



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:03 PM GMT

PDB ID : 3VT2
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

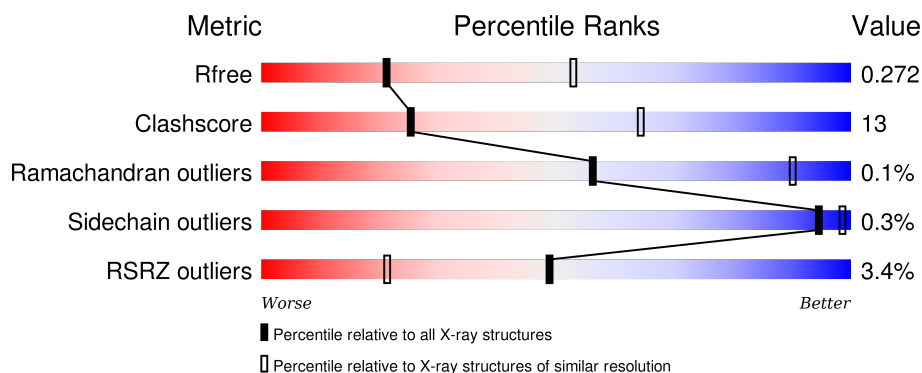
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	526	<div> <div></div> <div>67% 21% 12%</div> </div>
1	B	526	<div> <div>2%</div> <div>61% 26% 12%</div> </div>
1	C	526	<div> <div></div> <div>71% 20% 8%</div> </div>
1	D	526	<div> <div>16%</div> <div>56% 32% 12%</div> </div>
1	E	526	<div> <div></div> <div>67% 21% 12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	526	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IPT	D	601	-	-	-	X
2	IPT	F	601	-	-	-	X
2	IPT	F	602	-	-	-	X
3	GOL	C	602	-	-	-	X
3	GOL	C	603	-	-	-	X
3	GOL	E	602	-	-	-	X
3	GOL	F	603	-	-	-	X

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

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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

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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

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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

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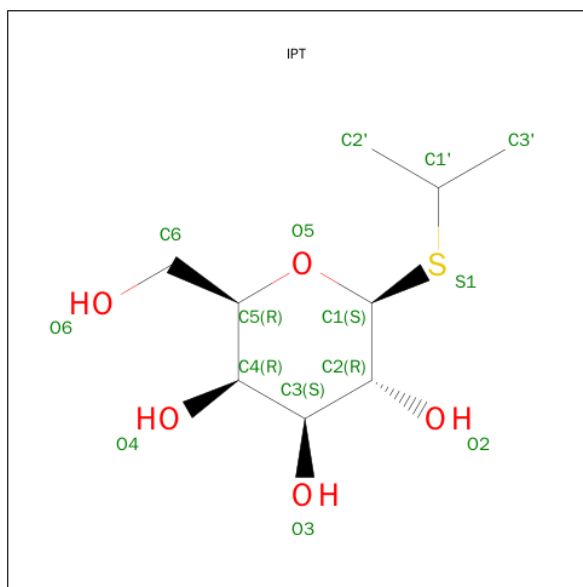
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PHE	-	EXPRESSION TAG	UNP A3DD67
E	-35	MET	-	EXPRESSION TAG	UNP A3DD67
E	-34	GLY	-	EXPRESSION TAG	UNP A3DD67
E	-33	SER	-	EXPRESSION TAG	UNP A3DD67
E	-32	SER	-	EXPRESSION TAG	UNP A3DD67
E	-31	HIS	-	EXPRESSION TAG	UNP A3DD67
E	-30	HIS	-	EXPRESSION TAG	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

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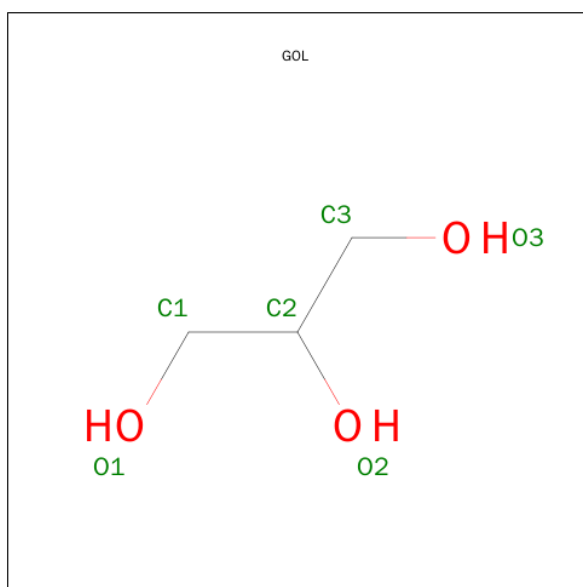
Chain	Residue	Modelled	Actual	Comment	Reference
F	-30	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-29	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-28	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-27	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-26	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-25	SER	-	EXPRESSION TAG	UNP A3DD67
F	-24	SER	-	EXPRESSION TAG	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 ISOPROPYL-1-BETA-D-THIOGALACTOSIDE (three-letter code: IPT) (formula: C₉H₁₈O₅S).



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 (three-letter code: GOL) (formula: C₃H₈O₃).

