



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:58 am BST

PDB ID : 5OVW
Title : Nanobody-bound BtuF, the vitamin B12 binding protein in Escherichia coli
Authors : Mireku, S.A.; Sauer, M.M.; Glockshuber, R.; Locher, K.P.
Deposited on : 2017-08-30
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 2.11
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) : 2.11

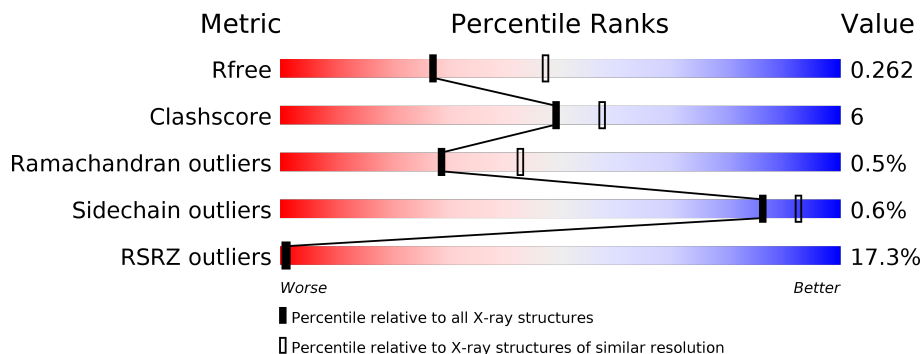
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	289	
1	B	289	
1	C	289	
1	D	289	
1	E	289	
1	F	289	

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Mol	Chain	Length	Quality of chain
2	G	159	<p>30% 66% 13% 21%</p>
2	H	159	<p>11% 68% 11% 21%</p>
2	I	159	<p>53% 64% 15% 21%</p>
2	J	159	<p>4% 69% 10% 21%</p>
2	K	159	<p>14% 69% 11% 21%</p>
2	L	159	<p>22% 67% 13% 21%</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17352 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 Vitamin B12-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	245	1907	1216	332	355	4	0	0	0
1	B	245	1907	1216	332	355	4	0	0	0
1	C	245	1907	1216	332	355	4	0	0	0
1	D	245	1907	1216	332	355	4	0	0	0
1	E	245	1907	1216	332	355	4	0	0	0
1	F	245	1907	1216	332	355	4	0	0	0

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP P37028
A	-1	LYS	-	expression tag	UNP P37028
A	0	LYS	-	expression tag	UNP P37028
A	1	THR	-	expression tag	UNP P37028
A	2	ALA	-	expression tag	UNP P37028
A	3	ILE	-	expression tag	UNP P37028
A	4	ALA	-	expression tag	UNP P37028
A	5	ILE	-	expression tag	UNP P37028
A	6	ALA	-	expression tag	UNP P37028
A	7	VAL	-	expression tag	UNP P37028
A	8	ALA	-	expression tag	UNP P37028
A	9	LEU	-	expression tag	UNP P37028
A	10	ALA	-	expression tag	UNP P37028
A	11	GLY	-	expression tag	UNP P37028
A	12	PHE	-	expression tag	UNP P37028
A	13	ALA	-	expression tag	UNP P37028
A	14	THR	-	expression tag	UNP P37028

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	VAL	-	expression tag	UNP P37028
A	16	ALA	-	expression tag	UNP P37028
A	17	GLN	-	expression tag	UNP P37028
A	18	ALA	-	expression tag	UNP P37028
A	19	ALA	-	expression tag	UNP P37028
A	20	SER	-	expression tag	UNP P37028
A	21	MET	-	expression tag	UNP P37028
A	267	SER	-	expression tag	UNP P37028
A	268	GLY	-	expression tag	UNP P37028
A	269	SER	-	expression tag	UNP P37028
A	270	LEU	-	expression tag	UNP P37028
A	271	GLU	-	expression tag	UNP P37028
A	272	VAL	-	expression tag	UNP P37028
A	273	LEU	-	expression tag	UNP P37028
A	274	PHE	-	expression tag	UNP P37028
A	275	GLN	-	expression tag	UNP P37028
A	276	GLY	-	expression tag	UNP P37028
A	277	PRO	-	expression tag	UNP P37028
A	278	GLY	-	expression tag	UNP P37028
A	279	GLY	-	expression tag	UNP P37028
A	280	SER	-	expression tag	UNP P37028
A	281	HIS	-	expression tag	UNP P37028
A	282	HIS	-	expression tag	UNP P37028
A	283	HIS	-	expression tag	UNP P37028
A	284	HIS	-	expression tag	UNP P37028
A	285	HIS	-	expression tag	UNP P37028
A	286	HIS	-	expression tag	UNP P37028
B	-2	MET	-	initiating methionine	UNP P37028
B	-1	LYS	-	expression tag	UNP P37028
B	0	LYS	-	expression tag	UNP P37028
B	1	THR	-	expression tag	UNP P37028
B	2	ALA	-	expression tag	UNP P37028
B	3	ILE	-	expression tag	UNP P37028
B	4	ALA	-	expression tag	UNP P37028
B	5	ILE	-	expression tag	UNP P37028
B	6	ALA	-	expression tag	UNP P37028
B	7	VAL	-	expression tag	UNP P37028
B	8	ALA	-	expression tag	UNP P37028
B	9	LEU	-	expression tag	UNP P37028
B	10	ALA	-	expression tag	UNP P37028
B	11	GLY	-	expression tag	UNP P37028
B	12	PHE	-	expression tag	UNP P37028

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Chain	Residue	Modelled	Actual	Comment	Reference
B	13	ALA	-	expression tag	UNP P37028
B	14	THR	-	expression tag	UNP P37028
B	15	VAL	-	expression tag	UNP P37028
B	16	ALA	-	expression tag	UNP P37028
B	17	GLN	-	expression tag	UNP P37028
B	18	ALA	-	expression tag	UNP P37028
B	19	ALA	-	expression tag	UNP P37028
B	20	SER	-	expression tag	UNP P37028
B	21	MET	-	expression tag	UNP P37028
B	267	SER	-	expression tag	UNP P37028
B	268	GLY	-	expression tag	UNP P37028
B	269	SER	-	expression tag	UNP P37028
B	270	LEU	-	expression tag	UNP P37028
B	271	GLU	-	expression tag	UNP P37028
B	272	VAL	-	expression tag	UNP P37028
B	273	LEU	-	expression tag	UNP P37028
B	274	PHE	-	expression tag	UNP P37028
B	275	GLN	-	expression tag	UNP P37028
B	276	GLY	-	expression tag	UNP P37028
B	277	PRO	-	expression tag	UNP P37028
B	278	GLY	-	expression tag	UNP P37028
B	279	GLY	-	expression tag	UNP P37028
B	280	SER	-	expression tag	UNP P37028
B	281	HIS	-	expression tag	UNP P37028
B	282	HIS	-	expression tag	UNP P37028
B	283	HIS	-	expression tag	UNP P37028
B	284	HIS	-	expression tag	UNP P37028
B	285	HIS	-	expression tag	UNP P37028
B	286	HIS	-	expression tag	UNP P37028
C	-2	MET	-	initiating methionine	UNP P37028
C	-1	LYS	-	expression tag	UNP P37028
C	0	LYS	-	expression tag	UNP P37028
C	1	THR	-	expression tag	UNP P37028
C	2	ALA	-	expression tag	UNP P37028
C	3	ILE	-	expression tag	UNP P37028
C	4	ALA	-	expression tag	UNP P37028
C	5	ILE	-	expression tag	UNP P37028
C	6	ALA	-	expression tag	UNP P37028
C	7	VAL	-	expression tag	UNP P37028
C	8	ALA	-	expression tag	UNP P37028
C	9	LEU	-	expression tag	UNP P37028
C	10	ALA	-	expression tag	UNP P37028

