



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4QQV
Title : Extracellular domains of mouse IL-3 beta receptor
Authors : Jackson, C.J.; Young, I.G.; Murphy, J.M.; Carr, P.D.; Ewens, C.L.; Dai, J.;
Ollis, D.L.
Deposited on : 2014-06-30
Resolution : 3.45 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

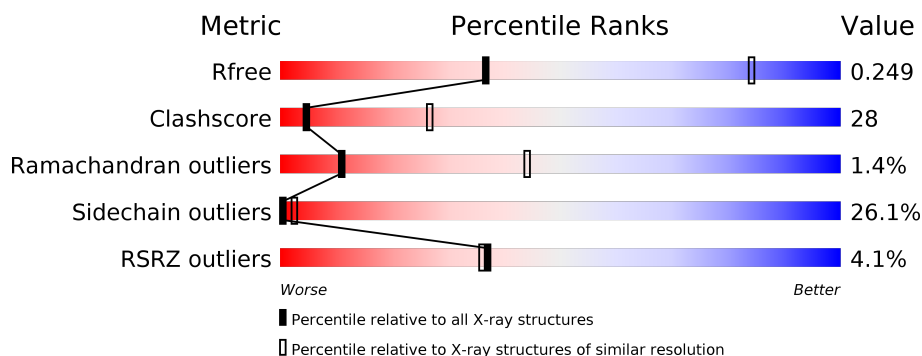
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 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	416	<div> <div>4%</div> <div> <div>42%</div> <div>40%</div> <div>13%</div> <div>• •</div> </div> </div>
1	B	416	<div> <div>6%</div> <div> <div>40%</div> <div>40%</div> <div>14%</div> <div>5%</div> </div> </div>
1	C	416	<div> <div>4%</div> <div> <div>39%</div> <div>40%</div> <div>17%</div> <div>•</div> </div> </div>
1	D	416	<div> <div>%</div> <div> <div>33%</div> <div>33%</div> <div>10%</div> <div>24%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12274 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 Interleukin-3 receptor class 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3229	2045	548	619	17			
1	B	395	Total	C	N	O	S	0	0	0
			3195	2023	543	612	17			
1	C	402	Total	C	N	O	S	0	0	0
			3252	2058	552	625	17			
1	D	316	Total	C	N	O	S	0	0	0
			2542	1609	433	485	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	GLN	ASN	engineered mutation	UNP P26954
A	331	ALA	LYS	engineered mutation	UNP P26954
A	333	ALA	ARG	engineered mutation	UNP P26954
A	334	ALA	ASP	engineered mutation	UNP P26954
B	328	GLN	ASN	engineered mutation	UNP P26954
B	331	ALA	LYS	engineered mutation	UNP P26954
B	333	ALA	ARG	engineered mutation	UNP P26954
B	334	ALA	ASP	engineered mutation	UNP P26954
C	328	GLN	ASN	engineered mutation	UNP P26954
C	331	ALA	LYS	engineered mutation	UNP P26954
C	333	ALA	ARG	engineered mutation	UNP P26954
C	334	ALA	ASP	engineered mutation	UNP P26954
D	328	GLN	ASN	engineered mutation	UNP P26954
D	331	ALA	LYS	engineered mutation	UNP P26954
D	333	ALA	ARG	engineered mutation	UNP P26954
D	334	ALA	ASP	engineered mutation	UNP P26954

