



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:14 PM UTC

PDB ID : 3VT2 / pdb_00003vt2
Title : Crystal structure of Ct1,3Gal43A in complex with isopropyl-beta-D-thiogalactoside
Authors : Jiang, D.; Fan, J.; Wang, X.; Zhao, Y.; Huang, B.; Zhang, X.C.
Deposited on : 2012-05-18
Resolution : 3.00 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

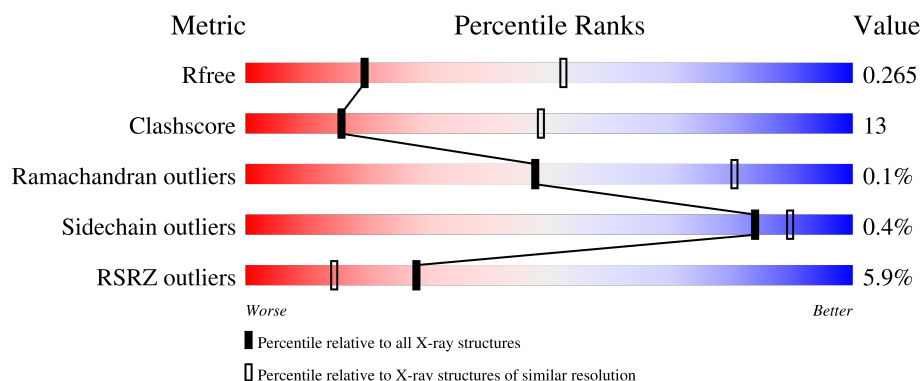
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 ≥ 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	526	3% 65% 23% 12%
1	B	526	3% 59% 28% 12%
1	C	526	2% 71% 21% 8%
1	D	526	18% 55% 32% 12%
1	E	526	0% 65% 23% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	526	4% 67% 20% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22274 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 Ricin B lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3664	2323	623	703	15			
1	B	461	Total	C	N	O	S	0	0	0
			3664	2323	623	703	15			
1	C	482	Total	C	N	O	S	0	0	0
			3807	2406	651	732	18			
1	D	461	Total	C	N	O	S	0	0	0
			3664	2323	623	703	15			
1	E	461	Total	C	N	O	S	0	0	0
			3664	2323	623	703	15			
1	F	461	Total	C	N	O	S	0	0	0
			3664	2323	623	703	15			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	expression tag	UNP A3DD67
A	-34	GLY	-	expression tag	UNP A3DD67
A	-33	SER	-	expression tag	UNP A3DD67
A	-32	SER	-	expression tag	UNP A3DD67
A	-31	HIS	-	expression tag	UNP A3DD67
A	-30	HIS	-	expression tag	UNP A3DD67
A	-29	HIS	-	expression tag	UNP A3DD67
A	-28	HIS	-	expression tag	UNP A3DD67
A	-27	HIS	-	expression tag	UNP A3DD67
A	-26	HIS	-	expression tag	UNP A3DD67
A	-25	SER	-	expression tag	UNP A3DD67
A	-24	SER	-	expression tag	UNP A3DD67
A	-23	GLY	-	expression tag	UNP A3DD67
A	-22	LEU	-	expression tag	UNP A3DD67
A	-21	VAL	-	expression tag	UNP A3DD67
A	-20	PRO	-	expression tag	UNP A3DD67
A	-19	ARG	-	expression tag	UNP A3DD67

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP A3DD67
A	-17	SER	-	expression tag	UNP A3DD67
A	-16	HIS	-	expression tag	UNP A3DD67
A	-15	MET	-	expression tag	UNP A3DD67
A	-14	ALA	-	expression tag	UNP A3DD67
A	-13	SER	-	expression tag	UNP A3DD67
A	-12	MET	-	expression tag	UNP A3DD67
A	-11	THR	-	expression tag	UNP A3DD67
A	-10	GLY	-	expression tag	UNP A3DD67
A	-9	GLY	-	expression tag	UNP A3DD67
A	-8	GLN	-	expression tag	UNP A3DD67
A	-7	GLN	-	expression tag	UNP A3DD67
A	-6	MET	-	expression tag	UNP A3DD67
A	-5	GLY	-	expression tag	UNP A3DD67
A	-4	ARG	-	expression tag	UNP A3DD67
A	-3	GLY	-	expression tag	UNP A3DD67
A	-2	SER	-	expression tag	UNP A3DD67
A	-1	GLU	-	expression tag	UNP A3DD67
A	0	PHE	-	expression tag	UNP A3DD67
B	-35	MET	-	expression tag	UNP A3DD67
B	-34	GLY	-	expression tag	UNP A3DD67
B	-33	SER	-	expression tag	UNP A3DD67
B	-32	SER	-	expression tag	UNP A3DD67
B	-31	HIS	-	expression tag	UNP A3DD67
B	-30	HIS	-	expression tag	UNP A3DD67
B	-29	HIS	-	expression tag	UNP A3DD67
B	-28	HIS	-	expression tag	UNP A3DD67
B	-27	HIS	-	expression tag	UNP A3DD67
B	-26	HIS	-	expression tag	UNP A3DD67
B	-25	SER	-	expression tag	UNP A3DD67
B	-24	SER	-	expression tag	UNP A3DD67
B	-23	GLY	-	expression tag	UNP A3DD67
B	-22	LEU	-	expression tag	UNP A3DD67
B	-21	VAL	-	expression tag	UNP A3DD67
B	-20	PRO	-	expression tag	UNP A3DD67
B	-19	ARG	-	expression tag	UNP A3DD67
B	-18	GLY	-	expression tag	UNP A3DD67
B	-17	SER	-	expression tag	UNP A3DD67
B	-16	HIS	-	expression tag	UNP A3DD67
B	-15	MET	-	expression tag	UNP A3DD67
B	-14	ALA	-	expression tag	UNP A3DD67
B	-13	SER	-	expression tag	UNP A3DD67

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	MET	-	expression tag	UNP A3DD67
B	-11	THR	-	expression tag	UNP A3DD67
B	-10	GLY	-	expression tag	UNP A3DD67
B	-9	GLY	-	expression tag	UNP A3DD67
B	-8	GLN	-	expression tag	UNP A3DD67
B	-7	GLN	-	expression tag	UNP A3DD67
B	-6	MET	-	expression tag	UNP A3DD67
B	-5	GLY	-	expression tag	UNP A3DD67
B	-4	ARG	-	expression tag	UNP A3DD67
B	-3	GLY	-	expression tag	UNP A3DD67
B	-2	SER	-	expression tag	UNP A3DD67
B	-1	GLU	-	expression tag	UNP A3DD67
B	0	PHE	-	expression tag	UNP A3DD67
C	-35	MET	-	expression tag	UNP A3DD67
C	-34	GLY	-	expression tag	UNP A3DD67
C	-33	SER	-	expression tag	UNP A3DD67
C	-32	SER	-	expression tag	UNP A3DD67
C	-31	HIS	-	expression tag	UNP A3DD67
C	-30	HIS	-	expression tag	UNP A3DD67
C	-29	HIS	-	expression tag	UNP A3DD67
C	-28	HIS	-	expression tag	UNP A3DD67
C	-27	HIS	-	expression tag	UNP A3DD67
C	-26	HIS	-	expression tag	UNP A3DD67
C	-25	SER	-	expression tag	UNP A3DD67
C	-24	SER	-	expression tag	UNP A3DD67
C	-23	GLY	-	expression tag	UNP A3DD67
C	-22	LEU	-	expression tag	UNP A3DD67
C	-21	VAL	-	expression tag	UNP A3DD67
C	-20	PRO	-	expression tag	UNP A3DD67
C	-19	ARG	-	expression tag	UNP A3DD67
C	-18	GLY	-	expression tag	UNP A3DD67
C	-17	SER	-	expression tag	UNP A3DD67
C	-16	HIS	-	expression tag	UNP A3DD67
C	-15	MET	-	expression tag	UNP A3DD67
C	-14	ALA	-	expression tag	UNP A3DD67
C	-13	SER	-	expression tag	UNP A3DD67
C	-12	MET	-	expression tag	UNP A3DD67
C	-11	THR	-	expression tag	UNP A3DD67
C	-10	GLY	-	expression tag	UNP A3DD67
C	-9	GLY	-	expression tag	UNP A3DD67
C	-8	GLN	-	expression tag	UNP A3DD67
C	-7	GLN	-	expression tag	UNP A3DD67

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MET	-	expression tag	UNP A3DD67
C	-5	GLY	-	expression tag	UNP A3DD67
C	-4	ARG	-	expression tag	UNP A3DD67
C	-3	GLY	-	expression tag	UNP A3DD67
C	-2	SER	-	expression tag	UNP A3DD67
C	-1	GLU	-	expression tag	UNP A3DD67
C	0	PHE	-	expression tag	UNP A3DD67
D	-35	MET	-	expression tag	UNP A3DD67
D	-34	GLY	-	expression tag	UNP A3DD67
D	-33	SER	-	expression tag	UNP A3DD67
D	-32	SER	-	expression tag	UNP A3DD67
D	-31	HIS	-	expression tag	UNP A3DD67
D	-30	HIS	-	expression tag	UNP A3DD67
D	-29	HIS	-	expression tag	UNP A3DD67
D	-28	HIS	-	expression tag	UNP A3DD67
D	-27	HIS	-	expression tag	UNP A3DD67
D	-26	HIS	-	expression tag	UNP A3DD67
D	-25	SER	-	expression tag	UNP A3DD67
D	-24	SER	-	expression tag	UNP A3DD67
D	-23	GLY	-	expression tag	UNP A3DD67
D	-22	LEU	-	expression tag	UNP A3DD67
D	-21	VAL	-	expression tag	UNP A3DD67
D	-20	PRO	-	expression tag	UNP A3DD67
D	-19	ARG	-	expression tag	UNP A3DD67
D	-18	GLY	-	expression tag	UNP A3DD67
D	-17	SER	-	expression tag	UNP A3DD67
D	-16	HIS	-	expression tag	UNP A3DD67
D	-15	MET	-	expression tag	UNP A3DD67
D	-14	ALA	-	expression tag	UNP A3DD67
D	-13	SER	-	expression tag	UNP A3DD67
D	-12	MET	-	expression tag	UNP A3DD67
D	-11	THR	-	expression tag	UNP A3DD67
D	-10	GLY	-	expression tag	UNP A3DD67
D	-9	GLY	-	expression tag	UNP A3DD67
D	-8	GLN	-	expression tag	UNP A3DD67
D	-7	GLN	-	expression tag	UNP A3DD67
D	-6	MET	-	expression tag	UNP A3DD67
D	-5	GLY	-	expression tag	UNP A3DD67
D	-4	ARG	-	expression tag	UNP A3DD67
D	-3	GLY	-	expression tag	UNP A3DD67
D	-2	SER	-	expression tag	UNP A3DD67
D	-1	GLU	-	expression tag	UNP A3DD67

Continued on next page...

Continued from previous page...