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Chain	Residue	Modelled	Actual	Comment	Reference
C	11	GLY	-	expression tag	UNP P37028
C	12	PHE	-	expression tag	UNP P37028
C	13	ALA	-	expression tag	UNP P37028
C	14	THR	-	expression tag	UNP P37028
C	15	VAL	-	expression tag	UNP P37028
C	16	ALA	-	expression tag	UNP P37028
C	17	GLN	-	expression tag	UNP P37028
C	18	ALA	-	expression tag	UNP P37028
C	19	ALA	-	expression tag	UNP P37028
C	20	SER	-	expression tag	UNP P37028
C	21	MET	-	expression tag	UNP P37028
C	267	SER	-	expression tag	UNP P37028
C	268	GLY	-	expression tag	UNP P37028
C	269	SER	-	expression tag	UNP P37028
C	270	LEU	-	expression tag	UNP P37028
C	271	GLU	-	expression tag	UNP P37028
C	272	VAL	-	expression tag	UNP P37028
C	273	LEU	-	expression tag	UNP P37028
C	274	PHE	-	expression tag	UNP P37028
C	275	GLN	-	expression tag	UNP P37028
C	276	GLY	-	expression tag	UNP P37028
C	277	PRO	-	expression tag	UNP P37028
C	278	GLY	-	expression tag	UNP P37028
C	279	GLY	-	expression tag	UNP P37028
C	280	SER	-	expression tag	UNP P37028
C	281	HIS	-	expression tag	UNP P37028
C	282	HIS	-	expression tag	UNP P37028
C	283	HIS	-	expression tag	UNP P37028
C	284	HIS	-	expression tag	UNP P37028
C	285	HIS	-	expression tag	UNP P37028
C	286	HIS	-	expression tag	UNP P37028
D	-2	MET	-	initiating methionine	UNP P37028
D	-1	LYS	-	expression tag	UNP P37028
D	0	LYS	-	expression tag	UNP P37028
D	1	THR	-	expression tag	UNP P37028
D	2	ALA	-	expression tag	UNP P37028
D	3	ILE	-	expression tag	UNP P37028
D	4	ALA	-	expression tag	UNP P37028
D	5	ILE	-	expression tag	UNP P37028
D	6	ALA	-	expression tag	UNP P37028
D	7	VAL	-	expression tag	UNP P37028
D	8	ALA	-	expression tag	UNP P37028

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Chain	Residue	Modelled	Actual	Comment	Reference
D	9	LEU	-	expression tag	UNP P37028
D	10	ALA	-	expression tag	UNP P37028
D	11	GLY	-	expression tag	UNP P37028
D	12	PHE	-	expression tag	UNP P37028
D	13	ALA	-	expression tag	UNP P37028
D	14	THR	-	expression tag	UNP P37028
D	15	VAL	-	expression tag	UNP P37028
D	16	ALA	-	expression tag	UNP P37028
D	17	GLN	-	expression tag	UNP P37028
D	18	ALA	-	expression tag	UNP P37028
D	19	ALA	-	expression tag	UNP P37028
D	20	SER	-	expression tag	UNP P37028
D	21	MET	-	expression tag	UNP P37028
D	267	SER	-	expression tag	UNP P37028
D	268	GLY	-	expression tag	UNP P37028
D	269	SER	-	expression tag	UNP P37028
D	270	LEU	-	expression tag	UNP P37028
D	271	GLU	-	expression tag	UNP P37028
D	272	VAL	-	expression tag	UNP P37028
D	273	LEU	-	expression tag	UNP P37028
D	274	PHE	-	expression tag	UNP P37028
D	275	GLN	-	expression tag	UNP P37028
D	276	GLY	-	expression tag	UNP P37028
D	277	PRO	-	expression tag	UNP P37028
D	278	GLY	-	expression tag	UNP P37028
D	279	GLY	-	expression tag	UNP P37028
D	280	SER	-	expression tag	UNP P37028
D	281	HIS	-	expression tag	UNP P37028
D	282	HIS	-	expression tag	UNP P37028
D	283	HIS	-	expression tag	UNP P37028
D	284	HIS	-	expression tag	UNP P37028
D	285	HIS	-	expression tag	UNP P37028
D	286	HIS	-	expression tag	UNP P37028
E	-2	MET	-	initiating methionine	UNP P37028
E	-1	LYS	-	expression tag	UNP P37028
E	0	LYS	-	expression tag	UNP P37028
E	1	THR	-	expression tag	UNP P37028
E	2	ALA	-	expression tag	UNP P37028
E	3	ILE	-	expression tag	UNP P37028
E	4	ALA	-	expression tag	UNP P37028
E	5	ILE	-	expression tag	UNP P37028
E	6	ALA	-	expression tag	UNP P37028

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Chain	Residue	Modelled	Actual	Comment	Reference
E	7	VAL	-	expression tag	UNP P37028
E	8	ALA	-	expression tag	UNP P37028
E	9	LEU	-	expression tag	UNP P37028
E	10	ALA	-	expression tag	UNP P37028
E	11	GLY	-	expression tag	UNP P37028
E	12	PHE	-	expression tag	UNP P37028
E	13	ALA	-	expression tag	UNP P37028
E	14	THR	-	expression tag	UNP P37028
E	15	VAL	-	expression tag	UNP P37028
E	16	ALA	-	expression tag	UNP P37028
E	17	GLN	-	expression tag	UNP P37028
E	18	ALA	-	expression tag	UNP P37028
E	19	ALA	-	expression tag	UNP P37028
E	20	SER	-	expression tag	UNP P37028
E	21	MET	-	expression tag	UNP P37028
E	267	SER	-	expression tag	UNP P37028
E	268	GLY	-	expression tag	UNP P37028
E	269	SER	-	expression tag	UNP P37028
E	270	LEU	-	expression tag	UNP P37028
E	271	GLU	-	expression tag	UNP P37028
E	272	VAL	-	expression tag	UNP P37028
E	273	LEU	-	expression tag	UNP P37028
E	274	PHE	-	expression tag	UNP P37028
E	275	GLN	-	expression tag	UNP P37028
E	276	GLY	-	expression tag	UNP P37028
E	277	PRO	-	expression tag	UNP P37028
E	278	GLY	-	expression tag	UNP P37028
E	279	GLY	-	expression tag	UNP P37028
E	280	SER	-	expression tag	UNP P37028
E	281	HIS	-	expression tag	UNP P37028
E	282	HIS	-	expression tag	UNP P37028
E	283	HIS	-	expression tag	UNP P37028
E	284	HIS	-	expression tag	UNP P37028
E	285	HIS	-	expression tag	UNP P37028
E	286	HIS	-	expression tag	UNP P37028
F	-2	MET	-	initiating methionine	UNP P37028
F	-1	LYS	-	expression tag	UNP P37028
F	0	LYS	-	expression tag	UNP P37028
F	1	THR	-	expression tag	UNP P37028
F	2	ALA	-	expression tag	UNP P37028
F	3	ILE	-	expression tag	UNP P37028
F	4	ALA	-	expression tag	UNP P37028

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Chain	Residue	Modelled	Actual	Comment	Reference
F	5	ILE	-	expression tag	UNP P37028
F	6	ALA	-	expression tag	UNP P37028
F	7	VAL	-	expression tag	UNP P37028
F	8	ALA	-	expression tag	UNP P37028
F	9	LEU	-	expression tag	UNP P37028
F	10	ALA	-	expression tag	UNP P37028
F	11	GLY	-	expression tag	UNP P37028
F	12	PHE	-	expression tag	UNP P37028
F	13	ALA	-	expression tag	UNP P37028
F	14	THR	-	expression tag	UNP P37028
F	15	VAL	-	expression tag	UNP P37028
F	16	ALA	-	expression tag	UNP P37028
F	17	GLN	-	expression tag	UNP P37028
F	18	ALA	-	expression tag	UNP P37028
F	19	ALA	-	expression tag	UNP P37028
F	20	SER	-	expression tag	UNP P37028
F	21	MET	-	expression tag	UNP P37028
F	267	SER	-	expression tag	UNP P37028
F	268	GLY	-	expression tag	UNP P37028
F	269	SER	-	expression tag	UNP P37028
F	270	LEU	-	expression tag	UNP P37028
F	271	GLU	-	expression tag	UNP P37028
F	272	VAL	-	expression tag	UNP P37028
F	273	LEU	-	expression tag	UNP P37028
F	274	PHE	-	expression tag	UNP P37028
F	275	GLN	-	expression tag	UNP P37028
F	276	GLY	-	expression tag	UNP P37028
F	277	PRO	-	expression tag	UNP P37028
F	278	GLY	-	expression tag	UNP P37028
F	279	GLY	-	expression tag	UNP P37028
F	280	SER	-	expression tag	UNP P37028
F	281	HIS	-	expression tag	UNP P37028
F	282	HIS	-	expression tag	UNP P37028
F	283	HIS	-	expression tag	UNP P37028
F	284	HIS	-	expression tag	UNP P37028
F	285	HIS	-	expression tag	UNP P37028
F	286	HIS	-	expression tag	UNP P37028

- Molecule 2 is a protein called Nanobody.

