



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:02 PM UTC

PDB ID : 8BLJ / pdb\_00008blj  
Title : Crystal structure of the ligand-binding domain (LBD) of human iGluR Delta-1 (GluD1), apo state  
Authors : Heroven, C.; Malinauskas, T.; Aricescu, A.R.  
Deposited on : 2022-11-09  
Resolution : 2.18 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

<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>.

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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

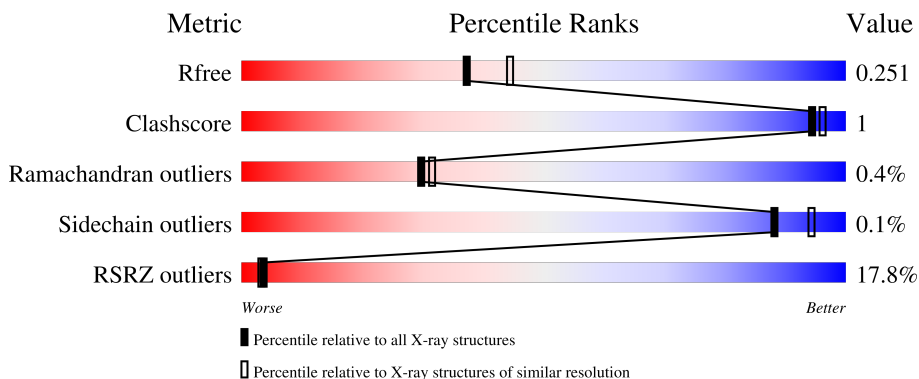
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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.



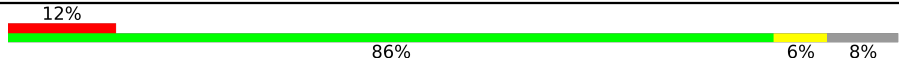
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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  $\geq 3$ , 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	282	 11% 91% 6%
1	B	282	 16% 90% 6%
1	C	282	 13% 90% 7%
1	D	282	 21% 90% 6%
1	E	282	 27% 86% 6% 9%

