



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 27, 2024 – 08:12 PM EDT

PDB ID : 1DE4  
Title : HEMOCHROMATOSIS PROTEIN HFE COMPLEXED WITH TRANSFERRIN RECEPTOR  
Authors : Bennett, M.J.; Lebron, J.A.; Bjorkman, P.J.  
Deposited on : 1999-11-12  
Resolution : 2.80 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

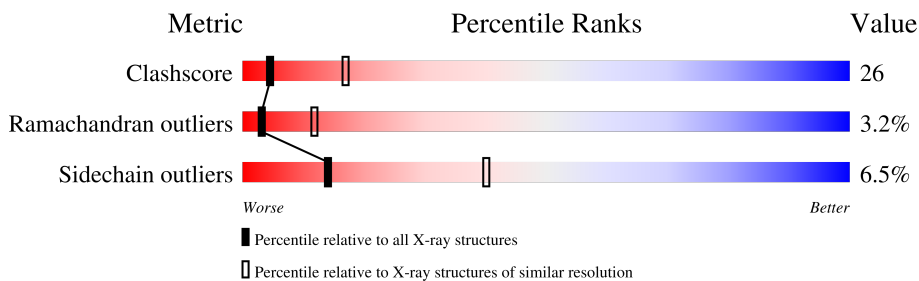
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)

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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	275	50% 41% 8% .
1	D	275	51% 40% 7% .
1	G	275	51% 41% 7% ..
2	B	99	52% 42% 6%
2	E	99	49% 43% 7%
2	H	99	52% 41% 7%
3	C	640	55% 39% 5% .
3	F	640	56% 39% 5% .

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Mol	Chain	Length	Quality of chain
3	I	640	<div><div></div><div>58%</div><div>36%</div><div>5% •</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24315 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 HEMOCHROMATOSIS PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2242	1424	390	416	12			
1	D	272	Total	C	N	O	S	0	0	0
			2242	1424	390	416	12			
1	G	272	Total	C	N	O	S	0	0	0
			2242	1424	390	416	12			

- Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	522	138	158	3			
2	E	99	Total	C	N	O	S	0	0	0
			821	522	138	158	3			
2	H	99	Total	C	N	O	S	0	0	0
			821	522	138	158	3			

- Molecule 3 is a protein called TRANSFERRIN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	635	Total	C	N	O	S	0	0	0
			5022	3223	845	940	14			
3	F	635	Total	C	N	O	S	0	0	0
			5022	3223	845	940	14			
3	I	635	Total	C	N	O	S	0	0	0
			5022	3223	845	940	14			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	I	1	Total	Ca	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

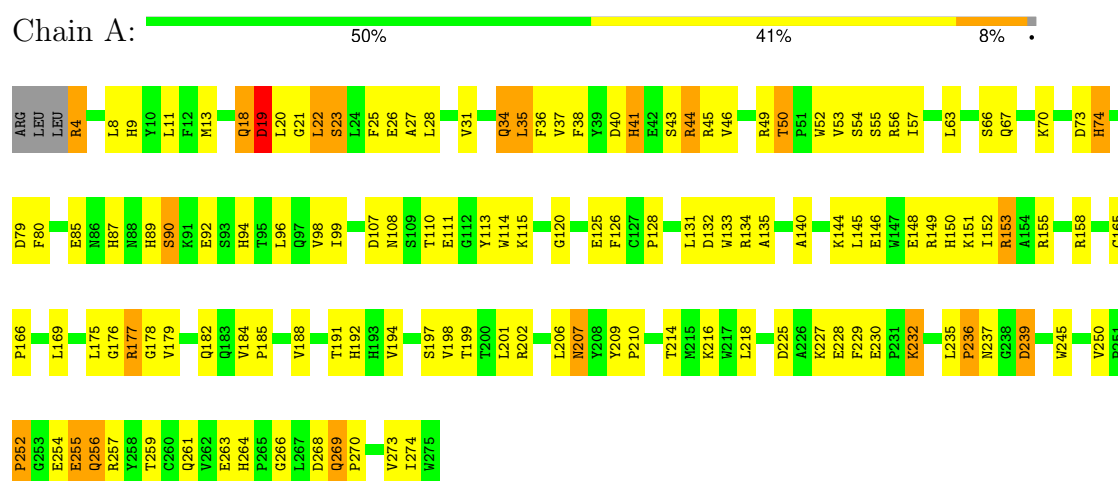
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	4	Total	O	0	0
			4	4		
7	F	2	Total	O	0	0
			2	2		
7	I	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