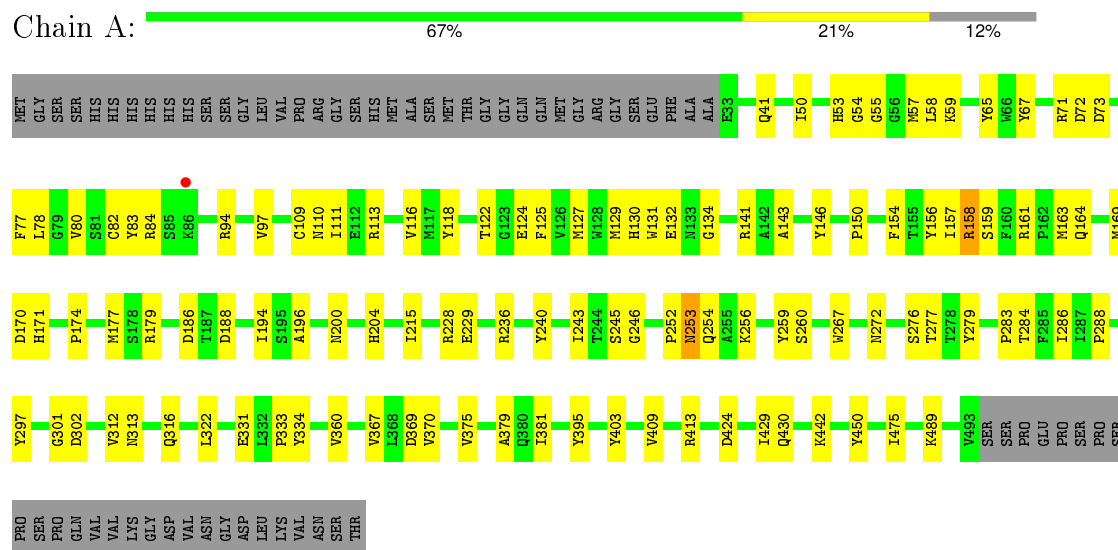


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

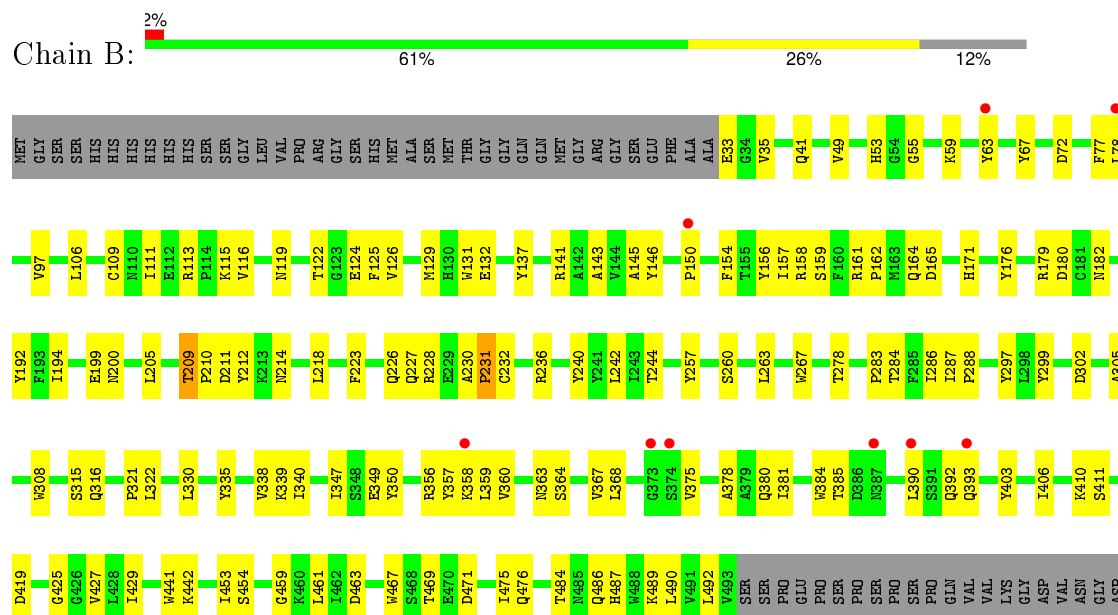
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ricin B lectin



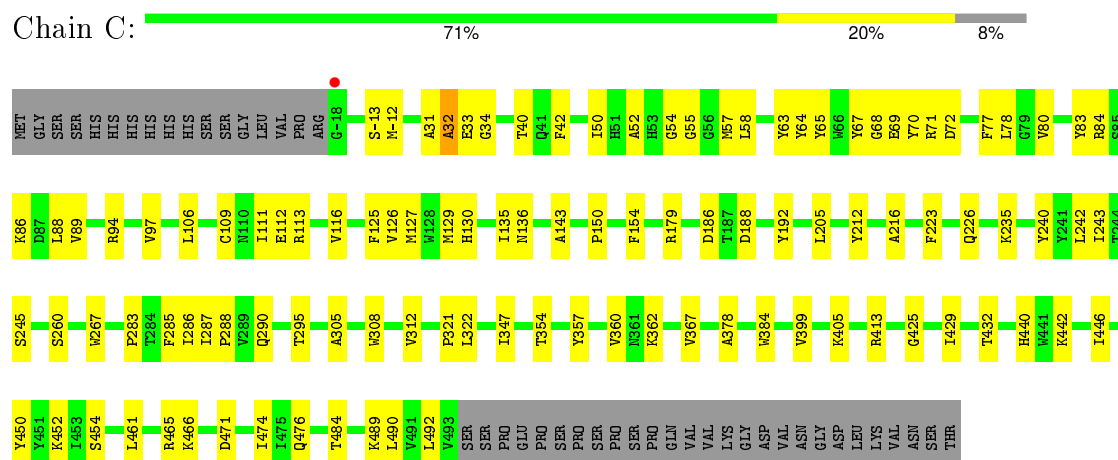
• Molecule 1: Ricin B lectin



LEU
LYS
VAL
ASN
SER
THR

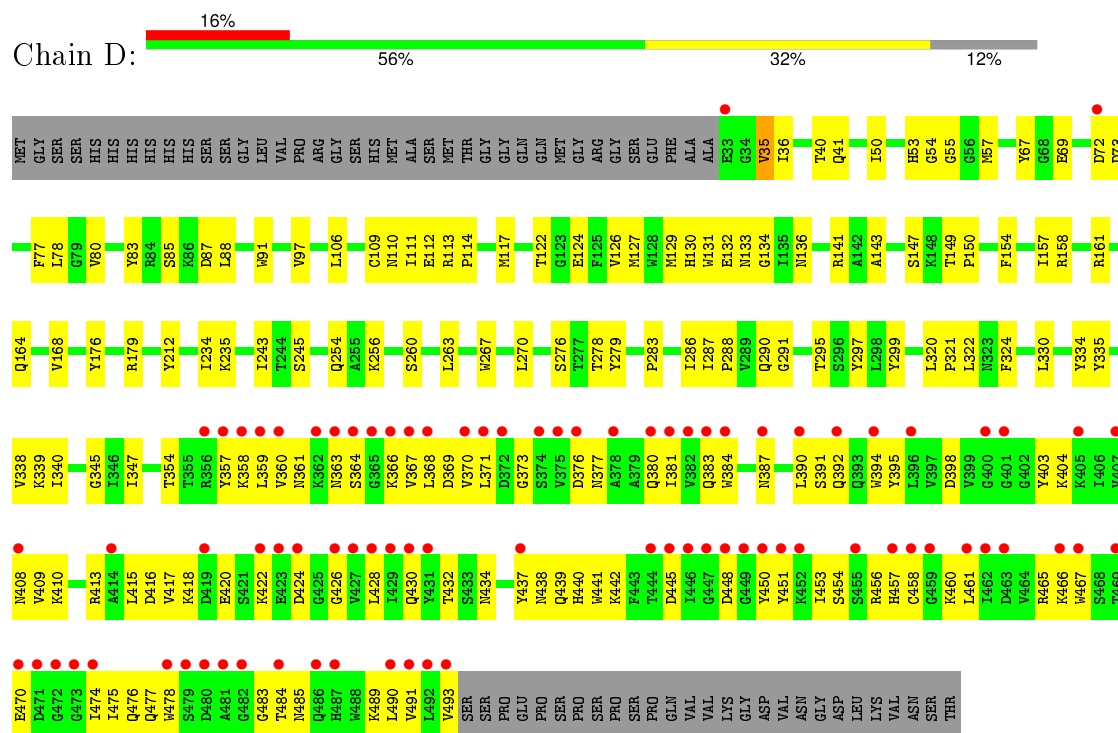
• Molecule 1: Ricin B lectin

Chain C:



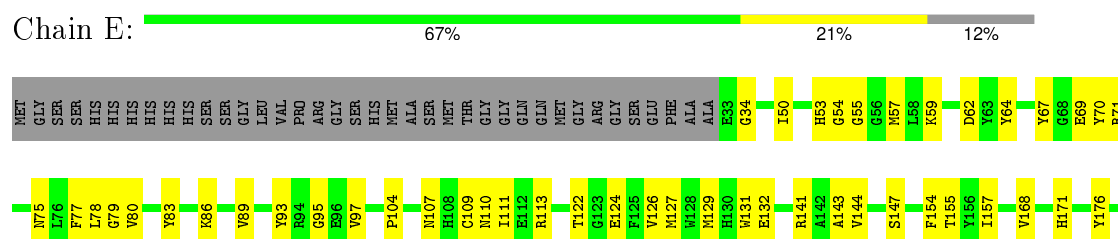
• Molecule 1: Ricin B lectin

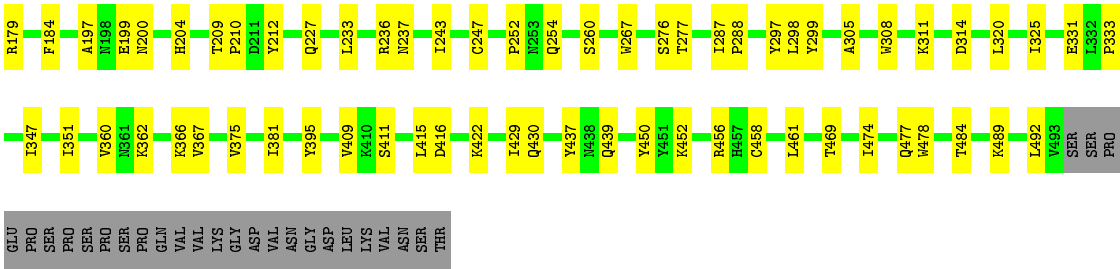
Chain D:



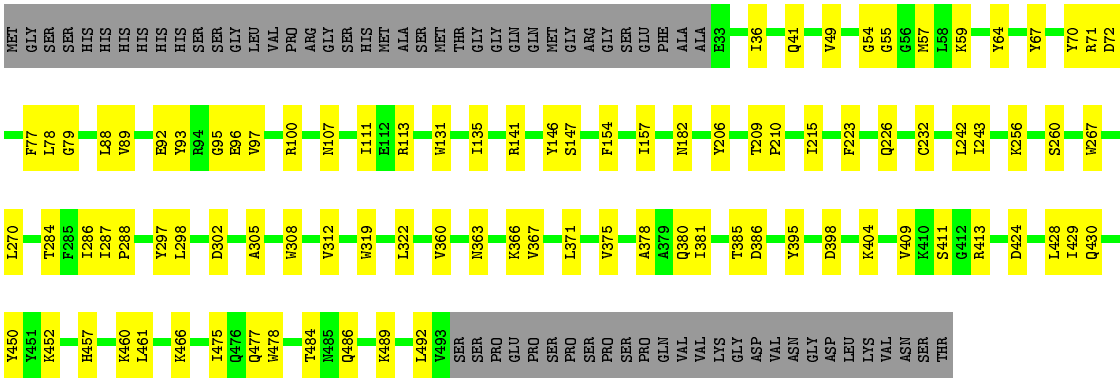
• Molecule 1: Ricin B lectin

Chain E:





● 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 47.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.0 (44.71-3.00) 83.0 (47.00-3.00)	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 (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.245 , 0.271 0.245 , 0.272	Depositor DCC
R_{free} test set	1586 reflections (1.82%)	DCC
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 88879 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.20	0/3762	0.34	0/5104
1	B	0.20	0/3762	0.34	0/5104
1	C	0.20	0/3907	0.34	0/5295
1	D	0.20	0/3762	0.34	0/5104
1	E	0.20	0/3762	0.34	0/5104
1	F	0.20	0/3762	0.35	0/5104
All	All	0.20	0/22717	0.34	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	88	0
1	B	3664	0	3480	104	0
1	C	3807	0	3613	85	0
1	D	3664	0	3480	140	0
1	E	3664	0	3480	72	0
1	F	3664	0	3480	65	0
2	A	15	0	18	0	0