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

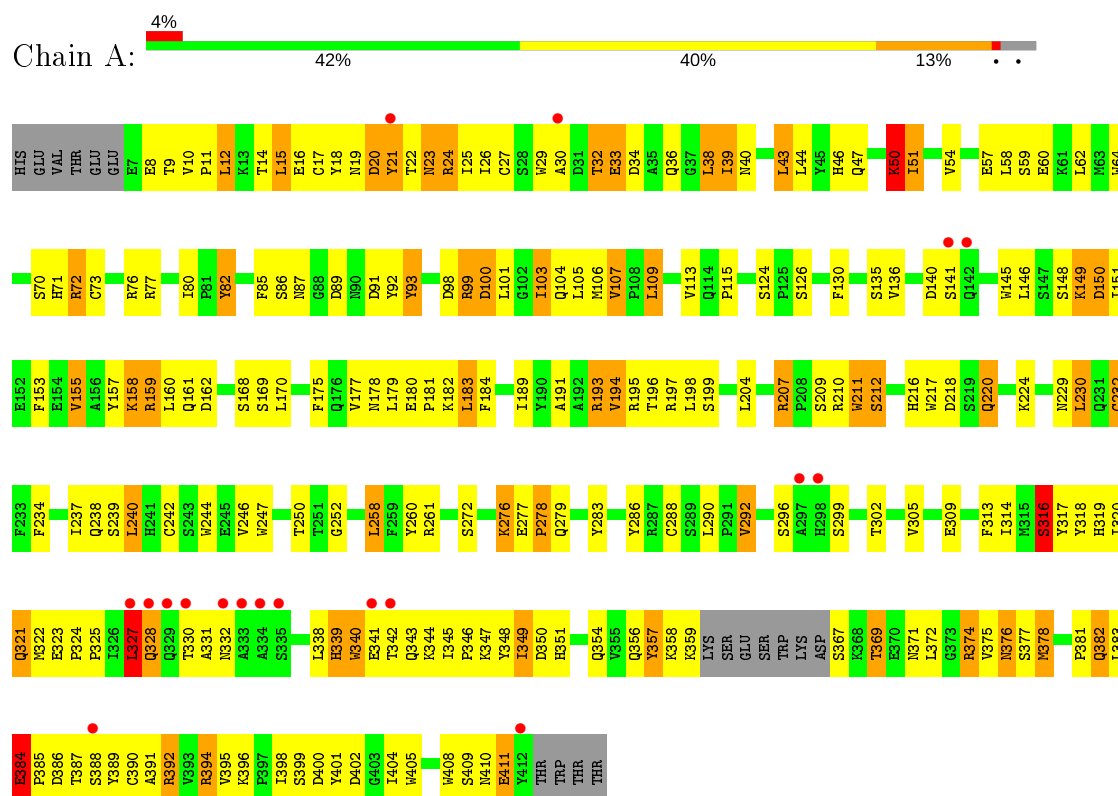


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

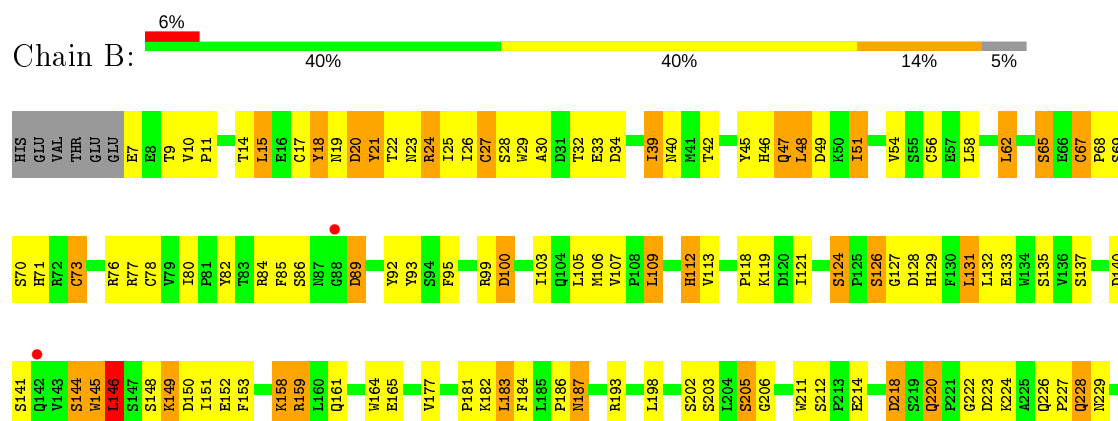
3 Residue-property plots

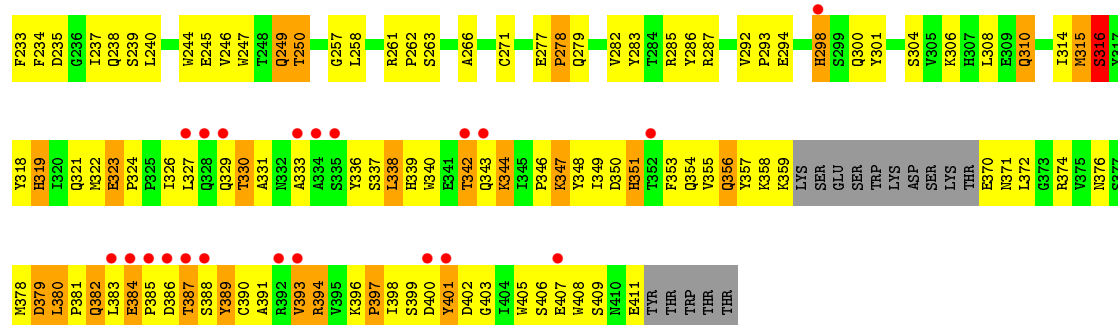
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Interleukin-3 receptor class 2 subunit beta

