



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:04 am GMT

PDB ID : 2ICE
Title : CRIG bound to C3c
Authors : Wiesmann, C.
Deposited on : 2006-09-12
Resolution : 3.10 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

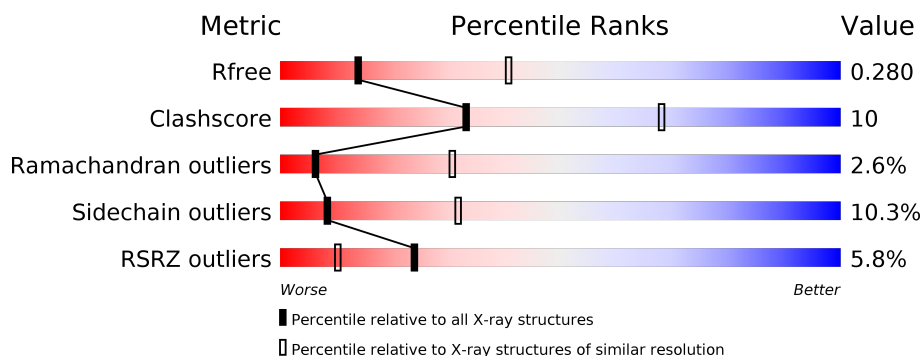
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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 $\leq 5\%$. 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	642	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 70%, yellow 70%, yellow 95%, orange 95%, orange 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 70% 25% 5% </div> </div>
1	D	642	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 5%, green 5%, green 70%, yellow 70%, yellow 95%, orange 95%, orange 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 70% 25% • • </div> </div>
2	B	206	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 0%, green 63%, yellow 63%, yellow 87%, grey 87%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 63% 24% • 11% </div> </div>
2	E	206	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 58%, yellow 58%, yellow 87%, orange 87%, orange 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 58% 29% • 11% </div> </div>
3	C	343	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 56%, yellow 56%, yellow 82%, orange 82%, orange 85%, orange 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 56% 26% • • 14% </div> </div>
3	F	343	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 26%, green 26%, green 64%, yellow 64%, yellow 83%, orange 83%, orange 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 26% 64% 19% • 14% </div> </div>

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Mol	Chain	Length	Quality of chain
4	S	119	<div><div></div><div>72%</div><div>26%</div><div></div></div>
4	T	119	<div><div>2%</div><div></div><div>73%</div><div>24%</div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19619 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 Complement C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5008	3188	848	957	15			
1	D	630	Total	C	N	O	S	0	0	0
			4907	3127	828	937	15			

- Molecule 2 is a protein called Complement C3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	0	0
			1480	950	249	276	5			
2	E	183	Total	C	N	O	S	0	0	0
			1480	950	249	276	5			

- Molecule 3 is a protein called Complement C3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	296	Total	C	N	O	S	0	0	0
			2407	1517	395	475	20			
3	F	296	Total	C	N	O	S	0	0	0
			2407	1517	395	475	20			

- Molecule 4 is a protein called V-set and immunoglobulin domain-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S	119	Total	C	N	O	S	0	0	0
			950	595	169	183	3			
4	T	119	Total	C	N	O	S	0	0	0
			950	595	169	183	3			

