



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:26 PM GMT

PDB ID : 4EXN  
Title : Crystal structure of mouse Interleukin-34  
Authors : Liu, H.; Leo, C.; Chen, X.; Wong, B.R.; Williams, L.T.; Lin, H.; He, X.  
Deposited on : 2012-04-30  
Resolution : 2.70 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 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

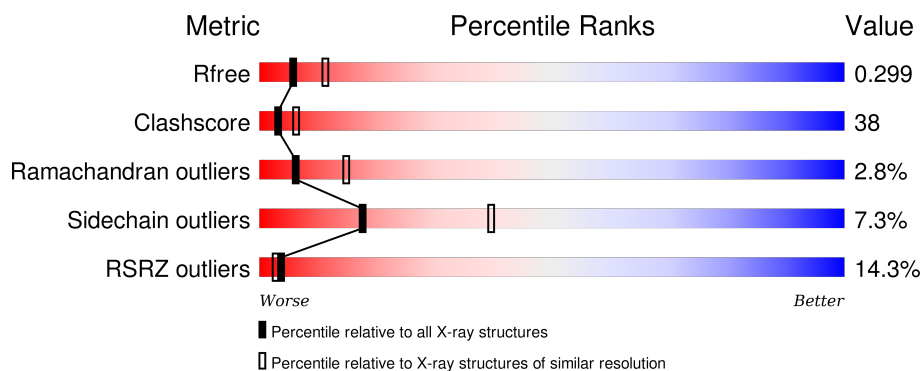
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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	175	<div> <div>5%</div> <div>49%</div> <div>43%</div> <div>6%</div> <div>••</div> </div>
1	B	175	<div> <div>9%</div> <div>46%</div> <div>41%</div> <div>6%</div> <div>• 7%</div> </div>
1	E	175	<div> <div>33%</div> <div>46%</div> <div>44%</div> <div>6%</div> <div>••</div> </div>
1	F	175	<div> <div>10%</div> <div>49%</div> <div>42%</div> <div>7%</div> <div>••</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	206	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6461 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 Interleukin-34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1408	906	240	252	10			
1	B	162	Total	C	N	O	S	0	0	0
			1322	851	227	234	10			
1	E	171	Total	C	N	O	S	0	0	0
			1397	899	238	250	10			
1	F	172	Total	C	N	O	S	0	0	0
			1408	906	240	252	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	-	EXPRESSION TAG	UNP Q8R1R4
B	195	ALA	-	EXPRESSION TAG	UNP Q8R1R4
E	195	ALA	-	EXPRESSION TAG	UNP Q8R1R4
F	195	ALA	-	EXPRESSION TAG	UNP Q8R1R4

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		
3	B	3	Total	C	N	O	0	0
			39	22	2	15		
3	E	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	5	Total	C	N	O	0	0
			61	34	2	25		
4	E	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	5	Total	C	N	O	0	0
			61	34	2	25		

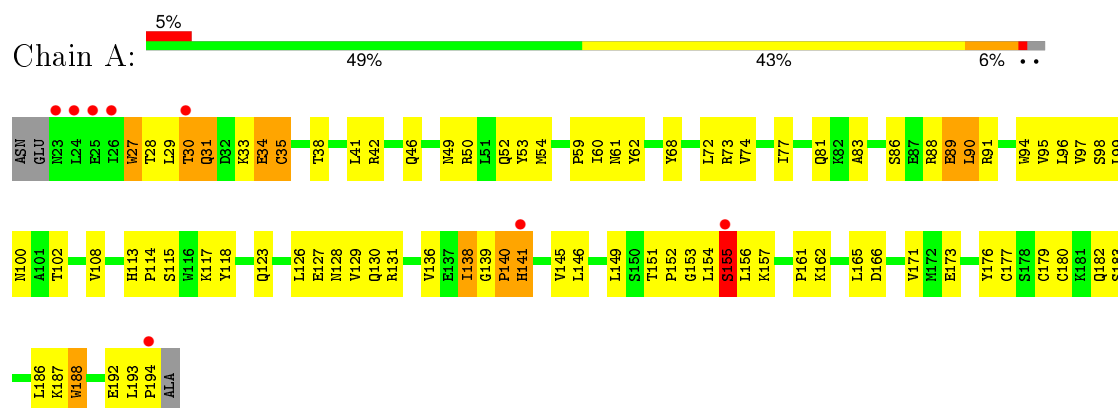
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	148	Total	O	0	0
			148	148		
6	B	139	Total	O	0	0
			139	139		
6	E	92	Total	O	0	0
			92	92		
6	F	147	Total	O	0	0
			147	147		

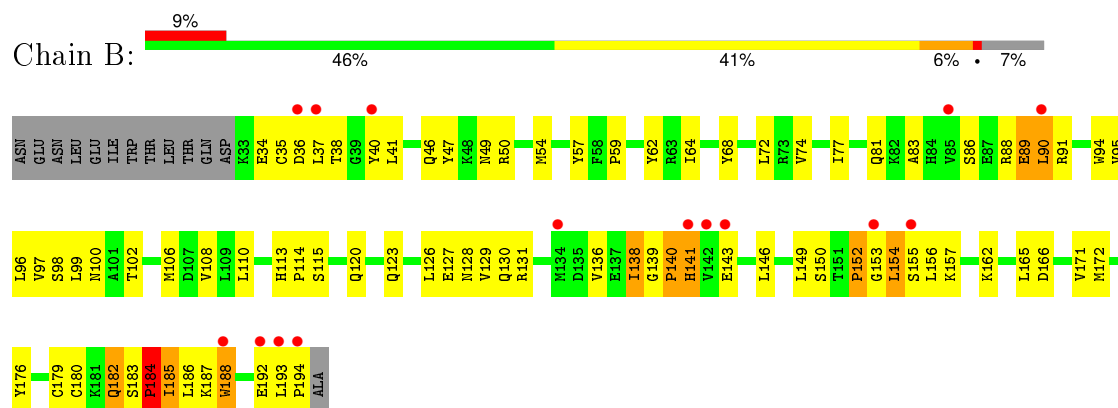
### 3 Residue-property plots

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.