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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	546	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 (546) 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: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:-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:D:57:MET:HE2	1:D:287:ILE:HG21	1.65	0.79
1:B:72:ASP:HB3	1:B:78:LEU:HG	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:375:VAL:C	1:A:413:ARG:HH22	1.96	0.67
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:E:54:GLY:O	1:E:113:ARG:HA	1.95	0.67
1:D:403:TYR:HB3	1:D:440:HIS:HB3	1.75	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:A:229:GLU:HG2	1:A:246:GLY:O	1.96	0.66
1:F:182:ASN:HD22	1:F:232:CYS:HA	1.61	0.66
1:B:364:SER:HA	1:B:469:THR:HG23	1.77	0.66
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:E:416:ASP:CB	1:E:439:GLN:HG2	2.27	0.64
1:B:378:ALA:HA	1:B:429:ILE:HD12	1.78	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
1:E:144:VAL:HG13	1:E:157:ILE:HB	1.78	0.64
1:E:57:MET:HE2	1:E:287:ILE:HD13	1.79	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:358:LYS:HE3	1:D:493:VAL:HG21	1.81	0.62
1:B:122:THR:HG23	1:B:124:GLU:H	1.65	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:C:57:MET:HE2	1:C:287:ILE:HD13	1.81	0.61
1:D:465:ARG:HD3	1:D:474:ILE:HB	1.81	0.61
1:B:223:PHE:HE2	1:B:242:LEU:HD23	1.63	0.61
1:B:97:VAL:HB	1:B:154:PHE:CD2	2.35	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:D:321:PRO:HD3	1:D:338:VAL:HG11	1.82	0.60
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:F:450:TYR:CE1	1:F:489:LYS:HB2	2.37	0.60
1:D:245:SER:HB3	1:D:283:PRO:HD2	1.82	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:D:72:ASP:CG	1:D:73:ASP:H	2.05	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:117:MET:HE3	1:D:212:TYR:HB3	1.84	0.59
1:D:35:VAL:HG22	1:D:36:ILE:N	2.14	0.59
1:C:80:VAL:HG11	1:C:127:MET:HE3	1.84	0.59
1:B:406:ILE:HD13	1:B:441:TRP:CD1	2.39	0.58
1:D:426:GLY:O	1:D:476:GLN:HB2	2.03	0.58
1:A:84:ARG:HD3	1:A:94:ARG:HH11	1.66	0.58
1:F:286:ILE:HD13	1:F:322:LEU:HD22	1.83	0.58
1:F:57:MET:HE2	1:F:287:ILE:HD13	1.85	0.58
1:A:130:HIS:CD2	1:A:179:ARG:HA	2.39	0.58
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:F:375:VAL:HG12	1:F:411:SER:HB3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:284:THR:HG21	1:F:302:ASP:OD2	2.03	0.58
1:B:171:HIS:CE1	1:B:199:GLU:HB2	2.39	0.58
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:D:366:LYS:HB2	1:D:383:GLN:OE1	2.04	0.57
1:F:366:LYS:HE3	1:F:385:THR:HG22	1.87	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:D:260:SER:HB2	1:D:267:TRP:HA	1.87	0.57
1:D:460:LYS:C	1:D:461:LEU:HD23	2.24	0.57
1:E:171:HIS:CE1	1:E:199:GLU:HB2	2.40	0.57
1:D:450:TYR:HB3	1:D:489:LYS:HG2	1.86	0.57
1:A:157:ILE:HG22	1:A:158:ARG:HG2	1.87	0.57
1:D:359:LEU:HD22	1:D:490:LEU:HA	1.86	0.57
1:A:228:ARG:NH1	1:A:256:LYS:HD2	2.20	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:A:450:TYR:CE1	1:A:489:LYS:HB2	2.39	0.56
1:D:129:MET:HG3	1:D:143:ALA:HB3	1.87	0.56
1:C:54:GLY:O	1:C:113:ARG:HA	2.05	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:A:67:TYR:HE1	1:A:82:CYS:HG	1.53	0.56
1:E:168:VAL:HG11	1:E:176:TYR:CE1	2.40	0.56
1:E:80:VAL:HG11	1:E:127:MET:HE3	1.88	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:D:454:SER:HA	1:D:461:LEU:HD22	1.88	0.56
1:B:182:ASN:HB2	1:B:231:PRO:HG2	1.87	0.56
1:A:288:PRO:HG3	1:A:297:TYR:CE1	2.41	0.56
1:D:340:ILE:HG22	1:D:347:ILE:HG23	1.87	0.56
1:A:71:ARG:NH1	1:A:312:VAL:HG11	2.21	0.56
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:C:125:PHE:CZ	1:C:150:PRO:HG3	2.42	0.55
1:D:381:ILE:HD11	1:D:430:GLN:CD	2.26	0.55
1:D:377:ASN:HA	1:D:413:ARG:NH2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:LYS:HD3	1:F:64:TYR:CE1	2.42	0.55
1:C:106:LEU:HD22	1:C:111:ILE:HD11	1.89	0.55
1:F:395:TYR:CE2	1:F:409:VAL:HG22	2.42	0.55
1:E:366:LYS:HE2	1:E:469:THR:O	2.06	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:F:100:ARG:HD2	1:F:107:ASN:O	2.07	0.54
1:D:417:VAL:HG21	1:D:477:GLN:NE2	2.23	0.54
1:D:448:ASP:HB2	1:D:450:TYR:CD2	2.43	0.54
1:B:97:VAL:HB	1:B:154:PHE:HD2	1.72	0.54
1:A:110:ASN:HB2	1:A:132:GLU:HB2	1.89	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: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: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: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:F:54:GLY:O	1:F:113:ARG:HA	2.08	0.53
1:A:116:VAL:HG22	1:A:127:MET:HB2	1.90	0.53
1:B:368:LEU:CD1	1:B:475:ILE:HD12	2.38	0.53
1:A:129:MET:HG2	1:A:143:ALA:HB3	1.90	0.53
1:D:437:TYR:O	1:D:456:ARG:HB3	2.09	0.53
1:A:118:TYR:CD1	1:A:125:PHE:HE1	2.26	0.53
1:D:110:ASN:HB2	1:D:132:GLU:HB2	1.89	0.53
1:B:230:ALA:O	1:B:244:THR:HA	2.08	0.53
1:A:256:LYS:HE2	1:A:272:ASN:ND2	2.23	0.53
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:106:LEU:HD11	1:B:156:TYR:CD2	2.44	0.53
1:B:41:GLN:HB3	1:B:49:VAL:HG23	1.89	0.53
1:B:284:THR:HG21	1:B:302:ASP:OD2	2.08	0.53
1:B:146:TYR:HD2	1:B:157:ILE:HD11	1.74	0.53
1:A:97:VAL:HB	1:A:154:PHE:CD2	2.44	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:F:131:TRP:HB3	1:F:141:ARG:HG3	1.91	0.52
1:B:59:LYS:HZ3	1:B:63:TYR:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ILE:HD11	1:D:286:ILE:O	2.08	0.52
1:B:55:GLY:HA3	1:B:67:TYR:O	2.09	0.52
1:A:395:TYR:CE2	1:A:409:VAL:HG22	2.44	0.52
1:A:80:VAL:HG11	1:A:127:MET:HE3	1.91	0.52
1:E:71:ARG:HH11	1:E:75:ASN:ND2	2.07	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:93:TYR:CZ	1:F:95:GLY:HA2	2.44	0.52
1:A:77:PHE:CD1	1:A:111:ILE:HB	2.45	0.52
1:C:63:TYR:CG	1:C:84:ARG:HD2	2.44	0.52
1:A:118:TYR:CD1	1:A:125:PHE:CE1	2.96	0.52
1:B:484:THR:HA	1:B:487:HIS:HD2	1.73	0.52
1:B:156:TYR:OH	1:B:159:SER:HB3	2.10	0.52
1:B:125:PHE:CZ	1:B:150:PRO:HG3	2.44	0.52
1:C:442:LYS:HE3	1:F:100:ARG:CZ	2.39	0.52
1:C:55:GLY:HA3	1:C:67:TYR:O	2.09	0.52
1:D:448:ASP:HB2	1:D:450:TYR:CE2	2.45	0.52
1:D:291:GLY:HA3	1:D:345:GLY:HA3	1.90	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:F:41:GLN:HB3	1:F:49:VAL:HG13	1.91	0.51
1:C:69:GLU:OE1	1:C:112:GLU:HA	2.10	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:321:PRO:HB3	1:B:347:ILE:HG22	1.92	0.51
1:B:41:GLN:HG3	1:B:316:GLN:HG2	1.93	0.51
1:B:363:ASN:HD22	1:B:467:TRP:HE3	1.58	0.51