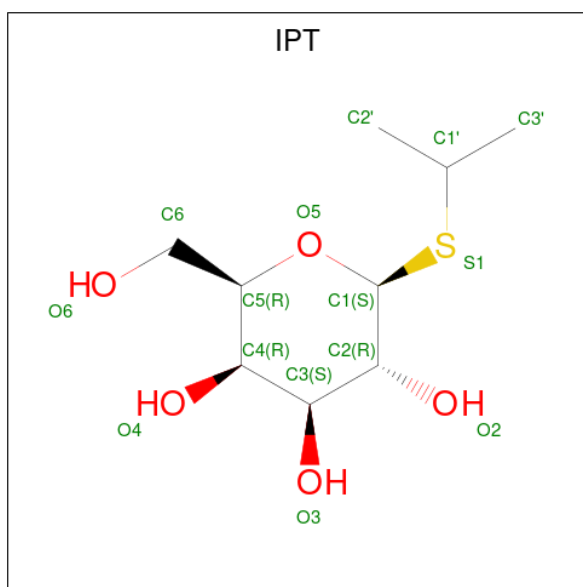
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PHE	-	expression tag	UNP A3DD67
E	-35	MET	-	expression tag	UNP A3DD67
E	-34	GLY	-	expression tag	UNP A3DD67
E	-33	SER	-	expression tag	UNP A3DD67
E	-32	SER	-	expression tag	UNP A3DD67
E	-31	HIS	-	expression tag	UNP A3DD67
E	-30	HIS	-	expression tag	UNP A3DD67
E	-29	HIS	-	expression tag	UNP A3DD67
E	-28	HIS	-	expression tag	UNP A3DD67
E	-27	HIS	-	expression tag	UNP A3DD67
E	-26	HIS	-	expression tag	UNP A3DD67
E	-25	SER	-	expression tag	UNP A3DD67
E	-24	SER	-	expression tag	UNP A3DD67
E	-23	GLY	-	expression tag	UNP A3DD67
E	-22	LEU	-	expression tag	UNP A3DD67
E	-21	VAL	-	expression tag	UNP A3DD67
E	-20	PRO	-	expression tag	UNP A3DD67
E	-19	ARG	-	expression tag	UNP A3DD67
E	-18	GLY	-	expression tag	UNP A3DD67
E	-17	SER	-	expression tag	UNP A3DD67
E	-16	HIS	-	expression tag	UNP A3DD67
E	-15	MET	-	expression tag	UNP A3DD67
E	-14	ALA	-	expression tag	UNP A3DD67
E	-13	SER	-	expression tag	UNP A3DD67
E	-12	MET	-	expression tag	UNP A3DD67
E	-11	THR	-	expression tag	UNP A3DD67
E	-10	GLY	-	expression tag	UNP A3DD67
E	-9	GLY	-	expression tag	UNP A3DD67
E	-8	GLN	-	expression tag	UNP A3DD67
E	-7	GLN	-	expression tag	UNP A3DD67
E	-6	MET	-	expression tag	UNP A3DD67
E	-5	GLY	-	expression tag	UNP A3DD67
E	-4	ARG	-	expression tag	UNP A3DD67
E	-3	GLY	-	expression tag	UNP A3DD67
E	-2	SER	-	expression tag	UNP A3DD67
E	-1	GLU	-	expression tag	UNP A3DD67
E	0	PHE	-	expression tag	UNP A3DD67
F	-35	MET	-	expression tag	UNP A3DD67
F	-34	GLY	-	expression tag	UNP A3DD67
F	-33	SER	-	expression tag	UNP A3DD67
F	-32	SER	-	expression tag	UNP A3DD67
F	-31	HIS	-	expression tag	UNP A3DD67

Continued on next page...

Continued from previous page...

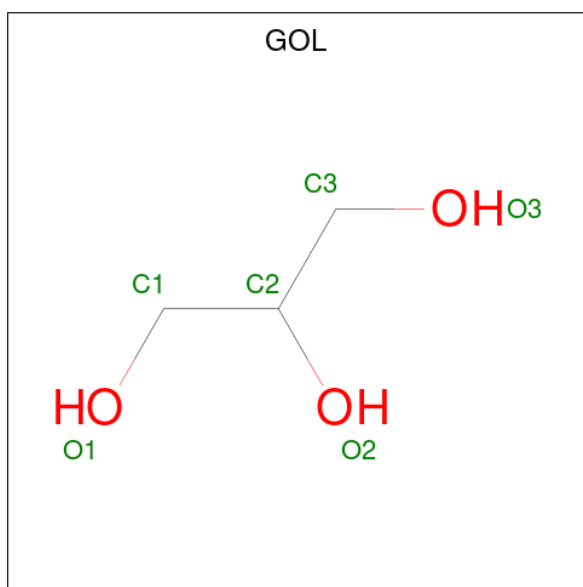
Chain	Residue	Modelled	Actual	Comment	Reference
F	-30	HIS	-	expression tag	UNP A3DD67
F	-29	HIS	-	expression tag	UNP A3DD67
F	-28	HIS	-	expression tag	UNP A3DD67
F	-27	HIS	-	expression tag	UNP A3DD67
F	-26	HIS	-	expression tag	UNP A3DD67
F	-25	SER	-	expression tag	UNP A3DD67
F	-24	SER	-	expression tag	UNP A3DD67
F	-23	GLY	-	expression tag	UNP A3DD67
F	-22	LEU	-	expression tag	UNP A3DD67
F	-21	VAL	-	expression tag	UNP A3DD67
F	-20	PRO	-	expression tag	UNP A3DD67
F	-19	ARG	-	expression tag	UNP A3DD67
F	-18	GLY	-	expression tag	UNP A3DD67
F	-17	SER	-	expression tag	UNP A3DD67
F	-16	HIS	-	expression tag	UNP A3DD67
F	-15	MET	-	expression tag	UNP A3DD67
F	-14	ALA	-	expression tag	UNP A3DD67
F	-13	SER	-	expression tag	UNP A3DD67
F	-12	MET	-	expression tag	UNP A3DD67
F	-11	THR	-	expression tag	UNP A3DD67
F	-10	GLY	-	expression tag	UNP A3DD67
F	-9	GLY	-	expression tag	UNP A3DD67
F	-8	GLN	-	expression tag	UNP A3DD67
F	-7	GLN	-	expression tag	UNP A3DD67
F	-6	MET	-	expression tag	UNP A3DD67
F	-5	GLY	-	expression tag	UNP A3DD67
F	-4	ARG	-	expression tag	UNP A3DD67
F	-3	GLY	-	expression tag	UNP A3DD67
F	-2	SER	-	expression tag	UNP A3DD67
F	-1	GLU	-	expression tag	UNP A3DD67
F	0	PHE	-	expression tag	UNP A3DD67

- Molecule 2 is 1-methylethyl 1-thio-beta-D-galactopyranoside (CCD ID: IPT) (formula: $C_9H_{18}O_5S$).

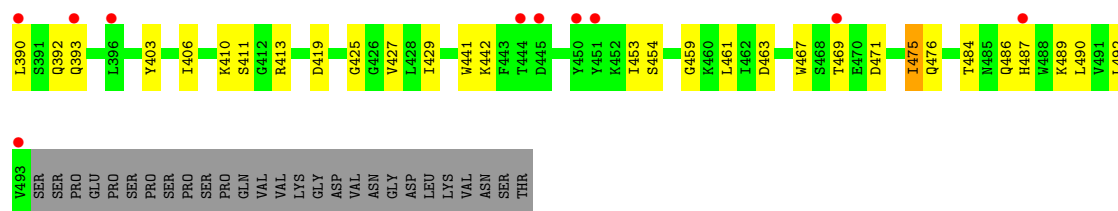


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			15	9	5	1		
2	B	1	Total	C	O	S	0	0
			15	9	5	1		
2	C	1	Total	C	O	S	0	0
			15	9	5	1		
2	D	1	Total	C	O	S	0	0
			15	9	5	1		
2	E	1	Total	C	O	S	0	0
			15	9	5	1		
2	F	1	Total	C	O	S	0	0
			15	9	5	1		
2	F	1	Total	C	O	S	0	0
			15	9	5	1		

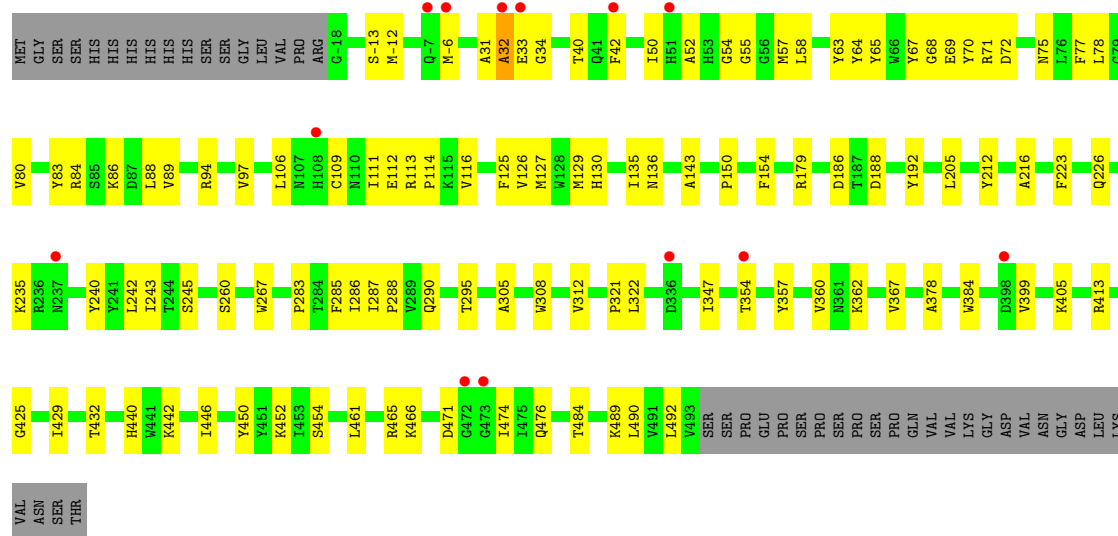
- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



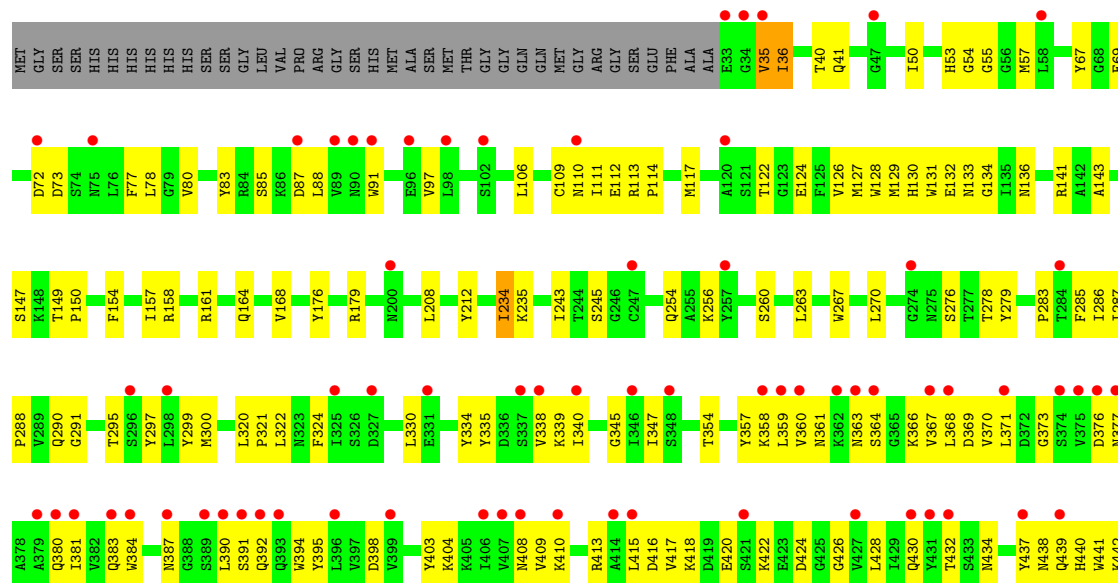
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