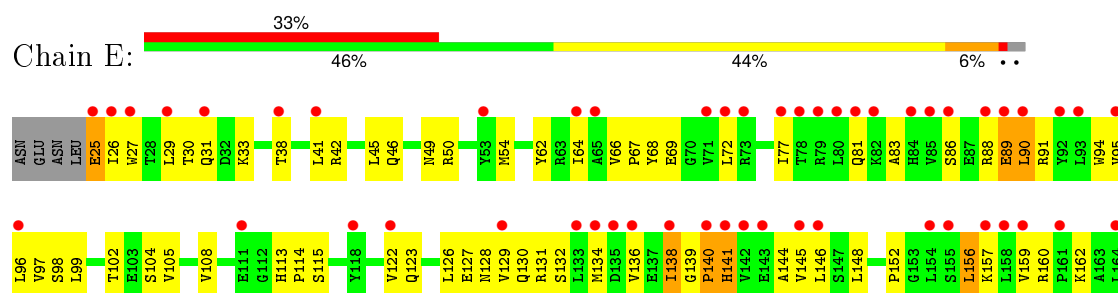
#### • Molecule 1: Interleukin-34

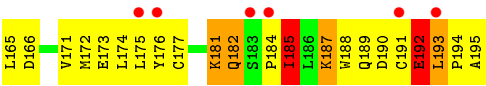


#### • Molecule 1: Interleukin-34

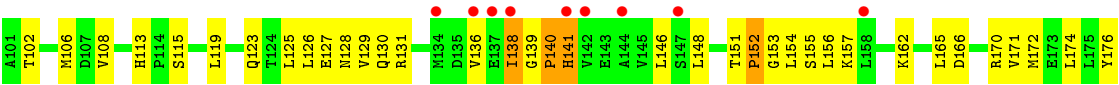


#### • Molecule 1: Interleukin-34





● Molecule 1: Interleukin-34



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.30 Å 80.04 Å 164.18 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 44.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-2.70) 97.7 (44.67-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 2.69 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.244 , 0.288 0.256 , 0.299	Depositor DCC
$R_{free}$ test set	1248 reflections (4.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.8	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 93.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25841 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6461	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: BMA, NAG, MAN

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	0.57	0/1438	0.82	3/1952 (0.2%)
1	B	0.45	0/1350	0.81	4/1830 (0.2%)
1	E	0.35	0/1427	0.72	2/1937 (0.1%)
1	F	0.44	0/1438	0.72	2/1952 (0.1%)
All	All	0.46	0/5653	0.77	11/7671 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	LEU	N-CA-C	13.31	146.95	111.00
1	E	192	GLU	N-CA-C	9.16	135.75	111.00
1	B	152	PRO	N-CA-C	-8.76	89.34	112.10
1	A	155	SER	N-CA-C	-7.62	90.43	111.00
1	A	83	ALA	N-CA-C	-5.89	95.09	111.00
1	E	83	ALA	N-CA-C	-5.81	95.32	111.00
1	A	35	CYS	N-CA-C	-5.80	95.34	111.00
1	F	83	ALA	N-CA-C	-5.76	95.44	111.00
1	F	31	GLN	N-CA-C	-5.75	95.47	111.00
1	B	83	ALA	N-CA-C	-5.73	95.52	111.00
1	B	155	SER	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1408	0	1436	111	0
1	B	1322	0	1355	96	0
1	E	1397	0	1424	101	0
1	F	1408	0	1436	117	0
2	A	61	0	52	3	0
3	A	39	0	34	9	0
3	B	39	0	34	6	0
3	E	39	0	34	5	0
3	F	39	0	34	6	0
4	B	61	0	52	4	0
4	E	61	0	52	7	0
5	F	61	0	52	9	0
6	A	148	0	0	35	0
6	B	139	0	0	24	0
6	E	92	0	0	35	0
6	F	147	0	0	34	0
All	All	6461	0	5995	451	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 38.