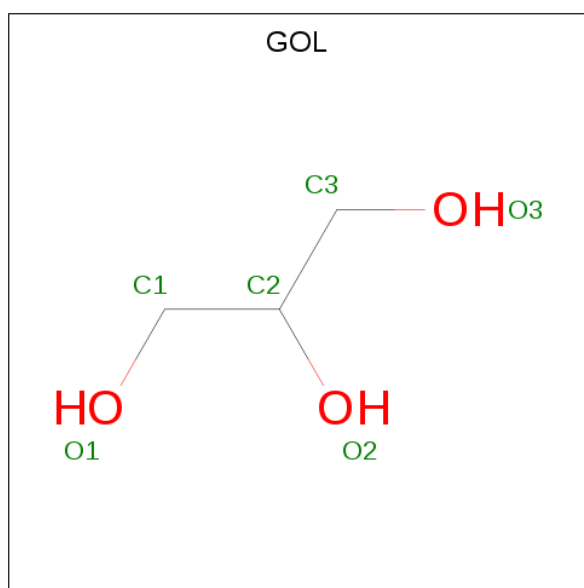
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	126	936	578	165	187	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	126	Total	C	N	O	S	0	0	0
			936	578	165	187	6			
2	I	126	Total	C	N	O	S	0	0	0
			936	578	165	187	6			
2	J	126	Total	C	N	O	S	0	0	0
			936	578	165	187	6			
2	K	126	Total	C	N	O	S	0	0	0
			936	578	165	187	6			
2	L	126	Total	C	N	O	S	0	0	0
			936	578	165	187	6			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

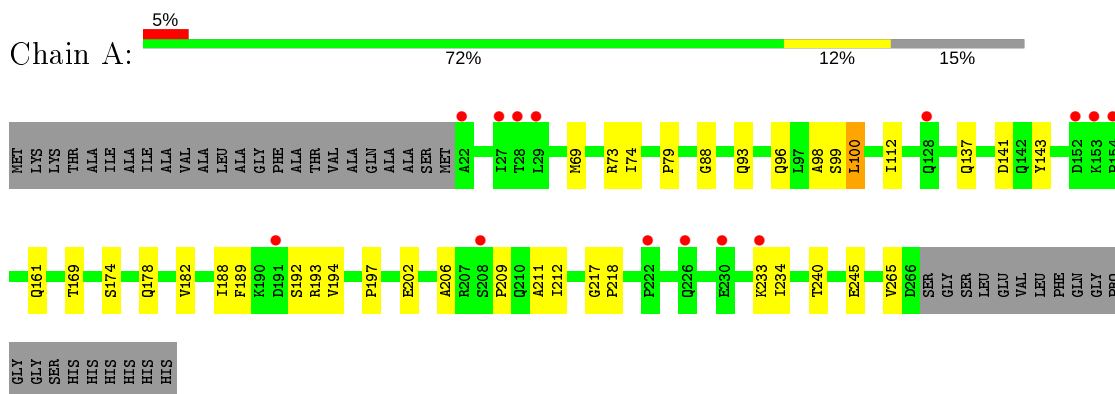
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	42	Total O 42 42	0	0
4	B	37	Total O 37 37	0	0
4	C	10	Total O 10 10	0	0
4	D	66	Total O 66 66	0	0
4	E	25	Total O 25 25	0	0
4	F	17	Total O 17 17	0	0
4	G	4	Total O 4 4	0	0
4	H	14	Total O 14 14	0	0
4	I	2	Total O 2 2	0	0
4	J	27	Total O 27 27	0	0
4	K	13	Total O 13 13	0	0
4	L	7	Total O 7 7	0	0

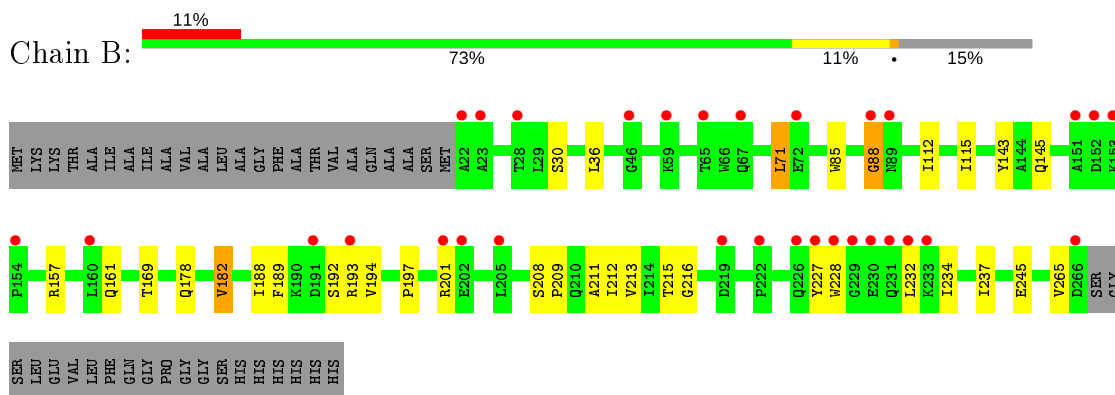
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

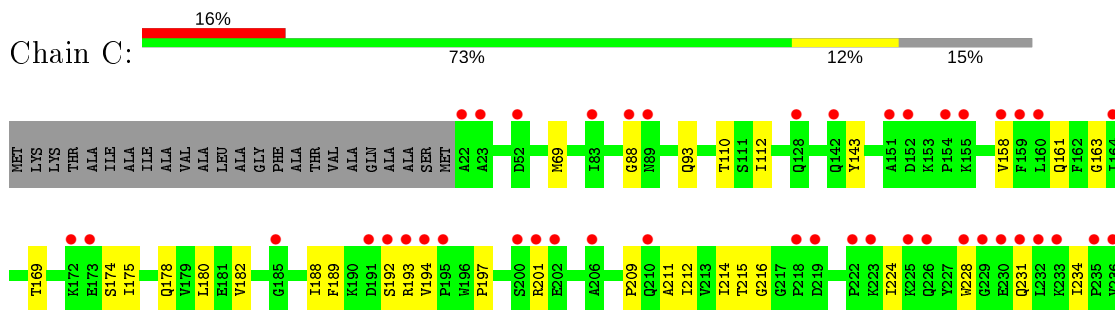
- Molecule 1: Vitamin B12-binding protein

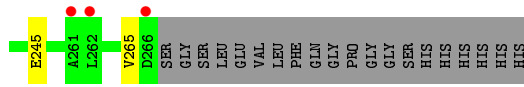


- Molecule 1: Vitamin B12-binding protein

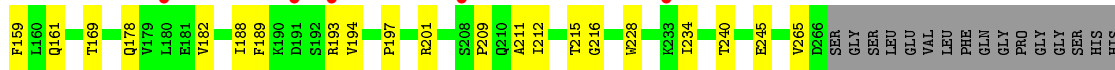
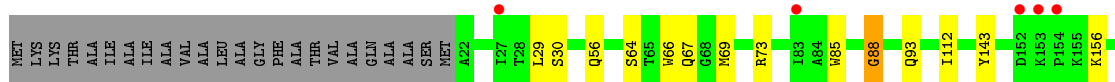
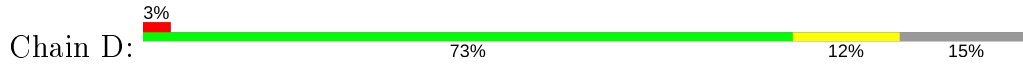


