



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:00 PM GMT

PDB ID : 1I3R
Title : CRYSTAL STRUCTURE OF A MUTANT IEK CLASS II MHC MOLECULE
Authors : Kappler, J.W.; Wilson, N.
Deposited on : 2001-02-15
Resolution : 2.40 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

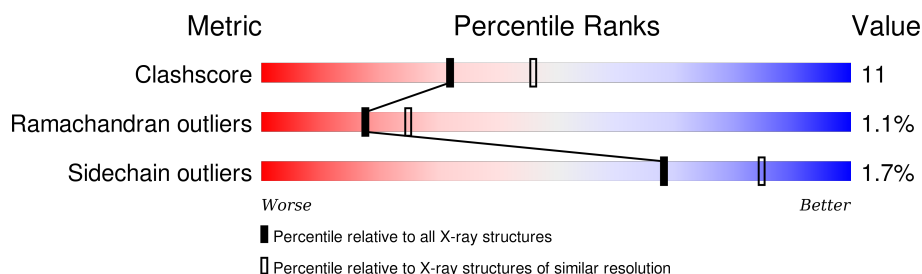
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)


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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	192	
1	C	192	
1	E	192	
1	G	192	
2	B	228	
2	D	228	
2	F	228	

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Mol	Chain	Length	Quality of chain
2	H	228	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: a green segment representing 68%, a yellow segment representing 26%, and a small grey segment representing 5%.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13325 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 H-2 CLASS II HISTOCOMPATIBILITY ANTIGEN, E-K ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1495	963	247	281	4			
1	C	182	Total	C	N	O	S	0	0	0
			1491	961	247	279	4			
1	E	182	Total	C	N	O	S	0	0	0
			1491	961	247	279	4			
1	G	182	Total	C	N	O	S	0	0	0
			1491	961	247	279	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLN	GLU	engineered	UNP P04224
A	66	ASN	ASP	engineered	UNP P04224
C	11	GLN	GLU	engineered	UNP P04224
C	66	ASN	ASP	engineered	UNP P04224
E	11	GLN	GLU	engineered	UNP P04224
E	66	ASN	ASP	engineered	UNP P04224
G	11	GLN	GLU	engineered	UNP P04224
G	66	ASN	ASP	engineered	UNP P04224

- Molecule 2 is a protein called FUSION PROTEIN CONSISTING OF MHC E-BETA-K PRECURSOR, GLYCINE RICH LINKER, AND HEMOGLOBIN BETA-2 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1701	1076	295	324	6			
2	D	216	Total	C	N	O	S	0	0	0
			1711	1082	299	324	6			
2	F	216	Total	C	N	O	S	0	0	0
			1701	1076	295	324	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1701	1076	295	324	6			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	ARG	-	CLONING ARTIFACT	UNP P02089
B	-2	ASP	-	CLONING ARTIFACT	UNP P02089
B	-1	SER	-	CLONING ARTIFACT	UNP P02089
B	0	ARG	-	CLONING ARTIFACT	UNP P02089
D	-3	ARG	-	CLONING ARTIFACT	UNP P02089
D	-2	ASP	-	CLONING ARTIFACT	UNP P02089
D	-1	SER	-	CLONING ARTIFACT	UNP P02089
D	0	ARG	-	CLONING ARTIFACT	UNP P02089
F	-3	ARG	-	CLONING ARTIFACT	UNP P02089
F	-2	ASP	-	CLONING ARTIFACT	UNP P02089
F	-1	SER	-	CLONING ARTIFACT	UNP P02089
F	0	ARG	-	CLONING ARTIFACT	UNP P02089
H	-3	ARG	-	CLONING ARTIFACT	UNP P02089
H	-2	ASP	-	CLONING ARTIFACT	UNP P02089
H	-1	SER	-	CLONING ARTIFACT	UNP P02089
H	0	ARG	-	CLONING ARTIFACT	UNP P02089
B	14	GLY	-	linker	UNP P02089
B	15	GLY	-	linker	UNP P02089
B	16	GLY	-	linker	UNP P02089
B	17	GLY	-	linker	UNP P02089
B	18	SER	-	linker	UNP P02089
B	19	LEU	-	linker	UNP P02089
B	20	VAL	-	linker	UNP P02089
B	21	GLY	-	linker	UNP P02089
B	22	GLY	-	linker	UNP P02089
B	23	GLY	-	linker	UNP P02089
B	24	SER	-	linker	UNP P02089
B	25	GLY	-	linker	UNP P02089
B	26	GLY	-	linker	UNP P02089
B	27	GLY	-	linker	UNP P02089
B	28	GLY	-	linker	UNP P02089
D	14	GLY	-	linker	UNP P02089
D	15	GLY	-	linker	UNP P02089
D	16	GLY	-	linker	UNP P02089
D	17	GLY	-	linker	UNP P02089
D	18	SER	-	linker	UNP P02089