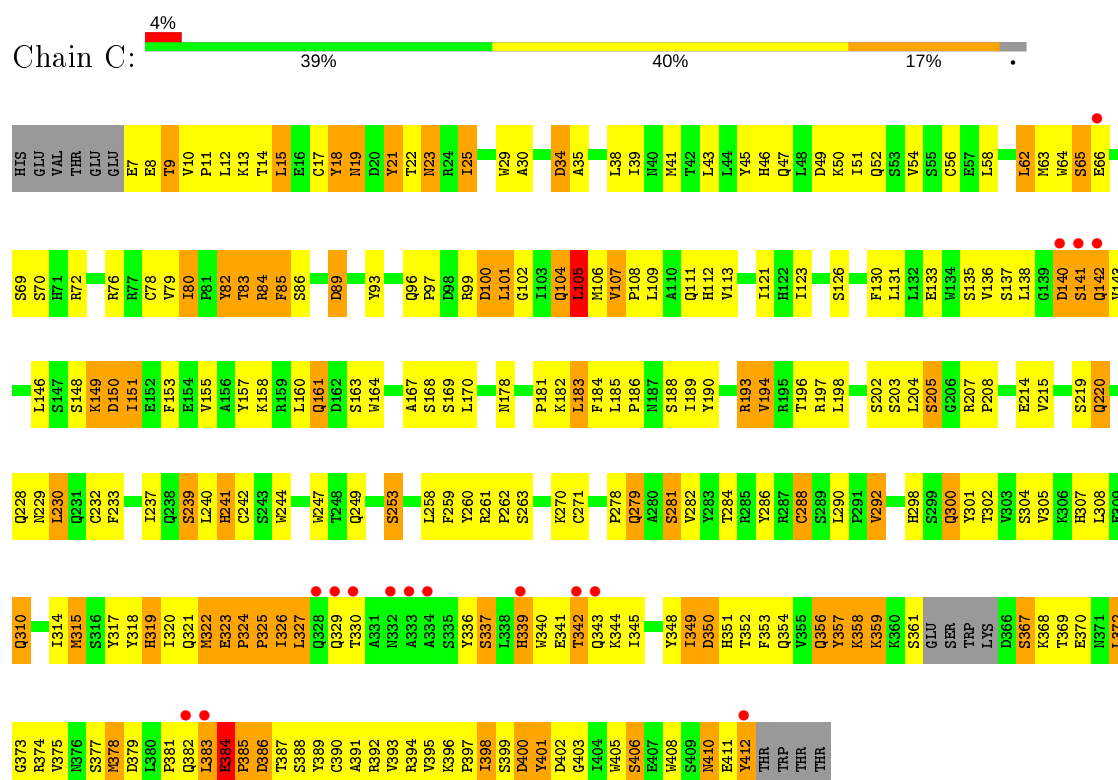


- Molecule 1: Interleukin-3 receptor class 2 subunit beta

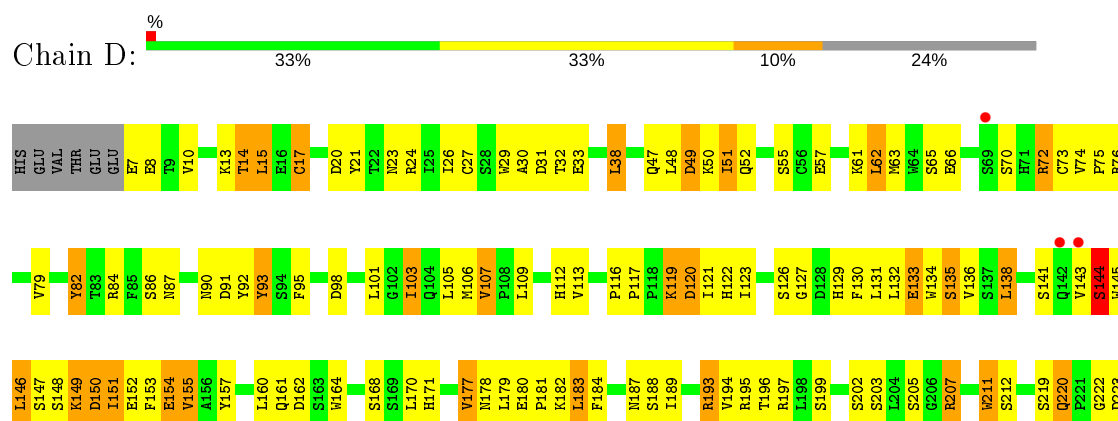




• Molecule 1: Interleukin-3 receptor class 2 subunit beta



• Molecule 1: Interleukin-3 receptor class 2 subunit beta



K224	A225	Q226	N229	L230	Q231	C232	F233	F234	L237	Q238	S239	L240	H241	C242	S243	H244	W247	T248	Q249	G252	F256	G257	L258	R261	P262	S263	P264	A265	A266	E269	P273	V274	V275	K276	E277	A280	R285	Y286	R287	C288	S289	L290	P291	V292	P293	E294	P295	S296	A297								
H298	S299	Q300	Y301	V302	S304	V305	K306	H307	L308	F309	Q310	G311	K312	F313	I314	Y317	Y318	H319	T320	Q321	K322	GLU	PRO	PRO	ILE	LEU	GLN	GLN	THR	ALA	ALA	ASN	ALA	ALA	SER	TYR	SER	LEU	HIS	TRP	TRP	GLU	THR	GLN	VAL	GLN	TYR	LYS									
LYS	LYS	SER	GLU	SER	TRP	LYS	ASP	SER	LYS	THR	GLU	ASN	LEU	GLY	ARG	VAL	ASN	SER	MET	ASP	LEU	PRO	GLN	LEU	GLU	PRO	ASP	THR	SER	TYR	CYS	ALA	ARG	VAL	VAL	ARG	VAL	LYS	PRO	ILE	SER	ASP	TYR	ASP	GLY	ILE	TRP	SER	GLU	TRP	SER	ASN	GLU	TYR	THR	THR	THR

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.15Å 166.46Å 128.00Å 90.00° 122.77° 90.00°	Depositor
Resolution (Å)	19.91 – 3.45 19.91 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.91-3.45) 99.5 (19.91-3.45)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 3.44Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1558)	Depositor