- Molecule 1: Vitamin B12-binding protein

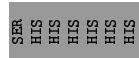
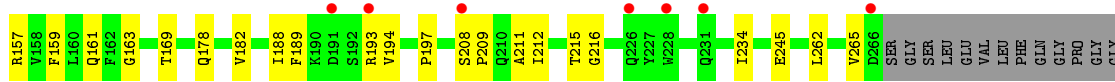
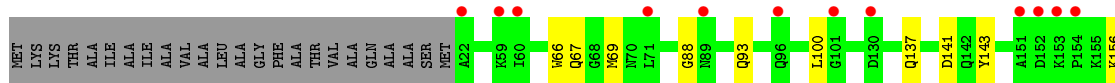
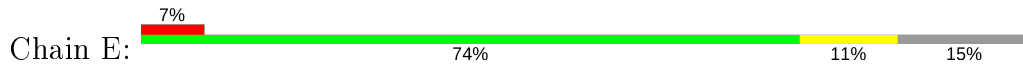




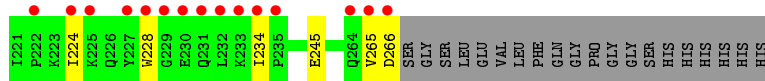
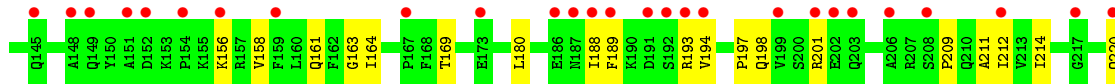
- Molecule 1: Vitamin B12-binding protein



- Molecule 1: Vitamin B12-binding protein



- Molecule 1: Vitamin B12-binding protein

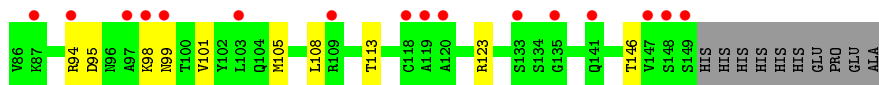
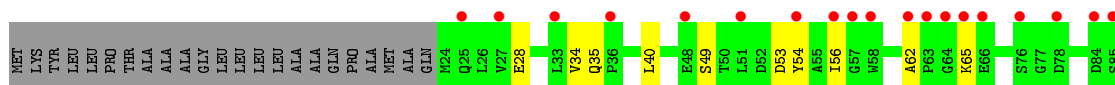


- Molecule 2: Nanobody





• Molecule 2: Nanobody



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.80Å 141.00Å 216.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 20.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	85.3 (20.00-2.65) 85.3 (20.00-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.95 (at 2.67Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.223 , 0.259 0.228 , 0.262	Depositor DCC
R_{free} test set	3239 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtrriage
Anisotropy	0.028	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17352	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.25	0/1951	0.43	0/2661
1	B	0.25	0/1951	0.42	0/2661
1	C	0.26	0/1951	0.42	0/2661
1	D	0.26	0/1951	0.42	0/2661
1	E	0.25	0/1951	0.42	0/2661
1	F	0.26	0/1951	0.41	0/2661
2	G	0.25	0/955	0.44	0/1295
2	H	0.26	0/955	0.44	0/1295
2	I	0.24	0/955	0.43	0/1295
2	J	0.27	0/955	0.45	0/1295
2	K	0.25	0/955	0.44	0/1295
2	L	0.25	0/955	0.45	0/1295
All	All	0.26	0/17436	0.43	0/23736

There are no bond length outliers.

There are no bond angle outliers.

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	1907	0	1924	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1907	0	1924	26	0
1	C	1907	0	1924	25	0
1	D	1907	0	1924	23	0
1	E	1907	0	1924	19	0
1	F	1907	0	1924	25	0
2	G	936	0	888	12	0
2	H	936	0	888	10	0
2	I	936	0	888	13	0
2	J	936	0	888	11	0
2	K	936	0	888	11	0
2	L	936	0	888	12	0
3	B	6	0	8	1	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	1	0
3	H	6	0	8	0	0
4	A	42	0	0	0	0
4	B	37	0	0	0	0
4	C	10	0	0	0	0
4	D	66	0	0	1	0
4	E	25	0	0	0	0
4	F	17	0	0	0	0
4	G	4	0	0	0	0
4	H	14	0	0	0	0
4	I	2	0	0	0	0
4	J	27	0	0	2	0
4	K	13	0	0	0	0
4	L	7	0	0	0	0
All	All	17352	0	16912	200	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 6.