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Mol	Chain	Length	Quality of chain
1	F	282	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '12%', a large green segment labeled '86%', a small yellow segment labeled '6%', and a grey segment on the far right labeled '8%'.</p>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25266 atoms, of which 12413 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 Glutamate receptor ionotropic, delta-1, Isoform 2 of Glutamate receptor ionotropic, delta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	265	4162	1331	2069	353	401	8	0	1	0
1	B	264	4162	1329	2073	355	397	8	0	1	0
1	C	261	4111	1315	2045	350	393	8	0	1	0
1	D	266	4190	1338	2085	359	400	8	0	1	0
1	E	258	4046	1294	2012	344	388	8	0	0	0
1	F	260	4117	1318	2045	354	392	8	0	3	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	548	GLY	-	linker	UNP Q9ULK0
A	549	THR	-	linker	UNP Q9ULK0
A	824	GLY	-	expression tag	UNP Q9ULK0-2
A	825	THR	-	expression tag	UNP Q9ULK0-2
A	826	LEU	-	expression tag	UNP Q9ULK0-2
A	827	GLU	-	expression tag	UNP Q9ULK0-2
A	828	VAL	-	expression tag	UNP Q9ULK0-2
A	829	LEU	-	expression tag	UNP Q9ULK0-2
A	830	PHE	-	expression tag	UNP Q9ULK0-2
A	831	GLN	-	expression tag	UNP Q9ULK0-2
B	548	GLY	-	linker	UNP Q9ULK0
B	549	THR	-	linker	UNP Q9ULK0
B	824	GLY	-	expression tag	UNP Q9ULK0-2
B	825	THR	-	expression tag	UNP Q9ULK0-2
B	826	LEU	-	expression tag	UNP Q9ULK0-2
B	827	GLU	-	expression tag	UNP Q9ULK0-2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	828	VAL	-	expression tag	UNP Q9ULK0-2
B	829	LEU	-	expression tag	UNP Q9ULK0-2
B	830	PHE	-	expression tag	UNP Q9ULK0-2
B	831	GLN	-	expression tag	UNP Q9ULK0-2
C	548	GLY	-	linker	UNP Q9ULK0
C	549	THR	-	linker	UNP Q9ULK0
C	824	GLY	-	expression tag	UNP Q9ULK0-2
C	825	THR	-	expression tag	UNP Q9ULK0-2
C	826	LEU	-	expression tag	UNP Q9ULK0-2
C	827	GLU	-	expression tag	UNP Q9ULK0-2
C	828	VAL	-	expression tag	UNP Q9ULK0-2
C	829	LEU	-	expression tag	UNP Q9ULK0-2
C	830	PHE	-	expression tag	UNP Q9ULK0-2
C	831	GLN	-	expression tag	UNP Q9ULK0-2
D	548	GLY	-	linker	UNP Q9ULK0
D	549	THR	-	linker	UNP Q9ULK0
D	824	GLY	-	expression tag	UNP Q9ULK0-2
D	825	THR	-	expression tag	UNP Q9ULK0-2
D	826	LEU	-	expression tag	UNP Q9ULK0-2
D	827	GLU	-	expression tag	UNP Q9ULK0-2
D	828	VAL	-	expression tag	UNP Q9ULK0-2
D	829	LEU	-	expression tag	UNP Q9ULK0-2
D	830	PHE	-	expression tag	UNP Q9ULK0-2
D	831	GLN	-	expression tag	UNP Q9ULK0-2
E	548	GLY	-	linker	UNP Q9ULK0
E	549	THR	-	linker	UNP Q9ULK0
E	824	GLY	-	expression tag	UNP Q9ULK0-2
E	825	THR	-	expression tag	UNP Q9ULK0-2
E	826	LEU	-	expression tag	UNP Q9ULK0-2
E	827	GLU	-	expression tag	UNP Q9ULK0-2
E	828	VAL	-	expression tag	UNP Q9ULK0-2
E	829	LEU	-	expression tag	UNP Q9ULK0-2
E	830	PHE	-	expression tag	UNP Q9ULK0-2
E	831	GLN	-	expression tag	UNP Q9ULK0-2
F	548	GLY	-	linker	UNP Q9ULK0
F	549	THR	-	linker	UNP Q9ULK0
F	824	GLY	-	expression tag	UNP Q9ULK0-2
F	825	THR	-	expression tag	UNP Q9ULK0-2
F	826	LEU	-	expression tag	UNP Q9ULK0-2
F	827	GLU	-	expression tag	UNP Q9ULK0-2
F	828	VAL	-	expression tag	UNP Q9ULK0-2
F	829	LEU	-	expression tag	UNP Q9ULK0-2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	830	PHE	-	expression tag	UNP Q9ULK0-2
F	831	GLN	-	expression tag	UNP Q9ULK0-2

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Ca 3 3	0	0
2	B	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	2	Total Ca 2 2	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0
3	C	2	Total Cl 2 2	0	0
3	E	1	Total Cl 1 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	E	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	F	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	C	1	10	2	6	2	0	0

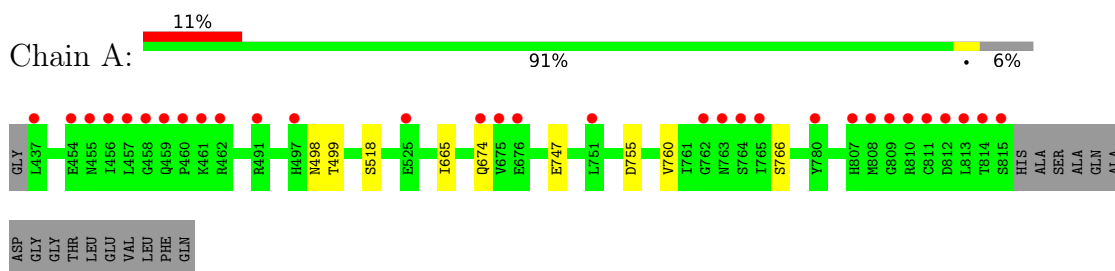
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	70	Total	O	0	0
			70	70		
6	B	41	Total	O	0	0
			41	41		
6	C	55	Total	O	0	0
			55	55		
6	D	42	Total	O	0	0
			42	42		
6	E	29	Total	O	0	0
			29	29		
6	F	53	Total	O	0	0
			53	53		