1:D:363:ASN:OD1	1:D:484:THR:HB	2.11	0.51
1:C:290:GLN:HG3	1:C:295:THR:HG22	1.91	0.51
1:D:55:GLY:HA3	1:D:67:TYR:O	2.10	0.51
1:A:146:TYR:CD2	1:A:157:ILE:HD11	2.46	0.51
1:A:72:ASP:CG	1:A:73:ASP:H	2.13	0.51
1:C:-13:SER:HA	1:C:492:LEU:HD11	1.93	0.51
1:D:394:TRP:HH2	1:D:430:GLN:HE21	1.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:C	1:A:253:ASN:HD22	2.14	0.50
1:B:356:ARG:HG2	1:B:393:GLN:OE1	2.11	0.50
1:C:399:VAL:O	1:C:399:VAL:HG12	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:D:381:ILE:HD11	1:D:430:GLN:NE2	2.27	0.50
1:D:358:LYS:O	1:D:491:VAL:HB	2.11	0.50
1:B:283:PRO:HB3	1:B:299:TYR:HE1	1.76	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:B:157:ILE:HD12	1:B:157:ILE:N	2.27	0.49
1:A:54:GLY:O	1:A:113:ARG:HA	2.12	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:256:LYS:HE2	1:A:272:ASN:HD21	1.76	0.49
1:A:125:PHE:HE2	1:A:150:PRO:HB3	1.78	0.49
1:D:234:ILE:HD11	1:D:286:ILE:C	2.33	0.49
1:D:445:ASP:HA	1:D:451:TYR:HB3	1.93	0.49
1:C:129:MET:HG2	1:C:143:ALA:HB3	1.94	0.49
1:E:236:ARG:HG2	1:E:237:ASN:OD1	2.13	0.49
1:E:375:VAL:HG12	1:E:411:SER:HB3	1.95	0.49
1:B:200:ASN:O	1:B:227:GLN:HA	2.12	0.49
1:D:442:LYS:HB3	1:D:454:SER:OG	2.12	0.49
1:A:245:SER:CB	1:A:283:PRO:HD2	2.40	0.49
1:D:361:ASN:HB3	1:D:364:SER:OG	2.13	0.49
1:C:223:PHE:HE2	1:C:242:LEU:HD23	1.77	0.49
1:D:465:ARG:O	1:D:466:LYS:HG2	2.11	0.49
1:A:55:GLY:HA3	1:A:67:TYR:O	2.13	0.49
1:E:131:TRP:CE3	1:E:141:ARG:HD2	2.48	0.49
1:F:70:TYR:HD1	1:F:96:GLU:OE2	1.96	0.48
1:A:196:ALA:HB1	1:A:200:ASN:HA	1.95	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:F:223:PHE:CE2	1:F:242:LEU:HD23	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:TYR:HB3	1:E:320:LEU:O	2.13	0.48
1:D:338:VAL:O	1:D:340:ILE:HG23	2.13	0.48
1:F:430:GLN:O	1:F:430:GLN:HG3	2.14	0.48
1:D:114:PRO:HB2	1:D:127:MET:HE3	1.94	0.48
1:F:55:GLY:HA3	1:F:67:TYR:O	2.13	0.48
1:E:260:SER:HB2	1:E:267:TRP:HA	1.96	0.48
1:A:110:ASN:OD1	1:A:134:GLY:HA2	2.14	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:156:TYR:OH	1:A:159:SER:HB3	2.13	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:298:LEU:HD11	1:F:319:TRP:HB3	1.96	0.48
1:F:71:ARG:HD3	1:F:312:VAL:HG11	1.96	0.48
1:D:416:ASP:CG	1:D:439:GLN:HG3	2.34	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:D:364:SER:HB2	1:D:383:GLN:OE1	2.14	0.47
1:C:378:ALA:HA	1:C:429:ILE:HD12	1.96	0.47
1:C:40:THR:HB	1:F:92:GLU:OE2	2.14	0.47
1:D:149:THR:HG23	1:D:150:PRO:HD2	1.96	0.47
1:A:381:ILE:HD13	1:A:429:ILE:HA	1.94	0.47
1:D:131:TRP:CE3	1:D:141:ARG:HD2	2.49	0.47
1:B:286:ILE:HD13	1:B:322:LEU:HD22	1.95	0.47
1:A:360:VAL:CG2	1:A:489:LYS:HB3	2.43	0.47
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:B:109:CYS:HB2	1:B:132:GLU:O	2.15	0.47
1:C:80:VAL:HG21	1:C:127:MET:HE1	1.97	0.47
1:F:147:SER:HB2	1:F:154:PHE:HA	1.96	0.47
1:C:362:LYS:HE3	1:C:484:THR:HG22	1.96	0.47
1:D:147:SER:HB2	1:D:154:PHE:HA	1.96	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:71:ARG:HH11	1:A:312:VAL:HG11	1.79	0.47
1:F:182:ASN:ND2	1:F:232:CYS:HA	2.27	0.47
1:A:53:HIS:HE2	1:A:313:ASN:HA	1.79	0.47
1:E:70:TYR:O	1:E:78:LEU:HB3	2.15	0.47
1:D:106:LEU:HA	1:D:109:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ARG:NH1	1:C:312:VAL:HG11	2.30	0.47
1:B:339:LYS:HB2	1:B:350:TYR:HB2	1.97	0.47
1:D:387:ASN:N	1:D:392:GLN:HE22	2.05	0.47
1:A:413:ARG:HE	1:A:430:GLN:HG3	1.79	0.47
1:B:453:ILE:N	1:B:453:ILE:HD12	2.30	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:D:278:THR:O	1:D:278:THR:HG22	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:321:PRO:HB3	1:D:347:ILE:CG2	2.45	0.46
1:C:31:ALA:O	1:C:32:ALA:C	2.54	0.46
1:D:234:ILE:HG22	1:D:235:LYS:N	2.31	0.46
1:D:77:PHE:HB2	1:D:111:ILE:H	1.80	0.46
1:E:70:TYR:HB3	1:E:79:GLY:O	2.16	0.46
1:C:354:THR:O	1:C:354:THR:HG22	2.16	0.46
1:A:131:TRP:CE3	1:A:141:ARG:HD2	2.51	0.46
1:C:80:VAL:HG21	1:C:127:MET:CE	2.45	0.46
1:A:169:MET:HE2	1:A:174:PRO:HA	1.97	0.46
1:F:72:ASP:HB3	1:F:78:LEU:HD11	1.97	0.46
1:F:70:TYR:CD1	1:F:96:GLU:OE2	2.69	0.46
1:B:335:TYR:HB2	1:B:338:VAL:HG22	1.98	0.46
1:A:254:GLN:OE1	1:A:276:SER:HA	2.16	0.46
1:C:106:LEU:HA	1:C:109:CYS:SG	2.56	0.46
1:D:80:VAL:HG21	1:D:127:MET:HE1	1.98	0.46
1:D:97:VAL:HB	1:D:154:PHE:CD2	2.50	0.46
1:C:192:TYR:HB3	1:C:205:LEU:HD11	1.98	0.46
1:D:390:LEU:O	1:D:410:LYS:HB2	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:F:64:TYR:CG	1:F:88:LEU:HD21	2.51	0.45
1:B:226:GLN:HB3	1:B:228:ARG:HG2	1.98	0.45
1:F:461:LEU:CD1	1:F:486:GLN:HB3	2.43	0.45
1:E:57:MET:CE	1:E:287:ILE:HG21	2.46	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: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:E:325:ILE:HD11	1:E:331:GLU:OE2	2.16	0.45
1:F:413:ARG:HB2	1:F:430:GLN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:381:ILE:HG12	1:E:429:ILE:HA	1.97	0.45
1:E:351:ILE:N	1:E:351:ILE:HD12	2.32	0.45
1:E:34:GLY:HA2	1:E:89:VAL:HG21	1.97	0.45
1:C:77:PHE:CZ	1:C:111:ILE:HD12	2.51	0.45
1:A:97:VAL:HB	1:A:154:PHE:HD2	1.81	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:403:TYR:CE1	1:B:442:LYS:HG2	2.52	0.45
1:B:288:PRO:HG3	1:B:297:TYR:CE1	2.52	0.45
1:F:492:LEU:HD12	1:F:492:LEU:N	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:D:161:ARG:O	1:D:164:GLN:HB3	2.16	0.45
1:C:-13:SER:HA	1:C:492:LEU:CD1	2.47	0.45
1:A:194:ILE:HD12	1:A:204:HIS:O	2.17	0.45
1:B:359:LEU:HD12	1:B:368:LEU:HD22	1.98	0.45
1:B:145:ALA:HA	1:B:157:ILE:CD1	2.47	0.45
1:B:119:ASN:HB2	1:B:212:TYR:CD2	2.52	0.45
1:E:252:PRO:HB2	1:E:277:THR:CG2	2.47	0.45
1:D:87:ASP:O	1:D:88:LEU:HB2	2.16	0.45
1:C:126:VAL:HG21	1:C:212:TYR:HB2	1.98	0.45
1:D:376:ASP:C	1:D:413:ARG:HH12	2.21	0.44
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:E:277:THR:HG22	1:E:277:THR:O	2.17	0.44
1:B:463:ASP:OD1	3:B:602:GOL:H11	2.18	0.44
1:B:257:TYR:CE2	1:B:330:LEU:HD13	2.52	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
1:C:57:MET:HE2	1:C:287:ILE:HG21	2.00	0.44
1:E:474:ILE:N	1:E:474:ILE:HD12	2.31	0.44
1:E:62:ASP:O	1:E:86:LYS:HG2	2.17	0.44
1:D:243:ILE:N	1:D:243:ILE:HD12	2.32	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:B:230:ALA:CB	1:B:283:PRO:HG2	2.48	0.44
1:B:218:LEU:HD12	1:B:218:LEU:O	2.17	0.44
1:B:209:THR:OG1	1:B:210:PRO:HD2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:TYR:CE2	1:A:334:TYR:HB2	2.52	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:E:59:LYS:HD3	1:E:64:TYR:CE1	2.52	0.44