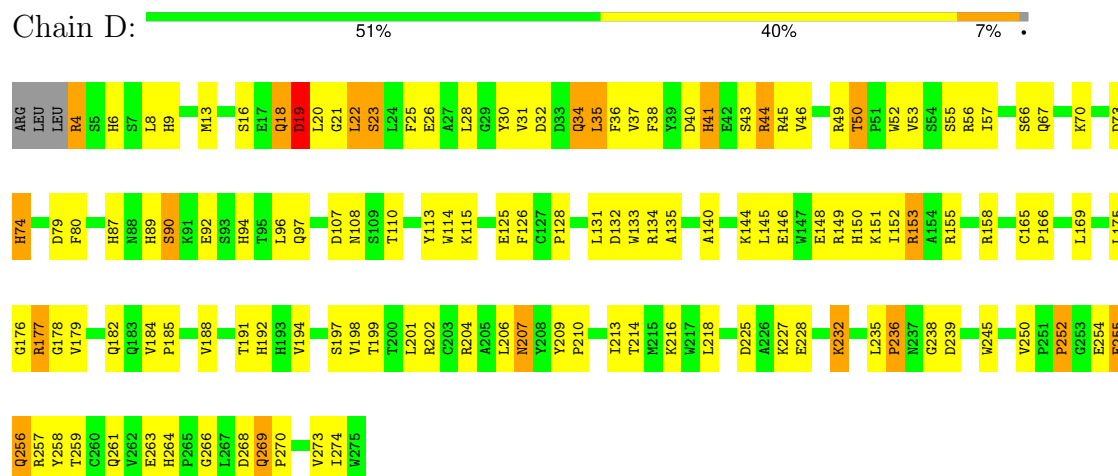
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: HEMOCHROMATOSIS PROTEIN