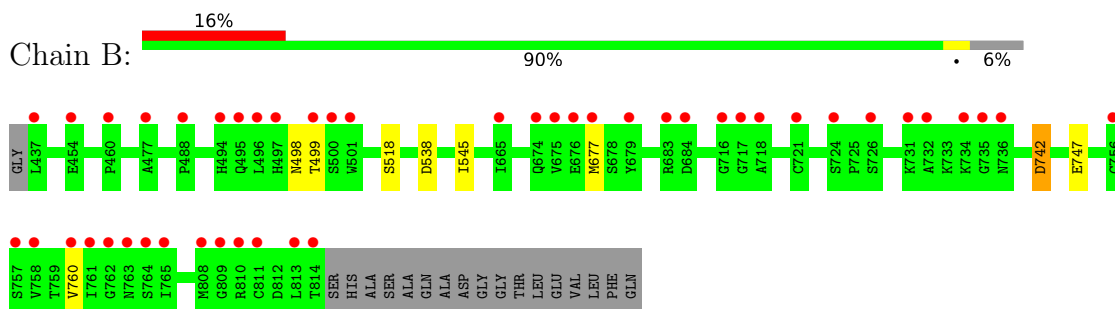
### 3 Residue-property plots [i](#)

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.

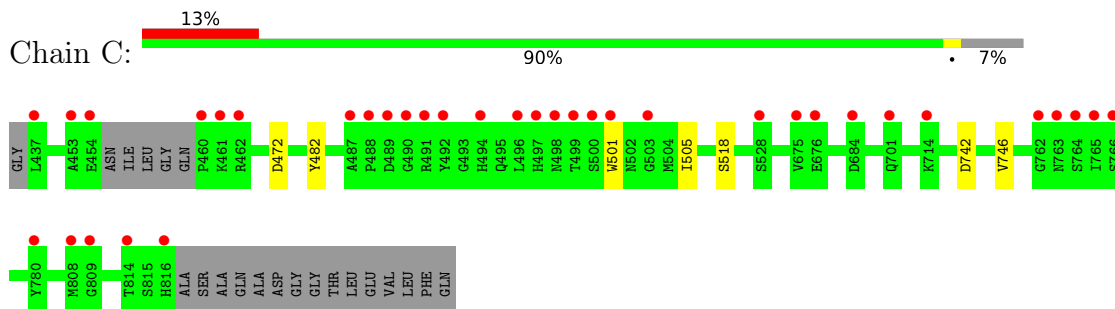
- Molecule 1: Glutamate receptor ionotropic, delta-1,Isoform 2 of Glutamate receptor ionotropic, delta-1



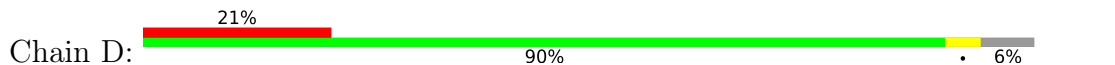
- Molecule 1: Glutamate receptor ionotropic, delta-1,Isoform 2 of Glutamate receptor ionotropic, delta-1