All (200) 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:E:156:LYS:NZ	1:E:265:VAL:O	2.06	0.88
2:J:41:ARG:NH1	4:J:201:HOH:O	2.12	0.77
1:F:156:LYS:HZ1	1:F:266:ASP:CG	1.89	0.76
1:C:201:ARG:NH1	1:C:231:GLN:OE1	2.24	0.70
2:L:54:TYR:O	2:L:94:ARG:NH2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ARG:HH12	1:C:228:TRP:HA	1.57	0.67
1:F:69:MET:HE2	1:F:93:GLN:HB3	1.77	0.65
1:D:69:MET:HE2	1:D:93:GLN:HB3	1.78	0.64
2:H:36:PRO:HD2	2:H:149:SER:HB3	1.79	0.64
2:L:34:VAL:HG21	2:L:40:LEU:HG	1.81	0.63
1:A:211:ALA:HB2	1:A:265:VAL:HG11	1.81	0.62
2:H:56:ILE:HG13	2:H:101:VAL:HG21	1.81	0.62
1:E:143:TYR:OH	1:E:178:GLN:NE2	2.32	0.61
2:K:56:ILE:HG13	2:K:101:VAL:HG21	1.83	0.60
1:F:245:GLU:OE2	2:L:123:ARG:HD2	2.01	0.59
1:C:69:MET:HE2	1:C:93:GLN:HB3	1.85	0.59
1:F:156:LYS:NZ	1:F:266:ASP:OD1	2.36	0.59
1:C:245:GLU:OE1	2:G:123:ARG:NH1	2.34	0.59
1:C:201:ARG:NH1	1:C:228:TRP:HA	2.18	0.59
1:D:143:TYR:CE1	1:D:182:VAL:HG11	2.38	0.59
2:K:36:PRO:HD2	2:K:149:SER:HB3	1.85	0.59
2:J:56:ILE:HG13	2:J:101:VAL:HG21	1.85	0.58
1:B:201:ARG:NH1	1:B:228:TRP:H	2.01	0.58
1:F:156:LYS:NZ	1:F:266:ASP:CG	2.57	0.58
2:G:54:TYR:O	2:G:94:ARG:NH2	2.37	0.58
1:A:178:GLN:O	1:A:182:VAL:HG13	2.05	0.57
2:H:105:MET:HB3	2:H:108:LEU:HD21	1.87	0.57
2:K:105:MET:HB3	2:K:108:LEU:HD21	1.87	0.57
1:B:209:PRO:O	1:B:234:ILE:HG21	2.06	0.56
2:L:105:MET:HB3	2:L:108:LEU:HD21	1.87	0.56
1:A:69:MET:HE2	1:A:93:GLN:HB3	1.88	0.55
1:D:245:GLU:OE1	2:J:123:ARG:NH1	2.38	0.55
1:E:211:ALA:HB2	1:E:265:VAL:HG11	1.87	0.55
2:L:28:GLU:OE1	2:L:28:GLU:N	2.39	0.55
2:I:36:PRO:HD2	2:I:149:SER:HB3	1.88	0.55
1:C:174:SER:O	1:C:178:GLN:NE2	2.40	0.55
2:I:113:THR:HG23	2:I:146:THR:HA	1.89	0.55
2:J:105:MET:HB3	2:J:108:LEU:HD21	1.90	0.54
1:F:137:GLN:NE2	1:F:141:ASP:OD1	2.39	0.54
1:B:169:THR:HG21	1:B:189:PHE:CD1	2.43	0.54
1:C:211:ALA:HB2	1:C:265:VAL:HG11	1.91	0.53
1:C:209:PRO:O	1:C:234:ILE:HG21	2.08	0.53
2:H:54:TYR:O	2:H:94:ARG:NH2	2.41	0.53
2:L:56:ILE:HG13	2:L:101:VAL:HG21	1.90	0.53
2:G:56:ILE:HG13	2:G:101:VAL:HG21	1.90	0.53
1:E:137:GLN:NE2	1:E:141:ASP:OD1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:28:GLU:N	2:J:28:GLU:OE1	2.42	0.53
1:B:112:ILE:HD12	1:B:143:TYR:HD1	1.74	0.53
1:D:56:GLN:NE2	4:D:403:HOH:O	2.42	0.53
1:A:245:GLU:OE1	2:H:123:ARG:NH1	2.41	0.53
1:E:143:TYR:CE1	1:E:182:VAL:HG11	2.44	0.52
1:E:169:THR:HG21	1:E:189:PHE:CD1	2.44	0.52
1:D:85:TRP:CZ2	1:D:88:GLY:HA3	2.45	0.52
1:F:161:GLN:OE1	1:F:212:ILE:HD11	2.10	0.52
1:F:198:GLN:HE21	3:F:301:GOL:H11	1.75	0.52
2:G:28:GLU:OE1	2:G:28:GLU:N	2.42	0.52
2:G:49:SER:O	2:G:99:ASN:ND2	2.41	0.52
1:B:178:GLN:O	1:B:182:VAL:HG13	2.10	0.52
2:H:28:GLU:N	2:H:28:GLU:OE1	2.43	0.52
1:D:201:ARG:NH1	1:D:228:TRP:H	2.08	0.52
1:A:143:TYR:CE1	1:A:182:VAL:HG11	2.45	0.51
1:F:209:PRO:O	1:F:234:ILE:HG21	2.11	0.51
2:K:28:GLU:N	2:K:28:GLU:OE1	2.43	0.51
1:B:201:ARG:HH12	1:B:228:TRP:H	1.58	0.51
1:C:143:TYR:CE1	1:C:182:VAL:HG11	2.46	0.51
2:K:113:THR:HG23	2:K:146:THR:HA	1.92	0.51
1:E:209:PRO:O	1:E:234:ILE:HG21	2.11	0.51
1:B:211:ALA:HB2	1:B:265:VAL:HG11	1.93	0.51
2:I:73:ILE:HD11	2:I:77:GLY:HA2	1.93	0.51
2:I:56:ILE:HG13	2:I:101:VAL:HG21	1.92	0.50
1:B:85:TRP:CZ2	1:B:88:GLY:HA3	2.47	0.50
2:I:105:MET:HB3	2:I:108:LEU:HD21	1.94	0.50
1:F:86:ARG:O	1:F:89:ASN:HB3	2.11	0.50
2:G:105:MET:HB3	2:G:108:LEU:HD21	1.94	0.50
1:F:163:GLY:HA2	2:L:53:ASP:OD2	2.12	0.50
1:C:175:ILE:HA	1:C:178:GLN:HE21	1.76	0.49
1:B:143:TYR:CE1	1:B:182:VAL:HG11	2.47	0.49
1:A:112:ILE:HD12	1:A:143:TYR:HD1	1.77	0.49
1:D:211:ALA:HB2	1:D:265:VAL:HG11	1.94	0.49
1:B:161:GLN:OE1	1:B:212:ILE:HD11	2.12	0.49
1:E:66:TRP:CE2	1:E:67:GLN:HG3	2.47	0.49
1:B:201:ARG:HH11	1:B:228:TRP:HA	1.78	0.49
1:D:66:TRP:CE2	1:D:67:GLN:HG3	2.48	0.48
1:D:209:PRO:O	1:D:234:ILE:HG21	2.13	0.48
2:I:28:GLU:OE1	2:I:28:GLU:N	2.47	0.48
2:J:94:ARG:NH1	4:J:203:HOH:O	2.40	0.48
1:A:209:PRO:O	1:A:234:ILE:HG21	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:49:SER:O	2:H:99:ASN:ND2	2.47	0.48
1:E:188:ILE:HD13	1:E:209:PRO:HG3	1.96	0.48
1:B:112:ILE:HD12	1:B:143:TYR:CD1	2.49	0.48
1:F:36:LEU:HD21	1:F:115:ILE:HG23	1.96	0.48
2:J:36:PRO:HD2	2:J:149:SER:HB2	1.96	0.48
1:F:158:VAL:HB	1:F:180:LEU:HD21	1.96	0.48
2:H:130:VAL:HB	2:H:134:SER:HB2	1.96	0.47
1:C:169:THR:HG21	1:C:189:PHE:CD1	2.49	0.47
1:C:175:ILE:HA	1:C:178:GLN:NE2	2.29	0.47
2:G:62:ALA:HB3	2:G:65:LYS:HE3	1.96	0.47
1:B:157:ARG:NE	1:B:208:SER:O	2.44	0.47
1:C:161:GLN:OE1	1:C:212:ILE:HD11	2.15	0.47
2:J:54:TYR:O	2:J:94:ARG:NH2	2.48	0.47
1:C:214:ILE:HD12	1:C:224:ILE:HD12	1.96	0.47
1:F:169:THR:HG21	1:F:189:PHE:CD1	2.49	0.47
1:D:169:THR:HG21	1:D:189:PHE:CD1	2.49	0.47
1:B:227:TYR:HD1	1:B:228:TRP:CD1	2.33	0.46
1:F:214:ILE:HD12	1:F:224:ILE:HD12	1.97	0.46
1:D:112:ILE:HD12	1:D:143:TYR:HD1	1.80	0.46
1:F:164:ILE:HD11	1:F:220:GLN:HB2	1.97	0.46
1:F:66:TRP:CE2	1:F:67:GLN:HG3	2.51	0.46
1:C:178:GLN:O	1:C:182:VAL:HG13	2.15	0.46
2:I:98:LYS:HD2	2:I:102:TYR:OH	2.16	0.46
1:D:188:ILE:HD13	1:D:209:PRO:HG3	1.98	0.46
1:F:211:ALA:HB2	1:F:265:VAL:HG11	1.97	0.45
1:A:137:GLN:NE2	1:A:141:ASP:OD1	2.49	0.45
1:E:245:GLU:OE1	2:K:123:ARG:NH1	2.46	0.45
1:E:66:TRP:CD1	2:K:81:ASN:HB3	2.51	0.45
2:G:113:THR:HG23	2:G:146:THR:HA	1.98	0.45
1:D:159:PHE:CE2	1:D:161:GLN:HB2	2.51	0.45
1:F:188:ILE:HD13	1:F:209:PRO:HG3	1.98	0.45
2:J:49:SER:O	2:J:99:ASN:ND2	2.47	0.45
1:D:178:GLN:O	1:D:182:VAL:HG13	2.17	0.45
1:D:161:GLN:OE1	1:D:212:ILE:HD11	2.17	0.45
2:I:54:TYR:O	2:I:94:ARG:NH2	2.50	0.45
1:D:85:TRP:CE2	1:D:88:GLY:HA3	2.52	0.45
2:J:62:ALA:HB3	2:J:65:LYS:HE3	1.99	0.44
2:L:113:THR:HG23	2:L:146:THR:HA	1.98	0.44
1:A:161:GLN:OE1	1:A:212:ILE:HD11	2.16	0.44
1:A:192:SER:O	1:A:194:VAL:N	2.51	0.44
2:L:95:ASP:OD2	2:L:98:LYS:HE3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:SER:O	1:B:194:VAL:N	2.51	0.44
1:D:73:ARG:HD2	1:D:73:ARG:HA	1.72	0.44
1:F:86:ARG:HD3	1:F:91:GLU:OE2	2.18	0.44
1:A:169:THR:HG21	1:A:189:PHE:CD1	2.51	0.44
1:F:73:ARG:HD2	1:F:73:ARG:HA	1.73	0.44
2:J:34:VAL:HG11	2:J:108:LEU:HD12	2.00	0.44
1:C:194:VAL:HG13	1:C:197:PRO:HB3	2.00	0.44
2:L:49:SER:O	2:L:99:ASN:ND2	2.47	0.44
1:F:156:LYS:HZ2	1:F:266:ASP:HA	1.83	0.43
2:K:53:ASP:N	2:K:53:ASP:OD1	2.42	0.43
1:B:188:ILE:HG13	1:B:189:PHE:CD1	2.54	0.43
1:E:69:MET:HE2	1:E:93:GLN:HB3	1.99	0.43
1:C:158:VAL:HB	1:C:180:LEU:HD21	2.00	0.43
2:H:62:ALA:HB3	2:H:65:LYS:HE3	2.01	0.43
1:E:157:ARG:NE	1:E:208:SER:O	2.42	0.43
1:A:188:ILE:HG13	1:A:189:PHE:CD1	2.53	0.43
1:B:188:ILE:HD13	1:B:209:PRO:HG3	2.01	0.43
1:D:215:THR:HA	1:D:216:GLY:HA2	1.84	0.43
2:L:62:ALA:HB3	2:L:65:LYS:HE3	1.99	0.43
1:F:194:VAL:HG13	1:F:197:PRO:HB3	2.01	0.43
1:B:194:VAL:HG13	1:B:197:PRO:HB3	2.01	0.43
3:B:301:GOL:O3	3:B:301:GOL:O1	2.32	0.42
1:B:36:LEU:HD21	1:B:115:ILE:HG23	2.01	0.42
1:C:192:SER:OG	1:C:197:PRO:HG3	2.20	0.42
1:A:174:SER:O	1:A:178:GLN:NE2	2.52	0.42
1:C:192:SER:O	1:C:194:VAL:N	2.52	0.42
1:D:188:ILE:HG13	1:D:189:PHE:CD1	2.55	0.42
1:D:156:LYS:NZ	1:D:265:VAL:O	2.46	0.42
1:F:201:ARG:NH1	1:F:228:TRP:H	2.16	0.42
1:A:98:ALA:C	1:A:100:LEU:H	2.23	0.42
2:I:57:GLY:HA2	2:I:72:CYS:HA	2.00	0.42
2:K:49:SER:O	2:K:99:ASN:ND2	2.50	0.42
1:A:202:GLU:O	1:A:206:ALA:N	2.52	0.42
1:C:163:GLY:HA2	2:G:53:ASP:OD2	2.20	0.42
2:I:62:ALA:HB3	2:I:65:LYS:HE3	2.01	0.42
1:A:73:ARG:HD2	1:A:73:ARG:HA	1.77	0.42
1:D:29:LEU:HD22	1:D:64:SER:HB2	2.02	0.42
1:E:156:LYS:HD2	1:E:262:LEU:HG	2.01	0.42
1:A:188:ILE:HD13	1:A:209:PRO:HG3	2.02	0.41
1:E:194:VAL:HG13	1:E:197:PRO:HB3	2.01	0.41
1:E:163:GLY:HA2	2:K:53:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:SER:HB3	1:B:85:TRP:CD1	2.55	0.41
1:E:161:GLN:OE1	1:E:212:ILE:HD11	2.21	0.41
1:B:215:THR:HA	1:B:216:GLY:HA2	1.83	0.41
1:C:188:ILE:HG13	1:C:189:PHE:CD1	2.55	0.41
1:A:112:ILE:HD12	1:A:143:TYR:CD1	2.54	0.41
1:B:228:TRP:CB	1:B:232:LEU:HG	2.51	0.41
2:H:113:THR:HG23	2:H:146:THR:HA	2.02	0.41
1:D:30:SER:HB3	1:D:85:TRP:CD1	2.55	0.41
1:F:188:ILE:HG13	1:F:189:PHE:CD1	2.56	0.41
1:B:71:LEU:H	1:B:71:LEU:HG	1.73	0.41
1:A:194:VAL:HG13	1:A:197:PRO:HB3	2.02	0.41
2:G:89:ARG:HH22	2:G:112:ASP:CG	2.24	0.41
1:C:112:ILE:HD12	1:C:143:TYR:HD1	1.86	0.41
2:G:57:GLY:HA2	2:G:72:CYS:HA	2.03	0.41
1:B:232:LEU:HD23	1:B:232:LEU:HA	1.84	0.41
1:B:213:VAL:HG22	1:B:237:ILE:HB	2.03	0.41
1:B:245:GLU:OE1	2:I:123:ARG:NH1	2.48	0.41
1:C:188:ILE:HD13	1:C:209:PRO:HG3	2.01	0.41
1:C:110:THR:O	1:C:178:GLN:NE2	2.54	0.40
1:C:215:THR:HA	1:C:216:GLY:HA2	1.84	0.40
2:L:34:VAL:HG12	2:L:35:GLN:O	2.20	0.40
1:A:217:GLY:HA2	1:A:218:PRO:HD3	1.93	0.40
1:D:194:VAL:HG13	1:D:197:PRO:HB3	2.03	0.40
1:E:159:PHE:CE2	1:E:161:GLN:HB2	2.55	0.40
1:E:215:THR:HA	1:E:216:GLY:HA2	1.84	0.40
2:G:36:PRO:HD2	2:G:149:SER:HB2	2.03	0.40
2:I:49:SER:O	2:I:99:ASN:ND2	2.53	0.40
2:I:53:ASP:N	2:I:53:ASP:OD1	2.41	0.40
2:K:54:TYR:O	2:K:94:ARG:NH2	2.53	0.40
1:A:74:ILE:O	1:A:79:PRO:HD3	2.22	0.40
1:A:93:GLN:HA	1:A:96:GLN:HE21	1.86	0.40