All (451) 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:A:31:GLN:N	1:A:31:GLN:HE21	1.59	1.00
1:A:113:HIS:HD2	1:A:115:SER:H	1.02	1.00
1:F:90:LEU:HG	6:F:417:HOH:O	1.64	0.96
1:A:90:LEU:HG	6:A:415:HOH:O	1.66	0.94
1:A:62:TYR:OH	1:A:108:VAL:HG11	1.68	0.93
1:E:102:THR:HG21	6:E:338:HOH:O	1.69	0.92
1:F:113:HIS:HD2	1:F:115:SER:H	1.05	0.92
1:B:113:HIS:HD2	1:B:115:SER:H	1.02	0.92
1:E:113:HIS:HD2	1:E:115:SER:H	1.02	0.92
1:E:64:ILE:HG21	6:E:368:HOH:O	1.72	0.90
1:E:62:TYR:OH	1:E:108:VAL:HG11	1.72	0.89
1:F:165:LEU:HD13	6:F:439:HOH:O	1.72	0.88
1:A:34:GLU:OE2	1:A:34:GLU:N	2.06	0.88
1:A:72:LEU:HG	6:A:444:HOH:O	1.72	0.88
1:F:62:TYR:OH	1:F:108:VAL:HG11	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:VAL:HG23	6:B:342:HOH:O	1.74	0.86
1:B:62:TYR:OH	1:B:108:VAL:HG11	1.73	0.86
1:F:37:LEU:HG	6:F:404:HOH:O	1.76	0.85
1:E:95:VAL:HA	6:E:381:HOH:O	1.77	0.85
1:F:27:TRP:HA	1:F:27:TRP:CE3	2.11	0.85
1:B:36:ASP:HB3	6:B:416:HOH:O	1.78	0.84
1:F:68:TYR:HA	6:F:406:HOH:O	1.78	0.83
1:F:91:ARG:HD3	1:F:176:TYR:CZ	2.14	0.83
1:B:113:HIS:CD2	1:B:115:SER:H	1.95	0.81
1:E:88:ARG:NH1	1:E:136:VAL:HG22	1.96	0.81
1:E:173:GLU:HA	6:E:361:HOH:O	1.81	0.81
1:A:31:GLN:N	1:A:31:GLN:NE2	2.30	0.80
1:F:88:ARG:NH1	1:F:136:VAL:HG22	1.97	0.80
1:A:113:HIS:CD2	1:A:115:SER:H	1.94	0.80
1:A:88:ARG:NH1	1:A:136:VAL:HG22	1.96	0.80
1:A:53:TYR:HA	6:A:411:HOH:O	1.80	0.80
1:B:162:LYS:HD2	6:B:421:HOH:O	1.81	0.80
1:F:27:TRP:HA	1:F:27:TRP:HE3	1.46	0.79
1:B:88:ARG:NH1	1:B:136:VAL:HG22	1.98	0.79
1:F:140:PRO:HA	6:F:402:HOH:O	1.83	0.78
1:E:45:LEU:HD22	6:E:371:HOH:O	1.84	0.78
1:B:108:VAL:O	1:B:108:VAL:HG12	1.83	0.78
1:F:77:ILE:HG23	6:F:417:HOH:O	1.83	0.77
1:B:141:HIS:HB2	6:B:427:HOH:O	1.83	0.77
1:F:119:LEU:HB3	6:F:423:HOH:O	1.85	0.77
1:E:188:TRP:HZ3	6:E:361:HOH:O	1.67	0.77
1:E:113:HIS:CD2	1:E:115:SER:H	1.95	0.76
1:F:106:MET:HG3	6:F:423:HOH:O	1.85	0.76
1:F:138:ILE:H	1:F:138:ILE:HD13	1.52	0.75
1:B:34:GLU:HG3	6:B:353:HOH:O	1.84	0.75
4:B:204:BMA:H2	6:B:405:HOH:O	1.87	0.75
1:F:179:CYS:HB3	6:F:378:HOH:O	1.85	0.74
1:B:138:ILE:HD13	1:B:138:ILE:H	1.53	0.74
1:F:108:VAL:O	1:F:108:VAL:HG12	1.86	0.73
1:E:88:ARG:HH12	1:E:136:VAL:HG22	1.53	0.73
1:A:138:ILE:H	1:A:138:ILE:HD13	1.53	0.73
1:B:192:GLU:OE2	1:B:194:PRO:HD2	1.89	0.73
5:F:204:BMA:H5	6:F:321:HOH:O	1.88	0.73
1:E:122:VAL:HG12	6:E:338:HOH:O	1.89	0.73
1:F:113:HIS:CD2	1:F:115:SER:H	1.97	0.73
1:E:195:ALA:HB2	6:E:353:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:VAL:O	1:E:108:VAL:HG12	1.90	0.72
1:E:138:ILE:HD13	1:E:138:ILE:H	1.53	0.72
3:A:206:NAG:H62	3:A:207:NAG:C8	2.19	0.71
3:E:207:NAG:H5	6:E:363:HOH:O	1.90	0.71
1:B:88:ARG:HH12	1:B:136:VAL:HG22	1.55	0.71
1:A:100:ASN:OD1	3:A:206:NAG:N2	2.22	0.71
1:F:88:ARG:HH12	1:F:136:VAL:HG22	1.54	0.71
1:B:113:HIS:HD2	1:B:115:SER:N	1.85	0.71
5:F:201:NAG:H62	5:F:202:NAG:C8	2.21	0.70
1:F:193:LEU:HB2	1:F:194:PRO:HD3	1.73	0.70
1:A:88:ARG:HH12	1:A:136:VAL:HG22	1.55	0.70
1:A:108:VAL:O	1:A:108:VAL:HG12	1.92	0.70
1:E:67:PRO:HD2	6:E:376:HOH:O	1.92	0.70
3:F:206:NAG:H61	3:F:207:NAG:N2	2.07	0.69
3:A:207:NAG:H81	6:A:429:HOH:O	1.92	0.69
1:B:176:TYR:O	1:B:180:CYS:HB2	1.92	0.69
1:A:31:GLN:HA	6:A:322:HOH:O	1.92	0.69
4:E:205:MAN:H2	6:E:307:HOH:O	1.93	0.69
1:E:174:LEU:HD22	1:E:192:GLU:HB3	1.76	0.68
1:F:38:THR:HG1	1:F:188:TRP:HZ3	1.41	0.68
1:E:159:VAL:HB	6:E:352:HOH:O	1.92	0.68
1:A:117:LYS:HD3	6:A:401:HOH:O	1.94	0.68
1:A:157:LYS:HG3	6:A:440:HOH:O	1.92	0.68
1:B:120:GLN:HA	6:B:403:HOH:O	1.93	0.67
1:B:193:LEU:HB2	1:B:194:PRO:HD3	1.76	0.67
1:B:150:SER:HB2	3:B:207:NAG:O3	1.95	0.66
1:B:95:VAL:HG11	1:B:130:GLN:HB2	1.77	0.66
1:A:113:HIS:HD2	1:A:115:SER:N	1.84	0.66
1:F:31:GLN:HE22	1:F:184:PRO:HD2	1.59	0.66
5:F:205:BMA:H3	6:F:313:HOH:O	1.95	0.66
1:B:36:ASP:OD1	1:B:185:ILE:HG13	1.95	0.66
3:A:206:NAG:H62	3:A:207:NAG:H82	1.78	0.66
1:E:193:LEU:HB3	1:E:194:PRO:HA	1.78	0.66
1:E:95:VAL:HG11	1:E:130:GLN:HB2	1.78	0.65
1:A:73:ARG:HB3	6:A:346:HOH:O	1.96	0.65
1:F:95:VAL:HG11	1:F:130:GLN:HB2	1.78	0.64
1:F:140:PRO:HG2	6:F:403:HOH:O	1.97	0.64
3:F:207:NAG:H62	3:F:208:BMA:H2	1.79	0.64
1:B:50:ARG:HD2	1:B:166:ASP:OD1	1.97	0.64
1:A:31:GLN:HB3	1:A:33:LYS:H	1.61	0.64
1:E:113:HIS:HD2	1:E:115:SER:N	1.85	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:ARG:HB3	6:F:436:HOH:O	1.98	0.64
1:B:157:LYS:HD3	6:B:317:HOH:O	1.96	0.64
1:F:162:LYS:HG2	6:F:436:HOH:O	1.98	0.63
1:F:113:HIS:HD2	1:F:115:SER:N	1.87	0.63
1:E:181:LYS:HE2	1:E:181:LYS:HA	1.80	0.63
1:F:138:ILE:N	1:F:138:ILE:HD13	2.13	0.63
1:B:100:ASN:OD1	3:B:206:NAG:C2	2.47	0.63
1:F:27:TRP:HB3	6:F:386:HOH:O	1.98	0.63
1:B:138:ILE:HD13	1:B:138:ILE:N	2.13	0.63
3:F:206:NAG:H61	3:F:207:NAG:C7	2.29	0.63
1:E:96:LEU:HD22	3:E:206:NAG:O3	1.98	0.63
4:B:201:NAG:H62	6:B:422:HOH:O	1.98	0.63
1:B:106:MET:HE1	6:B:403:HOH:O	1.97	0.63
1:E:26:ILE:N	1:E:26:ILE:HD12	2.14	0.63
1:A:194:PRO:HB3	6:A:412:HOH:O	1.99	0.63
1:F:31:GLN:HG3	1:F:36:ASP:OD1	1.99	0.62