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Chain	Residue	Modelled	Actual	Comment	Reference
D	19	LEU	-	linker	UNP P02089
D	20	VAL	-	linker	UNP P02089
D	21	GLY	-	linker	UNP P02089
D	22	GLY	-	linker	UNP P02089
D	23	GLY	-	linker	UNP P02089
D	24	SER	-	linker	UNP P02089
D	25	GLY	-	linker	UNP P02089
D	26	GLY	-	linker	UNP P02089
D	27	GLY	-	linker	UNP P02089
D	28	GLY	-	linker	UNP P02089
F	14	GLY	-	linker	UNP P02089
F	15	GLY	-	linker	UNP P02089
F	16	GLY	-	linker	UNP P02089
F	17	GLY	-	linker	UNP P02089
F	18	SER	-	linker	UNP P02089
F	19	LEU	-	linker	UNP P02089
F	20	VAL	-	linker	UNP P02089
F	21	GLY	-	linker	UNP P02089
F	22	GLY	-	linker	UNP P02089
F	23	GLY	-	linker	UNP P02089
F	24	SER	-	linker	UNP P02089
F	25	GLY	-	linker	UNP P02089
F	26	GLY	-	linker	UNP P02089
F	27	GLY	-	linker	UNP P02089
F	28	GLY	-	linker	UNP P02089
H	14	GLY	-	linker	UNP P02089
H	15	GLY	-	linker	UNP P02089
H	16	GLY	-	linker	UNP P02089
H	17	GLY	-	linker	UNP P02089
H	18	SER	-	linker	UNP P02089
H	19	LEU	-	linker	UNP P02089
H	20	VAL	-	linker	UNP P02089
H	21	GLY	-	linker	UNP P02089
H	22	GLY	-	linker	UNP P02089
H	23	GLY	-	linker	UNP P02089
H	24	SER	-	linker	UNP P02089
H	25	GLY	-	linker	UNP P02089
H	26	GLY	-	linker	UNP P02089
H	27	GLY	-	linker	UNP P02089
H	28	GLY	-	linker	UNP P02089

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



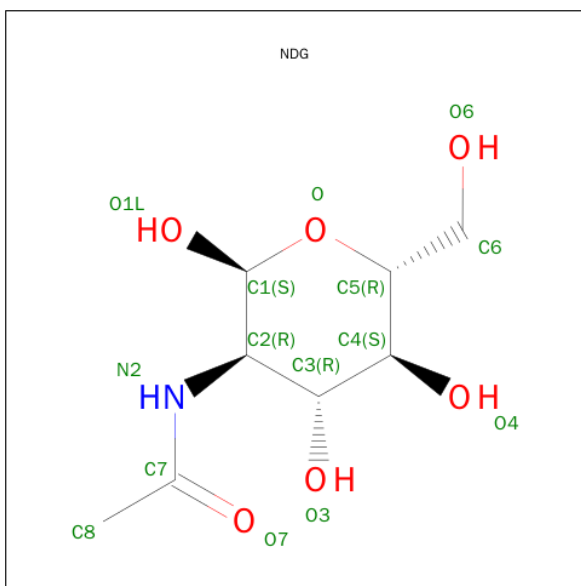
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

- Molecule 5 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE)

(three-letter code: NDG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is water.

