



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:26 PM GMT

PDB ID : 4EI5  
Title : Crystal Structure of XV19 TCR in complex with CD1d-sulfatide C24:1  
Authors : Patel, O.; Gras, S.; Rossjohn, J.  
Deposited on : 2012-04-04  
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](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

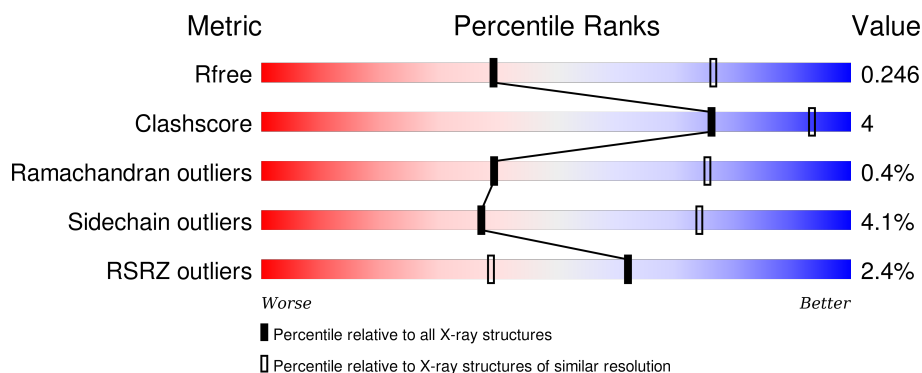
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	302	<div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	E	302	<div> <div>3%</div> <div>79%</div> <div>14%</div> <div>7%</div> </div>
2	B	99	<div> <div>83%</div> <div>15%</div> <div>..</div> </div>
2	F	99	<div> <div>2%</div> <div>81%</div> <div>15%</div> <div>.</div> </div>
3	C	208	<div> <div>2%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	208	
4	D	245	
4	H	245	

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
8	FLC	A	408	-	-	X	-
9	CIS	A	409	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13206 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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2346	1493	408	432	13			
1	E	280	Total	C	N	O	S	0	0	0
			2229	1420	387	410	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	GLY	-	EXPRESSION TAG	UNP P11609
A	281	SER	-	EXPRESSION TAG	UNP P11609
A	282	LEU	-	EXPRESSION TAG	UNP P11609
A	283	HIS	-	EXPRESSION TAG	UNP P11609
A	284	HIS	-	EXPRESSION TAG	UNP P11609
A	285	ILE	-	EXPRESSION TAG	UNP P11609
A	286	LEU	-	EXPRESSION TAG	UNP P11609
A	287	ASP	-	EXPRESSION TAG	UNP P11609
A	288	ALA	-	EXPRESSION TAG	UNP P11609
A	289	GLN	-	EXPRESSION TAG	UNP P11609
A	290	LYS	-	EXPRESSION TAG	UNP P11609
A	291	MET	-	EXPRESSION TAG	UNP P11609
A	292	VAL	-	EXPRESSION TAG	UNP P11609
A	293	TRP	-	EXPRESSION TAG	UNP P11609
A	294	ASN	-	EXPRESSION TAG	UNP P11609
A	295	HIS	-	EXPRESSION TAG	UNP P11609
A	296	ARG	-	EXPRESSION TAG	UNP P11609
A	297	HIS	-	EXPRESSION TAG	UNP P11609
A	298	HIS	-	EXPRESSION TAG	UNP P11609
A	299	HIS	-	EXPRESSION TAG	UNP P11609
A	300	HIS	-	EXPRESSION TAG	UNP P11609
A	301	HIS	-	EXPRESSION TAG	UNP P11609
A	302	HIS	-	EXPRESSION TAG	UNP P11609
E	201	HIS	ASP	SEE REMARK 999	UNP P11609