1:F:81:GLN:HA	6:F:302:HOH:O	1.97	0.62
1:A:183:SER:CB	6:A:422:HOH:O	2.48	0.62
1:A:146:LEU:HB3	6:A:426:HOH:O	1.99	0.62
1:A:180:CYS:HB3	6:A:422:HOH:O	1.99	0.62
1:F:181:LYS:HA	1:F:188:TRP:O	2.00	0.62
1:A:68:TYR:HD2	1:A:155:SER:HB3	1.64	0.62
1:A:95:VAL:O	1:A:99:LEU:HD23	1.99	0.62
1:F:138:ILE:H	1:F:138:ILE:CD1	2.12	0.62
1:B:138:ILE:CD1	1:B:138:ILE:H	2.12	0.62
1:B:110:LEU:HG	6:B:419:HOH:O	1.99	0.62
1:F:33:LYS:HB2	6:F:426:HOH:O	1.99	0.62
1:E:90:LEU:HG	6:E:388:HOH:O	1.99	0.62
1:A:77:ILE:HG23	6:A:415:HOH:O	1.99	0.61
5:F:201:NAG:H62	5:F:202:NAG:H83	1.82	0.61
1:A:95:VAL:HG11	1:A:130:GLN:HB2	1.83	0.61
1:E:138:ILE:N	1:E:138:ILE:HD13	2.14	0.60
1:A:52:GLN:HG2	6:A:411:HOH:O	2.01	0.60
1:A:50:ARG:HD2	1:A:166:ASP:OD1	2.01	0.60
1:A:138:ILE:N	1:A:138:ILE:HD13	2.16	0.60
1:E:138:ILE:CD1	1:E:138:ILE:H	2.14	0.60
1:A:173:GLU:HA	6:A:325:HOH:O	1.99	0.60
1:B:95:VAL:O	1:B:99:LEU:HD23	2.01	0.60
1:A:149:LEU:HD12	6:A:432:HOH:O	2.01	0.60
1:F:38:THR:HB	1:F:172:MET:SD	2.41	0.60
1:B:154:LEU:HB3	6:B:324:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ASN:OD1	3:B:206:NAG:H2	2.01	0.59
1:B:64:ILE:HG21	6:B:409:HOH:O	2.02	0.59
1:A:98:SER:O	1:A:102:THR:HG23	2.01	0.59
1:E:50:ARG:HD2	1:E:166:ASP:OD1	2.03	0.59
1:F:50:ARG:HD2	1:F:166:ASP:OD1	2.02	0.59
1:A:29:LEU:HG	1:A:30:THR:N	2.18	0.59
1:B:94:TRP:CH2	1:B:172:MET:HE2	2.37	0.59
1:B:149:LEU:O	3:B:206:NAG:H3	2.01	0.59
1:A:29:LEU:HG	1:A:30:THR:H	1.68	0.59
1:E:95:VAL:O	1:E:99:LEU:HD23	2.03	0.59
1:A:138:ILE:H	1:A:138:ILE:CD1	2.14	0.59
1:E:134:MET:HE1	6:E:323:HOH:O	2.02	0.59
1:B:179:CYS:HA	1:B:182:GLN:HE22	1.67	0.59
1:E:156:LEU:HG	6:E:351:HOH:O	2.02	0.58
1:E:171:VAL:O	1:E:175:LEU:HG	2.03	0.58
1:E:94:TRP:CZ2	1:E:172:MET:HB2	2.38	0.58
1:B:41:LEU:HD13	1:B:172:MET:CE	2.33	0.58
4:E:204:BMA:H61	6:E:379:HOH:O	2.03	0.58
1:B:41:LEU:HB2	1:B:172:MET:HE1	1.85	0.58
1:A:28:THR:O	1:A:28:THR:HG22	2.03	0.58
2:A:201:NAG:H62	2:A:202:NAG:H82	1.84	0.58
1:A:151:THR:O	1:A:153:GLY:N	2.36	0.58
1:F:38:THR:OG1	1:F:188:TRP:CZ3	2.53	0.58
1:F:69:GLU:HG3	5:F:201:NAG:H82	1.86	0.57
1:B:186:LEU:HD22	1:B:186:LEU:H	1.68	0.57
1:F:96:LEU:HD12	1:F:146:LEU:HD11	1.87	0.57
1:A:68:TYR:CD2	1:A:155:SER:HB3	2.39	0.57
1:A:27:TRP:C	1:A:29:LEU:H	2.08	0.56
1:B:140:PRO:HG2	1:B:141:HIS:H	1.69	0.56
1:A:61:ASN:HB2	6:A:313:HOH:O	2.05	0.56
3:F:208:BMA:H62	6:F:353:HOH:O	2.05	0.56
1:A:81:GLN:HG3	6:A:415:HOH:O	2.06	0.56
1:B:68:TYR:CD1	1:B:157:LYS:HE3	2.41	0.56
1:E:96:LEU:HD12	1:E:146:LEU:HD11	1.87	0.56
1:E:127:GLU:HA	6:E:358:HOH:O	2.05	0.55
1:E:140:PRO:HG2	1:E:141:HIS:H	1.70	0.55
1:F:29:LEU:O	1:F:30:THR:C	2.44	0.55
1:B:86:SER:O	1:B:90:LEU:HD22	2.07	0.55
1:A:74:VAL:HG23	6:A:346:HOH:O	2.07	0.55
1:F:98:SER:O	1:F:102:THR:HG23	2.07	0.55
1:F:86:SER:O	1:F:90:LEU:HD22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LEU:HD12	1:B:146:LEU:HD11	1.89	0.55
1:E:98:SER:O	1:E:102:THR:HG23	2.06	0.55
5:F:203:BMA:H3	5:F:205:BMA:O2	2.06	0.55
3:A:207:NAG:H61	6:A:338:HOH:O	2.07	0.55
1:A:154:LEU:HG	6:A:424:HOH:O	2.07	0.55
1:A:96:LEU:HD12	1:A:146:LEU:HD11	1.88	0.55
1:A:171:VAL:HB	6:A:420:HOH:O	2.05	0.54
1:A:35:CYS:N	6:A:437:HOH:O	2.41	0.54
5:F:201:NAG:H62	5:F:202:NAG:H82	1.89	0.54
1:F:91:ARG:HD3	1:F:176:TYR:OH	2.07	0.54
1:F:95:VAL:O	1:F:99:LEU:HD23	2.07	0.54
1:A:100:ASN:OD1	3:A:206:NAG:C2	2.54	0.54
1:A:35:CYS:SG	6:A:437:HOH:O	2.58	0.54
1:E:86:SER:O	1:E:90:LEU:HD22	2.08	0.54
1:B:98:SER:O	1:B:102:THR:HG23	2.08	0.54
1:A:27:TRP:CD1	1:A:27:TRP:N	2.76	0.54
1:F:100:ASN:CG	3:F:206:NAG:HN2	2.10	0.54
1:A:183:SER:HB3	6:A:422:HOH:O	2.08	0.54
1:A:145:VAL:HG13	2:A:201:NAG:H81	1.90	0.54
1:E:99:LEU:CD2	1:E:126:LEU:HB3	2.37	0.54
4:B:204:BMA:H61	6:B:361:HOH:O	2.07	0.53
1:A:91:ARG:O	1:A:95:VAL:HG23	2.08	0.53
1:B:41:LEU:CB	1:B:172:MET:HE1	2.38	0.53
1:F:170:ARG:O	1:F:174:LEU:HD23	2.08	0.53
1:E:104:SER:C	6:E:368:HOH:O	2.46	0.53
1:A:53:TYR:CA	6:A:411:HOH:O	2.45	0.53
1:A:68:TYR:CD1	1:A:157:LYS:HE3	2.43	0.53
1:F:26:ILE:C	1:F:26:ILE:HD13	2.27	0.53
1:B:86:SER:HB3	1:B:89:GLU:HB2	1.90	0.53
1:E:68:TYR:CD1	1:E:157:LYS:HE3	2.43	0.53
1:B:54:MET:HG3	1:B:165:LEU:HD12	1.91	0.53
1:E:54:MET:HG3	1:E:165:LEU:HD12	1.91	0.53
1:B:108:VAL:CG1	1:B:108:VAL:O	2.55	0.53
1:A:140:PRO:HG2	1:A:141:HIS:H	1.73	0.53
3:B:208:BMA:H2	6:B:398:HOH:O	2.09	0.53
1:E:41:LEU:HB2	1:E:172:MET:HE1	1.91	0.52
1:E:162:LYS:HB2	6:E:383:HOH:O	2.07	0.52
1:F:185:ILE:HD12	1:F:185:ILE:N	2.24	0.52
1:A:94:TRP:HA	6:A:444:HOH:O	2.08	0.52
1:F:62:TYR:HH	1:F:108:VAL:HG11	1.74	0.52
1:F:54:MET:HG3	1:F:165:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:SER:HB3	1:E:89:GLU:HB2	1.91	0.52
1:A:54:MET:HG3	1:A:165:LEU:HD12	1.91	0.52
1:B:89:GLU:OE1	1:B:139:GLY:N	2.43	0.52
1:F:72:LEU:CD1	1:F:171:VAL:HG21	2.39	0.52
1:A:53:TYR:N	6:A:411:HOH:O	2.42	0.52
1:A:86:SER:HB3	1:A:89:GLU:HB2	1.91	0.52
1:F:181:LYS:HB2	1:F:191:CYS:SG	2.50	0.52
1:F:26:ILE:O	1:F:26:ILE:HD13	2.09	0.52