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	243/289 (84%)	228 (94%)	12 (5%)	3 (1%)	13	19
1	B	243/289 (84%)	228 (94%)	13 (5%)	2 (1%)	19	29
1	C	243/289 (84%)	229 (94%)	12 (5%)	2 (1%)	19	29
1	D	243/289 (84%)	230 (95%)	11 (4%)	2 (1%)	19	29
1	E	243/289 (84%)	230 (95%)	11 (4%)	2 (1%)	19	29
1	F	243/289 (84%)	228 (94%)	14 (6%)	1 (0%)	34	48
2	G	124/159 (78%)	120 (97%)	4 (3%)	0	100	100
2	H	124/159 (78%)	120 (97%)	4 (3%)	0	100	100
2	I	124/159 (78%)	120 (97%)	4 (3%)	0	100	100
2	J	124/159 (78%)	120 (97%)	4 (3%)	0	100	100
2	K	124/159 (78%)	120 (97%)	4 (3%)	0	100	100
2	L	124/159 (78%)	120 (97%)	4 (3%)	0	100	100
All	All	2202/2688 (82%)	2093 (95%)	97 (4%)	12 (0%)	29	43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	SER
1	A	193	ARG
1	B	193	ARG
1	C	193	ARG
1	E	193	ARG
1	F	193	ARG
1	A	88	GLY
1	D	193	ARG
1	E	88	GLY
1	C	88	GLY
1	B	88	GLY
1	D	88	GLY

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	205/235 (87%)	202 (98%)	3 (2%)	65	80
1	B	205/235 (87%)	202 (98%)	3 (2%)	65	80
1	C	205/235 (87%)	205 (100%)	0	100	100
1	D	205/235 (87%)	204 (100%)	1 (0%)	88	94
1	E	205/235 (87%)	204 (100%)	1 (0%)	88	94
1	F	205/235 (87%)	204 (100%)	1 (0%)	88	94
2	G	100/124 (81%)	100 (100%)	0	100	100
2	H	100/124 (81%)	100 (100%)	0	100	100
2	I	100/124 (81%)	99 (99%)	1 (1%)	76	86
2	J	100/124 (81%)	100 (100%)	0	100	100
2	K	100/124 (81%)	99 (99%)	1 (1%)	76	86
2	L	100/124 (81%)	100 (100%)	0	100	100
All	All	1830/2154 (85%)	1819 (99%)	11 (1%)	86	92

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	233	LYS
1	A	240	THR
1	B	71	LEU
1	B	145	GLN
1	B	182	VAL
1	D	240	THR
1	E	100	LEU
1	F	89	ASN
2	I	34	VAL
2	K	34	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	B	178	GLN
1	C	177	ASN