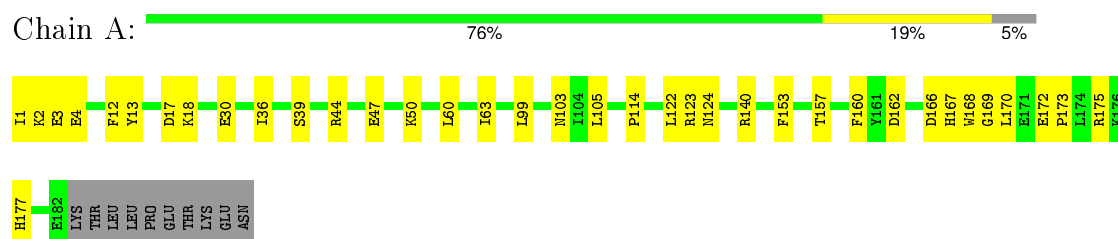
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	42	Total	O	0	0
			42	42		
6	B	31	Total	O	0	0
			31	31		
6	C	46	Total	O	0	0
			46	46		
6	D	35	Total	O	0	0
			35	35		
6	E	35	Total	O	0	0
			35	35		
6	F	41	Total	O	0	0
			41	41		
6	G	58	Total	O	0	0
			58	58		
6	H	31	Total	O	0	0
			31	31		

3 Residue-property plots [i](#)

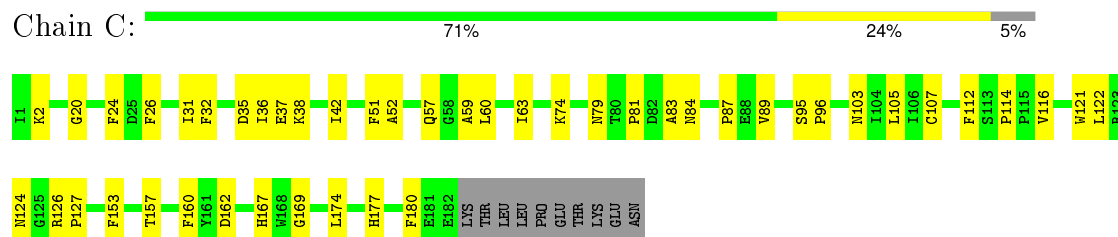
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

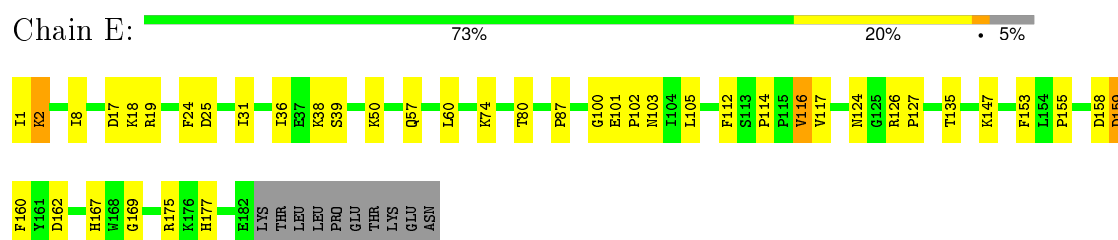
• Molecule 1: H-2 CLASS II HISTOCOMPATIBILITY ANTIGEN, E-K ALPHA CHAIN



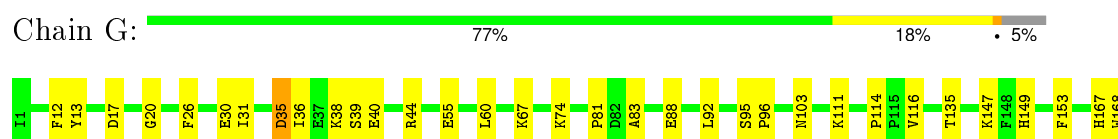
• Molecule 1: H-2 CLASS II HISTOCOMPATIBILITY ANTIGEN, E-K ALPHA CHAIN

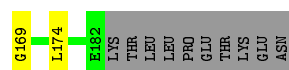


• Molecule 1: H-2 CLASS II HISTOCOMPATIBILITY ANTIGEN, E-K ALPHA CHAIN

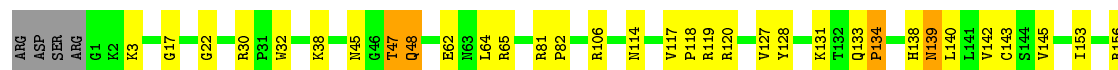


• Molecule 1: H-2 CLASS II HISTOCOMPATIBILITY ANTIGEN, E-K ALPHA CHAIN





- Molecule 2: FUSION PROTEIN CONSISTING OF MHC E-BETA-K PRECURSOR, GLYCINE RICH LINKER, AND HEMOGLOBIN BETA-2 CHAIN



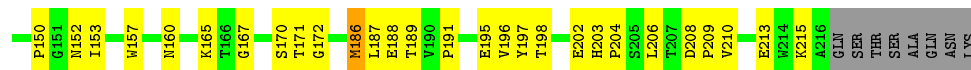
- Molecule 2: FUSION PROTEIN CONSISTING OF MHC E-BETA-K PRECURSOR, GLYCINE RICH LINKER, AND HEMOGLOBIN BETA-2 CHAIN