R, R_{free}	0.203 , 0.248 0.208 , 0.249	Depositor DCC
R_{free} test set	2269 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	96.7	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12274	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: 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	0.59	0/3327	0.81	3/4535 (0.1%)
1	B	0.61	2/3292 (0.1%)	0.81	1/4488 (0.0%)
1	C	0.54	0/3350	0.81	3/4565 (0.1%)
1	D	0.55	0/2620	0.74	0/3572
All	All	0.57	2/12589 (0.0%)	0.79	7/17160 (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	4
1	B	0	3
1	C	0	2
1	D	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	CYS	CB-SG	7.60	1.95	1.82
1	B	67	CYS	CB-SG	6.36	1.93	1.82

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	324	PRO	C-N-CD	-8.99	100.83	120.60
1	C	384	GLU	C-N-CD	-8.64	101.58	120.60
1	A	50	LYS	N-CA-C	5.69	126.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	LEU	CA-CB-CG	-5.62	102.38	115.30
1	A	22	THR	N-CA-C	-5.60	95.87	111.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	277	GLU	Peptide
1	A	278	PRO	Peptide
1	A	316	SER	Peptide
1	A	384	GLU	Peptide
1	B	278	PRO	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	3229	0	3067	173	0
1	B	3195	0	3035	212	0
1	C	3252	0	3089	211	0
1	D	2542	0	2413	134	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
All	All	12274	0	11656	671	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 28.