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		

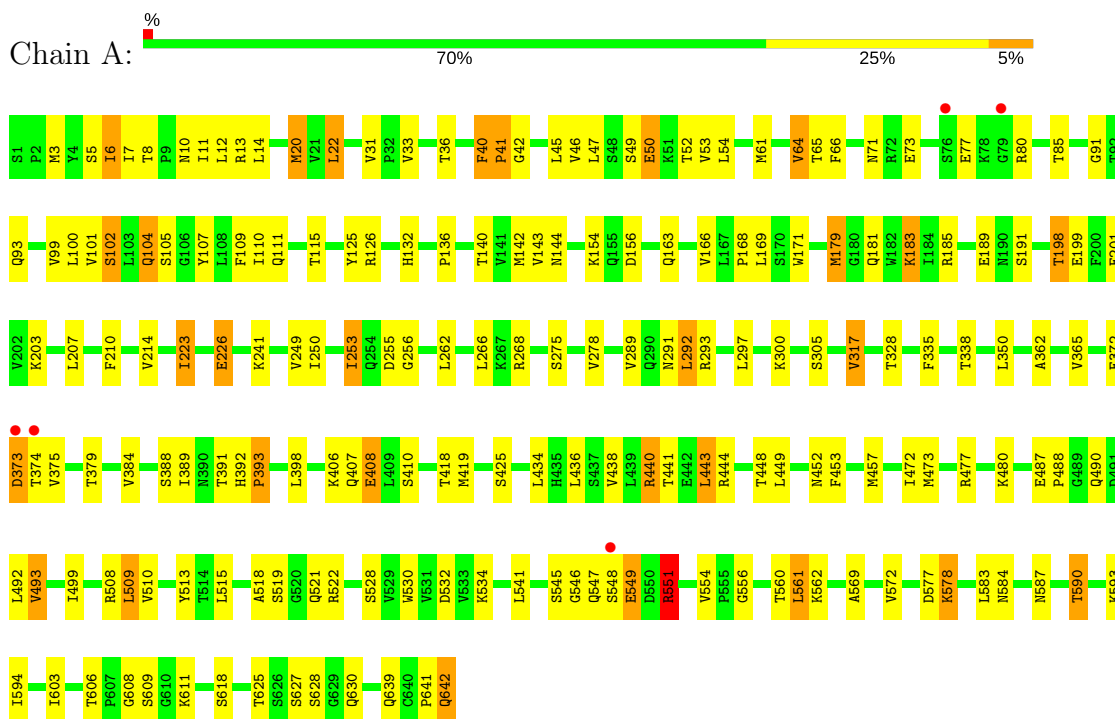
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		

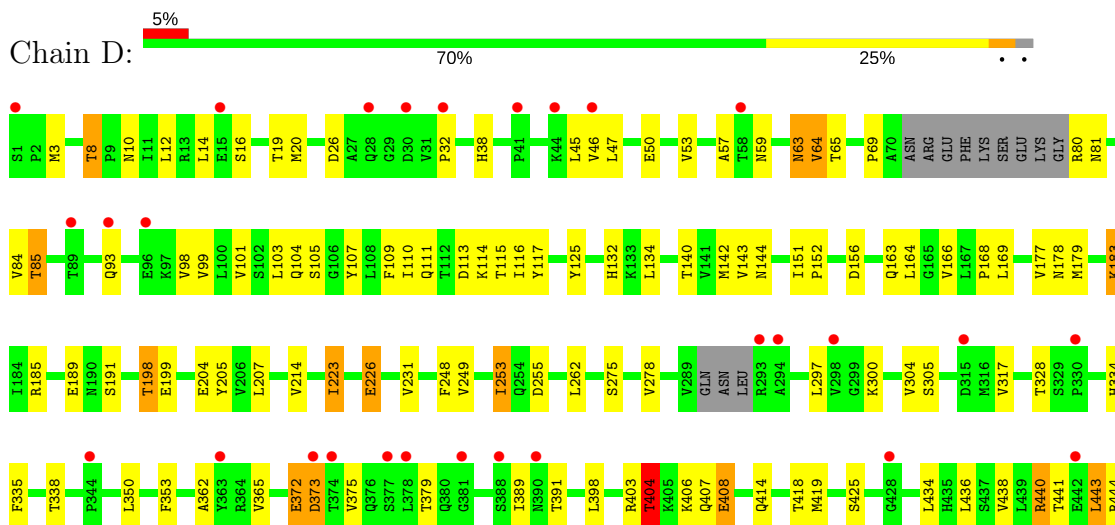
3 Residue-property plots

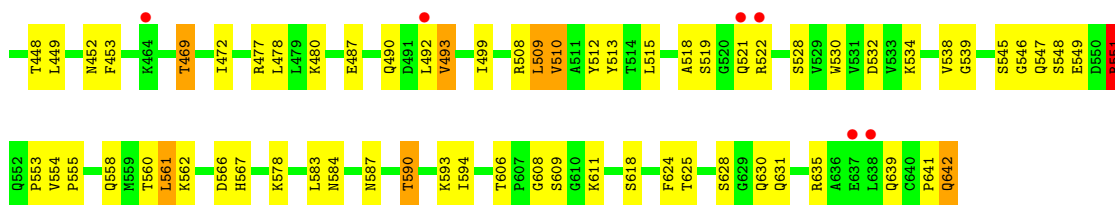
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Complement C3 beta chain