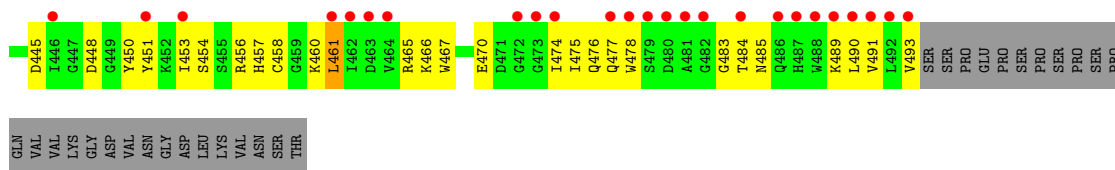


● Molecule 1: Ricin B lectin

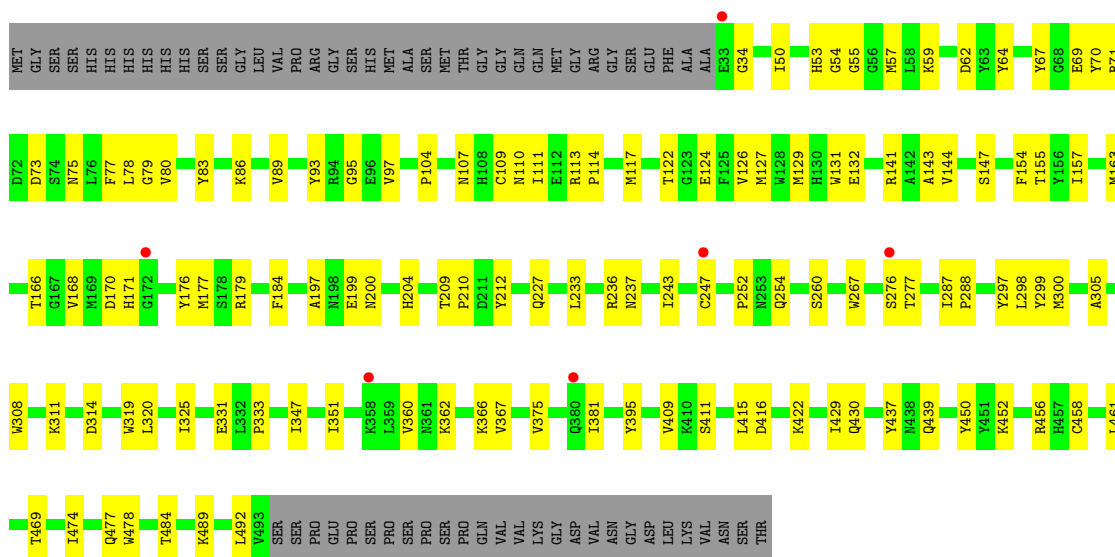


● Molecule 1: Ricin B lectin

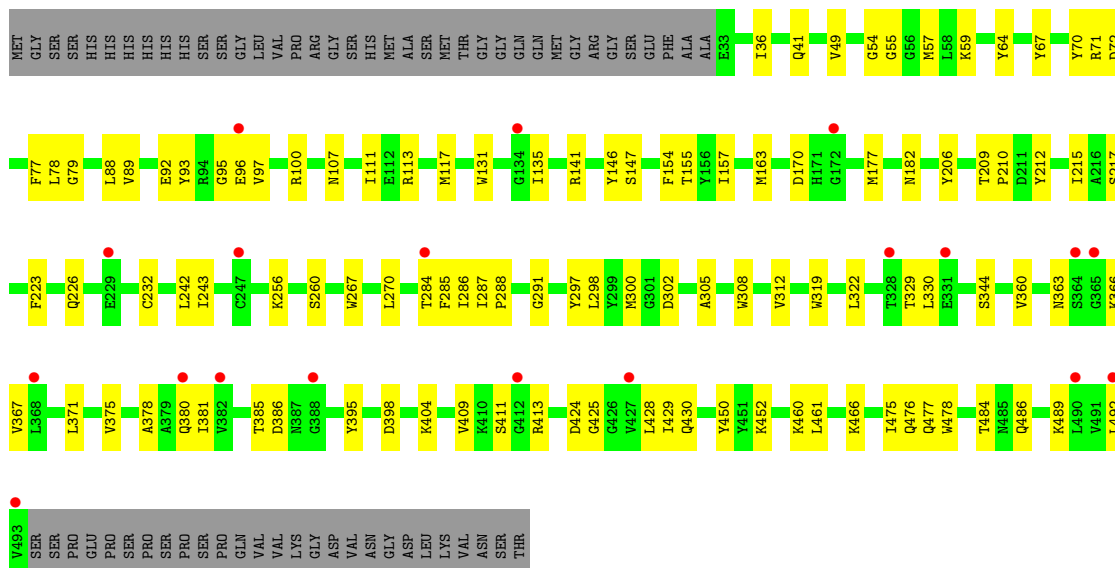




- Molecule 1: Ricin B lectin



- Molecule 1: Ricin B lectin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.23Å 121.97Å 405.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.71 – 3.00 44.71 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.0 (44.71-3.00) 83.0 (44.71-3.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.245 , 0.271 0.239 , 0.265	Depositor DCC
R_{free} test set	1586 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22274	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, IPT

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	0.23	0/3762	0.65	0/5104
1	B	0.23	0/3762	0.63	0/5104
1	C	0.23	0/3907	0.64	0/5295
1	D	0.23	0/3762	0.64	0/5104
1	E	0.23	0/3762	0.65	0/5104
1	F	0.23	0/3762	0.65	0/5104
All	All	0.23	0/22717	0.64	0/30815

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	3664	0	3480	96	0
1	B	3664	0	3480	109	0
1	C	3807	0	3613	85	0
1	D	3664	0	3480	147	0
1	E	3664	0	3480	76	0
1	F	3664	0	3480	73	0
2	A	15	0	18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	18	2	0
2	C	15	0	18	0	0
2	D	15	0	18	2	0
2	E	15	0	18	0	0
2	F	30	0	36	0	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
3	C	12	0	16	1	0
3	E	12	0	16	1	0
3	F	6	0	8	1	0
All	All	22274	0	21195	577	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 13.