1:F:194:PRO:HB2	6:F:350:HOH:O	2.10	0.52
1:F:86:SER:HB3	1:F:89:GLU:HB2	1.92	0.52
1:E:123:GLN:O	1:E:127:GLU:HG3	2.10	0.51
1:E:192:GLU:O	1:E:193:LEU:HB2	2.10	0.51
1:F:193:LEU:CB	1:F:194:PRO:HD3	2.39	0.51
1:E:25:GLU:HB2	6:E:335:HOH:O	2.11	0.51
1:F:89:GLU:OE1	1:F:139:GLY:N	2.44	0.51
1:A:113:HIS:CD2	1:A:115:SER:HB2	2.46	0.51
1:F:68:TYR:CD1	1:F:157:LYS:HE3	2.46	0.51
1:E:89:GLU:OE1	1:E:139:GLY:N	2.43	0.51
1:A:72:LEU:CD1	1:A:171:VAL:HG21	2.42	0.50
1:B:72:LEU:CD1	1:B:171:VAL:HG21	2.42	0.50
1:F:99:LEU:HB3	3:F:206:NAG:O7	2.12	0.50
1:B:91:ARG:HD3	1:B:176:TYR:CE1	2.47	0.50
1:E:174:LEU:HD23	6:E:391:HOH:O	2.10	0.50
1:E:42:ARG:NH1	1:E:173:GLU:HB2	2.27	0.50
1:A:35:CYS:SG	6:A:422:HOH:O	2.59	0.50
1:F:140:PRO:CD	6:F:403:HOH:O	2.58	0.50
1:A:89:GLU:OE1	1:A:139:GLY:N	2.45	0.50
1:E:72:LEU:CD1	1:E:171:VAL:HG21	2.42	0.50
4:E:204:BMA:H5	6:E:379:HOH:O	2.11	0.50
1:B:113:HIS:CD2	1:B:115:SER:HB2	2.47	0.49
1:F:99:LEU:HD22	1:F:126:LEU:HB3	1.94	0.49
3:A:206:NAG:H62	3:A:207:NAG:H83	1.94	0.49
4:E:205:MAN:H3	6:E:339:HOH:O	2.11	0.49
1:A:91:ARG:HD3	1:A:176:TYR:CZ	2.46	0.49
1:B:186:LEU:HD22	1:B:186:LEU:N	2.27	0.49
1:F:140:PRO:HG2	1:F:141:HIS:H	1.77	0.49
1:A:114:PRO:HD3	1:B:57:TYR:CD2	2.47	0.49
1:F:34:GLU:N	1:F:34:GLU:OE1	2.46	0.49
3:A:207:NAG:H83	6:A:418:HOH:O	2.13	0.49
1:B:35:CYS:HB2	1:B:185:ILE:HG12	1.95	0.49
1:F:99:LEU:CD2	1:F:126:LEU:HB3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LEU:N	1:B:193:LEU:HD12	2.28	0.49
1:F:38:THR:OG1	1:F:188:TRP:HZ3	1.94	0.49
1:E:123:GLN:HA	6:E:338:HOH:O	2.13	0.49
1:E:38:THR:HG1	1:E:188:TRP:HH2	1.61	0.49
1:B:152:PRO:HD2	1:B:154:LEU:HB2	1.94	0.49
1:E:30:THR:HG21	1:E:132:SER:HB3	1.93	0.49
1:B:35:CYS:HB2	1:B:185:ILE:CG1	2.42	0.48
1:F:123:GLN:O	1:F:127:GLU:HG3	2.12	0.48
1:E:187:LYS:NZ	6:E:375:HOH:O	2.44	0.48
1:A:86:SER:O	1:A:90:LEU:HD22	2.13	0.48
1:B:36:ASP:OD1	1:B:185:ILE:CG1	2.61	0.48
1:B:68:TYR:CE1	1:B:157:LYS:HE3	2.48	0.48
1:F:45:LEU:CD2	6:F:439:HOH:O	2.61	0.48
1:B:99:LEU:CD2	1:B:126:LEU:HB3	2.42	0.48
1:B:77:ILE:HG13	1:B:171:VAL:HG13	1.95	0.48
1:E:174:LEU:HG	6:E:309:HOH:O	2.14	0.48
1:B:172:MET:O	1:B:172:MET:HG2	2.14	0.48
1:A:118:TYR:N	6:A:409:HOH:O	2.43	0.48
3:E:206:NAG:H2	3:E:206:NAG:H62	1.96	0.48
1:E:72:LEU:HB2	1:E:97:VAL:HG11	1.95	0.48
1:E:105:VAL:N	6:E:368:HOH:O	2.46	0.48
1:E:99:LEU:HD22	1:E:126:LEU:HB3	1.93	0.48
1:A:59:PRO:HB3	1:B:108:VAL:HG12	1.96	0.48
1:A:173:GLU:OE2	1:A:192:GLU:HB3	2.13	0.48
1:A:114:PRO:HG3	1:B:114:PRO:HG3	1.95	0.48
1:F:34:GLU:CA	6:F:404:HOH:O	2.61	0.47
1:F:68:TYR:CD2	1:F:155:SER:HB2	2.49	0.47
1:E:181:LYS:HE3	1:E:188:TRP:O	2.13	0.47
1:F:174:LEU:HD13	6:F:329:HOH:O	2.14	0.47
1:F:113:HIS:CD2	1:F:115:SER:HB2	2.48	0.47
1:E:108:VAL:O	1:E:108:VAL:CG1	2.61	0.47
1:E:172:MET:HG2	6:E:361:HOH:O	2.15	0.47
1:B:46:GLN:HG2	1:B:49:ASN:ND2	2.29	0.47
1:F:68:TYR:CE1	1:F:157:LYS:HE3	2.49	0.47
1:E:26:ILE:H	1:E:26:ILE:HD12	1.77	0.47
1:B:110:LEU:N	6:B:419:HOH:O	2.47	0.47
1:A:68:TYR:CE1	1:A:157:LYS:HE3	2.49	0.47
1:E:77:ILE:HG13	1:E:171:VAL:HG13	1.97	0.47
1:E:128:ASN:HD22	1:E:131:ARG:HH11	1.63	0.47
1:E:91:ARG:O	1:E:95:VAL:HG23	2.14	0.47
1:F:91:ARG:O	1:F:95:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:HD22	6:B:407:HOH:O	2.14	0.47
1:E:189:GLN:HB3	1:E:190:ASP:H	1.47	0.47
1:F:42:ARG:HG2	1:F:187:LYS:O	2.14	0.47
1:F:152:PRO:HB3	6:F:381:HOH:O	2.14	0.47
1:F:41:LEU:HB3	1:F:172:MET:HE1	1.97	0.47
1:E:68:TYR:CE1	1:E:157:LYS:HE3	2.50	0.47
1:A:60:ILE:HD11	6:B:425:HOH:O	2.15	0.47
1:B:91:ARG:O	1:B:95:VAL:HG23	2.14	0.46
1:F:140:PRO:HD2	6:F:403:HOH:O	2.16	0.46
3:E:207:NAG:C7	3:E:207:NAG:O3	2.63	0.46
1:B:99:LEU:HD22	1:B:126:LEU:HB3	1.96	0.46
1:A:38:THR:OG1	1:A:188:TRP:CH2	2.60	0.46
1:A:38:THR:HG1	1:A:188:TRP:HZ3	1.50	0.46
1:E:30:THR:HA	1:E:33:LYS:HB2	1.97	0.46
1:A:128:ASN:HD22	1:A:131:ARG:HH11	1.62	0.46
1:F:183:SER:HB2	1:F:184:PRO:CD	2.46	0.46
1:A:108:VAL:HG12	1:B:59:PRO:HB3	1.98	0.46
1:E:41:LEU:HD13	1:E:172:MET:CE	2.46	0.46
1:E:46:GLN:HG2	1:E:49:ASN:ND2	2.30	0.46
1:A:99:LEU:CD2	1:A:126:LEU:HB3	2.45	0.46
1:B:128:ASN:HD22	1:B:131:ARG:HH11	1.62	0.46
1:A:46:GLN:HG2	1:A:49:ASN:ND2	2.31	0.46
1:A:72:LEU:HB2	1:A:97:VAL:HG11	1.98	0.46
1:A:38:THR:HA	1:A:41:LEU:HD12	1.97	0.46
1:E:126:LEU:HA	1:E:129:VAL:HG12	1.98	0.46
1:F:140:PRO:CG	6:F:403:HOH:O	2.61	0.46
1:E:182:GLN:NE2	1:E:182:GLN:H	2.13	0.46
1:F:77:ILE:HG13	1:F:171:VAL:HG13	1.97	0.45
1:F:108:VAL:CG1	1:F:108:VAL:O	2.58	0.45
1:F:26:ILE:HD11	1:F:37:LEU:HD11	1.98	0.45
1:F:45:LEU:HD22	6:F:439:HOH:O	2.16	0.45
1:F:119:LEU:HD22	6:F:423:HOH:O	2.15	0.45
1:B:37:LEU:HG	6:B:353:HOH:O	2.15	0.45
1:A:33:LYS:HB2	6:A:437:HOH:O	2.17	0.45
1:A:77:ILE:HG13	1:A:171:VAL:HG13	1.97	0.45
1:B:179:CYS:HA	1:B:182:GLN:NE2	2.31	0.45
1:A:123:GLN:O	1:A:127:GLU:HG3	2.16	0.45
1:F:26:ILE:HD11	1:F:37:LEU:HD21	1.96	0.45
1:E:68:TYR:HB2	6:E:355:HOH:O	2.16	0.45
1:B:40:TYR:CE1	1:B:187:LYS:NZ	2.85	0.45