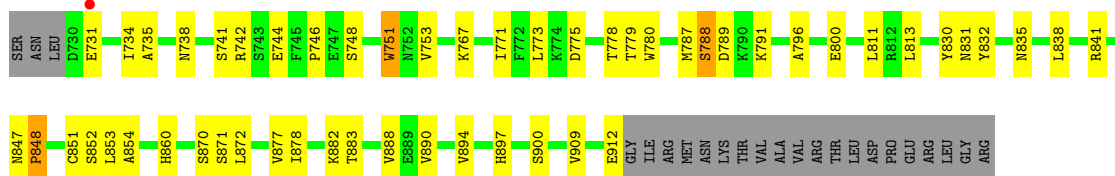


• Molecule 1: Complement C3 beta chain

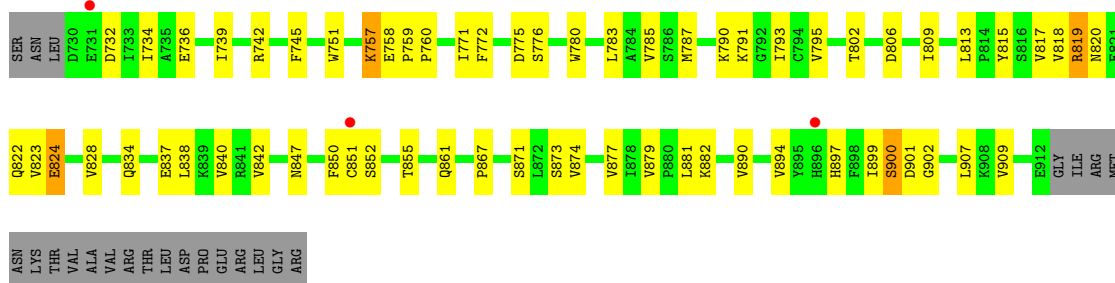




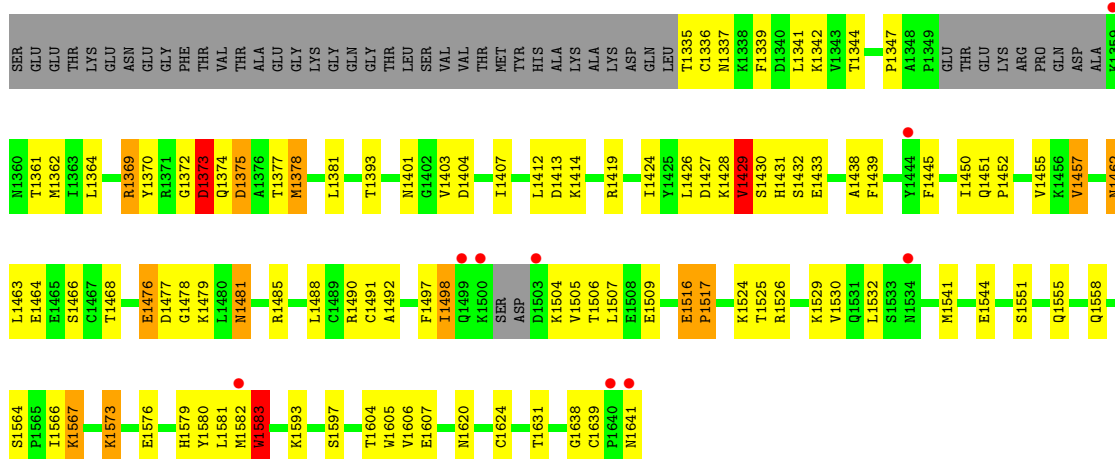
• Molecule 2: Complement C3 alpha chain



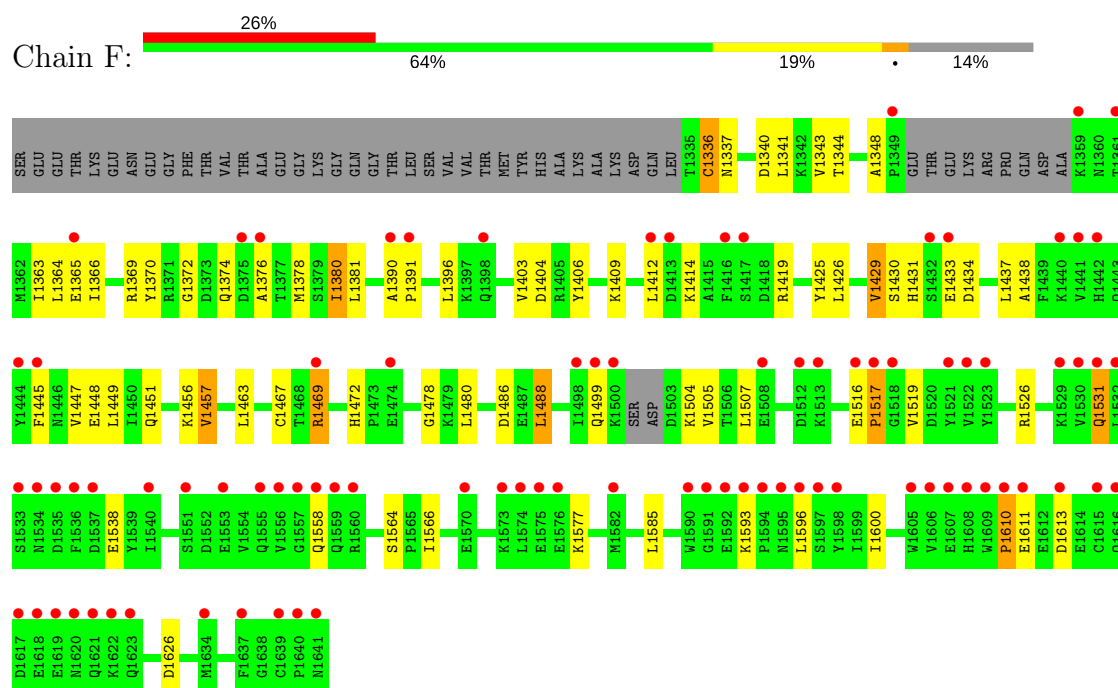
• Molecule 2: Complement C3 alpha chain



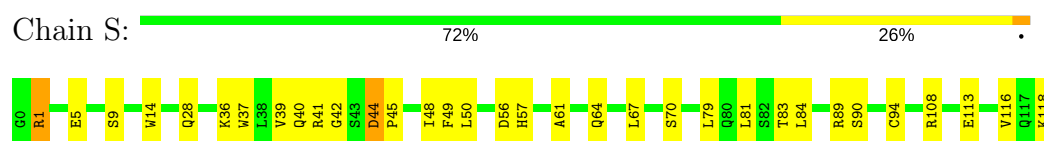
• Molecule 3: Complement C3 alpha chain



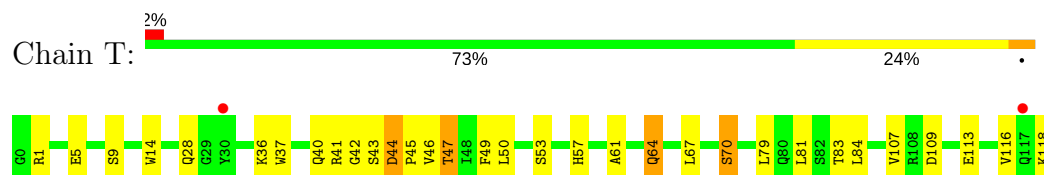
• Molecule 3: Complement C3 alpha chain



- Molecule 4: V-set and immunoglobulin domain-containing protein 4



- Molecule 4: V-set and immunoglobulin domain-containing protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	384.94Å 65.21Å 147.68Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 19.96 – 3.11	Depositor EDS
% Data completeness (in resolution range)	95.8 (20.00-3.10) 95.3 (19.96-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 3.09Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.236 , 0.295 0.229 , 0.280	Depositor DCC
R_{free} test set	3112 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19619	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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

5.1 Standard geometry

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