All (577) 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:416:ASP:HB3	1:E:439:GLN:HG2	1.54	0.89
1:E:57:MET:HE2	1:E:287:ILE:HG21	1.55	0.89
1:D:35:VAL:HG22	1:D:36:ILE:H	1.38	0.88
1:A:360:VAL:HG12	1:A:367:VAL:HG12	1.55	0.87
1:B:360:VAL:HG12	1:B:367:VAL:HG12	1.56	0.86
1:D:370:VAL:HG12	1:D:430:GLN:HE22	1.43	0.83
1:F:360:VAL:HG22	1:F:367:VAL:HG12	1.60	0.83
1:D:335:TYR:HB2	1:D:338:VAL:HG22	1.61	0.83
1:C:57:MET:HE2	1:C:287:ILE:HG21	1.59	0.82
1:C:-12:MET:HG3	1:E:155:THR:HG22	1.63	0.81
1:B:360:VAL:HG22	1:B:489:LYS:HB3	1.63	0.81
1:D:387:ASN:H	1:D:392:GLN:HE22	1.29	0.81
1:D:72:ASP:HB3	1:D:78:LEU:HD22	1.63	0.81
1:F:57:MET:HE2	1:F:287:ILE:HG21	1.63	0.78
1:B:72:ASP:HB3	1:B:78:LEU:HG	1.66	0.78
1:D:57:MET:HE2	1:D:287:ILE:HG21	1.66	0.78
1:B:390:LEU:O	1:B:410:LYS:HB2	1.85	0.77
1:D:35:VAL:HB	1:D:339:LYS:HA	1.65	0.77
1:C:216:ALA:HA	1:D:164:GLN:HE22	1.48	0.75
1:C:360:VAL:HG22	1:C:367:VAL:HG12	1.67	0.75
1:E:422:LYS:HD2	1:E:458:CYS:HB3	1.67	0.75
1:D:451:TYR:HE2	1:D:490:LEU:HB2	1.53	0.74
1:F:461:LEU:HD11	1:F:486:GLN:HB3	1.68	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:VAL:C	1:A:413:ARG:HH22	1.96	0.73
1:B:146:TYR:CD2	1:B:157:ILE:HD11	2.24	0.72
1:B:53:HIS:HD2	1:B:315:SER:HB2	1.53	0.72
1:A:228:ARG:HH12	1:A:256:LYS:HD2	1.54	0.72
1:C:80:VAL:HG21	1:C:127:MET:HE1	1.72	0.71
1:F:371:LEU:HD12	1:F:380:GLN:HB3	1.72	0.71
1:D:398:ASP:HA	1:D:404:LYS:HA	1.73	0.70
1:A:381:ILE:HG22	1:A:475:ILE:HB	1.74	0.70
1:D:371:LEU:HD22	1:D:380:GLN:HB2	1.74	0.70
1:D:322:LEU:HD21	1:D:330:LEU:HD23	1.74	0.70
1:A:228:ARG:HH21	1:A:246:GLY:H	1.38	0.69
1:C:34:GLY:HA2	1:C:89:VAL:HG21	1.73	0.69
1:D:418:LYS:HA	2:D:601:IPT:H61	1.73	0.69
1:C:72:ASP:HB3	1:C:78:LEU:HD22	1.74	0.69
1:E:360:VAL:HG22	1:E:367:VAL:HG12	1.75	0.68
1:D:451:TYR:CE2	1:D:490:LEU:HB2	2.27	0.68
1:A:260:SER:HB2	1:A:267:TRP:HA	1.76	0.68
1:A:284:THR:HG21	1:A:302:ASP:OD2	1.94	0.67
1:D:416:ASP:OD1	1:D:439:GLN:HG3	1.94	0.67
1:B:137:TYR:HB3	1:B:179:ARG:HH21	1.59	0.67
1:A:331:GLU:HG2	1:A:333:PRO:HD3	1.75	0.67
1:D:403:TYR:HB3	1:D:440:HIS:HB3	1.75	0.67
1:E:54:GLY:O	1:E:113:ARG:HA	1.95	0.67
1:B:161:ARG:O	1:B:164:GLN:HG3	1.95	0.66
1:C:442:LYS:HG3	1:F:100:ARG:NH2	2.10	0.66
1:B:59:LYS:HZ1	1:B:61:GLY:C	2.02	0.66
1:A:229:GLU:HG2	1:A:246:GLY:O	1.96	0.66
1:B:364:SER:HA	1:B:469:THR:HG23	1.77	0.66
1:F:182:ASN:HD22	1:F:232:CYS:HA	1.61	0.66
1:D:117:MET:HE3	1:D:212:TYR:HB3	1.76	0.65
1:C:442:LYS:HG3	1:F:100:ARG:HH22	1.62	0.65
1:D:69:GLU:OE1	1:D:112:GLU:HA	1.96	0.65
1:D:53:HIS:O	1:D:69:GLU:HG2	1.97	0.65
1:A:413:ARG:HH21	1:A:430:GLN:NE2	1.95	0.64
1:B:378:ALA:HA	1:B:429:ILE:HD12	1.78	0.64
1:D:72:ASP:CG	1:D:73:ASP:H	2.05	0.64
1:E:416:ASP:CB	1:E:439:GLN:HG2	2.27	0.64
1:D:453:ILE:O	1:D:461:LEU:HD22	1.97	0.64
1:A:245:SER:HB3	1:A:283:PRO:HD2	1.78	0.64
1:B:137:TYR:HB3	1:B:179:ARG:NH2	2.13	0.64
1:E:53:HIS:O	1:E:69:GLU:HG2	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:VAL:HG13	1:E:157:ILE:HB	1.78	0.64
1:C:260:SER:HB2	1:C:267:TRP:HA	1.79	0.64
1:B:461:LEU:HD11	1:B:486:GLN:HB3	1.78	0.63
1:A:72:ASP:HB3	1:A:78:LEU:HD12	1.80	0.63
1:A:285:PHE:HB3	1:A:300:MET:HE3	1.80	0.63
1:B:285:PHE:HB3	1:B:300:MET:HE3	1.80	0.63
1:C:65:TYR:CE2	1:C:84:ARG:HD3	2.33	0.63
1:B:340:ILE:HG22	1:B:347:ILE:HG23	1.80	0.62
1:C:413:ARG:NH1	1:C:432:THR:HG22	2.13	0.62
1:E:77:PHE:CD2	1:E:111:ILE:HB	2.33	0.62
1:B:122:THR:HG23	1:B:124:GLU:H	1.65	0.62
1:D:358:LYS:HE3	1:D:493:VAL:HG21	1.81	0.62
1:D:460:LYS:C	1:D:461:LEU:HD23	2.24	0.62
1:D:370:VAL:HG12	1:D:430:GLN:NE2	2.13	0.62
1:D:359:LEU:HD21	1:D:490:LEU:HD12	1.82	0.61
1:C:413:ARG:HH12	1:C:432:THR:HG22	1.64	0.61
1:F:113:ARG:HH12	1:F:284:THR:HG22	1.65	0.61
1:B:368:LEU:HD12	1:B:475:ILE:HD12	1.82	0.61
1:D:465:ARG:HD3	1:D:474:ILE:HB	1.81	0.61
1:B:97:VAL:HB	1:B:154:PHE:CD2	2.35	0.61
1:B:223:PHE:HE2	1:B:242:LEU:HD23	1.63	0.61
1:D:381:ILE:HD11	1:D:430:GLN:CD	2.26	0.61
1:F:97:VAL:HB	1:F:154:PHE:CD2	2.36	0.61
1:D:424:ASP:OD2	1:D:478:TRP:HA	2.01	0.61
1:B:157:ILE:HG22	1:B:158:ARG:HG2	1.82	0.60
1:C:465:ARG:HH21	1:C:474:ILE:HG21	1.66	0.60
1:D:321:PRO:HD3	1:D:338:VAL:HG11	1.82	0.60
1:D:245:SER:HB3	1:D:283:PRO:HD2	1.82	0.60
1:F:450:TYR:CE1	1:F:489:LYS:HB2	2.37	0.60
1:D:35:VAL:HG21	1:D:338:VAL:O	2.02	0.60
1:D:395:TYR:CE2	1:D:409:VAL:HG22	2.36	0.60
1:D:387:ASN:H	1:D:392:GLN:NE2	1.98	0.60
1:D:370:VAL:HG22	1:D:391:SER:HB3	1.83	0.60
1:A:360:VAL:HG22	1:A:489:LYS:HB3	1.84	0.59
1:B:53:HIS:CD2	1:B:315:SER:HB2	2.36	0.59
1:D:35:VAL:HG22	1:D:36:ILE:N	2.14	0.59
1:B:406:ILE:HD13	1:B:441:TRP:CD1	2.39	0.58
1:A:84:ARG:HD3	1:A:94:ARG:HH11	1.66	0.58
1:D:426:GLY:O	1:D:476:GLN:HB2	2.03	0.58
1:F:286:ILE:HD13	1:F:322:LEU:HD22	1.83	0.58
1:A:130:HIS:CD2	1:A:179:ARG:HA	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ALA:O	1:C:33:GLU:HG3	2.01	0.58
1:F:260:SER:HB2	1:F:267:TRP:HA	1.86	0.58
1:B:403:TYR:CE1	1:B:442:LYS:HE2	2.38	0.58
1:D:130:HIS:CD2	1:D:179:ARG:HA	2.38	0.58
1:F:375:VAL:HG12	1:F:411:SER:HB3	1.85	0.58
1:B:171:HIS:CE1	1:B:199:GLU:HB2	2.39	0.58
1:F:284:THR:HG21	1:F:302:ASP:OD2	2.03	0.58
1:D:366:LYS:HB2	1:D:383:GLN:OE1	2.04	0.57
1:D:408:ASN:HD22	1:D:430:GLN:NE2	2.01	0.57
1:D:467:TRP:HA	1:D:485:ASN:ND2	2.19	0.57
1:B:260:SER:HB2	1:B:267:TRP:HA	1.87	0.57
1:D:420:GLU:HB3	1:D:457:HIS:CE1	2.40	0.57
1:F:366:LYS:HE3	1:F:385:THR:HG22	1.87	0.57
1:B:117:MET:HE3	1:B:185:VAL:HG22	1.86	0.57
1:D:260:SER:HB2	1:D:267:TRP:HA	1.87	0.57
1:D:450:TYR:HB3	1:D:489:LYS:HG2	1.86	0.57
1:E:171:HIS:CE1	1:E:199:GLU:HB2	2.40	0.57
1:A:157:ILE:HG22	1:A:158:ARG:HG2	1.87	0.57
1:A:228:ARG:NH1	1:A:256:LYS:HD2	2.20	0.57
1:D:359:LEU:HD22	1:D:490:LEU:HA	1.86	0.57
1:E:114:PRO:HB2	1:E:127:MET:HE3	1.87	0.57
1:D:420:GLU:HG2	1:D:438:ASN:ND2	2.19	0.56
1:E:474:ILE:HD12	1:E:474:ILE:H	1.69	0.56
1:F:285:PHE:HB3	1:F:300:MET:HE3	1.87	0.56
1:A:450:TYR:CE1	1:A:489:LYS:HB2	2.39	0.56
1:C:54:GLY:O	1:C:113:ARG:HA	2.05	0.56
1:D:129:MET:HG3	1:D:143:ALA:HB3	1.87	0.56
1:F:163:MET:HE1	1:F:217:SER:HA	1.87	0.56
1:A:67:TYR:HE1	1:A:82:CYS:HG	1.53	0.56
1:B:163:MET:HE3	1:B:166:THR:HG21	1.87	0.56
1:C:63:TYR:CE1	1:C:86:LYS:HE3	2.40	0.56
1:E:129:MET:HG2	1:E:143:ALA:HB3	1.88	0.56
1:E:168:VAL:HG11	1:E:176:TYR:CE1	2.40	0.56
1:A:161:ARG:O	1:A:164:GLN:HG3	2.06	0.56
1:D:54:GLY:O	1:D:113:ARG:HA	2.05	0.56
1:F:223:PHE:HE2	1:F:242:LEU:HD23	1.69	0.56
1:B:182:ASN:HB2	1:B:231:PRO:HG2	1.87	0.56
1:D:454:SER:HA	1:D:461:LEU:HD22	1.88	0.56
1:A:288:PRO:HG3	1:A:297:TYR:CE1	2.41	0.56
1:A:71:ARG:NH1	1:A:312:VAL:HG11	2.21	0.56
1:D:340:ILE:HG22	1:D:347:ILE:HG23	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:PHE:CD2	1:C:50:ILE:HD12	2.41	0.56
1:E:252:PRO:HB2	1:E:277:THR:HG23	1.87	0.56
1:A:72:ASP:CG	1:A:73:ASP:H	2.13	0.55
1:C:125:PHE:CZ	1:C:150:PRO:HG3	2.42	0.55
1:D:377:ASN:HA	1:D:413:ARG:NH2	2.21	0.55
1:E:80:VAL:HG21	1:E:127:MET:HE1	1.88	0.55
1:A:253:ASN:C	1:A:253:ASN:HD22	2.14	0.55
1:D:126:VAL:HG21	1:D:212:TYR:HB2	1.89	0.55
1:D:254:GLN:HG2	1:D:276:SER:HA	1.89	0.55
1:E:179:ARG:HG3	1:E:200:ASN:OD1	2.07	0.55
1:C:106:LEU:HD22	1:C:111:ILE:HD11	1.89	0.55
1:F:59:LYS:HD3	1:F:64:TYR:CE1	2.42	0.55
1:E:366:LYS:HE2	1:E:469:THR:O	2.06	0.55
1:F:395:TYR:CE2	1:F:409:VAL:HG22	2.42	0.55
1:B:119:ASN:HB3	1:B:122:THR:HG22	1.89	0.54
1:D:366:LYS:HB3	1:D:384:TRP:O	2.08	0.54
1:C:97:VAL:HB	1:C:154:PHE:CD2	2.42	0.54
1:F:77:PHE:CD1	1:F:111:ILE:HB	2.41	0.54
1:D:417:VAL:HG21	1:D:477:GLN:NE2	2.23	0.54
1:F:100:ARG:HD2	1:F:107:ASN:O	2.07	0.54
1:D:448:ASP:HB2	1:D:450:TYR:CD2	2.43	0.54
1:D:234:ILE:HD11	1:D:286:ILE:C	2.33	0.54
1:A:110:ASN:HB2	1:A:132:GLU:HB2	1.89	0.54
1:B:97:VAL:HB	1:B:154:PHE:HD2	1.72	0.54
1:D:50:ILE:HG23	1:D:83:TYR:CZ	2.43	0.54
1:B:360:VAL:CG2	1:B:489:LYS:HB3	2.36	0.54
1:C:84:ARG:HH21	1:C:94:ARG:CZ	2.21	0.54
1:D:420:GLU:O	1:D:457:HIS:HE1	1.90	0.54
1:D:441:TRP:HA	1:D:454:SER:O	2.07	0.54
1:D:453:ILE:HG22	1:D:454:SER:H	1.71	0.54
1:D:357:TYR:CD1	1:D:490:LEU:HD11	2.43	0.53
1:F:305:ALA:HA	1:F:308:TRP:CZ2	2.43	0.53
1:A:116:VAL:HG22	1:A:127:MET:HB2	1.90	0.53
1:F:54:GLY:O	1:F:113:ARG:HA	2.08	0.53
1:A:129:MET:HG2	1:A:143:ALA:HB3	1.90	0.53
1:B:368:LEU:CD1	1:B:475:ILE:HD12	2.38	0.53
1:A:118:TYR:CD1	1:A:125:PHE:HE1	2.26	0.53
1:B:230:ALA:O	1:B:244:THR:HA	2.08	0.53
1:D:110:ASN:HB2	1:D:132:GLU:HB2	1.89	0.53
1:D:437:TYR:O	1:D:456:ARG:HB3	2.09	0.53
1:A:256:LYS:HE2	1:A:272:ASN:ND2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:MET:HG2	1:B:143:ALA:HB3	1.90	0.53
1:F:223:PHE:HB3	1:F:226:GLN:HG3	1.90	0.53
1:B:41:GLN:HB3	1:B:49:VAL:HG23	1.89	0.53