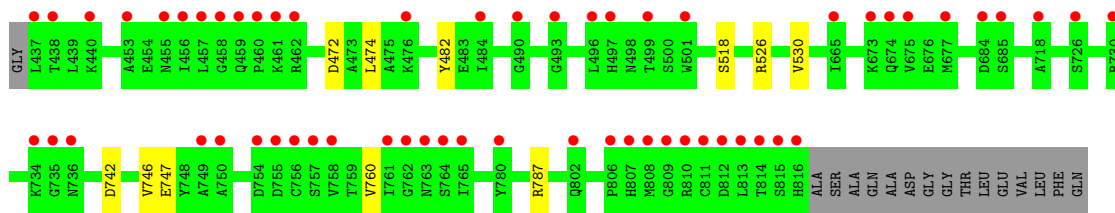


- Molecule 1: Glutamate receptor ionotropic, delta-1,Isoform 2 of Glutamate receptor ionotropic, delta-1

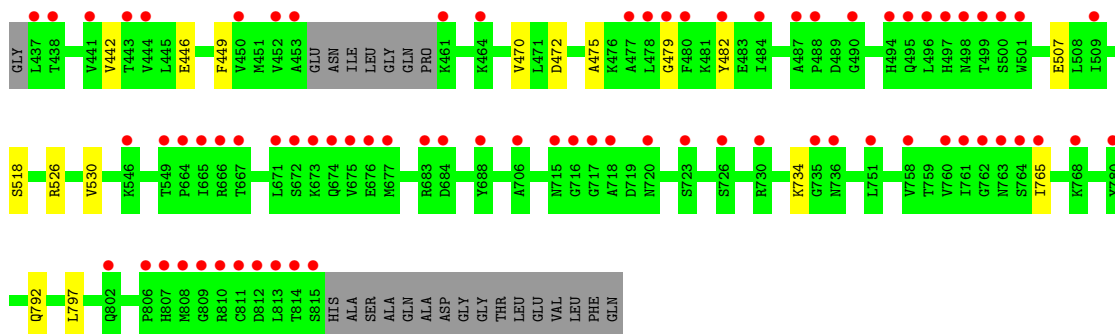
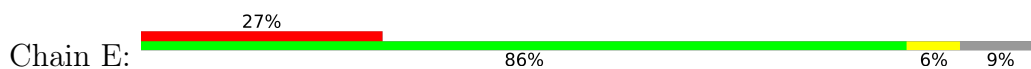


- Molecule 1: Glutamate receptor ionotropic, delta-1,Isoform 2 of Glutamate receptor ionotropic, delta-1

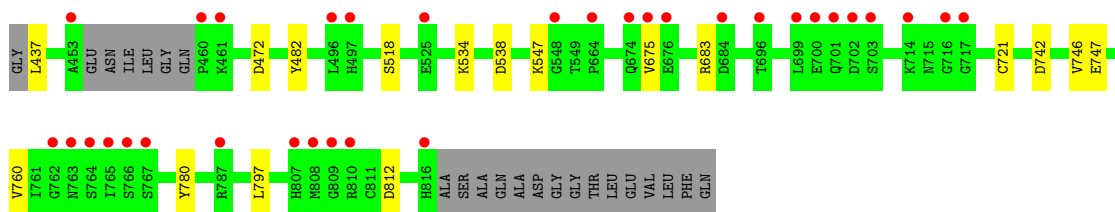
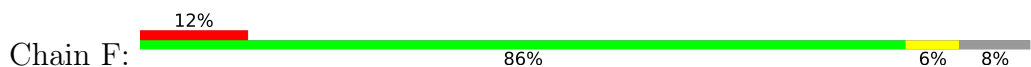




- Molecule 1: Glutamate receptor ionotropic, delta-1, Isoform 2 of Glutamate receptor ionotropic, delta-1



- Molecule 1: Glutamate receptor ionotropic, delta-1, Isoform 2 of Glutamate receptor ionotropic, delta-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.29Å 107.57Å 98.56Å 90.00° 94.08° 90.00°	Depositor
Resolution (Å)	62.59 – 2.18 62.59 – 2.18	Depositor EDS
% Data completeness (in resolution range)	59.8 (62.59-2.18) 56.7 (62.59-2.18)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 2.18Å)	Xtrriage
Refinement program	REFMAC 5.8.0270, PHENIX dev_4761	Depositor
R, $R_{free}$	0.206 , 0.244 0.216 , 0.251	Depositor DCC
$R_{free}$ test set	2698 reflections (2.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtrriage
Anisotropy	0.005	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	25266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.62% 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, 0.333 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: EDO, NAG, CL, CA