The worst 5 of 671 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:357:TYR:HE1	1:B:391:ALA:CB	1.40	1.35
1:B:357:TYR:CE1	1:B:391:ALA:CB	2.16	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:TYR:CE1	1:B:391:ALA:HB2	1.79	1.18
1:C:14:THR:HG23	1:C:62:LEU:HD11	1.19	1.12
1:C:169:SER:C	1:C:170:LEU:HD12	1.70	1.11

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	395/416 (95%)	354 (90%)	36 (9%)	5 (1%)	12	46
1	B	391/416 (94%)	353 (90%)	33 (8%)	5 (1%)	12	46
1	C	398/416 (96%)	355 (89%)	35 (9%)	8 (2%)	7	37
1	D	314/416 (76%)	291 (93%)	20 (6%)	3 (1%)	15	52
All	All	1498/1664 (90%)	1353 (90%)	124 (8%)	21 (1%)	11	44

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	PRO
1	C	323	GLU
1	C	385	PRO
1	A	384	GLU
1	B	51	ILE

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	368/385 (96%)	274 (74%)	94 (26%)	0	2
1	B	364/385 (94%)	277 (76%)	87 (24%)	0	3
1	C	371/385 (96%)	264 (71%)	107 (29%)	0	2
1	D	291/385 (76%)	215 (74%)	76 (26%)	0	2
All	All	1394/1540 (90%)	1030 (74%)	364 (26%)	0	2

5 of 364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	347	LYS
1	C	82	TYR
1	D	182	LYS
1	B	379	ASP
1	C	18	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	382	GLN
1	C	249	GLN
1	D	112	HIS
1	B	328	GLN
1	B	329	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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	NAG	A	501	1	14,14,15	0.66	0	17,19,21	0.58	1 (5%)
2	NAG	B	501	1	14,14,15	1.13	1 (7%)	17,19,21	0.66	0
2	NAG	C	501	1	14,14,15	0.66	0	17,19,21	0.56	0
2	NAG	D	501	1	14,14,15	0.50	0	17,19,21	0.37	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	NAG	A	501	1	-	2/6/23/26	0/1/1/1
2	NAG	B	501	1	-	4/6/23/26	0/1/1/1
2	NAG	C	501	1	-	2/6/23/26	0/1/1/1
2	NAG	D	501	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAG	C1-C2	3.72	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAG	C1-O5-C5	2.12	115.07	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	NAG	O5-C5-C6-O6
2	C	501	NAG	C4-C5-C6-O6
2	C	501	NAG	O5-C5-C6-O6
2	A	501	NAG	O5-C5-C6-O6
2	A	501	NAG	C4-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, 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	399/416 (95%)	-0.01	18 (4%) 33 32	59, 121, 191, 245	0
1	B	395/416 (94%)	0.04	23 (5%) 23 23	54, 100, 229, 299	0
1	C	402/416 (96%)	-0.05	16 (3%) 38 36	58, 113, 195, 262	0
1	D	316/416 (75%)	-0.32	5 (1%) 72 69	62, 99, 153, 240	0
All	All	1512/1664 (90%)	-0.07	62 (4%) 37 36	54, 107, 200, 299	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	GLN	14.2
1	A	334	ALA	9.9
1	B	342	THR	8.4
1	B	387	THR	6.2
1	C	334	ALA	6.2

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(\AA^2)	Q<0.9
2	NAG	D	501	14/15	0.81	0.30	141,157,168,168	0
2	NAG	B	501	14/15	0.82	0.20	125,145,155,157	0
2	NAG	A	501	14/15	0.82	0.23	136,149,152,153	0
2	NAG	C	501	14/15	0.88	0.29	134,148,158,160	0

6.5 Other polymers [i](#)

There are no such residues in this entry.