1:B:106:LEU:HD11	1:B:156:TYR:CD2	2.44	0.53
1:B:284:THR:HG21	1:B:302:ASP:OD2	2.08	0.53
1:A:97:VAL:HB	1:A:154:PHE:CD2	2.44	0.53
1:B:146:TYR:HD2	1:B:157:ILE:HD11	1.74	0.53
1:B:454:SER:HA	1:B:461:LEU:HA	1.90	0.53
1:D:133:ASN:HD21	1:D:136:ASN:ND2	2.06	0.52
1:D:416:ASP:CG	1:D:439:GLN:HG3	2.34	0.52
1:F:131:TRP:HB3	1:F:141:ARG:HG3	1.91	0.52
1:A:395:TYR:CE2	1:A:409:VAL:HG22	2.44	0.52
1:B:55:GLY:HA3	1:B:67:TYR:O	2.09	0.52
1:D:234:ILE:HD11	1:D:286:ILE:O	2.08	0.52
1:A:114:PRO:HB2	1:A:127:MET:HE3	1.91	0.52
1:E:71:ARG:HH11	1:E:75:ASN:ND2	2.07	0.52
1:A:77:PHE:CD1	1:A:111:ILE:HB	2.45	0.52
1:B:403:TYR:HE1	1:B:442:LYS:HE2	1.74	0.52
1:C:235:LYS:HD2	1:C:240:TYR:CE2	2.44	0.52
1:F:57:MET:HB2	1:F:300:MET:HE1	1.91	0.52
1:F:93:TYR:CZ	1:F:95:GLY:HA2	2.44	0.52
1:A:118:TYR:CD1	1:A:125:PHE:CE1	2.96	0.52
1:C:63:TYR:CG	1:C:84:ARG:HD2	2.44	0.52
1:D:114:PRO:HB2	1:D:127:MET:HE3	1.91	0.52
1:B:484:THR:HA	1:B:487:HIS:HD2	1.73	0.52
1:B:125:PHE:CZ	1:B:150:PRO:HG3	2.44	0.52
1:B:156:TYR:OH	1:B:159:SER:HB3	2.10	0.52
1:C:55:GLY:HA3	1:C:67:TYR:O	2.09	0.52
1:C:442:LYS:HE3	1:F:100:ARG:CZ	2.39	0.52
1:D:291:GLY:HA3	1:D:345:GLY:HA3	1.90	0.52
1:D:448:ASP:HB2	1:D:450:TYR:CE2	2.45	0.52
1:F:428:LEU:HD12	1:F:475:ILE:HG22	1.90	0.52
1:C:50:ILE:HG23	1:C:83:TYR:CE1	2.45	0.51
1:C:69:GLU:OE1	1:C:112:GLU:HA	2.10	0.51
1:F:41:GLN:HB3	1:F:49:VAL:HG13	1.91	0.51
1:A:379:ALA:HB3	1:A:430:GLN:HE21	1.75	0.51
1:B:363:ASN:ND2	1:B:467:TRP:HE3	2.09	0.51
1:B:41:GLN:HG3	1:B:316:GLN:HG2	1.93	0.51
1:B:321:PRO:HB3	1:B:347:ILE:HG22	1.92	0.51
1:B:363:ASN:HD22	1:B:467:TRP:HE3	1.58	0.51
1:C:290:GLN:HG3	1:C:295:THR:HG22	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:GLY:HA3	1:D:67:TYR:O	2.10	0.51
1:D:363:ASN:OD1	1:D:484:THR:HB	2.11	0.51
1:A:146:TYR:CD2	1:A:157:ILE:HD11	2.46	0.51
1:C:31:ALA:O	1:C:32:ALA:C	2.54	0.51
1:C:-13:SER:HA	1:C:492:LEU:HD11	1.93	0.51
1:C:-6:MET:HE1	1:F:155:THR:HG21	1.92	0.51
1:A:254:GLN:NE2	1:A:272:ASN:HB3	2.26	0.51
1:B:113:ARG:NH1	1:B:284:THR:HG22	2.26	0.51
1:D:77:PHE:CD1	1:D:111:ILE:HB	2.46	0.51
1:D:394:TRP:HH2	1:D:430:GLN:HE21	1.59	0.51
1:E:97:VAL:HB	1:E:154:PHE:CD2	2.46	0.51
1:C:454:SER:HB3	1:C:461:LEU:HD23	1.92	0.51
1:D:110:ASN:OD1	1:D:134:GLY:HA2	2.11	0.50
1:E:478:TRP:CZ3	3:E:602:GOL:H31	2.46	0.50
1:B:356:ARG:HG2	1:B:393:GLN:OE1	2.11	0.50
1:C:399:VAL:HG12	1:C:399:VAL:O	2.11	0.50
1:E:331:GLU:HG2	1:E:333:PRO:HD3	1.94	0.50
1:A:109:CYS:HB2	1:A:132:GLU:O	2.10	0.50
1:C:130:HIS:CD2	1:C:179:ARG:HA	2.46	0.50
1:B:283:PRO:HB3	1:B:299:TYR:HE1	1.76	0.50
1:D:358:LYS:O	1:D:491:VAL:HB	2.11	0.50
1:D:381:ILE:HD11	1:D:430:GLN:NE2	2.27	0.50
1:D:157:ILE:HG22	1:D:158:ARG:HG2	1.93	0.50
1:C:77:PHE:CD1	1:C:111:ILE:HB	2.47	0.50
1:E:126:VAL:HG21	1:E:212:TYR:HB2	1.92	0.50
1:B:67:TYR:CE2	1:B:116:VAL:HG21	2.47	0.50
1:B:380:GLN:HE22	1:B:427:VAL:HG13	1.77	0.50
1:A:54:GLY:O	1:A:113:ARG:HA	2.12	0.49
1:B:157:ILE:N	1:B:157:ILE:HD12	2.27	0.49
1:A:369:ASP:OD1	1:A:370:VAL:N	2.44	0.49
1:B:33:GLU:HG2	1:B:35:VAL:HG12	1.95	0.49
1:B:381:ILE:HG12	1:B:429:ILE:HA	1.94	0.49
1:D:422:LYS:HA	1:D:458:CYS:HB3	1.95	0.49
1:A:125:PHE:HE2	1:A:150:PRO:HB3	1.78	0.49
1:A:256:LYS:HE2	1:A:272:ASN:HD21	1.76	0.49
1:D:376:ASP:C	1:D:413:ARG:HH12	2.21	0.49
1:C:129:MET:HG2	1:C:143:ALA:HB3	1.94	0.49
1:D:445:ASP:HA	1:D:451:TYR:HB3	1.93	0.49
1:E:236:ARG:HG2	1:E:237:ASN:OD1	2.13	0.49
1:B:200:ASN:O	1:B:227:GLN:HA	2.12	0.49
1:E:375:VAL:HG12	1:E:411:SER:HB3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:SER:CB	1:A:283:PRO:HD2	2.40	0.49
1:C:223:PHE:HE2	1:C:242:LEU:HD23	1.77	0.49
1:D:361:ASN:HB3	1:D:364:SER:OG	2.13	0.49
1:D:442:LYS:HB3	1:D:454:SER:OG	2.12	0.49
1:A:55:GLY:HA3	1:A:67:TYR:O	2.13	0.49
1:A:117:MET:HE3	1:A:185:VAL:HG22	1.95	0.49
1:D:465:ARG:O	1:D:466:LYS:HG2	2.11	0.49
1:E:131:TRP:CE3	1:E:141:ARG:HD2	2.48	0.49
1:A:196:ALA:HB1	1:A:200:ASN:HA	1.95	0.48
1:F:70:TYR:HD1	1:F:96:GLU:OE2	1.96	0.48
1:C:70:TYR:CE2	1:C:78:LEU:HD23	2.47	0.48
1:C:321:PRO:HB3	1:C:347:ILE:HG22	1.95	0.48
1:E:93:TYR:CZ	1:E:95:GLY:HA2	2.48	0.48
1:E:299:TYR:HB3	1:E:320:LEU:O	2.13	0.48
1:F:223:PHE:CE2	1:F:242:LEU:HD23	2.47	0.48
1:D:338:VAL:O	1:D:340:ILE:HG23	2.13	0.48
1:E:163:MET:HE3	1:E:166:THR:HG21	1.93	0.48
1:E:260:SER:HB2	1:E:267:TRP:HA	1.96	0.48
1:F:55:GLY:HA3	1:F:67:TYR:O	2.13	0.48
1:A:110:ASN:OD1	1:A:134:GLY:HA2	2.14	0.48
1:A:156:TYR:OH	1:A:159:SER:HB3	2.13	0.48
1:A:424:ASP:O	1:C:136:ASN:HB2	2.14	0.48
1:E:450:TYR:CE1	1:E:489:LYS:HB2	2.49	0.48
1:F:135:ILE:HD12	1:F:135:ILE:N	2.29	0.48
1:A:284:THR:HG23	1:A:301:GLY:HA2	1.94	0.48
1:F:256:LYS:HD3	1:F:270:LEU:HB3	1.95	0.48
1:F:71:ARG:HD3	1:F:312:VAL:HG11	1.96	0.48
1:F:298:LEU:HD11	1:F:319:TRP:HB3	1.96	0.48
1:B:357:TYR:HB3	1:B:490:LEU:HD11	1.95	0.48
1:C:446:ILE:HG21	1:C:452:LYS:HG3	1.96	0.48
1:A:53:HIS:HD2	1:A:312:VAL:HG12	1.79	0.48
1:A:57:MET:HB2	1:A:300:MET:HE1	1.96	0.47
1:C:40:THR:HB	1:F:92:GLU:OE2	2.14	0.47
1:C:378:ALA:HA	1:C:429:ILE:HD12	1.96	0.47
1:D:149:THR:HG23	1:D:150:PRO:HD2	1.96	0.47
1:D:364:SER:HB2	1:D:383:GLN:OE1	2.14	0.47
1:A:381:ILE:HD13	1:A:429:ILE:HA	1.94	0.47
1:B:286:ILE:HD13	1:B:322:LEU:HD22	1.95	0.47
1:D:131:TRP:CE3	1:D:141:ARG:HD2	2.49	0.47
1:A:360:VAL:CG2	1:A:489:LYS:HB3	2.43	0.47
1:B:109:CYS:HB2	1:B:132:GLU:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:ALA:HA	1:E:308:TRP:CZ2	2.49	0.47
1:F:206:TYR:HB3	1:F:215:ILE:HG23	1.96	0.47
1:C:362:LYS:HE3	1:C:484:THR:HG22	1.96	0.47
1:D:117:MET:HE2	1:D:128:TRP:CD1	2.49	0.47
1:D:147:SER:HB2	1:D:154:PHE:HA	1.96	0.47
1:F:147:SER:HB2	1:F:154:PHE:HA	1.96	0.47
1:F:430:GLN:O	1:F:430:GLN:HG3	2.14	0.47
1:A:71:ARG:HH11	1:A:312:VAL:HG11	1.79	0.47
1:D:363:ASN:HB2	1:D:485:ASN:HB3	1.96	0.47
1:D:437:TYR:HE1	1:D:457:HIS:CD2	2.33	0.47
1:A:80:VAL:HG21	1:A:127:MET:HE1	1.97	0.47
1:D:106:LEU:HA	1:D:109:CYS:SG	2.55	0.47
1:E:70:TYR:O	1:E:78:LEU:HB3	2.15	0.47
1:F:182:ASN:ND2	1:F:232:CYS:HA	2.27	0.47
1:B:339:LYS:HB2	1:B:350:TYR:HB2	1.97	0.47
1:C:71:ARG:NH1	1:C:312:VAL:HG11	2.30	0.47
1:A:413:ARG:HE	1:A:430:GLN:HG3	1.79	0.47
1:B:453:ILE:HD12	1:B:453:ILE:N	2.30	0.47
1:D:387:ASN:N	1:D:392:GLN:HE22	2.05	0.47
1:D:467:TRP:HA	1:D:485:ASN:HD21	1.78	0.47
1:F:363:ASN:HB2	1:F:484:THR:OG1	2.14	0.47
1:A:118:TYR:HD1	1:A:125:PHE:CE1	2.33	0.46
1:D:234:ILE:CG2	1:D:235:LYS:N	2.77	0.46
1:E:184:PHE:CG	1:E:233:LEU:HD22	2.50	0.46
1:D:278:THR:HG22	1:D:278:THR:O	2.14	0.46
1:D:234:ILE:HG22	1:D:235:LYS:N	2.31	0.46
1:D:321:PRO:HB3	1:D:347:ILE:CG2	2.45	0.46
1:D:77:PHE:HB2	1:D:111:ILE:H	1.80	0.46
1:A:131:TRP:CE3	1:A:141:ARG:HD2	2.51	0.46
1:C:354:THR:HG22	1:C:354:THR:O	2.16	0.46
1:E:70:TYR:HB3	1:E:79:GLY:O	2.16	0.46
1:B:335:TYR:HB2	1:B:338:VAL:HG22	1.98	0.46
1:F:70:TYR:CD1	1:F:96:GLU:OE2	2.69	0.46
1:F:72:ASP:HB3	1:F:78:LEU:HD11	1.97	0.46
1:A:254:GLN:OE1	1:A:276:SER:HA	2.16	0.46
1:A:286:ILE:HD13	1:A:322:LEU:HD22	1.98	0.46
1:B:384:TRP:CZ3	1:B:471:ASP:HB3	2.51	0.46
1:C:106:LEU:HA	1:C:109:CYS:SG	2.56	0.46
1:C:192:TYR:HB3	1:C:205:LEU:HD11	1.98	0.46
1:D:97:VAL:HB	1:D:154:PHE:CD2	2.50	0.46
1:D:390:LEU:O	1:D:410:LYS:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:GLN:HB3	1:B:228:ARG:HG2	1.98	0.45
1:F:64:TYR:CG	1:F:88:LEU:HD21	2.51	0.45
1:A:58:LEU:HD13	1:A:59:LYS:N	2.32	0.45
1:B:192:TYR:HB3	1:B:205:LEU:HD11	1.98	0.45
1:C:77:PHE:HB2	1:C:111:ILE:H	1.81	0.45
1:E:122:THR:OG1	1:E:124:GLU:HG2	2.15	0.45
1:F:461:LEU:CD1	1:F:486:GLN:HB3	2.43	0.45
1:C:114:PRO:HB2	1:C:127:MET:HE3	1.98	0.45
1:D:366:LYS:HB3	1:D:384:TRP:C	2.41	0.45
1:E:34:GLY:HA2	1:E:89:VAL:HG21	1.97	0.45
1:E:325:ILE:HD11	1:E:331:GLU:OE2	2.16	0.45
1:E:351:ILE:N	1:E:351:ILE:HD12	2.32	0.45
1:E:381:ILE:HG12	1:E:429:ILE:HA	1.97	0.45
1:F:413:ARG:HB2	1:F:430:GLN:HB2	1.99	0.45
1:A:97:VAL:HB	1:A:154:PHE:HD2	1.81	0.45
1:C:77:PHE:CZ	1:C:111:ILE:HD12	2.51	0.45
1:D:434:ASN:HD21	2:D:601:IPT:H3	1.81	0.45
1:D:437:TYR:HE1	1:D:457:HIS:CG	2.35	0.45
1:E:55:GLY:HA3	1:E:67:TYR:O	2.16	0.45
1:B:288:PRO:HG3	1:B:297:TYR:CE1	2.52	0.45
1:B:403:TYR:CE1	1:B:442:LYS:HG2	2.52	0.45
1:C:425:GLY:HA2	1:C:476:GLN:CD	2.42	0.45
1:F:492:LEU:N	1:F:492:LEU:HD12	2.32	0.45
1:A:72:ASP:CB	1:A:78:LEU:HD12	2.47	0.45
1:A:170:ASP:OD1	1:A:177:MET:HG3	2.16	0.45
1:A:194:ILE:HD12	1:A:204:HIS:O	2.17	0.45
1:C:-13:SER:HA	1:C:492:LEU:CD1	2.47	0.45
1:D:161:ARG:O	1:D:164:GLN:HB3	2.16	0.45
1:B:119:ASN:HB2	1:B:212:TYR:CD2	2.52	0.45
1:B:145:ALA:HA	1:B:157:ILE:CD1	2.47	0.45
1:B:359:LEU:HD12	1:B:368:LEU:HD22	1.98	0.45
1:C:126:VAL:HG21	1:C:212:TYR:HB2	1.98	0.45
1:D:87:ASP:O	1:D:88:LEU:HB2	2.16	0.45