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	0.08	0/2140	0.22	0/2896
1	B	0.07	0/2136	0.21	0/2890
1	C	0.07	0/2113	0.21	0/2856
1	D	0.07	0/2153	0.21	0/2913
1	E	0.07	0/2076	0.21	0/2807
1	F	0.07	0/2125	0.22	0/2872
All	All	0.07	0/12743	0.21	0/17234

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	2093	2069	2071	5	0
1	B	2089	2073	2073	5	0
1	C	2066	2045	2045	3	0
1	D	2105	2085	2085	5	0
1	E	2034	2012	2012	9	0
1	F	2072	2045	2056	9	0
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
3	E	1	0	0	1	0
4	A	14	13	13	0	0
4	B	14	13	13	0	0
4	C	14	13	13	0	0
4	D	14	13	13	0	0
4	E	14	13	13	0	0
4	F	14	13	13	0	0
5	C	4	6	6	0	0
6	A	70	0	0	0	0
6	B	41	0	0	0	0
6	C	55	0	0	0	0
6	D	42	0	0	0	0
6	E	29	0	0	0	0
6	F	53	0	0	0	0
All	All	12853	12413	12426	33	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.

The worst 5 of 33 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:472:ASP:OD1	1:F:482:TYR:OH	2.09	0.67
1:F:742:ASP:O	1:F:746:VAL:HG22	1.95	0.67
1:E:472:ASP:OD1	1:E:482:TYR:OH	2.13	0.64
1:D:747:GLU:HA	1:D:760:VAL:HG21	1.81	0.61
1:D:472:ASP:OD1	1:D:482:TYR:OH	2.19	0.57

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	264/282 (94%)	258 (98%)	5 (2%)	1 (0%)	30	31
1	B	263/282 (93%)	258 (98%)	4 (2%)	1 (0%)	30	31
1	C	258/282 (92%)	252 (98%)	5 (2%)	1 (0%)	30	31
1	D	265/282 (94%)	260 (98%)	4 (2%)	1 (0%)	30	31
1	E	254/282 (90%)	248 (98%)	5 (2%)	1 (0%)	30	31
1	F	259/282 (92%)	254 (98%)	4 (2%)	1 (0%)	30	31
All	All	1563/1692 (92%)	1530 (98%)	27 (2%)	6 (0%)	30	31

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	SER
1	C	518	SER
1	D	518	SER
1	E	518	SER
1	F	518	SER

### 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	227/237 (96%)	227 (100%)	0	100	100
1	B	226/237 (95%)	225 (100%)	1 (0%)	84	91
1	C	224/237 (94%)	224 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	228/237 (96%)	228 (100%)	0	100	100
1	E	220/237 (93%)	220 (100%)	0	100	100
1	F	225/237 (95%)	224 (100%)	1 (0%)	84	91
All	All	1350/1422 (95%)	1348 (100%)	2 (0%)	88	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	742	ASP
1	F	797	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	486	GLN
1	F	669	GLN
1	C	786	GLN
1	D	494	HIS
1	E	701	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 oligosaccharides in this entry.

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

Of 23 ligands modelled in this entry, 16 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	D	902	1	14,14,15	0.47	0	17,19,21	0.93	0
5	EDO	C	906	-	3,3,3	0.25	0	2,2,2	0.29	0
4	NAG	F	903	1	14,14,15	0.41	0	17,19,21	1.20	1 (5%)
4	NAG	E	903	1	14,14,15	0.45	0	17,19,21	0.94	0
4	NAG	B	903	1	14,14,15	0.41	0	17,19,21	1.80	3 (17%)
4	NAG	C	905	1	14,14,15	0.41	0	17,19,21	1.11	1 (5%)
4	NAG	A	906	1	14,14,15	0.51	0	17,19,21	0.97	1 (5%)