- Molecule 2: FUSION PROTEIN CONSISTING OF MHC E-BETA-K PRECURSOR, GLYCINE RICH LINKER, AND HEMOGLOBIN BETA-2 CHAIN



- Molecule 2: FUSION PROTEIN CONSISTING OF MHC E-BETA-K PRECURSOR, GLYCINE RICH LINKER, AND HEMOGLOBIN BETA-2 CHAIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.06 Å 58.02 Å 143.22 Å 90.00° 93.24° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40	Depositor
% Data completeness (in resolution range)	96.9 (25.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.229 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13325	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.39	0/1538	0.62	0/2091
1	C	0.40	0/1534	0.61	0/2086
1	E	0.41	0/1534	0.63	0/2086
1	G	0.43	0/1534	0.65	0/2086
2	B	0.36	0/1743	0.61	1/2368 (0.0%)
2	D	0.37	0/1755	0.61	1/2384 (0.0%)
2	F	0.38	0/1743	0.63	1/2368 (0.0%)
2	H	0.37	0/1743	0.61	1/2368 (0.0%)
All	All	0.39	0/13124	0.62	4/17837 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	134	PRO	N-CA-CB	5.71	110.15	103.30
2	B	134	PRO	N-CA-CB	5.57	109.99	103.30
2	F	134	PRO	N-CA-CB	5.42	109.81	103.30
2	D	134	PRO	N-CA-CB	5.38	109.76	103.30

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	1495	0	1421	30	0
1	C	1491	0	1417	33	0
1	E	1491	0	1417	32	0
1	G	1491	0	1417	23	0
2	B	1701	0	1602	38	0
2	D	1711	0	1613	38	0
2	F	1701	0	1603	40	0
2	H	1701	0	1603	44	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	E	14	0	13	0	0
3	F	14	0	13	0	0
3	G	14	0	13	0	0
3	H	14	0	13	1	0
4	A	28	0	25	5	0
4	C	28	0	25	2	0
4	E	28	0	25	1	0
4	G	28	0	25	2	0
5	D	14	0	13	0	0
6	A	42	0	0	0	0
6	B	31	0	0	0	0
6	C	46	0	0	1	0
6	D	35	0	0	0	0
6	E	35	0	0	2	0
6	F	41	0	0	0	0
6	G	58	0	0	1	0
6	H	31	0	0	0	0
All	All	13325	0	12297	267	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 11.

The worst 5 of 267 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)
2:F:196:VAL:HG22	2:F:215:LYS:HG2	1.56	0.86
2:F:78:GLU:OE1	2:H:172:GLY:HA3	1.78	0.84
2:H:3:LYS:HE3	2:H:3:LYS:HA	1.62	0.82
1:A:2:LYS:H	1:A:2:LYS:HD2	1.44	0.81
2:B:3:LYS:HE3	2:B:114:ASN:HD21	1.46	0.81

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	180/192 (94%)	174 (97%)	5 (3%)	1 (1%)	30	43
1	C	180/192 (94%)	170 (94%)	9 (5%)	1 (1%)	30	43
1	E	180/192 (94%)	168 (93%)	11 (6%)	1 (1%)	30	43
1	G	180/192 (94%)	171 (95%)	9 (5%)	0	100	100
2	B	214/228 (94%)	193 (90%)	17 (8%)	4 (2%)	10	12
2	D	214/228 (94%)	191 (89%)	18 (8%)	5 (2%)	8	8
2	F	214/228 (94%)	193 (90%)	16 (8%)	5 (2%)	8	8
2	H	214/228 (94%)	196 (92%)	17 (8%)	1 (0%)	34	48
All	All	1576/1680 (94%)	1456 (92%)	102 (6%)	18 (1%)	17	25