1:E:252:PRO:HB2	1:E:277:THR:CG2	2.47	0.45
1:F:425:GLY:HA2	1:F:476:GLN:CD	2.42	0.45
1:A:163:MET:SD	1:B:165:ASP:HB2	2.57	0.44
1:A:240:TYR:O	1:A:259:TYR:HA	2.16	0.44
1:B:257:TYR:CE2	1:B:330:LEU:HD13	2.52	0.44
1:B:463:ASP:OD1	3:B:602:GOL:H11	2.18	0.44
1:D:299:TYR:HB3	1:D:320:LEU:O	2.18	0.44
1:D:428:LEU:HD22	1:D:475:ILE:HG22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:THR:HG22	1:E:277:THR:O	2.17	0.44
1:F:117:MET:HE2	1:F:212:TYR:CD2	2.52	0.44
1:D:243:ILE:N	1:D:243:ILE:HD12	2.32	0.44
1:E:62:ASP:O	1:E:86:LYS:HG2	2.17	0.44
1:E:474:ILE:HD12	1:E:474:ILE:N	2.31	0.44
1:F:291:GLY:HA3	1:F:344:SER:C	2.42	0.44
1:B:209:THR:OG1	1:B:210:PRO:HD2	2.17	0.44
1:B:218:LEU:O	1:B:218:LEU:HD12	2.17	0.44
1:B:230:ALA:CB	1:B:283:PRO:HG2	2.48	0.44
1:D:358:LYS:HG3	1:D:392:GLN:HB3	2.00	0.44
1:E:129:MET:CG	1:E:143:ALA:HB3	2.47	0.44
1:F:57:MET:HE2	1:F:287:ILE:HD13	1.99	0.44
1:A:279:TYR:CE2	1:A:334:TYR:HB2	2.52	0.44
1:B:484:THR:HA	1:B:487:HIS:CD2	2.52	0.44
1:D:168:VAL:HG21	1:D:176:TYR:CE1	2.52	0.44
1:E:170:ASP:CG	1:E:177:MET:HG3	2.43	0.44
1:D:285:PHE:HB3	1:D:300:MET:HE3	1.98	0.44
1:D:321:PRO:HB3	1:D:347:ILE:HG22	1.99	0.44
1:D:367:VAL:HG12	1:D:368:LEU:N	2.32	0.44
1:F:381:ILE:HG12	1:F:429:ILE:HA	1.98	0.44
1:C:129:MET:CG	1:C:143:ALA:HB3	2.48	0.44
1:D:263:LEU:HD12	1:D:263:LEU:H	1.83	0.44
1:E:59:LYS:HD3	1:E:64:TYR:CE1	2.52	0.44
1:B:129:MET:CG	1:B:143:ALA:HB3	2.48	0.44
1:B:278:THR:HG22	1:B:278:THR:O	2.18	0.44
1:D:111:ILE:HD11	1:D:131:TRP:HD1	1.81	0.44
1:A:57:MET:HA	1:A:65:TYR:O	2.18	0.44
1:A:125:PHE:HD2	1:A:150:PRO:HA	1.83	0.44
1:C:245:SER:HB3	1:C:283:PRO:HD2	2.00	0.44
1:C:399:VAL:HG11	1:C:440:HIS:CE1	2.53	0.44
1:D:297:TYR:CD2	1:D:324:PHE:CE2	3.06	0.44
1:E:109:CYS:HB2	1:E:132:GLU:O	2.17	0.44
1:A:129:MET:CG	1:A:143:ALA:HB3	2.47	0.43
1:B:209:THR:HG23	1:B:211:ASP:OD1	2.18	0.43
1:B:419:ASP:HA	2:B:601:IPT:S1	2.57	0.43
1:C:42:PHE:CE2	1:C:50:ILE:HD12	2.53	0.43
1:C:126:VAL:HG11	1:C:212:TYR:O	2.18	0.43
1:F:329:THR:C	1:F:330:LEU:HD12	2.42	0.43
1:D:451:TYR:OH	1:D:490:LEU:HD13	2.18	0.43
1:B:115:LYS:HG3	1:B:182:ASN:HA	2.00	0.43
1:D:288:PRO:HG3	1:D:297:TYR:CE1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:LEU:O	1:D:367:VAL:HG13	2.18	0.43
1:D:361:ASN:HD21	1:D:485:ASN:C	2.26	0.43
1:E:362:LYS:HG2	1:E:484:THR:HB	1.99	0.43
1:E:452:LYS:HG2	1:E:461:LEU:HD22	2.00	0.43
1:F:70:TYR:O	1:F:78:LEU:HB2	2.18	0.43
1:A:279:TYR:CD2	1:A:334:TYR:HB2	2.52	0.43
1:C:223:PHE:CE2	1:C:242:LEU:HD23	2.52	0.43
1:F:288:PRO:HB3	1:F:297:TYR:CE1	2.54	0.43
1:B:131:TRP:CE3	1:B:141:ARG:HD2	2.54	0.43
1:C:135:ILE:HG13	1:C:136:ASN:ND2	2.34	0.43
1:D:80:VAL:HG21	1:D:127:MET:HE1	2.01	0.43
1:A:252:PRO:HB2	1:A:277:THR:HB	2.01	0.43
1:C:286:ILE:HD13	1:C:322:LEU:HD22	2.00	0.43
1:C:399:VAL:HG21	1:C:405:LYS:HB2	2.00	0.43
1:D:57:MET:HE3	1:D:287:ILE:HD13	2.01	0.43
1:D:83:TYR:HB3	1:D:91:TRP:HB3	2.00	0.43
1:D:117:MET:HE1	1:D:208:LEU:CD1	2.48	0.43
1:D:364:SER:HB2	1:D:383:GLN:CD	2.44	0.43
1:B:321:PRO:HB3	1:B:347:ILE:CG2	2.48	0.43
1:C:58:LEU:HD22	1:C:116:VAL:HG12	2.00	0.43
1:C:287:ILE:HA	1:C:288:PRO:HD3	1.88	0.43
1:D:340:ILE:CG2	1:D:347:ILE:HG23	2.47	0.43
1:E:110:ASN:HB3	1:E:132:GLU:HB2	2.01	0.43
1:E:395:TYR:CE2	1:E:409:VAL:HG22	2.54	0.43
1:A:50:ILE:HG23	1:A:83:TYR:CE1	2.53	0.43
1:C:63:TYR:CE1	1:C:84:ARG:NH1	2.86	0.43
1:D:122:THR:OG1	1:D:124:GLU:HG2	2.17	0.43
1:D:369:ASP:OD1	1:D:391:SER:HB2	2.19	0.43
1:E:197:ALA:HB3	1:E:204:HIS:CE1	2.54	0.43
1:C:127:MET:HG2	1:C:129:MET:HE2	2.01	0.43
1:D:415:LEU:HD21	1:D:428:LEU:HD21	2.00	0.43
1:A:67:TYR:HE1	1:A:82:CYS:SG	2.41	0.43
1:B:240:TYR:CZ	1:B:263:LEU:HD11	2.54	0.43
1:D:256:LYS:HD3	1:D:270:LEU:HB3	2.00	0.43
1:E:147:SER:HB2	1:E:154:PHE:HA	2.01	0.43
1:F:146:TYR:HD2	1:F:157:ILE:HD11	1.84	0.43
1:A:125:PHE:CE2	1:A:150:PRO:HB3	2.54	0.42
1:C:466:LYS:H	3:C:602:GOL:C1	2.32	0.42
1:D:40:THR:HG22	1:D:41:GLN:N	2.34	0.42
1:D:50:ILE:HG23	1:D:83:TYR:CE1	2.54	0.42
1:D:354:THR:HG22	1:D:354:THR:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:ARG:HG2	1:D:432:THR:HA	2.00	0.42
1:A:370:VAL:HG11	1:A:430:GLN:NE2	2.34	0.42
1:B:335:TYR:CD2	1:B:349:GLU:HB2	2.54	0.42
1:B:375:VAL:HG12	1:B:411:SER:HB3	2.00	0.42
1:B:411:SER:C	1:B:413:ARG:H	2.27	0.42
1:B:425:GLY:HA2	1:B:476:GLN:OE1	2.19	0.42
1:C:285:PHE:HE2	1:C:287:ILE:HB	1.85	0.42
1:E:144:VAL:HG22	1:E:157:ILE:HD12	2.02	0.42
1:A:122:THR:OG1	1:A:124:GLU:HG2	2.19	0.42
1:B:358:LYS:HE2	1:B:392:GLN:HB2	2.01	0.42
1:A:215:ILE:HD12	1:A:215:ILE:N	2.35	0.42
1:E:227:GLN:OE1	1:E:247:CYS:HB3	2.19	0.42
1:B:492:LEU:HD12	1:B:492:LEU:N	2.34	0.42
1:D:72:ASP:CG	1:D:73:ASP:N	2.71	0.42
1:D:130:HIS:NE2	1:D:179:ARG:HA	2.35	0.42
1:D:441:TRP:HB3	1:D:453:ILE:HG22	2.01	0.42
1:E:209:THR:HB	1:E:210:PRO:HD2	2.02	0.42
1:E:430:GLN:O	1:E:430:GLN:HG3	2.19	0.42
1:F:77:PHE:CZ	1:F:79:GLY:HA2	2.55	0.42
1:C:71:ARG:HD3	1:C:75:ASN:CG	2.44	0.42
1:C:305:ALA:HA	1:C:308:TRP:CZ2	2.54	0.42
1:E:381:ILE:HG13	1:E:415:LEU:CD1	2.50	0.42
1:F:209:THR:HB	1:F:210:PRO:HD2	2.02	0.42
1:F:466:LYS:H	3:F:603:GOL:C3	2.33	0.42
1:B:77:PHE:CE2	1:B:111:ILE:HD12	2.54	0.42
1:B:182:ASN:HD22	1:B:232:CYS:HA	1.85	0.42
1:D:370:VAL:CG2	1:D:373:GLY:HA2	2.50	0.42
1:D:441:TRP:HB3	1:D:453:ILE:CG2	2.50	0.42
1:E:254:GLN:OE1	1:E:276:SER:HA	2.19	0.42
1:B:57:MET:HE3	1:B:287:ILE:HG21	2.02	0.42
1:E:362:LYS:HB2	1:E:450:TYR:CE1	2.55	0.42
1:E:461:LEU:O	1:E:477:GLN:HA	2.20	0.42
1:F:378:ALA:HA	1:F:429:ILE:HD12	2.01	0.42
1:F:97:VAL:HB	1:F:154:PHE:HD2	1.80	0.41
1:A:41:GLN:HG3	1:A:316:GLN:HG2	2.02	0.41
1:A:186:ASP:HB3	1:A:188:ASP:OD1	2.20	0.41
1:A:243:ILE:N	1:A:243:ILE:HD12	2.36	0.41
1:B:236:ARG:HB2	1:B:297:TYR:OH	2.20	0.41
1:E:300:MET:HE3	1:E:319:TRP:CZ2	2.55	0.41
1:B:162:PRO:HD2	1:B:176:TYR:O	2.20	0.41
1:B:194:ILE:HG23	1:B:231:PRO:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ALA:HB1	1:C:68:GLY:HA3	2.01	0.41
1:D:85:SER:HB2	1:D:91:TRP:HA	2.02	0.41
1:D:394:TRP:CZ3	1:D:408:ASN:HB3	2.55	0.41
1:F:36:ILE:HD11	1:F:89:VAL:HG22	2.01	0.41
1:B:126:VAL:HG21	1:B:212:TYR:HB2	2.02	0.41
1:F:170:ASP:CG	1:F:177:MET:HG3	2.46	0.41
1:A:57:MET:CB	1:A:300:MET:HE1	2.51	0.41
1:A:169:MET:HE1	1:A:174:PRO:HA	2.02	0.41
1:C:243:ILE:N	1:C:243:ILE:HD12	2.35	0.41
1:C:362:LYS:HB2	1:C:450:TYR:CE1	2.55	0.41
1:F:424:ASP:HB3	1:F:478:TRP:CE3	2.55	0.41
1:E:50:ILE:HG23	1:E:83:TYR:CE1	2.56	0.41
1:A:170:ASP:O	1:A:171:HIS:HB2	2.20	0.41
1:D:279:TYR:CD2	1:D:334:TYR:HB2	2.56	0.41
1:E:197:ALA:HB3	1:E:204:HIS:ND1	2.35	0.41
1:E:492:LEU:HD12	1:E:492:LEU:N	2.35	0.41
1:A:78:LEU:C	1:A:78:LEU:HD23	2.46	0.41
1:A:428:LEU:HD13	1:A:476:GLN:C	2.45	0.41
1:B:305:ALA:HA	1:B:308:TRP:CH2	2.56	0.41
1:C:384:TRP:CZ3	1:C:471:ASP:HB3	2.55	0.41
1:A:168:VAL:O	1:A:169:MET:HE2	2.21	0.41
1:B:119:ASN:HB3	1:B:122:THR:CG2	2.51	0.41
1:B:254:GLN:CD	1:B:272:ASN:HD22	2.29	0.41
1:C:42:PHE:HD2	1:C:50:ILE:HD12	1.83	0.41
1:D:290:GLN:OE1	1:D:295:THR:HB	2.21	0.41
1:E:104:PRO:HA	1:E:107:ASN:OD1	2.21	0.41
1:E:298:LEU:HB2	1:E:347:ILE:CD1	2.51	0.41
1:E:437:TYR:CG	1:E:456:ARG:HD3	2.56	0.41
1:A:172:GLY:C	1:A:173:LEU:HD12	2.46	0.41
1:A:403:TYR:CD1	1:A:442:LYS:HB2	2.56	0.41
1:B:419:ASP:OD1	2:B:601:IPT:H3'2	2.21	0.41
1:B:454:SER:HB2	1:B:459:GLY:O	2.20	0.41
1:C:-13:SER:OG	1:C:490:LEU:HB3	2.20	0.41
1:E:243:ILE:HD12	1:E:243:ILE:N	2.36	0.41
1:A:125:PHE:O	1:A:146:TYR:HA	2.21	0.40
1:A:236:ARG:HG3	1:A:297:TYR:CZ	2.56	0.40
1:B:209:THR:HG22	1:B:214:ASN:O	2.22	0.40
1:B:359:LEU:O	1:B:367:VAL:HA	2.20	0.40
1:C:186:ASP:HB3	1:C:188:ASP:OD1	2.21	0.40
1:C:357:TYR:CD1	1:C:490:LEU:HG	2.56	0.40
1:C:399:VAL:HG11	1:C:440:HIS:NE2	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:TRP:CH2	1:D:483:GLY:HA2	2.56	0.40
1:B:385:THR:HG23	1:B:471:ASP:OD1	2.21	0.40
1:C:450:TYR:CE1	1:C:489:LYS:HB2	2.57	0.40
1:D:360:VAL:HG23	1:D:366:LYS:C	2.46	0.40
1:A:130:HIS:NE2	1:A:179:ARG:HA	2.36	0.40
1:C:223:PHE:HB3	1:C:226:GLN:HG3	2.03	0.40
1:E:73:ASP:C	1:E:75:ASN:H	2.28	0.40
1:E:117:MET:HE2	1:E:212:TYR:CD2	2.56	0.40
1:E:288:PRO:HB3	1:E:297:TYR:CE1	2.57	0.40
1:A:84:ARG:NE	1:A:94:ARG:HD3	2.36	0.40
1:C:64:TYR:CG	1:C:88:LEU:HD21	2.56	0.40
1:D:360:VAL:HG22	1:D:361:ASN:N	2.37	0.40
1:E:311:LYS:HG2	1:E:314:ASP:OD2	2.21	0.40
1:F:70:TYR:HB3	1:F:79:GLY:O	2.22	0.40
1:F:398:ASP:HA	1:F:404:LYS:HG2	2.04	0.40
1:F:452:LYS:HB2	1:F:461:LEU:HD22	2.04	0.40
1:B:119:ASN:HB2	1:B:212:TYR:CE2	2.57	0.40
1:B:287:ILE:HA	1:B:288:PRO:HD3	1.91	0.40
1:C:446:ILE:HG12	1:C:450:TYR:O	2.21	0.40
1:F:243:ILE:HD12	1:F:243:ILE:N	2.37	0.40
1:F:460:LYS:HB2	1:F:477:GLN:HG2	2.03	0.40