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	0/5108	0.67	0/6939
1	D	0.41	0/5004	0.59	0/6799
2	B	0.57	0/1512	0.66	0/2055
2	E	0.46	0/1512	0.59	0/2055
3	C	0.60	3/2453 (0.1%)	0.64	0/3305
3	F	0.38	0/2453	0.54	1/3305 (0.0%)
4	S	0.50	0/972	0.60	0/1323
4	T	0.41	0/972	0.64	1/1323 (0.1%)
All	All	0.49	3/19986 (0.0%)	0.62	2/27104 (0.0%)

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	D	0	3
2	B	0	1
3	C	0	1
4	S	0	1
4	T	0	2
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1607	GLU	CD-OE2	15.28	1.42	1.25
3	C	1607	GLU	CD-OE1	8.79	1.35	1.25
3	C	1620	ASN	CG-OD1	5.04	1.35	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	47	THR	N-CA-C	-9.05	86.56	111.00
3	F	1463	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	ASP	Peptide
1	A	372	GLU	Peptide
1	A	40	PHE	Peptide
2	B	751	TRP	Peptide
3	C	1373	ASP	Peptide

5.2 Too-close contacts

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	5008	0	5071	116	0
1	D	4907	0	4971	97	0
2	B	1480	0	1502	32	0
2	E	1480	0	1502	38	0
3	C	2407	0	2321	66	0
3	F	2407	0	2321	42	0
4	S	950	0	935	20	0
4	T	950	0	935	12	0
5	A	28	0	25	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
All	All	19619	0	19583	384	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 10.