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	133	GLN
2	D	134	PRO
2	F	133	GLN
2	F	134	PRO
2	H	137	HIS

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	164/175 (94%)	163 (99%)	1 (1%)	90	96
1	C	163/175 (93%)	161 (99%)	2 (1%)	78	90
1	E	163/175 (93%)	160 (98%)	3 (2%)	66	84
1	G	163/175 (93%)	158 (97%)	5 (3%)	47	69
2	B	181/200 (90%)	178 (98%)	3 (2%)	68	85
2	D	183/200 (92%)	180 (98%)	3 (2%)	70	86
2	F	181/200 (90%)	177 (98%)	4 (2%)	60	79
2	H	181/200 (90%)	179 (99%)	2 (1%)	80	92
All	All	1379/1500 (92%)	1356 (98%)	23 (2%)	68	85

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	116	VAL
2	F	115	PHE
2	H	3	LYS
1	E	159	ASP
2	F	139	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	114	ASN
1	E	57	GLN
2	H	96	GLN
2	D	137	HIS
1	E	149	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 ⓘ

8 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$
4	NAG	A	302	1,4	14,14,15	0.72	0	15,19,21	0.97	0
4	NAG	A	303	4	14,14,15	0.45	0	15,19,21	0.74	0
4	NAG	C	306	1,4	14,14,15	0.53	0	15,19,21	0.67	0
4	NAG	C	307	4	14,14,15	0.55	0	15,19,21	0.60	0
4	NAG	E	310	1,4	14,14,15	0.50	0	15,19,21	0.67	0
4	NAG	E	311	4	14,14,15	0.52	0	15,19,21	0.86	1 (6%)
4	NAG	G	314	1,4	14,14,15	0.43	0	15,19,21	0.93	1 (6%)
4	NAG	G	315	4	14,14,15	0.53	0	15,19,21	0.71	1 (6%)

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	A	302	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	303	4	-	0/6/23/26	0/1/1/1
4	NAG	C	306	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	307	4	-	0/6/23/26	0/1/1/1
4	NAG	E	310	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	311	4	-	0/6/23/26	0/1/1/1
4	NAG	G	314	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	315	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	314	NAG	C2-N2-C7	-2.49	119.85	123.04
4	E	311	NAG	C4-C3-C2	-2.13	107.92	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	315	NAG	C2-N2-C7	-2.07	120.38	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	NAG	3	0
4	A	303	NAG	4	0
4	C	306	NAG	1	0
4	C	307	NAG	2	0
4	E	310	NAG	1	0
4	E	311	NAG	1	0
4	G	314	NAG	2	0

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	301	1	14,14,15	0.67	0	15,19,21	0.70	1 (6%)
3	NAG	B	304	2	14,14,15	0.72	1 (7%)	15,19,21	0.86	1 (6%)
3	NAG	C	305	1	14,14,15	0.61	0	15,19,21	0.68	0
5	NDG	D	308	2	14,14,15	0.71	1 (7%)	15,19,21	0.64	0
3	NAG	E	309	1	14,14,15	0.61	0	15,19,21	0.77	1 (6%)
3	NAG	F	312	2	14,14,15	0.67	0	15,19,21	0.70	0
3	NAG	G	313	1	14,14,15	0.49	0	15,19,21	0.73	1 (6%)
3	NAG	H	316	2	14,14,15	0.50	0	15,19,21	0.77	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	304	2	-	0/6/23/26	0/1/1/1
3	NAG	C	305	1	-	0/6/23/26	0/1/1/1
5	NDG	D	308	2	-	0/6/23/26	0/1/1/1
3	NAG	E	309	1	-	0/6/23/26	0/1/1/1
3	NAG	F	312	2	-	0/6/23/26	0/1/1/1
3	NAG	G	313	1	-	0/6/23/26	0/1/1/1
3	NAG	H	316	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	308	NDG	C1-C2	2.03	1.55	1.52
3	B	304	NAG	C1-C2	2.08	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	304	NAG	C2-N2-C7	-2.40	119.95	123.04
3	E	309	NAG	C2-N2-C7	-2.33	120.04	123.04
3	H	316	NAG	C2-N2-C7	-2.24	120.16	123.04
3	G	313	NAG	C2-N2-C7	-2.23	120.18	123.04
3	A	301	NAG	C2-N2-C7	-2.09	120.35	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	316	NAG	1	0

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.