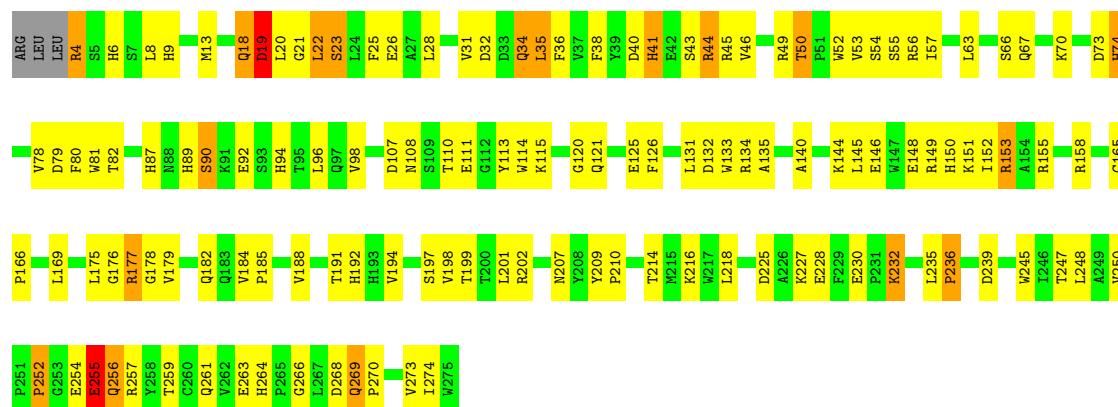


#### • Molecule 1: HEMOCHROMATOSIS PROTEIN

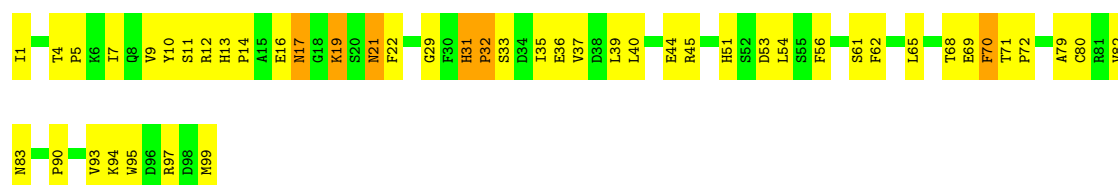


#### • Molecule 1: HEMOCHROMATOSIS PROTEIN

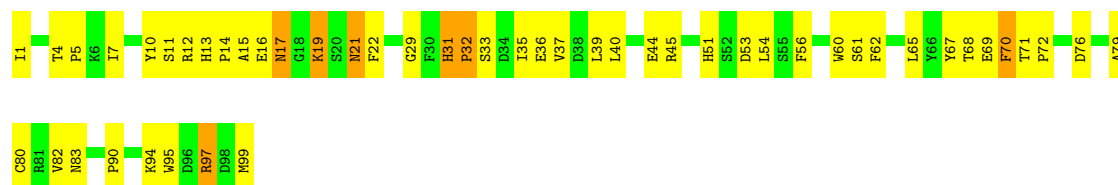




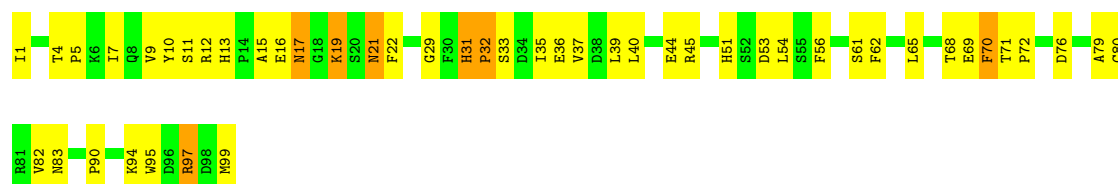
• Molecule 2: BETA-2-MICROGLOBULIN



• Molecule 2: BETA-2-MICROGLOBULIN

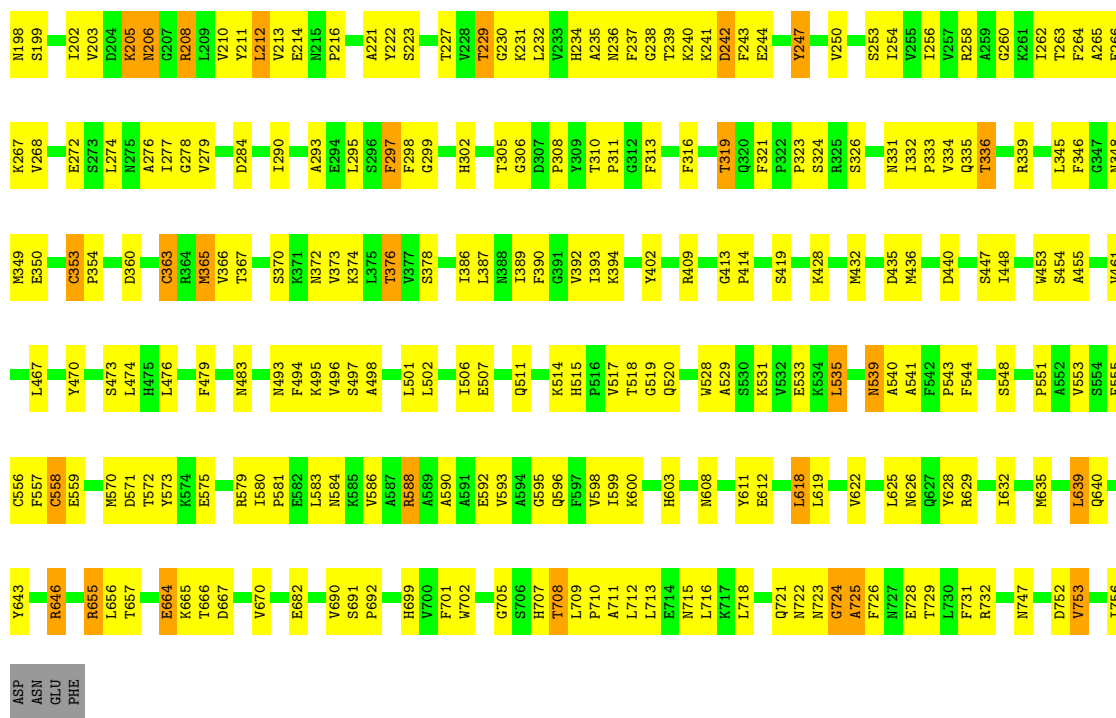


• Molecule 2: BETA-2-MICROGLOBULIN



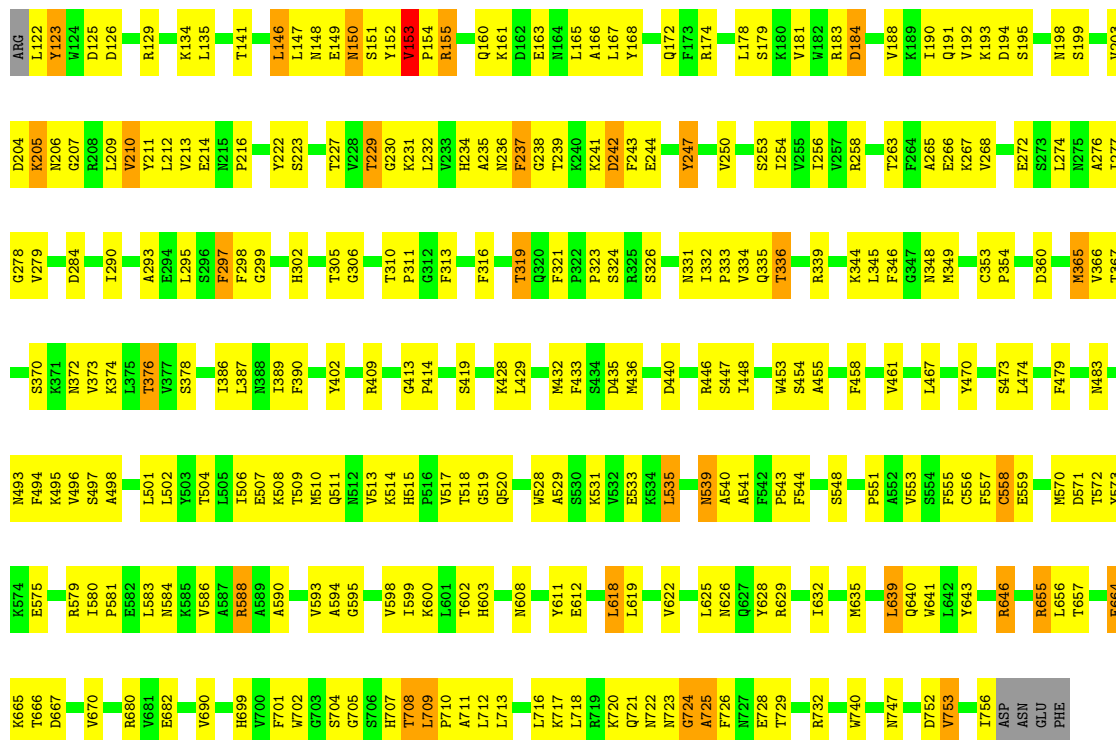
• Molecule 3: TRANSFERRIN RECEPTOR





### • Molecule 3: TRANSFERRIN RECEPTOR

Chain F: 56% 39% 5%



### • Molecule 3: TRANSFERRIN RECEPTOR

Chain I: 58% 36% 5%

H699	V586	L501	K371	D284	I202	ARG
V700	A587	L502	N372	D284	I202	L122
F701	R588		V373	I290	V203	Y123
W702	A589	L505	K374		D204	W124
G703	A590	L506	L375	A293	K205	D125
S704	A591	E507	T376	E294	N206	D126
G705	E592	R508	V377	L295	G207	
S706	V593	T509	S378	S296	R208	R129
W707	A594	T509	I386	F297	L209	
T708	G595	Q511		F298	Y211	K134
L709	Q596	Q511	I389	G299	Y211	L135
F710	F597	N512	F390	H302	L212	
P711	V598	W513	Y402		V213	T141
A711	I599	K514		T305	E214	
L712	K600	H515		P216		L146
L713		V517	R409	G306	Y222	L147
L716	H603	T518	G413	T310	S223	L148
K717	N608	Q519	P414	P311		E149
L718		Q520	S419	G312	T227	N150
Q721	Y611	W528		F313	V228	S151