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Mol	Chain	Res	Type
1	C	178	GLN
1	D	137	GLN
1	F	198	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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	$\# Z > 2$
3	GOL	F	301	-	5,5,5	0.37	0	5,5,5	0.35	0
3	GOL	E	301	-	5,5,5	0.34	0	5,5,5	0.29	0
3	GOL	B	301	-	5,5,5	0.38	0	5,5,5	0.33	0
3	GOL	H	201	-	5,5,5	0.36	0	5,5,5	0.29	0
3	GOL	D	301	-	5,5,5	0.35	0	5,5,5	0.30	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
3	GOL	F	301	-	-	0/4/4/4	-
3	GOL	E	301	-	-	2/4/4/4	-
3	GOL	B	301	-	-	2/4/4/4	-
3	GOL	H	201	-	-	2/4/4/4	-
3	GOL	D	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	GOL	O1-C1-C2-O2
3	B	301	GOL	O1-C1-C2-C3
3	H	201	GOL	O1-C1-C2-O2
3	H	201	GOL	O1-C1-C2-C3
3	D	301	GOL	O1-C1-C2-C3
3	E	301	GOL	O1-C1-C2-C3
3	D	301	GOL	O1-C1-C2-O2
3	E	301	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	301	GOL	1	0
3	B	301	GOL	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 [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	245/289 (84%)	0.40	14 (5%) 23 20	55, 77, 118, 156	0
1	B	245/289 (84%)	0.61	31 (12%) 3 2	50, 83, 139, 185	0
1	C	245/289 (84%)	1.01	46 (18%) 1 1	65, 102, 168, 201	0
1	D	245/289 (84%)	0.26	10 (4%) 37 33	49, 74, 116, 166	0
1	E	245/289 (84%)	0.60	19 (7%) 13 10	56, 88, 136, 170	0
1	F	245/289 (84%)	1.15	51 (20%) 1 1	59, 101, 163, 212	0
2	G	126/159 (79%)	2.13	48 (38%) 0 0	94, 146, 180, 216	0
2	H	126/159 (79%)	0.84	18 (14%) 2 1	61, 95, 138, 159	0
2	I	126/159 (79%)	3.05	85 (67%) 0 0	78, 158, 221, 252	0
2	J	126/159 (79%)	0.53	6 (4%) 30 27	53, 86, 132, 165	0
2	K	126/159 (79%)	1.01	22 (17%) 1 1	69, 103, 148, 182	0
2	L	126/159 (79%)	1.52	35 (27%) 0 0	79, 114, 163, 186	0
All	All	2226/2688 (82%)	0.96	385 (17%) 1 1	49, 95, 167, 252	0

All (385) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	230	GLU	9.7
1	C	154	PRO	8.5
2	G	32	GLY	8.3
2	I	140	GLY	8.1
1	F	152	ASP	8.1
2	I	142	GLY	7.9
2	I	110	PRO	7.8
2	I	146	THR	7.7
2	G	48	GLU	7.6
2	I	87	LYS	7.6
2	G	33	LEU	7.4

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Mol	Chain	Res	Type	RSRZ
1	E	193	ARG	7.2
2	G	78	ASP	7.1
2	I	65	LYS	7.1
1	F	233	LYS	6.9
2	I	98	LYS	6.6
2	L	63	PRO	6.6
1	C	151	ALA	6.6
2	I	144	PRO	6.6
2	L	148	SER	6.5
2	I	31	GLY	6.5
2	I	116	TYR	6.4
1	C	230	GLU	6.2
1	F	193	ARG	6.2
1	D	152	ASP	6.2
2	I	143	THR	6.0
2	I	29	SER	6.0
1	F	231	GLN	6.0
1	F	191	ASP	5.9
1	B	152	ASP	5.9
2	I	117	TYR	5.9
2	I	39	SER	5.9
2	K	149	SER	5.8
2	G	29	SER	5.7
2	I	149	SER	5.6
1	C	193	ARG	5.5
1	B	23	ALA	5.5
2	G	97	ALA	5.5
2	I	35	GLN	5.5
2	G	144	PRO	5.5
2	I	113	THR	5.5
2	G	147	VAL	5.4
2	I	25	GLN	5.3
2	I	147	VAL	5.3
2	G	110	PRO	5.3
2	I	84	ASP	5.3
2	I	64	GLY	5.3
2	J	148	SER	5.2
1	A	153	LYS	5.2
1	F	208	SER	5.2
2	I	148	SER	5.2
2	G	95	ASP	5.2
1	B	154	PRO	5.1