1:D:263:LEU:HD12	1:D:263:LEU:H	1.83	0.44
1:B:129:MET:CG	1:B:143:ALA:HB3	2.48	0.44
1:D:111:ILE:HD11	1:D:131:TRP:HD1	1.81	0.44
1:B:278:THR:O	1:B:278:THR:HG22	2.18	0.44
1:A:125:PHE:HD2	1:A:150:PRO:HA	1.83	0.44
1:C:399:VAL:HG11	1:C:440:HIS:CE1	2.53	0.44
1:E:109:CYS:HB2	1:E:132:GLU:O	2.17	0.44
1:C:245:SER:HB3	1:C:283:PRO:HD2	2.00	0.44
1:D:297:TYR:CD2	1:D:324:PHE:CE2	3.06	0.44
1:A:57:MET:HA	1:A:65:TYR:O	2.18	0.44
1:C:42:PHE:CE2	1:C:50:ILE:HD12	2.53	0.43
1:A:129:MET:CG	1:A:143:ALA:HB3	2.47	0.43
1:C:126:VAL:HG11	1:C:212:TYR:O	2.18	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:D:451:TYR:OH	1:D:490:LEU:HD13	2.18	0.43
1:D:359:LEU:O	1:D:367:VAL:HG13	2.18	0.43
1:B:115:LYS:HG3	1:B:182:ASN:HA	2.00	0.43
1:F:70:TYR:O	1:F:78:LEU:HB2	2.18	0.43
1:E:362:LYS:HG2	1:E:484:THR:HB	1.99	0.43
1:D:288:PRO:HG3	1:D:297:TYR:CE1	2.52	0.43
1:E:452:LYS:HG2	1:E:461:LEU:HD22	2.00	0.43
1:C:223:PHE:CE2	1:C:242:LEU:HD23	2.52	0.43
1:A:279:TYR:CD2	1:A:334:TYR:HB2	2.52	0.43
1:F:288:PRO:HB3	1:F:297:TYR:CE1	2.54	0.43
1:C:135:ILE:HG13	1:C:136:ASN:ND2	2.34	0.43
1:B:131:TRP:CE3	1:B:141:ARG:HD2	2.54	0.43
1:D:83:TYR:HB3	1:D:91:TRP:HB3	2.00	0.43
1:C:399:VAL:HG21	1:C:405:LYS:HB2	2.00	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:D:340:ILE:CG2	1:D:347:ILE:HG23	2.47	0.43
1:B:321:PRO:HB3	1:B:347:ILE:CG2	2.48	0.43
1:C:287:ILE:HA	1:C:288:PRO:HD3	1.88	0.43
1:E:110:ASN:HB3	1:E:132:GLU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:395:TYR:CE2	1:E:409:VAL:HG22	2.54	0.43
1:C:58:LEU:HD22	1:C:116:VAL:HG12	2.00	0.43
1:D:369:ASP:OD1	1:D:391:SER:HB2	2.19	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:E:197:ALA:HB3	1:E:204:HIS:CE1	2.54	0.43
1:A:50:ILE:HG23	1:A:83:TYR:CE1	2.53	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:E:147:SER:HB2	1:E:154:PHE:HA	2.01	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: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:D:413:ARG:HG2	1:D:432:THR:HA	2.00	0.42
1:D:50:ILE:HG23	1:D:83:TYR:CE1	2.54	0.42
1:C:466:LYS:H	3:C:602:GOL:C1	2.32	0.42
1:D:354:THR:O	1:D:354:THR:HG22	2.19	0.42
1:D:40:THR:HG22	1:D:41:GLN:N	2.34	0.42
1:A:370:VAL:HG11	1:A:430:GLN:NE2	2.34	0.42
1:E:144:VAL:HG22	1:E:157:ILE:HD12	2.02	0.42
1:C:285:PHE:HE2	1:C:287:ILE:HB	1.85	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:425:GLY:HA2	1:B:476:GLN:OE1	2.19	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:E:227:GLN:OE1	1:E:247:CYS:HB3	2.19	0.42
1:A:215:ILE:N	1:A:215:ILE:HD12	2.35	0.42
1:D:441:TRP:HB3	1:D:453:ILE:HG22	2.01	0.42
1:D:130:HIS:NE2	1:D:179:ARG:HA	2.35	0.42
1:F:77:PHE:CZ	1:F:79:GLY:HA2	2.55	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: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:E:381:ILE:HG13	1:E:415:LEU:CD1	2.50	0.42
1:C:305:ALA:HA	1:C:308:TRP:CZ2	2.54	0.42
1:F:466:LYS:H	3:F:603:GOL:C3	2.33	0.42
1:F:209:THR:HB	1:F:210:PRO:HD2	2.02	0.42
1:D:370:VAL:CG2	1:D:373:GLY:HA2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:TRP:HB3	1:D:453:ILE:CG2	2.50	0.42
1:C:57:MET:CE	1:C:287:ILE:HG21	2.50	0.42
1:B:182:ASN:HD22	1:B:232:CYS:HA	1.85	0.42
1:E:254:GLN:OE1	1:E:276:SER:HA	2.19	0.42
1:B:77:PHE:CE2	1:B:111:ILE:HD12	2.54	0.42
1:E:362:LYS:HB2	1:E:450:TYR:CE1	2.55	0.42
1:F:378:ALA:HA	1:F:429:ILE:HD12	2.01	0.42
1:E:461:LEU:O	1:E:477:GLN:HA	2.20	0.42
1:F:97:VAL:HB	1:F:154:PHE:HD2	1.80	0.41
1:E:57:MET:HE2	1:E:287:ILE:HG21	2.00	0.41
1:B:236:ARG:HB2	1:B:297:TYR:OH	2.20	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:A:41:GLN:HG3	1:A:316:GLN:HG2	2.02	0.41
1:D:394:TRP:CZ3	1:D:408:ASN:HB3	2.55	0.41
1:B:194:ILE:HG23	1:B:231:PRO:HB2	2.02	0.41
1:D:85:SER:HB2	1:D:91:TRP:HA	2.02	0.41
1:B:162:PRO:HD2	1:B:176:TYR:O	2.20	0.41
1:F:36:ILE:HD11	1:F:89:VAL:HG22	2.01	0.41
1:C:52:ALA:HB1	1:C:68:GLY:HA3	2.01	0.41
1:B:126:VAL:HG21	1:B:212:TYR:HB2	2.02	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:C:243:ILE:N	1:C:243:ILE:HD12	2.35	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: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:D:279:TYR:CD2	1:D:334:TYR:HB2	2.56	0.41
1:F:57:MET:HE1	1:F:287:ILE:HG21	2.02	0.41
1:C:384:TRP:CZ3	1:C:471:ASP:HB3	2.55	0.41
1:B:305:ALA:HA	1:B:308:TRP:CH2	2.56	0.41
1:B:119:ASN:HB3	1:B:122:THR:CG2	2.51	0.41
1:C:42:PHE:HD2	1:C:50:ILE:HD12	1.83	0.41
1:E:104:PRO:HA	1:E:107:ASN:OD1	2.21	0.41
1:E:437:TYR:CG	1:E:456:ARG:HD3	2.56	0.41
1:E:298:LEU:HB2	1:E:347:ILE:CD1	2.51	0.41
1:D:290:GLN:OE1	1:D:295:THR:HB	2.21	0.41
1:B:454:SER:HB2	1:B:459:GLY:O	2.20	0.41
1:D:366:LYS:HB3	1:D:384:TRP:C	2.41	0.41
1:C:-13:SER:OG	1:C:490:LEU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ASP:OD1	2:B:601:IPT:H3'2	2.21	0.41
1:E:243:ILE:HD12	1:E:243:ILE:N	2.36	0.41
1:A:403:TYR:CD1	1:A:442:LYS:HB2	2.56	0.41
1:B:359:LEU:O	1:B:367:VAL:HA	2.20	0.40
1:D:467:TRP:CH2	1:D:483:GLY:HA2	2.56	0.40
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: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
1:B:209:THR:HG22	1:B:214:ASN:O	2.22	0.40
1:C:186:ASP:HB3	1:C:188:ASP:OD1	2.21	0.40
1:C:450:TYR:CE1	1:C:489:LYS:HB2	2.57	0.40
1:B:385:THR:HG23	1:B:471:ASP:OD1	2.21	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:288:PRO:HB3	1:E:297:TYR:CE1	2.57	0.40
1:F:452:LYS:HB2	1:F:461:LEU:HD22	2.04	0.40
1:A:84:ARG:NE	1:A:94:ARG:HD3	2.36	0.40
1:D:360:VAL:HG22	1:D:361:ASN:N	2.37	0.40
1:F:70:TYR:HB3	1:F:79:GLY:O	2.22	0.40
1:C:64:TYR:CG	1:C:88:LEU:HD21	2.56	0.40
1:E:311:LYS:HG2	1:E:314:ASP:OD2	2.21	0.40
1:F:398:ASP:HA	1:F:404:LYS:HG2	2.04	0.40
1:C:425:GLY:HA2	1:C:476:GLN:CD	2.42	0.40
1:B:119:ASN:HB2	1:B:212:TYR:CE2	2.57	0.40
1:F:57:MET:CE	1:F:287:ILE:HG21	2.51	0.40
1:B:156:TYR:HH	1:B:159:SER:HB3	1.87	0.40
1:C:446:ILE:HG12	1:C:450:TYR:O	2.21	0.40
1:B:287:ILE:HA	1:B:288:PRO:HD3	1.91	0.40
1:F:460:LYS:HB2	1:F:477:GLN:HG2	2.03	0.40
1:F:243:ILE:N	1:F:243:ILE:HD12	2.37	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	459/526 (87%)	431 (94%)	28 (6%)	0	100	100
1	B	459/526 (87%)	424 (92%)	34 (7%)	1 (0%)	52	88
1	C	480/526 (91%)	453 (94%)	26 (5%)	1 (0%)	52	88
1	D	459/526 (87%)	423 (92%)	35 (8%)	1 (0%)	52	88
1	E	459/526 (87%)	439 (96%)	20 (4%)	0	100	100
1	F	459/526 (87%)	439 (96%)	19 (4%)	1 (0%)	52	88
All	All	2775/3156 (88%)	2609 (94%)	162 (6%)	4 (0%)	56	90