N722	E612	A529	K428		T229	Y152
N723	L618			F316	G230	P154
G724	L619	E533	M432	T319	K231	P155
A725		K534		Q320	L232	
F726	V622	L535	D435	F321	H233	Q160
N727	R623				H234	K161
E728	D624	N539	K439	S324	A235	D162
	L625	A540	D440	R325	N236	E163
R732	N626	A541	G441	S326	F237	N164
	Q627	F542			G238	L165
	Y628	P543	S447	I332	L239	A166
N747	R629	F544	I448	P333	L167	A166
D752				V334	K241	Y168
V753	I632	S548	W453	Q335	D242	Q172
	M635	P551	S454	T336	F243	F173
ASP		A552	A455		Y247	R174
ASN	L639	V553		R339		
GLU	Q640	S554	F458	L345	V250	L178
PHE	Y643	C556	V461	F346	S253	S179
	R646	F557	L467	G347	I254	K180
		C558		N348	R258	V181
	R655	E559	Y470	M349		W182
	L656		L474	E350	T263	R183
	T657	M570		C353	Q185	D184
		D571	F479	P354	H186	Q185
	E664	T572	N483	D360	F187	V188
	F665	Y573		C363	V188	K189
	T666	R574	N493	M364	A265	I190
	D667	E575	F494	V366	E266	V191
			K495	T367	K267	V192
	V670	R579	V496	S370	V268	K193
		I580	S497		L274	D194
	E682				W275	S195
	V690	L583			A276	
		N584			I277	N198
		K585			G278	S199
					V279	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.40Å 144.40Å 327.10Å 90.00° 93.60° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	94.3 (30.00-2.80)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.231 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24315	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