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Chain	Residue	Modelled	Actual	Comment	Reference
E	280	GLY	-	EXPRESSION TAG	UNP P11609
E	281	SER	-	EXPRESSION TAG	UNP P11609
E	282	LEU	-	EXPRESSION TAG	UNP P11609
E	283	HIS	-	EXPRESSION TAG	UNP P11609
E	284	HIS	-	EXPRESSION TAG	UNP P11609
E	285	ILE	-	EXPRESSION TAG	UNP P11609
E	286	LEU	-	EXPRESSION TAG	UNP P11609
E	287	ASP	-	EXPRESSION TAG	UNP P11609
E	288	ALA	-	EXPRESSION TAG	UNP P11609
E	289	GLN	-	EXPRESSION TAG	UNP P11609
E	290	LYS	-	EXPRESSION TAG	UNP P11609
E	291	MET	-	EXPRESSION TAG	UNP P11609
E	292	VAL	-	EXPRESSION TAG	UNP P11609
E	293	TRP	-	EXPRESSION TAG	UNP P11609
E	294	ASN	-	EXPRESSION TAG	UNP P11609
E	295	HIS	-	EXPRESSION TAG	UNP P11609
E	296	ARG	-	EXPRESSION TAG	UNP P11609
E	297	HIS	-	EXPRESSION TAG	UNP P11609
E	298	HIS	-	EXPRESSION TAG	UNP P11609
E	299	HIS	-	EXPRESSION TAG	UNP P11609
E	300	HIS	-	EXPRESSION TAG	UNP P11609
E	301	HIS	-	EXPRESSION TAG	UNP P11609
E	302	HIS	-	EXPRESSION TAG	UNP P11609

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			809	517	137	148	7			
2	F	95	Total	C	N	O	S	0	0	0
			782	502	131	143	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	ASP	SEE REMARK 999	UNP P01887
F	85	ALA	ASP	SEE REMARK 999	UNP P01887

- Molecule 3 is a protein called Valpha1 XV19 Type II Natural Killer T cell receptor (mouse variable domain, human constant domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	201	Total	C	N	O	S	0	0	0
			1578	985	268	316	9			
3	G	172	Total	C	N	O	S	0	1	0
			1364	855	229	273	7			

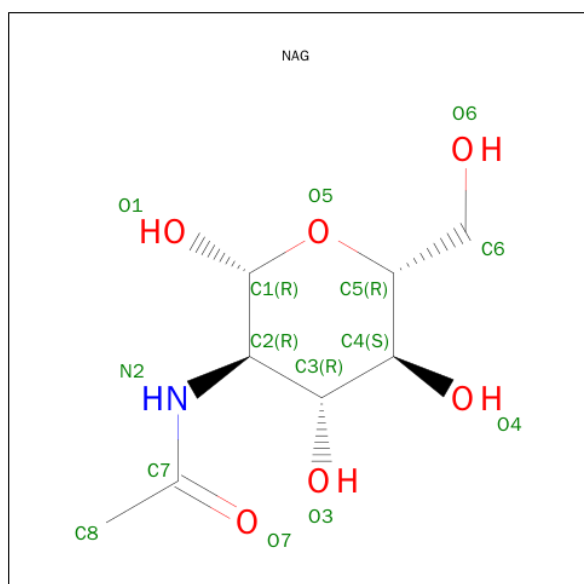
- Molecule 4 is a protein called Vbeta16 XV19 Type II Natural Killer T cell receptor (mouse variable domain, human constant domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1961	1262	327	363	9			
4	H	230	Total	C	N	O	S	0	0	0
			1862	1198	309	346	9			

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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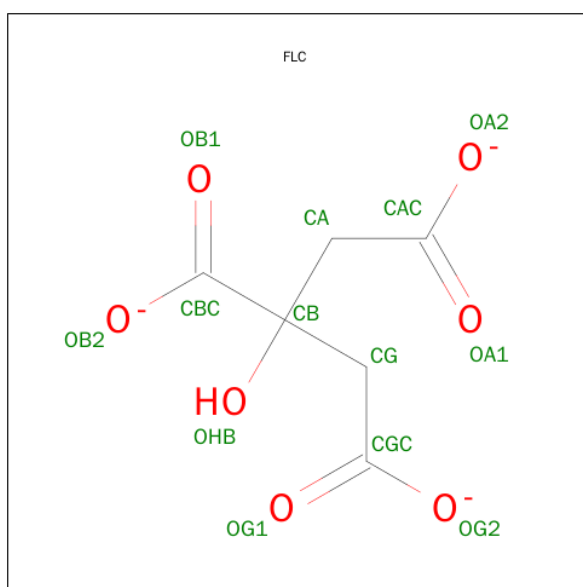
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