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%)	387 (100%)	2 (0%)	92	98
1	B	389/442 (88%)	387 (100%)	2 (0%)	92	98
1	C	402/442 (91%)	402 (100%)	0	100	100
1	D	389/442 (88%)	388 (100%)	1 (0%)	94	98
1	E	389/442 (88%)	389 (100%)	0	100	100
1	F	389/442 (88%)	388 (100%)	1 (0%)	94	98
All	All	2347/2652 (88%)	2341 (100%)	6 (0%)	94	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ARG
1	A	253	ASN
1	B	180	ASP
1	B	209	THR
1	D	470	GLU
1	F	457	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	272	ASN
1	A	430	GLN
1	B	53	HIS
1	B	171	HIS
1	B	272	ASN
1	B	430	GLN
1	B	487	HIS
1	C	200	ASN
1	D	38	ASN
1	D	119	ASN
1	D	136	ASN
1	D	164	GLN
1	D	392	GLN
1	D	430	GLN
1	D	457	HIS
1	D	477	GLN
1	E	108	HIS
1	E	171	HIS
1	F	171	HIS
1	F	269	GLN
1	F	476	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](#)

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	$\# Z > 2$
2	IPT	A	601	-	15,15,15	0.72	1 (6%)	19,21,21	0.77	0
3	GOL	A	602	-	5,5,5	0.34	0	5,5,5	0.24	0
2	IPT	B	601	-	15,15,15	0.73	1 (6%)	19,21,21	0.84	1 (5%)
3	GOL	B	602	-	5,5,5	0.34	0	5,5,5	0.26	0
2	IPT	C	601	-	15,15,15	0.74	1 (6%)	19,21,21	0.95	2 (10%)
3	GOL	C	602	-	5,5,5	0.34	0	5,5,5	0.26	0
3	GOL	C	603	-	5,5,5	0.33	0	5,5,5	0.21	0
2	IPT	D	601	-	15,15,15	0.72	1 (6%)	19,21,21	0.87	1 (5%)
2	IPT	E	601	-	15,15,15	0.74	1 (6%)	19,21,21	1.10	2 (10%)
3	GOL	E	602	-	5,5,5	0.36	0	5,5,5	0.22	0
3	GOL	E	603	-	5,5,5	0.34	0	5,5,5	0.23	0
2	IPT	F	601	-	15,15,15	0.74	1 (6%)	19,21,21	0.90	1 (5%)
2	IPT	F	602	-	15,15,15	0.74	1 (6%)	19,21,21	1.23	3 (15%)
3	GOL	F	603	-	5,5,5	0.34	0	5,5,5	0.23	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
2	IPT	A	601	-	-	0/6/26/26	0/1/1/1
3	GOL	A	602	-	-	0/4/4/4	0/0/0/0
2	IPT	B	601	-	-	0/6/26/26	0/1/1/1
3	GOL	B	602	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IPT	C	601	-	-	0/6/26/26	0/1/1/1
3	GOL	C	602	-	-	0/4/4/4	0/0/0/0
3	GOL	C	603	-	-	0/4/4/4	0/0/0/0
2	IPT	D	601	-	-	0/6/26/26	0/1/1/1
2	IPT	E	601	-	-	0/6/26/26	0/1/1/1
3	GOL	E	602	-	-	0/4/4/4	0/0/0/0
3	GOL	E	603	-	-	0/4/4/4	0/0/0/0
2	IPT	F	601	-	-	0/6/26/26	0/1/1/1
2	IPT	F	602	-	-	0/6/26/26	0/1/1/1
3	GOL	F	603	-	-	0/4/4/4	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	IPT	C1-S1	-2.21	1.77	1.80
2	C	601	IPT	C1-S1	-2.18	1.77	1.80
2	B	601	IPT	C1-S1	-2.17	1.77	1.80
2	A	601	IPT	C1-S1	-2.17	1.77	1.80
2	E	601	IPT	C1-S1	-2.15	1.77	1.80
2	D	601	IPT	C1-S1	-2.14	1.77	1.80
2	F	602	IPT	C1-S1	-2.09	1.77	1.80