1:E:66:VAL:HA	6:E:351:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:LEU:HD23	6:F:351:HOH:O	2.17	0.45
1:F:128:ASN:HD22	1:F:131:ARG:HH11	1.64	0.45
1:A:100:ASN:OD1	3:A:206:NAG:C7	2.65	0.45
1:F:157:LYS:HA	6:F:310:HOH:O	2.17	0.45
1:B:186:LEU:H	1:B:186:LEU:CD2	2.29	0.44
1:F:24:LEU:HD13	1:F:27:TRP:CE2	2.52	0.44
1:F:31:GLN:HE22	1:F:184:PRO:CD	2.30	0.44
1:B:72:LEU:HB2	1:B:97:VAL:HG11	1.98	0.44
1:F:68:TYR:CD1	5:F:202:NAG:H2	2.53	0.44
1:E:173:GLU:O	1:E:177:CYS:SG	2.75	0.44
1:E:193:LEU:HB3	1:E:194:PRO:CA	2.46	0.44
1:F:46:GLN:HG2	1:F:49:ASN:ND2	2.32	0.44
1:F:31:GLN:HE21	1:F:31:GLN:HB3	1.38	0.44
1:B:94:TRP:HH2	1:B:172:MET:HE2	1.78	0.44
1:F:73:ARG:HD3	6:F:352:HOH:O	2.18	0.44
1:F:72:LEU:HB2	1:F:97:VAL:HG11	1.99	0.44
1:B:88:ARG:HB3	1:B:88:ARG:CZ	2.48	0.44
1:B:123:GLN:HB3	6:B:403:HOH:O	2.17	0.44
1:F:94:TRP:HZ2	1:F:172:MET:HE3	1.83	0.44
1:A:68:TYR:CD1	2:A:202:NAG:H2	2.53	0.44
1:B:143:GLU:HA	6:B:407:HOH:O	2.17	0.44
1:F:157:LYS:HE3	6:F:406:HOH:O	2.18	0.44
1:B:126:LEU:HA	1:B:129:VAL:HG12	1.99	0.44
1:F:146:LEU:HB3	6:F:434:HOH:O	2.16	0.44
4:E:201:NAG:H61	4:E:202:NAG:O7	2.18	0.44
1:A:180:CYS:CB	6:A:422:HOH:O	2.63	0.43
1:A:154:LEU:O	1:A:155:SER:CB	2.66	0.43
1:B:123:GLN:O	1:B:127:GLU:HG3	2.18	0.43
1:E:88:ARG:CZ	1:E:88:ARG:HB3	2.48	0.43
1:E:146:LEU:HB3	3:E:207:NAG:H82	2.00	0.43
1:B:152:PRO:O	1:B:153:GLY:C	2.56	0.43
1:E:144:ALA:C	6:E:392:HOH:O	2.57	0.43
1:F:77:ILE:O	1:F:81:GLN:HG3	2.18	0.43
1:A:38:THR:O	1:A:42:ARG:HB2	2.18	0.43
4:B:201:NAG:H61	4:B:202:NAG:H82	2.01	0.43
1:E:68:TYR:CD1	4:E:202:NAG:H2	2.54	0.43
1:F:24:LEU:HD13	1:F:27:TRP:CZ2	2.53	0.43
1:A:88:ARG:CZ	1:A:88:ARG:HB3	2.48	0.43
1:A:194:PRO:HB2	6:A:448:HOH:O	2.18	0.43
1:F:139:GLY:CA	6:F:411:HOH:O	2.66	0.43
1:A:193:LEU:HB2	1:A:194:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ILE:O	1:A:81:GLN:HG3	2.19	0.42
1:F:126:LEU:HA	1:F:129:VAL:HG12	2.01	0.42
1:A:126:LEU:HA	1:A:129:VAL:HG12	2.01	0.42
1:E:185:ILE:N	1:E:185:ILE:HD13	2.34	0.42
1:F:54:MET:HB3	1:F:162:LYS:HA	2.02	0.42
1:A:99:LEU:HD22	1:A:126:LEU:HB3	2.01	0.42
1:B:47:TYR:HB3	6:B:413:HOH:O	2.19	0.42
1:B:126:LEU:HA	1:B:129:VAL:CG1	2.49	0.42
1:A:54:MET:HB3	1:A:162:LYS:HA	2.01	0.42
1:F:186:LEU:C	1:F:188:TRP:H	2.23	0.42
1:B:38:THR:HG1	1:B:188:TRP:HZ3	1.66	0.42
1:B:157:LYS:NZ	6:B:305:HOH:O	2.43	0.42
1:A:126:LEU:HA	1:A:129:VAL:CG1	2.50	0.42
1:A:173:GLU:O	1:A:177:CYS:HB2	2.18	0.42
1:E:54:MET:HB3	1:E:162:LYS:HA	2.02	0.42
1:E:69:GLU:HG2	1:E:148:LEU:CB	2.49	0.42
1:B:54:MET:HB3	1:B:162:LYS:HA	2.01	0.42
1:F:41:LEU:HD13	1:F:172:MET:HE2	2.01	0.42
1:F:31:GLN:OE1	1:F:184:PRO:HB2	2.20	0.42
1:F:154:LEU:HD12	5:F:205:BMA:O3	2.20	0.42
1:A:30:THR:C	1:A:31:GLN:NE2	2.72	0.42
1:F:38:THR:HA	1:F:41:LEU:HD12	2.01	0.42
1:E:30:THR:HA	1:E:33:LYS:CB	2.50	0.42
1:A:128:ASN:HD22	1:A:131:ARG:NH1	2.17	0.42
1:F:148:LEU:N	1:F:148:LEU:HD12	2.35	0.42
1:A:31:GLN:H	1:A:31:GLN:HE21	1.54	0.42
1:E:162:LYS:HD3	1:E:166:ASP:OD2	2.20	0.42
1:B:94:TRP:CZ2	1:B:172:MET:HB2	2.55	0.42
1:E:138:ILE:HB	6:E:364:HOH:O	2.20	0.42
1:B:100:ASN:OD1	3:B:206:NAG:C7	2.67	0.42
1:A:54:MET:HE3	1:A:161:PRO:HB2	2.02	0.42
1:E:145:VAL:CG2	6:E:392:HOH:O	2.68	0.42
1:E:126:LEU:HA	1:E:129:VAL:CG1	2.49	0.41
1:E:114:PRO:HD3	1:F:57:TYR:CD2	2.55	0.41
1:A:31:GLN:C	1:A:33:LYS:N	2.72	0.41
1:A:31:GLN:CA	1:A:31:GLN:NE2	2.74	0.41
1:F:38:THR:O	1:F:42:ARG:HB2	2.21	0.41
4:E:205:MAN:H5	6:E:341:HOH:O	2.19	0.41
1:B:72:LEU:HD13	1:B:171:VAL:HG21	2.02	0.41
1:E:128:ASN:HD22	1:E:131:ARG:NH1	2.17	0.41
1:B:162:LYS:HD3	1:B:166:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:CD2	6:A:424:HOH:O	2.68	0.41
1:F:151:THR:O	1:F:153:GLY:N	2.54	0.41
1:E:113:HIS:CD2	1:E:115:SER:HB2	2.55	0.41
1:F:162:LYS:HD3	1:F:166:ASP:OD2	2.21	0.41
1:B:194:PRO:HB3	6:B:355:HOH:O	2.20	0.41
1:A:28:THR:CG2	1:A:34:GLU:CD	2.89	0.41
1:A:27:TRP:C	1:A:29:LEU:N	2.74	0.41
1:E:38:THR:HA	1:E:41:LEU:HD12	2.03	0.41
1:F:128:ASN:HD22	1:F:131:ARG:NH1	2.18	0.41
1:E:69:GLU:HG2	1:E:148:LEU:HB3	2.02	0.41
1:F:88:ARG:CZ	1:F:88:ARG:HB3	2.51	0.41
1:F:181:LYS:HD2	1:F:193:LEU:HD11	2.03	0.41
1:A:54:MET:CG	1:A:165:LEU:HD12	2.51	0.41
1:F:126:LEU:HA	1:F:129:VAL:CG1	2.51	0.40
1:E:72:LEU:HD13	1:E:171:VAL:HG21	2.03	0.40
1:B:128:ASN:HD22	1:B:131:ARG:NH1	2.19	0.40
1:B:183:SER:O	1:B:184:PRO:C	2.59	0.40
1:B:184:PRO:O	1:B:185:ILE:C	2.60	0.40
1:E:77:ILE:O	1:E:81:GLN:HG3	2.21	0.40
1:A:151:THR:O	1:A:152:PRO:C	2.54	0.40
1:B:77:ILE:O	1:B:81:GLN:HG3	2.21	0.40
1:E:91:ARG:HD3	1:E:176:TYR:CZ	2.56	0.40
1:E:94:TRP:CH2	1:E:172:MET:HE2	2.57	0.40
1:E:160:ARG:HB3	6:E:383:HOH:O	2.20	0.40
1:E:41:LEU:HD13	1:E:172:MET:HE3	2.02	0.40
1:A:162:LYS:HD3	1:A:166:ASP:OD2	2.21	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	170/175 (97%)	153 (90%)	14 (8%)	3 (2%)	11	27
1	B	160/175 (91%)	139 (87%)	18 (11%)	3 (2%)	10	25
1	E	169/175 (97%)	147 (87%)	14 (8%)	8 (5%)	3	5
1	F	170/175 (97%)	149 (88%)	16 (9%)	5 (3%)	6	14
All	All	669/700 (96%)	588 (88%)	62 (9%)	19 (3%)	6	15