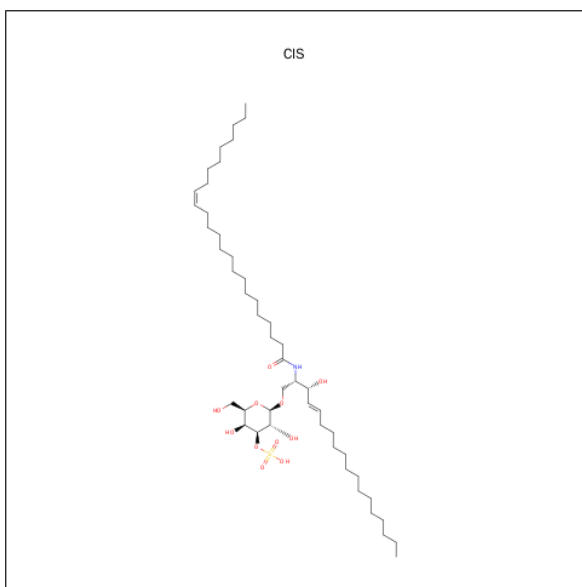
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	2	Total	C	N	O	0	0
			28	16	2	10		
7	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 9 is (15Z)-N-((1S,2R,3E)-2-HYDROXY-1-[(3-O-SULFO-BETA-D-GALACTOPYRANOSYL)OXY]METHYL}HEPTADEC-3-ENYL)TETRACOS-15-ENAMIDE (three-letter code: CIS) (formula:  $C_{48}H_{91}NO_{11}S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	S	0	0
			55	42	1	11	1		
9	E	1	Total	C	N	O	S	0	0
			34	21	1	11	1		

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

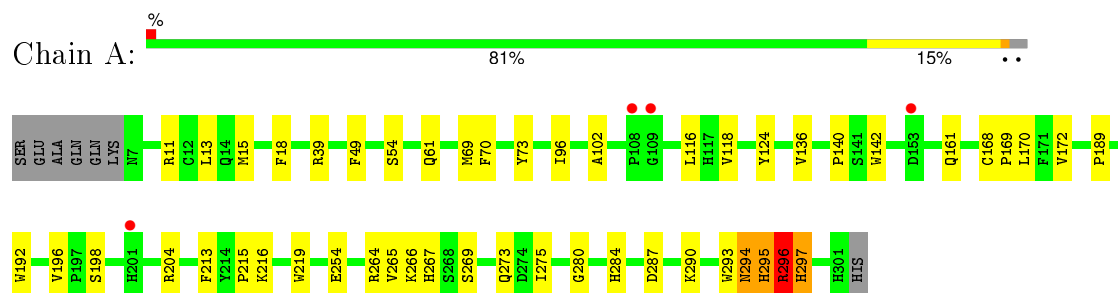
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	E	3	Total	C	N	O	0	0
			39	22	2	15		



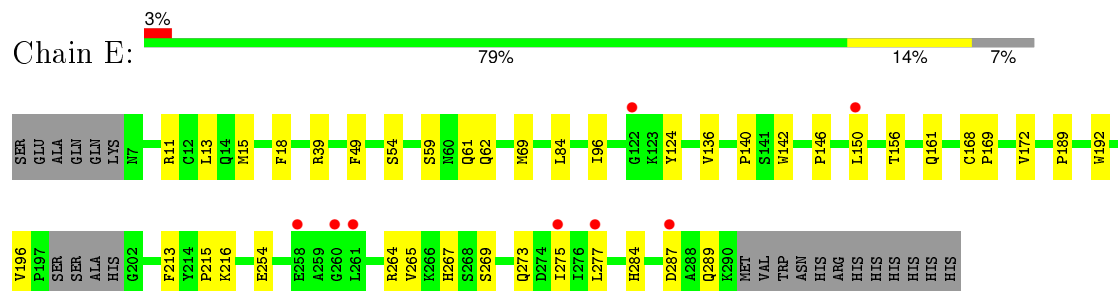
### 3 Residue-property plots [i](#)

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.