## 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: GOL, 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	0.34	0/2310	0.60	0/3143
1	D	0.34	0/2310	0.60	0/3143
1	G	0.35	0/2310	0.60	0/3143
2	B	0.33	0/844	0.56	0/1144
2	E	0.34	0/844	0.56	0/1144
2	H	0.33	0/844	0.56	0/1144
3	C	0.40	0/5142	0.65	2/6973 (0.0%)
3	F	0.40	0/5142	0.65	1/6973 (0.0%)
3	I	0.43	0/5142	0.66	2/6973 (0.0%)
All	All	0.38	0/24888	0.63	5/33780 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	557	PHE	N-CA-C	-6.66	93.01	111.00
3	F	557	PHE	N-CA-C	-6.58	93.23	111.00
3	I	557	PHE	N-CA-C	-6.44	93.61	111.00
3	C	363	CYS	CA-CB-SG	5.07	123.13	114.00
3	I	363	CYS	CA-CB-SG	5.03	123.05	114.00

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	2242	0	2126	136	0
1	D	2242	0	2126	139	0
1	G	2242	0	2126	133	0
2	B	821	0	772	51	0
2	E	821	0	772	55	0
2	H	821	0	772	50	0
3	C	5022	0	4965	253	0
3	F	5022	0	4965	250	0
3	I	5022	0	4965	238	0
4	C	14	0	13	0	0
4	F	14	0	13	0	0
4	I	14	0	13	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
6	G	6	0	8	3	0
7	C	4	0	0	0	0
7	F	2	0	0	0	0
7	I	3	0	0	0	0
All	All	24315	0	23636	1231	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 26.