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	602	IPT	O5-C5-C4	2.02	113.47	109.68
2	C	601	IPT	O5-C1-C2	2.07	113.00	110.19
2	D	601	IPT	C1-O5-C5	2.21	116.95	112.74
2	F	601	IPT	C1-O5-C5	2.22	116.97	112.74
2	B	601	IPT	C1-O5-C5	2.22	116.97	112.74
2	E	601	IPT	C1-O5-C5	2.32	117.17	112.74
2	C	601	IPT	C1-O5-C5	2.40	117.32	112.74
2	F	602	IPT	O5-C1-C2	2.69	113.84	110.19
2	E	601	IPT	O5-C1-C2	3.28	114.64	110.19
2	F	602	IPT	C1-O5-C5	3.40	119.22	112.74

There are no chirality outliers.

There are no torsion outliers.

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	B	602	GOL	1	0
3	C	602	GOL	1	0
2	D	601	IPT	2	0
3	E	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%)	-0.02	1 (0%) 95 87	55, 84, 107, 140	0
1	B	461/526 (87%)	0.10	9 (1%) 68 39	64, 94, 120, 138	0
1	C	482/526 (91%)	-0.19	1 (0%) 95 87	45, 62, 84, 132	0
1	D	461/526 (87%)	0.75	84 (18%) 2 1	54, 97, 178, 183	0
1	E	461/526 (87%)	-0.09	0 100 100	50, 72, 91, 115	0
1	F	461/526 (87%)	-0.14	0 100 100	43, 67, 89, 113	0
All	All	2787/3156 (88%)	0.07	95 (3%) 49 21	43, 78, 135, 183	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	430	GLN	6.8
1	D	383	GLN	6.6
1	D	380	GLN	6.4
1	D	490	LEU	6.2
1	D	374	SER	5.6
1	D	491	VAL	5.5
1	D	473	GLY	5.1
1	D	427	VAL	5.1
1	D	414	ALA	4.8
1	D	367	VAL	4.7
1	D	471	ASP	4.7
1	D	474	ILE	4.5
1	D	480	ASP	4.5
1	D	375	VAL	4.4
1	D	446	ILE	4.4
1	D	396	LEU	4.4
1	D	382	VAL	4.4
1	D	444	THR	4.3
1	D	492	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	459	GLY	4.3
1	D	423	GLU	4.2
1	D	452	LYS	4.2
1	D	484	THR	4.2
1	D	451	TYR	4.0
1	D	390	LEU	3.9
1	D	387	ASN	3.9
1	D	493	VAL	3.9
1	D	384	TRP	3.6
1	D	448	ASP	3.6
1	D	450	TYR	3.5
1	D	487	HIS	3.4
1	D	358	LYS	3.4
1	D	467	TRP	3.4
1	D	470	GLU	3.4
1	D	458	CYS	3.4
1	D	378	ALA	3.4
1	D	479	SER	3.3
1	D	364	SER	3.1
1	D	394	TRP	3.1
1	D	478	TRP	3.1
1	D	482	GLY	3.1
1	D	457	HIS	3.0
1	D	472	GLY	3.0
1	B	63	TYR	3.0
1	D	365	GLY	3.0
1	D	424	ASP	3.0
1	D	381	ILE	3.0
1	D	426	GLY	3.0
1	D	422	LYS	2.9
1	D	429	ILE	2.9
1	D	462	ILE	2.8
1	D	360	VAL	2.8
1	D	376	ASP	2.8
1	D	392	GLN	2.8
1	D	371	LEU	2.8
1	D	481	ALA	2.8
1	D	431	TYR	2.7
1	D	437	TYR	2.7
1	D	356	ARG	2.7
1	D	469	THR	2.7
1	D	466	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	366	LYS	2.7
1	B	393	GLN	2.6
1	D	33	GLU	2.6
1	D	370	VAL	2.5
1	D	359	LEU	2.5
1	D	445	ASP	2.5
1	D	461	LEU	2.5
1	D	363	ASN	2.5
1	D	372	ASP	2.5
1	D	357	TYR	2.5
1	D	401	GLY	2.5
1	D	428	LEU	2.5
1	D	407	VAL	2.4
1	D	72	ASP	2.3
1	A	86	LYS	2.3
1	D	447	GLY	2.3
1	D	368	LEU	2.3
1	D	419	ASP	2.3
1	B	78	LEU	2.2
1	B	390	LEU	2.2
1	D	449	GLY	2.2
1	B	387	ASN	2.2
1	B	150	PRO	2.2
1	D	405	LYS	2.2
1	D	362	LYS	2.2
1	D	463	ASP	2.2
1	B	374	SER	2.1
1	D	455	SER	2.1
1	D	486	GLN	2.1
1	D	408	ASN	2.1
1	C	-18	GLY	2.1
1	B	373	GLY	2.0
1	B	358	LYS	2.0
1	D	400	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	F	603	6/6	0.95	0.36	4.06	66,71,77,78	0
2	IPT	F	602	15/15	0.74	0.42	4.01	81,98,118,123	0
3	GOL	C	603	6/6	0.76	0.31	2.73	57,69,71,73	0
3	GOL	E	602	6/6	0.92	0.34	2.73	66,75,77,80	0
3	GOL	C	602	6/6	0.91	0.33	2.29	62,66,74,77	0
2	IPT	F	601	15/15	0.96	0.27	2.06	61,66,73,81	0
3	GOL	A	602	6/6	0.89	0.29	1.49	58,63,71,81	0
3	GOL	B	602	6/6	0.86	0.32	1.43	74,77,79,79	0
2	IPT	A	601	15/15	0.96	0.26	1.28	62,68,85,86	0
2	IPT	C	601	15/15	0.94	0.22	0.38	57,64,80,90	0
2	IPT	D	601	15/15	0.78	0.40	0.17	121,133,141,143	0
2	IPT	B	601	15/15	0.92	0.19	-0.23	75,81,88,100	0
2	IPT	E	601	15/15	0.95	0.17	-0.75	63,74,82,88	0
3	GOL	E	603	6/6	0.83	0.22	-	71,73,78,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.