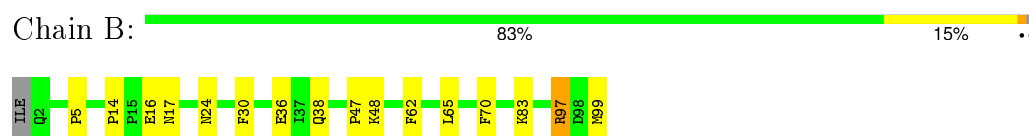
- Molecule 1: Antigen-presenting glycoprotein CD1d1



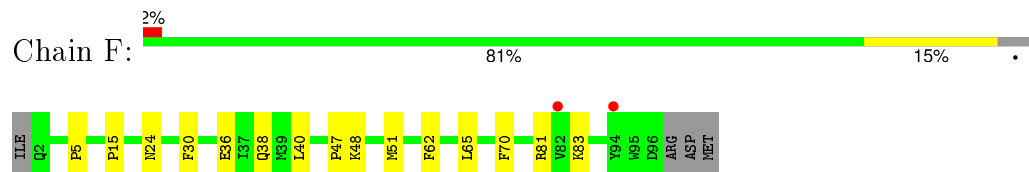
- Molecule 1: Antigen-presenting glycoprotein CD1d1



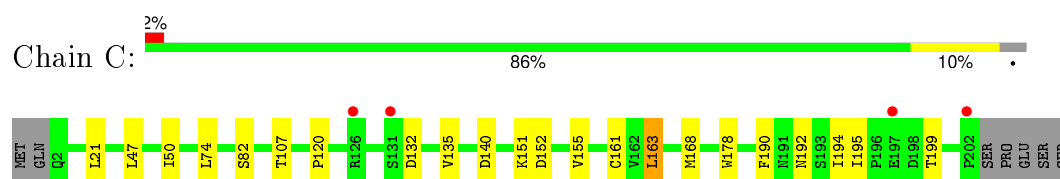
- Molecule 2: Beta-2-microglobulin



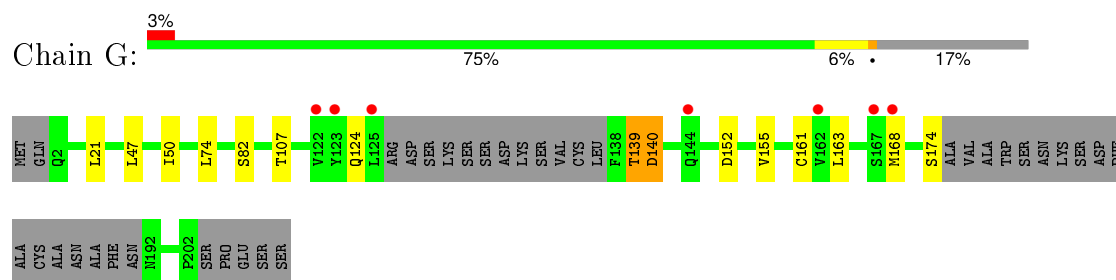
- Molecule 2: Beta-2-microglobulin



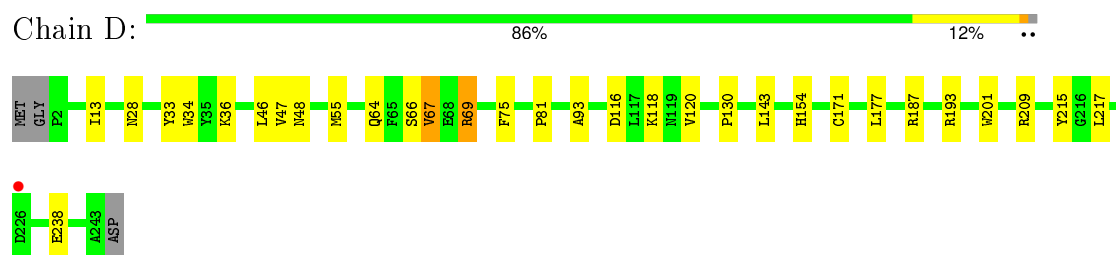
- Molecule 3: Valpha1 XV19 Type II Natural Killer T cell receptor (mouse variable domain, human constant domain)