The worst 5 of 384 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)
3:C:1370:TYR:O	3:C:1431:HIS:HB2	1.54	1.06
1:A:365:VAL:H	1:A:379:THR:HG22	1.22	1.02
1:D:365:VAL:H	1:D:379:THR:HG22	1.24	1.01
3:C:1516:GLU:HB3	3:C:1517:PRO:CD	1.98	0.93
4:S:44:ASP:HB2	4:S:45:PRO:HD3	1.51	0.91

There are no symmetry-related clashes.

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	640/642 (100%)	601 (94%)	23 (4%)	16 (2%)	6	31
1	D	624/642 (97%)	581 (93%)	27 (4%)	16 (3%)	6	31
2	B	181/206 (88%)	170 (94%)	9 (5%)	2 (1%)	17	54
2	E	181/206 (88%)	160 (88%)	20 (11%)	1 (1%)	28	67
3	C	290/343 (84%)	235 (81%)	42 (14%)	13 (4%)	3	17
3	F	290/343 (84%)	244 (84%)	35 (12%)	11 (4%)	4	22
4	S	117/119 (98%)	103 (88%)	13 (11%)	1 (1%)	20	60
4	T	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	6	31
All	All	2440/2620 (93%)	2194 (90%)	183 (8%)	63 (3%)	6	31

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	PRO
1	A	373	ASP
1	A	551	ARG
3	C	1373	ASP
3	C	1516	GLU

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	566/566 (100%)	499 (88%)	67 (12%)	6	25
1	D	555/566 (98%)	500 (90%)	55 (10%)	9	34
2	B	171/191 (90%)	157 (92%)	14 (8%)	13	45
2	E	171/191 (90%)	152 (89%)	19 (11%)	7	29
3	C	270/309 (87%)	234 (87%)	36 (13%)	4	20
3	F	270/309 (87%)	253 (94%)	17 (6%)	21	56
4	S	109/109 (100%)	100 (92%)	9 (8%)	13	45
4	T	109/109 (100%)	97 (89%)	12 (11%)	7	30
All	All	2221/2350 (94%)	1992 (90%)	229 (10%)	8	32

5 of 229 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	1506	THR
1	D	26	ASP
3	F	1507	LEU
3	C	1564	SER
3	C	1631	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	1462	ASN
4	S	28	GLN
4	T	59	GLN
3	C	1472	HIS
3	C	1558	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

2 carbohydrates 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	$\# Z > 2$
5	NAG	A	643	1,5	14,14,15	0.46	0	15,19,21	2.23	2 (13%)
5	NAG	A	644	5	14,14,15	0.52	0	15,19,21	0.91	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
5	NAG	A	643	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	644	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	643	NAG	C3-C4-C5	2.40	114.44	110.22
5	A	643	NAG	C1-O5-C5	7.53	122.54	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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, 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	642/642 (100%)	-0.43	5 (0%) 86 71	17, 47, 84, 126	0
1	D	630/642 (98%)	0.21	34 (5%) 26 12	17, 50, 123, 142	0
2	B	183/206 (88%)	-0.60	1 (0%) 90 80	13, 37, 64, 82	0
2	E	183/206 (88%)	-0.29	3 (1%) 72 51	12, 49, 91, 95	0
3	C	296/343 (86%)	-0.16	9 (3%) 51 27	19, 60, 94, 116	0
3	F	296/343 (86%)	1.47	89 (30%) 1 0	42, 133, 199, 223	0
4	S	119/119 (100%)	-0.49	0 100 100	22, 46, 68, 94	0
4	T	119/119 (100%)	-0.24	2 (1%) 70 49	22, 46, 68, 94	0
All	All	2468/2620 (94%)	-0.00	143 (5%) 24 10	12, 51, 161, 223	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1610	PRO	12.4
3	F	1608	HIS	9.1
1	D	1	SER	7.0
3	F	1607	GLU	6.7
1	D	374	THR	6.6

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 ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	A	643	14/15	0.95	0.16	-0.50	51,58,71,76	0
5	NAG	A	644	14/15	0.90	0.40	-	82,87,88,89	0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	CA	D	643	1/1	0.96	0.04	-2.26	64,64,64,64	0
6	CA	A	645	1/1	0.94	0.06	-2.66	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.