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	SER
1	B	184	PRO
1	E	184	PRO
1	E	185	ILE
1	E	192	GLU
1	F	27	TRP
1	E	27	TRP
1	F	30	THR
1	A	187	LYS
1	F	193	LEU
1	E	31	GLN
1	E	152	PRO
1	F	152	PRO
1	B	185	ILE
1	E	140	PRO
1	F	140	PRO
1	B	140	PRO
1	A	140	PRO
1	E	193	LEU

### 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	160/162 (99%)	147 (92%)	13 (8%)	15	33
1	B	150/162 (93%)	142 (95%)	8 (5%)	28	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	158/162 (98%)	145 (92%)	13 (8%)	14	32
1	F	160/162 (99%)	148 (92%)	12 (8%)	17	38
All	All	628/648 (97%)	582 (93%)	46 (7%)	17	39

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	TRP
1	A	30	THR
1	A	31	GLN
1	A	34	GLU
1	A	89	GLU
1	A	90	LEU
1	A	138	ILE
1	A	141	HIS
1	A	156	LEU
1	A	179	CYS
1	A	182	GLN
1	A	186	LEU
1	A	188	TRP
1	B	89	GLU
1	B	90	LEU
1	B	138	ILE
1	B	141	HIS
1	B	156	LEU
1	B	182	GLN
1	B	184	PRO
1	B	188	TRP
1	E	25	GLU
1	E	29	LEU
1	E	89	GLU
1	E	90	LEU
1	E	138	ILE
1	E	141	HIS
1	E	156	LEU
1	E	181	LYS
1	E	182	GLN
1	E	185	ILE
1	E	187	LYS
1	E	191	CYS
1	E	192	GLU

