	A	902	8/8	0.90	0.14	49,51,51,52	0
3	MPD	B	902	8/8	0.91	0.11	48,49,49,49	0
2	ACT	C	901	4/4	0.94	0.11	28,31,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.