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	459/526 (87%)	431 (94%)	28 (6%)	0	100	100
1	B	459/526 (87%)	424 (92%)	34 (7%)	1 (0%)	43	76
1	C	480/526 (91%)	453 (94%)	26 (5%)	1 (0%)	43	76
1	D	459/526 (87%)	423 (92%)	35 (8%)	1 (0%)	43	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	459/526 (87%)	439 (96%)	20 (4%)	0	100	100
1	F	459/526 (87%)	439 (96%)	19 (4%)	1 (0%)	43	76
All	All	2775/3156 (88%)	2609 (94%)	162 (6%)	4 (0%)	48	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	32	ALA
1	D	35	VAL
1	F	386	ASP
1	B	231	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	389/442 (88%)	388 (100%)	1 (0%)	86	91
1	B	389/442 (88%)	385 (99%)	4 (1%)	68	84
1	C	402/442 (91%)	402 (100%)	0	100	100
1	D	389/442 (88%)	385 (99%)	4 (1%)	68	84
1	E	389/442 (88%)	389 (100%)	0	100	100
1	F	389/442 (88%)	389 (100%)	0	100	100
All	All	2347/2652 (88%)	2338 (100%)	9 (0%)	84	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	B	209	THR
1	B	226	GLN
1	B	346	ILE
1	B	475	ILE
1	D	36	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	234	ILE
1	D	461	LEU
1	D	470	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	253	ASN
1	A	272	ASN
1	A	430	GLN
1	B	53	HIS
1	B	119	ASN
1	B	171	HIS
1	B	272	ASN
1	B	313	ASN
1	B	392	GLN
1	B	430	GLN
1	B	487	HIS
1	C	-8	GLN
1	C	101	ASN
1	C	139	GLN
1	C	164	GLN
1	C	383	GLN
1	D	60	HIS
1	D	119	ASN
1	D	133	ASN
1	D	164	GLN
1	D	392	GLN
1	D	430	GLN
1	D	457	HIS
1	E	108	HIS
1	E	171	HIS
1	E	361	ASN
1	E	457	HIS
1	F	60	HIS
1	F	101	ASN
1	F	107	ASN
1	F	269	GLN
1	F	282	GLN
1	F	380	GLN
1	F	476	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 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	C	603	-	5,5,5	0.36	0	5,5,5	0.28	0
2	IPT	B	601	-	15,15,15	0.69	0	18,21,21	0.90	1 (5%)
3	GOL	E	602	-	5,5,5	0.39	0	5,5,5	0.29	0
3	GOL	E	603	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	C	602	-	5,5,5	0.36	0	5,5,5	0.35	0
2	IPT	C	601	-	15,15,15	0.70	0	18,21,21	0.99	1 (5%)
2	IPT	F	601	-	15,15,15	0.70	0	18,21,21	0.94	1 (5%)
2	IPT	E	601	-	15,15,15	0.70	0	18,21,21	1.14	2 (11%)
2	IPT	D	601	-	15,15,15	0.69	0	18,21,21	0.93	1 (5%)
2	IPT	F	602	-	15,15,15	0.71	0	18,21,21	1.32	3 (16%)
2	IPT	A	601	-	15,15,15	0.69	0	18,21,21	0.81	0
3	GOL	A	602	-	5,5,5	0.37	0	5,5,5	0.31	0
3	GOL	B	602	-	5,5,5	0.37	0	5,5,5	0.34	0
3	GOL	F	603	-	5,5,5	0.37	0	5,5,5	0.34	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	C	603	-	-	2/4/4/4	-
2	IPT	B	601	-	-	1/6/26/26	0/1/1/1
3	GOL	E	602	-	-	2/4/4/4	-
3	GOL	E	603	-	-	2/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
2	IPT	C	601	-	-	1/6/26/26	0/1/1/1
2	IPT	F	601	-	-	1/6/26/26	0/1/1/1
2	IPT	E	601	-	-	2/6/26/26	0/1/1/1
2	IPT	D	601	-	-	0/6/26/26	0/1/1/1
2	IPT	F	602	-	-	1/6/26/26	0/1/1/1
2	IPT	A	601	-	-	0/6/26/26	0/1/1/1
3	GOL	A	602	-	-	2/4/4/4	-
3	GOL	B	602	-	-	2/4/4/4	-
3	GOL	F	603	-	-	4/4/4/4	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	602	IPT	C1-O5-C5	3.71	119.22	112.56
2	E	601	IPT	O5-C1-C2	3.14	114.64	110.32
2	C	601	IPT	C1-O5-C5	2.65	117.32	112.56
2	E	601	IPT	C1-O5-C5	2.57	117.17	112.56
2	F	602	IPT	O5-C1-C2	2.55	113.84	110.32
2	B	601	IPT	C1-O5-C5	2.46	116.97	112.56
2	F	601	IPT	C1-O5-C5	2.46	116.97	112.56
2	D	601	IPT	C1-O5-C5	2.44	116.95	112.56
2	F	602	IPT	O5-C5-C4	2.09	113.47	109.70