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
4	NAG	D	902	1	-	2/6/23/26	0/1/1/1
5	EDO	C	906	-	-	0/1/1/1	-
4	NAG	F	903	1	-	2/6/23/26	0/1/1/1
4	NAG	E	903	1	-	2/6/23/26	0/1/1/1
4	NAG	B	903	1	-	3/6/23/26	0/1/1/1
4	NAG	C	905	1	-	4/6/23/26	0/1/1/1
4	NAG	A	906	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	903	NAG	C1-C2-N2	4.79	117.97	110.43
4	F	903	NAG	C1-O5-C5	3.84	117.33	112.19
4	B	903	NAG	O5-C1-C2	-3.55	105.79	111.29
4	C	905	NAG	C1-O5-C5	3.24	116.52	112.19
4	B	903	NAG	C4-C3-C2	-2.29	107.67	111.02

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	906	NAG	O5-C5-C6-O6
4	C	905	NAG	O5-C5-C6-O6
4	D	902	NAG	O5-C5-C6-O6
4	E	903	NAG	O5-C5-C6-O6
4	F	903	NAG	O5-C5-C6-O6

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, 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	265/282 (93%)	0.61	31 (11%) 9 8	17, 36, 89, 140	1 (0%)
1	B	264/282 (93%)	1.10	46 (17%) 4 3	17, 51, 91, 139	1 (0%)
1	C	261/282 (92%)	0.95	36 (13%) 6 6	26, 46, 93, 152	1 (0%)
1	D	266/282 (94%)	1.30	58 (21%) 2 2	25, 55, 113, 165	1 (0%)
1	E	258/282 (91%)	1.57	76 (29%) 1 1	30, 63, 97, 147	0
1	F	260/282 (92%)	0.68	33 (12%) 8 7	19, 40, 81, 143	3 (1%)
All	All	1574/1692 (93%)	1.03	280 (17%) 4 3	17, 49, 96, 165	7 (0%)

The worst 5 of 280 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	457	LEU	8.0
1	B	765	ILE	8.0
1	D	457	LEU	7.8
1	C	765	ILE	7.3
1	F	765	ILE	7.3

### 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	B	903	14/15	0.44	0.21	82,102,123,129	0
4	NAG	C	905	14/15	0.48	0.21	101,115,137,142	0
4	NAG	F	903	14/15	0.62	0.18	60,81,107,111	0
4	NAG	D	902	14/15	0.63	0.22	52,89,106,108	0
4	NAG	E	903	14/15	0.71	0.21	77,92,111,111	0
4	NAG	A	906	14/15	0.79	0.13	57,79,98,101	0
2	CA	A	903	1/1	0.79	0.17	59,59,59,59	0
2	CA	B	902	1/1	0.81	0.12	65,65,65,65	0
2	CA	A	902	1/1	0.86	0.11	62,62,62,62	0
2	CA	F	902	1/1	0.90	0.08	41,41,41,41	0
5	EDO	C	906	4/4	0.90	0.15	37,46,53,53	0
3	CL	A	905	1/1	0.91	0.12	51,51,51,51	0
2	CA	C	902	1/1	0.91	0.09	43,43,43,43	0
3	CL	C	903	1/1	0.93	0.08	49,49,49,49	0
2	CA	E	901	1/1	0.95	0.08	52,52,52,52	0
2	CA	F	901	1/1	0.95	0.06	47,47,47,47	0
2	CA	C	901	1/1	0.95	0.05	50,50,50,50	0
2	CA	D	901	1/1	0.95	0.10	51,51,51,51	0
2	CA	A	901	1/1	0.96	0.04	39,39,39,39	0
2	CA	B	901	1/1	0.96	0.04	46,46,46,46	0
3	CL	E	902	1/1	0.97	0.04	44,44,44,44	0
3	CL	C	904	1/1	0.97	0.14	47,47,47,47	0
3	CL	A	904	1/1	0.98	0.06	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.