The worst 5 of 1231 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:708:THR:HG22	3:C:711:ALA:H	1.18	1.09
3:C:708:THR:HG23	3:C:710:PRO:HD2	1.29	1.08
3:I:708:THR:HG23	3:I:710:PRO:HD2	1.29	1.07
3:F:708:THR:HG23	3:F:710:PRO:HD2	1.31	1.04
3:I:708:THR:HG22	3:I:711:ALA:H	1.18	1.03

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	270/275 (98%)	233 (86%)	24 (9%)	13 (5%)	2	6
1	D	270/275 (98%)	230 (85%)	26 (10%)	14 (5%)	1	5
1	G	270/275 (98%)	230 (85%)	27 (10%)	13 (5%)	2	6
2	B	97/99 (98%)	83 (86%)	9 (9%)	5 (5%)	1	5
2	E	97/99 (98%)	84 (87%)	8 (8%)	5 (5%)	1	5
2	H	97/99 (98%)	84 (87%)	8 (8%)	5 (5%)	1	5
3	C	633/640 (99%)	575 (91%)	45 (7%)	13 (2%)	5	20
3	F	633/640 (99%)	572 (90%)	47 (7%)	14 (2%)	5	20
3	I	633/640 (99%)	573 (90%)	47 (7%)	13 (2%)	5	20
All	All	3000/3042 (99%)	2664 (89%)	241 (8%)	95 (3%)	3	12

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	22	LEU
1	A	44	ARG
2	B	31	HIS
3	C	153	VAL

### 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	244/249 (98%)	230 (94%)	14 (6%)	17	46
1	D	244/249 (98%)	230 (94%)	14 (6%)	17	46
1	G	244/249 (98%)	230 (94%)	14 (6%)	17	46
2	B	92/94 (98%)	88 (96%)	4 (4%)	25	57
2	E	92/94 (98%)	88 (96%)	4 (4%)	25	57
2	H	92/94 (98%)	88 (96%)	4 (4%)	25	57
3	C	544/549 (99%)	504 (93%)	40 (7%)	11	33
3	F	544/549 (99%)	506 (93%)	38 (7%)	12	36
3	I	544/549 (99%)	505 (93%)	39 (7%)	12	34
All	All	2640/2676 (99%)	2469 (94%)	171 (6%)	14	40

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	13	MET
3	I	229	THR
1	G	35	LEU
2	H	51	HIS
3	I	353	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	83	ASN
3	I	699	HIS
3	F	603	HIS
3	I	640	GLN
3	I	236	ASN

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	C	900	3	14,14,15	0.66	0	17,19,21	0.82	1 (5%)
4	NAG	F	901	3	14,14,15	0.59	0	17,19,21	0.87	1 (5%)
6	GOL	G	309	-	5,5,5	1.82	2 (40%)	5,5,5	0.99	0
4	NAG	I	902	3	14,14,15	0.46	0	17,19,21	1.04	2 (11%)

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	C	900	3	-	2/6/23/26	0/1/1/1
4	NAG	F	901	3	-	2/6/23/26	0/1/1/1
6	GOL	G	309	-	-	2/4/4/4	-
4	NAG	I	902	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	309	GOL	O2-C2	2.98	1.52	1.43
6	G	309	GOL	C3-C2	2.20	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	901	NAG	C2-N2-C7	-2.79	119.16	122.90
4	I	902	NAG	C2-N2-C7	-2.64	119.36	122.90
4	C	900	NAG	C2-N2-C7	-2.49	119.56	122.90
4	I	902	NAG	C4-C3-C2	-2.04	108.03	111.02

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	309	GOL	C1-C2-C3-O3
6	G	309	GOL	O2-C2-C3-O3
4	F	901	NAG	O5-C5-C6-O6
4	F	901	NAG	C4-C5-C6-O6
4	I	902	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	309	GOL	3	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.