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	IPT	C3'-C1'-S1-C1
2	F	601	IPT	C3'-C1'-S1-C1
2	F	602	IPT	C3'-C1'-S1-C1
3	B	602	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	603	GOL	O1-C1-C2-C3
3	E	602	GOL	O1-C1-C2-C3
3	E	603	GOL	O1-C1-C2-C3
3	F	603	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-C3
3	C	602	GOL	O1-C1-C2-C3
3	F	603	GOL	C1-C2-C3-O3
3	A	602	GOL	O1-C1-C2-O2
3	B	602	GOL	O1-C1-C2-O2
3	C	603	GOL	O1-C1-C2-O2
3	F	603	GOL	O1-C1-C2-O2
3	C	602	GOL	O1-C1-C2-O2
3	E	602	GOL	O1-C1-C2-O2
3	E	603	GOL	O1-C1-C2-O2
3	F	603	GOL	O2-C2-C3-O3
2	E	601	IPT	C4-C5-C6-O6
2	B	601	IPT	C3'-C1'-S1-C1
2	E	601	IPT	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	IPT	2	0
3	E	602	GOL	1	0
3	C	602	GOL	1	0
2	D	601	IPT	2	0
3	B	602	GOL	1	0
3	F	603	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

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, 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	461/526 (87%)	0.53	15 (3%)	49	28	55, 84, 107, 140	0
1	B	461/526 (87%)	0.66	17 (3%)	45	25	64, 94, 120, 138	0
1	C	482/526 (91%)	0.29	13 (2%)	56	33	45, 62, 84, 132	0
1	D	461/526 (87%)	1.23	95 (20%)	2	2	54, 97, 178, 183	0
1	E	461/526 (87%)	0.29	6 (1%)	75	53	50, 72, 91, 115	0
1	F	461/526 (87%)	0.39	19 (4%)	41	23	43, 67, 89, 113	0
All	All	2787/3156 (88%)	0.56	165 (5%)	28	14	43, 78, 135, 183	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	430	GLN	6.4
1	C	32	ALA	6.0
1	F	96	GLU	5.9
1	D	406	ILE	4.7
1	D	408	ASN	4.7
1	A	133	ASN	4.5
1	A	411	SER	4.4
1	D	464	VAL	4.4
1	D	481	ALA	4.3
1	D	414	ALA	4.1
1	F	493	VAL	4.1
1	F	388	GLY	4.0
1	D	491	VAL	3.9
1	D	390	LEU	3.9
1	B	445	ASP	3.9
1	D	451	TYR	3.8
1	A	245	SER	3.8
1	B	393	GLN	3.7
1	D	462	ILE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	72	ASP	3.7
1	D	493	VAL	3.6
1	D	490	LEU	3.6
1	D	415	LEU	3.6
1	D	387	ASN	3.5
1	D	35	VAL	3.5
1	C	33	GLU	3.4
1	D	484	THR	3.4
1	D	474	ILE	3.4
1	D	359	LEU	3.4
1	E	380	GLN	3.3
1	D	431	TYR	3.3
1	D	375	VAL	3.3
1	D	380	GLN	3.3
1	D	427	VAL	3.3
1	D	110	ASN	3.2
1	D	47	GLY	3.2
1	D	374	SER	3.2
1	D	463	ASP	3.2
1	D	453	ILE	3.2
1	D	34	GLY	3.1
1	D	284	THR	3.1
1	F	331	GLU	3.1
1	F	380	GLN	3.0
1	D	360	VAL	3.0
1	D	407	VAL	3.0
1	D	331	GLU	3.0
1	D	338	VAL	3.0
1	D	376	ASP	3.0
1	D	247	CYS	3.0
1	B	229	GLU	3.0
1	B	390	LEU	3.0
1	D	340	ILE	2.9
1	D	377	ASN	2.9
1	D	437	TYR	2.9
1	E	276	SER	2.9
1	F	412	GLY	2.9
1	B	451	TYR	2.9
1	D	439	GLN	2.8
1	D	477	GLN	2.8
1	D	381	ILE	2.8
1	D	379	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	247	CYS	2.8
1	F	229	GLU	2.8
1	D	473	GLY	2.8
1	A	69	GLU	2.8
1	C	354	THR	2.8
1	D	480	ASP	2.7
1	D	120	ALA	2.7
1	D	327	ASP	2.7
1	D	472	GLY	2.7
1	D	75	ASN	2.7
1	A	172	GLY	2.7
1	D	96	GLU	2.7
1	D	391	SER	2.7
1	D	257	TYR	2.6
1	C	42	PHE	2.6
1	C	-6	MET	2.6
1	D	486	GLN	2.6
1	D	325	ILE	2.6
1	A	72	ASP	2.6
1	D	274	GLY	2.6
1	D	488	TRP	2.5
1	D	102	SER	2.5
1	D	337	SER	2.5
1	D	393	GLN	2.5
1	D	371	LEU	2.5
1	D	479	SER	2.5
1	D	446	ILE	2.5
1	D	98	LEU	2.5
1	D	383	GLN	2.5
1	D	392	GLN	2.5
1	D	461	LEU	2.5
1	B	65	TYR	2.5
1	B	450	TYR	2.5
1	B	493	VAL	2.5
1	D	367	VAL	2.5
1	D	399	VAL	2.5
1	D	33	GLU	2.4
1	D	478	TRP	2.4
1	F	492	LEU	2.4
1	D	89	VAL	2.4
1	F	365	GLY	2.4
1	A	113	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	389	SER	2.4
1	B	150	PRO	2.4
1	D	410	LYS	2.4
1	D	296	SER	2.4
1	D	87	ASP	2.4
1	F	382	VAL	2.4
1	C	473	GLY	2.3
1	F	328	THR	2.3
1	D	58	LEU	2.3
1	E	358	LYS	2.3
1	D	492	LEU	2.3
1	D	346	ILE	2.3
1	D	432	THR	2.3
1	F	247	CYS	2.3
1	A	229	GLU	2.3
1	D	482	GLY	2.3
1	B	444	THR	2.3
1	C	336	ASP	2.3
1	E	33	GLU	2.3
1	C	472	GLY	2.3
1	D	368	LEU	2.3
1	D	348	SER	2.3
1	C	237	ASN	2.3
1	D	90	ASN	2.3
1	C	108	HIS	2.2
1	D	489	LYS	2.2
1	A	174	PRO	2.2
1	B	231	PRO	2.2
1	A	247	CYS	2.2
1	C	398	ASP	2.2
1	D	364	SER	2.2
1	D	298	LEU	2.2
1	B	469	THR	2.1
1	F	427	VAL	2.1
1	D	363	ASN	2.1
1	D	91	TRP	2.1
1	D	362	LYS	2.1
1	F	368	LEU	2.1
1	A	84	ARG	2.1
1	A	401	GLY	2.1
1	B	138	GLY	2.1
1	D	421	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	181	CYS	2.1
1	F	134	GLY	2.1
1	B	164	GLN	2.1
1	F	172	GLY	2.1
1	F	364	SER	2.1
1	D	200	ASN	2.1
1	D	384	TRP	2.1
1	D	396	LEU	2.1
1	B	487	HIS	2.1
1	D	487	HIS	2.1
1	B	220	ALA	2.1
1	E	172	GLY	2.1
1	D	358	LYS	2.0
1	F	490	LEU	2.0
1	C	-7	GLN	2.0
1	A	75	ASN	2.0
1	A	250	TRP	2.0
1	C	51	HIS	2.0
1	F	284	THR	2.0
1	B	396	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
2	IPT	F	602	15/15	0.62	0.27	81,98,118,123	0
2	IPT	D	601	15/15	0.64	0.20	121,133,141,143	0
3	GOL	C	603	6/6	0.81	0.26	57,69,71,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	E	603	6/6	0.84	0.13	71,73,78,80	0
3	GOL	B	602	6/6	0.86	0.17	74,77,79,79	0
3	GOL	A	602	6/6	0.88	0.19	58,63,71,81	0
2	IPT	E	601	15/15	0.90	0.13	63,74,82,88	0
2	IPT	B	601	15/15	0.90	0.14	75,81,88,100	0
3	GOL	E	602	6/6	0.91	0.14	66,75,77,80	0
3	GOL	C	602	6/6	0.91	0.20	62,66,74,77	0
2	IPT	C	601	15/15	0.93	0.13	57,64,80,90	0
2	IPT	A	601	15/15	0.94	0.10	62,68,85,86	0
3	GOL	F	603	6/6	0.96	0.18	66,71,77,78	0
2	IPT	F	601	15/15	0.97	0.10	61,66,73,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.