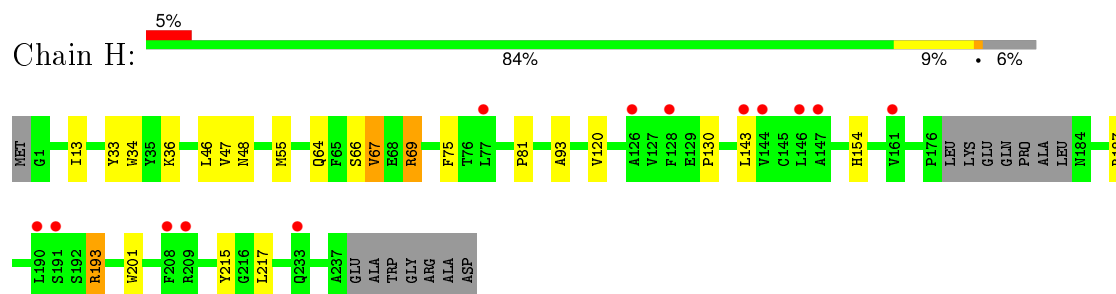
- Molecule 3: Valpha1 XV19 Type II Natural Killer T cell receptor (mouse variable domain, human constant domain)



- Molecule 4: Vbeta16 XV19 Type II Natural Killer T cell receptor (mouse variable domain, human constant domain)



- Molecule 4: Vbeta16 XV19 Type II Natural Killer T cell receptor (mouse variable domain, human constant domain)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.74Å 140.71Å 160.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.88 – 3.10 105.88 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (105.88-3.10) 98.6 (105.88-3.10)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.197 , 0.227 0.220 , 0.246	Depositor DCC
$R_{free}$ test set	2152 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.8	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 63.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 42391 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13206	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CIS, FLC, BMA, NAG, MAN

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	0.42	0/2417	0.67	2/3291 (0.1%)
1	E	0.40	0/2294	0.66	1/3121 (0.0%)
2	B	0.40	0/835	0.62	0/1133
2	F	0.37	0/808	0.61	0/1098
3	C	0.39	0/1617	0.63	0/2189
3	G	0.39	0/1400	0.64	0/1893
4	D	0.38	0/2021	0.60	0/2750
4	H	0.37	0/1918	0.59	0/2609
All	All	0.39	0/13310	0.63	3/18084 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	HIS	C-N-CA	6.47	137.87	121.70
1	E	284	HIS	C-N-CA	5.81	136.23	121.70
1	A	297	HIS	N-CA-C	5.07	124.69	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	2346	0	2208	31	0
1	E	2229	0	2112	20	0
2	B	809	0	783	9	0
2	F	782	0	757	6	0
3	C	1578	0	1471	8	0
3	G	1364	0	1272	6	0
4	D	1961	0	1872	13	0
4	H	1862	0	1773	12	0
5	A	50	0	43	1	0
6	A	14	0	13	0	0
6	E	14	0	13	0	0
7	A	28	0	25	0	0
7	E	28	0	25	0	0
8	A	13	0	5	5	0
9	A	55	0	75	3	0
9	E	34	0	32	1	0
10	E	39	0	34	1	0
All	All	13206	0	12513	97	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 4.

The worst 5 of 97 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:A:295:HIS:CD2	8:A:408:FLC:OB1	2.32	0.81
1:A:196:VAL:HG21	2:B:99:MET:HG3	1.66	0.78
1:A:15:MET:HG2	2:B:62:PHE:HE1	1.53	0.73
3:C:163:LEU:HD23	4:D:171:CYS:HB2	1.71	0.73
4:D:48:ASN:HD22	4:D:55:MET:HB2	1.57	0.69

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	293/302 (97%)	278 (95%)	14 (5%)	1 (0%)	46	80
1	E	276/302 (91%)	262 (95%)	13 (5%)	1 (0%)	39	75
2	B	96/99 (97%)	91 (95%)	4 (4%)	1 (1%)	19	58
2	F	93/99 (94%)	89 (96%)	3 (3%)	1 (1%)	17	55
3	C	199/208 (96%)	187 (94%)	10 (5%)	2 (1%)	19	58
3	G	167/208 (80%)	159 (95%)	7 (4%)	1 (1%)	30	68
4	D	240/245 (98%)	232 (97%)	8 (3%)	0	100	100
4	H	226/245 (92%)	218 (96%)	8 (4%)	0	100	100
All	All	1590/1708 (93%)	1516 (95%)	67 (4%)	7 (0%)	39	75