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Mol	Chain	Res	Type	RSRZ
2	G	148	SER	5.1
1	B	193	ARG	5.1
2	I	48	GLU	5.1
2	L	141	GLN	5.1
2	H	33	LEU	5.0
1	F	266	ASP	5.0
1	F	22	ALA	5.0
2	K	148	SER	4.9
2	L	48	GLU	4.9
2	I	34	VAL	4.9
1	C	152	ASP	4.9
1	F	154	PRO	4.9
1	C	191	ASP	4.8
2	I	30	GLY	4.8
2	I	119	ALA	4.8
2	G	98	LYS	4.8
2	I	85	SER	4.7
2	I	41	ARG	4.7
1	C	194	VAL	4.7
2	I	108	LEU	4.7
1	C	229	GLY	4.7
2	H	48	GLU	4.6
2	I	63	PRO	4.6
1	F	202	GLU	4.6
2	G	84	ASP	4.6
2	K	63	PRO	4.6
2	G	146	THR	4.6
1	B	191	ASP	4.6
2	I	105	MET	4.5
2	G	34	VAL	4.5
1	B	222	PRO	4.5
1	C	232	LEU	4.5
2	I	90	PHE	4.4
2	L	65	LYS	4.4
2	I	71	SER	4.4
2	H	149	SER	4.4
2	I	57	GLY	4.4
1	C	155	LYS	4.4
2	K	83	ALA	4.3
2	G	58	TRP	4.3
2	I	33	LEU	4.3
2	G	149	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	235	PRO	4.3
2	G	47	PRO	4.3
2	G	102	TYR	4.3
2	I	114	ALA	4.3
2	G	31	GLY	4.2
1	A	152	ASP	4.2
1	F	264	GLN	4.2
1	C	233	LYS	4.2
2	G	118	CYS	4.2
1	F	149	GLN	4.2
1	F	228	TRP	4.2
1	B	151	ALA	4.2
1	C	22	ALA	4.2
2	I	40	LEU	4.1
2	G	87	LYS	4.1
2	I	76	SER	4.1
2	I	109	ARG	4.1
2	J	149	SER	4.1
2	I	62	ALA	4.1
2	L	76	SER	4.1
2	I	120	ALA	4.1
1	F	222	PRO	4.0
2	I	60	ARG	4.0
1	C	206	ALA	3.9
1	B	232	LEU	3.9
2	L	58	TRP	3.9
1	E	266	ASP	3.9
1	F	167	PRO	3.9
2	I	118	CYS	3.8
2	K	66	GLU	3.8
1	F	229	GLY	3.8
2	G	141	GLN	3.8
2	G	116	TYR	3.8
2	I	88	GLY	3.8
1	F	130	ASP	3.8
2	L	118	CYS	3.8
1	B	22	ALA	3.8
2	I	112	ASP	3.7
2	I	106	ASN	3.7
2	I	49	SER	3.7
2	K	36	PRO	3.7
2	I	66	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	28	THR	3.7
1	C	231	GLN	3.7
2	I	47	PRO	3.7
2	I	107	ASP	3.6
2	I	42	LEU	3.6
2	I	141	GLN	3.6
2	I	59	PHE	3.6
2	K	62	ALA	3.6
2	L	149	SER	3.5
2	I	28	GLU	3.5
1	F	50	TYR	3.5
2	I	37	GLY	3.5
2	G	107	ASP	3.5
2	I	56	ILE	3.5
1	B	230	GLU	3.5
2	G	82	TYR	3.4
2	K	107	ASP	3.4
2	H	31	GLY	3.4
2	I	43	SER	3.4
2	K	118	CYS	3.4
2	K	31	GLY	3.4
2	I	58	TRP	3.4
1	B	153	LYS	3.4
1	A	154	PRO	3.4
2	I	26	LEU	3.4
1	F	212	ILE	3.3
2	H	65	LYS	3.3
1	F	151	ALA	3.3
2	H	97	ALA	3.3
1	F	89	ASN	3.3
2	G	57	GLY	3.3
2	L	97	ALA	3.3
2	I	27	VAL	3.3
1	F	159	PHE	3.2
1	F	148	ALA	3.2
2	I	104	GLN	3.2
1	C	200	SER	3.2
2	L	64	GLY	3.2
2	L	62	ALA	3.2
1	E	208	SER	3.2
2	L	133	SER	3.2
1	C	226	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	L	66	GLU	3.2
2	H	64	GLY	3.2
1	E	151	ALA	3.2
1	A	22	ALA	3.2
2	J	33	LEU	3.2
2	G	117	TYR	3.2
2	I	111	GLU	3.2
1	F	225	LYS	3.2
1	F	234	ILE	3.2
2	I	78	ASP	3.1
1	E	226	GLN	3.1
1	E	152	ASP	3.1
2	K	58	TRP	3.1
1	F	220	GLN	3.1
1	B	89	ASN	3.1
2	L	98	LYS	3.1
1	B	228	TRP	3.1
2	I	38	GLY	3.0
1	C	266	ASP	3.0
2	G	142	GLY	3.0
1	E	231	GLN	3.0
1	E	22	ALA	3.0
2	G	56	ILE	3.0
1	F	217	GLY	3.0
1	F	188	ILE	2.9
2	L	78	ASP	2.9
2	I	68	GLU	2.9
2	H	62	ALA	2.9
2	I	79	SER	2.9
1	E	154	PRO	2.9
2	L	147	VAL	2.9
2	I	97	ALA	2.9
1	C	89	ASN	2.9
2	H	84	ASP	2.9
2	H	66	GLU	2.9
1	B	266	ASP	2.9
1	C	128	GLN	2.9
1	E	153	LYS	2.9
1	E	191	ASP	2.9
1	F	127	PRO	2.9
1	C	225	LYS	2.9
2	G	27	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	I	36	PRO	2.9
1	B	229	GLY	2.9
1	C	192	SER	2.9
1	F	156	LYS	2.9
2	L	87	LYS	2.9
2	L	84	ASP	2.9
2	L	57	GLY	2.8
1	B	227	TYR	2.8
2	K	57	GLY	2.8
1	B	231	GLN	2.8
2	I	100	THR	2.8
2	K	84	ASP	2.8
1	C	261	ALA	2.8
1	E	228	TRP	2.8
1	C	159	PHE	2.8
2	L	51	LEU	2.8
2	L	135	GLY	2.8
1	C	236	VAL	2.8
1	F	206	ALA	2.8
2	G	119	ALA	2.8
2	J	118	CYS	2.8
1	C	218	PRO	2.8
2	K	33	LEU	2.7
1	E	89	ASN	2.7
1	C	228	TRP	2.7
1	C	52	ASP	2.7
2	G	105	MET	2.7
2	H	57	GLY	2.7
1	D	233	LYS	2.7
1	F	194	VAL	2.6
1	B	233	LYS	2.6
1	C	142	GLN	2.6
1	D	27	ILE	2.6
1	F	224	ILE	2.6
2	G	99	ASN	2.6
2	G	76	SER	2.6
1	D	83	ILE	2.6
1	C	201	ARG	2.6
2	G	67	ARG	2.6
2	L	109	ARG	2.6
1	D	153	LYS	2.6
1	C	222	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	102	TYR	2.6
2	I	45	ALA	2.6
1	C	223	LYS	2.6
2	G	30	GLY	2.6
1	C	173	GLU	2.5
1	F	265	VAL	2.5
2	H	87	LYS	2.5
1	F	145	GLN	2.5
2	L	54	TYR	2.5
2	H	141	GLN	2.5
2	L	25	GLN	2.5
1	F	187	ASN	2.5
2	L	99	ASN	2.5
2	L	119	ALA	2.5
1	D	180	LEU	2.5
1	E	59	LYS	2.5
2	L	56	ILE	2.5
2	L	85	SER	2.5
1	C	23	ALA	2.5
1	A	128	GLN	2.5
1	B	28	THR	2.5
1	B	205	LEU	2.5
2	I	103	LEU	2.5
2	G	41	ARG	2.5
2	I	67	ARG	2.4
1	B	67	GLN	2.4
2	I	61	GLN	2.4
1	B	160	LEU	2.4
1	C	83	ILE	2.4
1	F	232	LEU	2.4
1	C	160	LEU	2.4
1	B	88	GLY	2.4
2	G	54	TYR	2.4
1	A	222	PRO	2.4
1	D	154	PRO	2.4
1	A	233	LYS	2.4
2	I	70	VAL	2.4
1	C	88	GLY	2.4
2	I	83	ALA	2.4
1	E	130	ASP	2.4
2	H	78	ASP	2.4
2	I	99	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	189	PHE	2.4
2	I	77	GLY	2.4
2	H	63	PRO	2.3
2	I	136	TYR	2.3
2	G	51	LEU	2.3
2	K	64	GLY	2.3
2	G	59	PHE	2.3
1	E	96	GLN	2.3
1	B	226	GLN	2.3
1	F	128	GLN	2.3
1	F	46	GLY	2.3
2	H	148	SER	2.3
2	I	115	VAL	2.3
1	F	88	GLY	2.3
2	I	69	GLY	2.3
2	J	141	GLN	2.3
1	C	158	VAL	2.3
2	K	147	VAL	2.3
1	D	208	SER	2.3
1	F	201	ARG	2.3
1	C	172	LYS	2.3
1	C	210	GLN	2.2
2	K	116	TYR	2.2
2	H	118	CYS	2.2
1	A	27	ILE	2.2
1	A	226	GLN	2.2
1	A	208	SER	2.2
2	L	103	LEU	2.2
2	H	119	ALA	2.2
2	G	79	SER	2.2
1	C	195	PRO	2.2
1	E	101	GLY	2.2
2	I	145	VAL	2.2
1	C	202	GLU	2.2
2	L	27	VAL	2.2
2	G	35	GLN	2.2
1	B	46	GLY	2.2
1	A	230	GLU	2.2
2	L	36	PRO	2.2
1	D	191	ASP	2.2
1	F	192	SER	2.1
1	B	72	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	36	PRO	2.1
2	K	103	LEU	2.1
2	K	142	GLY	2.1
1	A	29	LEU	2.1
1	B	219	ASP	2.1
1	E	71	LEU	2.1
1	B	201	ARG	2.1
2	L	94	ARG	2.1
1	C	219	ASP	2.1
2	K	87	LYS	2.1
1	B	202	GLU	2.1
2	G	113	THR	2.1
2	I	89	ARG	2.1
1	F	199	VAL	2.1
2	L	33	LEU	2.1
2	G	46	ALA	2.1
2	J	70	VAL	2.1
1	F	227	TYR	2.1
2	L	120	ALA	2.1
1	C	185	GLY	2.1
1	F	173	GLU	2.1
1	C	164	ILE	2.1
2	K	117	TYR	2.1
2	G	94	ARG	2.1
1	B	65	THR	2.1
1	A	191	ASP	2.1
2	K	133	SER	2.1
1	B	59	LYS	2.0
1	F	186	GLU	2.0
2	G	83	ALA	2.0
2	I	46	ALA	2.0
1	C	262	LEU	2.0
1	C	235	PRO	2.0
1	E	60	ILE	2.0
1	F	27	ILE	2.0
2	I	32	GLY	2.0
1	F	203	GLN	2.0
1	D	193	ARG	2.0

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 [i](#)

There are no carbohydrates 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(Å ²)	Q<0.9
3	GOL	F	301	6/6	0.60	0.30	124,126,129,130	0
3	GOL	E	301	6/6	0.81	0.27	73,76,82,85	0
3	GOL	B	301	6/6	0.84	0.28	93,100,103,108	0
3	GOL	H	201	6/6	0.87	0.21	70,77,82,92	0
3	GOL	D	301	6/6	0.96	0.16	66,68,70,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.