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	289	GLN
3	C	132	ASP
1	A	296	ARG
2	B	47	PRO
2	F	47	PRO

### 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	250/264 (95%)	238 (95%)	12 (5%)	31	69
1	E	238/264 (90%)	230 (97%)	8 (3%)	44	79
2	B	92/93 (99%)	88 (96%)	4 (4%)	35	72
2	F	89/93 (96%)	85 (96%)	4 (4%)	34	70
3	C	178/185 (96%)	171 (96%)	7 (4%)	39	75
3	G	155/185 (84%)	148 (96%)	7 (4%)	34	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	214/216 (99%)	205 (96%)	9 (4%)	36	73
4	H	205/216 (95%)	198 (97%)	7 (3%)	44	79
All	All	1421/1516 (94%)	1363 (96%)	58 (4%)	37	74

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	67	VAL
1	E	61	GLN
4	H	67	VAL
4	D	69	ARG
4	D	177	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	154	HIS
1	E	62	GLN
4	H	48	ASN
1	E	14	GLN
1	E	117	HIS

### 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 ⓘ

11 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	401	1,5	14,14,15	1.78	5 (35%)	15,19,21	1.43	2 (13%)
5	NAG	A	402	5	14,14,15	1.78	4 (28%)	15,19,21	1.67	4 (26%)
5	BMA	A	403	5	11,11,12	1.82	3 (27%)	14,15,17	1.84	4 (28%)
5	MAN	A	404	5	11,11,12	1.92	3 (27%)	14,15,17	1.98	5 (35%)
7	NAG	A	406	1,7	14,14,15	1.83	3 (21%)	15,19,21	1.98	5 (33%)
7	NAG	A	407	7	14,14,15	1.85	3 (21%)	15,19,21	1.93	3 (20%)
10	NAG	E	401	1,10	14,14,15	1.81	4 (28%)	15,19,21	1.46	2 (13%)
10	NAG	E	402	10	14,14,15	1.79	4 (28%)	15,19,21	1.69	4 (26%)
10	BMA	E	403	10	11,11,12	1.82	3 (27%)	14,15,17	1.61	4 (28%)
7	NAG	E	405	1,7	14,14,15	1.81	3 (21%)	15,19,21	1.95	4 (26%)
7	NAG	E	406	7	14,14,15	1.82	3 (21%)	15,19,21	1.89	3 (20%)

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	401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	402	5	-	0/6/23/26	0/1/1/1
5	BMA	A	403	5	-	0/2/19/22	0/1/1/1
5	MAN	A	404	5	-	0/2/19/22	0/1/1/1
7	NAG	A	406	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	407	7	-	0/6/23/26	0/1/1/1
10	NAG	E	401	1,10	-	0/6/23/26	0/1/1/1
10	NAG	E	402	10	-	0/6/23/26	0/1/1/1
10	BMA	E	403	10	-	0/2/19/22	0/1/1/1
7	NAG	E	405	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	406	7	-	0/6/23/26	0/1/1/1

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	403	BMA	C4-C3	-4.27	1.41	1.52
5	A	403	BMA	C4-C3	-4.07	1.41	1.52
5	A	404	MAN	C4-C3	-3.91	1.42	1.52
5	A	404	MAN	C2-C3	-3.41	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	BMA	C2-C3	-2.95	1.48	1.52

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	403	BMA	O4-C4-C3	-2.15	105.49	110.34
5	A	401	NAG	C2-N2-C7	-2.03	120.43	123.04
5	A	402	NAG	O5-C5-C6	2.01	111.69	107.35
10	E	402	NAG	O6-C6-C5	2.04	118.06	111.33
5	A	404	MAN	O6-C6-C5	2.04	118.09	111.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	NAG	1	0
10	E	401	NAG	1	0

## 5.6 Ligand geometry [i](#)

5 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
6	NAG	A	405	1	14,14,15	1.87	4 (28%)	15,19,21	1.59	5 (33%)
8	FLC	A	408	-	3,12,12	0.50	0	3,17,17	0.76	0
9	CIS	A	409	-	54,55,61	1.63	8 (14%)	60,66,72	1.48	12 (20%)
6	NAG	E	404	1	14,14,15	1.98	5 (35%)	15,19,21	2.60	8 (53%)
9	CIS	E	407	-	33,34,61	2.08	7 (21%)	38,45,72	1.91	12 (31%)

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
6	NAG	A	405	1	-	0/6/23/26	0/1/1/1
8	FLC	A	408	-	-	0/6/16/16	0/0/0/0
9	CIS	A	409	-	-	0/52/72/78	0/1/1/1
6	NAG	E	404	1	-	0/6/23/26	0/1/1/1
9	CIS	E	407	-	-	0/31/51/78	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	409	CIS	C44-C45	-2.96	1.44	1.52
9	E	407	CIS	C44-C45	-2.65	1.44	1.52
9	A	409	CIS	O4-S	-2.37	1.49	1.57
6	A	405	NAG	C4-C3	-2.26	1.46	1.52
6	E	404	NAG	C1-C2	-2.26	1.49	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	409	CIS	O8-S-O9	-2.97	99.53	112.46
9	A	409	CIS	O3-C44-C43	-2.85	103.77	110.02
9	E	407	CIS	O8-S-O9	-2.70	100.70	112.46
9	E	407	CIS	O3-C44-C43	-2.57	104.39	110.02
9	E	407	CIS	C5-C4-C3	-2.48	117.69	125.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	408	FLC	5	0
9	A	409	CIS	3	0
9	E	407	CIS	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, 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	295/302 (97%)	0.08	4 (1%) 78 60	50, 76, 116, 158	0
1	E	280/302 (92%)	0.12	8 (2%) 55 31	60, 109, 167, 184	0
2	B	98/99 (98%)	0.03	0 100 100	52, 67, 92, 105	0
2	F	95/99 (95%)	0.16	2 (2%) 67 44	91, 117, 140, 153	0
3	C	201/208 (96%)	0.25	4 (1%) 68 46	48, 83, 164, 181	0
3	G	172/208 (82%)	0.27	7 (4%) 41 19	44, 77, 178, 190	0
4	D	242/245 (98%)	-0.01	1 (0%) 93 85	49, 97, 150, 173	0
4	H	230/245 (93%)	0.38	13 (5%) 27 11	58, 126, 173, 191	0
All	All	1613/1708 (94%)	0.16	39 (2%) 62 39	44, 96, 163, 191	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	147	ALA	5.3
4	H	126	ALA	4.7
4	H	208	PHE	4.2
3	C	126	ARG	3.7
1	E	277	LEU	3.7

### 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, 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
7	NAG	A	406	14/15	0.78	0.34	1.38	108,117,128,133	0
5	NAG	A	402	14/15	0.96	0.19	0.37	76,88,103,115	0
7	NAG	E	405	14/15	0.86	0.21	0.10	150,152,160,161	0
5	NAG	A	401	14/15	0.92	0.22	-0.21	64,70,78,83	0
10	NAG	E	401	14/15	0.90	0.20	-0.63	72,91,96,103	0
10	NAG	E	402	14/15	0.91	0.17	-0.66	108,112,125,133	0
7	NAG	A	407	14/15	0.73	0.39	-	139,147,152,152	0
5	BMA	A	403	11/12	0.67	0.17	-	127,139,145,146	0
7	NAG	E	406	14/15	0.67	0.31	-	162,171,175,177	0
10	BMA	E	403	11/12	0.72	0.18	-	141,149,153,156	0
5	MAN	A	404	11/12	0.86	0.26	-	151,156,163,163	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, 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
9	CIS	A	409	55/61	0.95	0.40	2.33	50,59,69,71	3
6	NAG	A	405	14/15	0.82	0.30	-0.05	106,118,138,139	0
9	CIS	E	407	34/61	0.96	0.27	-0.17	66,76,86,87	0
8	FLC	A	408	13/13	0.94	0.26	-0.87	35,63,70,77	0
6	NAG	E	404	14/15	0.70	0.27	-	142,156,161,161	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.