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Mol	Chain	Res	Type
1	F	26	ILE
1	F	27	TRP
1	F	28	THR
1	F	29	LEU
1	F	31	GLN
1	F	34	GLU
1	F	89	GLU
1	F	90	LEU
1	F	138	ILE
1	F	141	HIS
1	F	156	LEU
1	F	188	TRP

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	31	GLN
1	A	46	GLN
1	A	49	ASN
1	A	113	HIS
1	A	128	ASN
1	A	182	GLN
1	B	46	GLN
1	B	49	ASN
1	B	113	HIS
1	B	128	ASN
1	B	182	GLN
1	E	46	GLN
1	E	49	ASN
1	E	113	HIS
1	E	128	ASN
1	E	182	GLN
1	F	23	ASN
1	F	31	GLN
1	F	46	GLN
1	F	49	ASN
1	F	113	HIS
1	F	128	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

32 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	201	1,2	14,14,15	0.64	0	15,19,21	0.95	1 (6%)
2	NAG	A	202	2	14,14,15	0.72	0	15,19,21	0.93	1 (6%)
2	BMA	A	203	2	11,11,12	1.20	1 (9%)	14,15,17	1.16	1 (7%)
2	MAN	A	204	2	11,11,12	0.75	0	14,15,17	0.69	0
2	BMA	A	205	2	11,11,12	0.91	1 (9%)	14,15,17	1.28	1 (7%)
3	NAG	A	206	1,3	14,14,15	0.86	1 (7%)	15,19,21	0.89	1 (6%)
3	NAG	A	207	3	14,14,15	0.74	0	15,19,21	0.78	1 (6%)
3	BMA	A	208	3	11,11,12	0.62	0	14,15,17	0.74	1 (7%)
4	NAG	B	201	1,4	14,14,15	0.70	0	15,19,21	0.89	1 (6%)
4	NAG	B	202	4	14,14,15	0.66	0	15,19,21	0.87	1 (6%)
4	BMA	B	203	4	11,11,12	0.56	0	14,15,17	0.72	0
4	BMA	B	204	4	11,11,12	0.72	0	14,15,17	0.52	0
4	MAN	B	205	4	11,11,12	0.67	0	14,15,17	0.82	1 (7%)
3	NAG	B	206	1,3	14,14,15	0.91	1 (7%)	15,19,21	1.01	2 (13%)
3	NAG	B	207	3	14,14,15	0.85	1 (7%)	15,19,21	0.86	1 (6%)
3	BMA	B	208	3	11,11,12	0.51	0	14,15,17	0.48	0
4	NAG	E	201	1,4	14,14,15	0.55	0	15,19,21	0.79	1 (6%)
4	NAG	E	202	4	14,14,15	0.63	0	15,19,21	1.01	1 (6%)
4	BMA	E	203	4	11,11,12	0.70	0	14,15,17	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	E	204	4	11,11,12	0.70	0	14,15,17	0.65	0
4	MAN	E	205	4	11,11,12	0.66	0	14,15,17	0.94	1 (7%)
3	NAG	E	206	1,3	14,14,15	0.88	0	15,19,21	1.01	1 (6%)
3	NAG	E	207	3	14,14,15	0.75	0	15,19,21	0.66	0
3	BMA	E	208	3	11,11,12	0.68	0	14,15,17	0.65	0
5	NAG	F	201	1,5	14,14,15	0.56	0	15,19,21	0.69	0
5	NAG	F	202	5	14,14,15	0.55	0	15,19,21	0.91	1 (6%)
5	BMA	F	203	5	11,11,12	0.82	0	14,15,17	1.19	1 (7%)
5	BMA	F	204	5	11,11,12	0.58	0	14,15,17	0.60	0
5	BMA	F	205	5	11,11,12	0.57	0	14,15,17	0.42	0
3	NAG	F	206	1,3	14,14,15	0.64	0	15,19,21	0.99	1 (6%)
3	NAG	F	207	3	14,14,15	0.69	0	15,19,21	0.76	0
3	BMA	F	208	3	11,11,12	0.63	0	14,15,17	0.79	1 (7%)

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	NAG	A	201	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	202	2	-	0/6/23/26	0/1/1/1
2	BMA	A	203	2	-	0/2/19/22	0/1/1/1
2	MAN	A	204	2	-	0/2/19/22	0/1/1/1
2	BMA	A	205	2	-	0/2/19/22	0/1/1/1
3	NAG	A	206	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	207	3	-	0/6/23/26	0/1/1/1
3	BMA	A	208	3	-	0/2/19/22	0/1/1/1
4	NAG	B	201	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	202	4	-	0/6/23/26	0/1/1/1
4	BMA	B	203	4	-	0/2/19/22	0/1/1/1
4	BMA	B	204	4	-	0/2/19/22	0/1/1/1
4	MAN	B	205	4	-	0/2/19/22	0/1/1/1
3	NAG	B	206	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	207	3	-	0/6/23/26	0/1/1/1
3	BMA	B	208	3	-	0/2/19/22	0/1/1/1
4	NAG	E	201	1,4	-	1/6/23/26	0/1/1/1
4	NAG	E	202	4	-	0/6/23/26	0/1/1/1
4	BMA	E	203	4	-	0/2/19/22	0/1/1/1
4	BMA	E	204	4	-	0/2/19/22	0/1/1/1
4	MAN	E	205	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	206	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	207	3	-	0/6/23/26	0/1/1/1
3	BMA	E	208	3	-	0/2/19/22	0/1/1/1
5	NAG	F	201	1,5	-	2/6/23/26	0/1/1/1
5	NAG	F	202	5	-	0/6/23/26	0/1/1/1
5	BMA	F	203	5	-	0/2/19/22	0/1/1/1
5	BMA	F	204	5	-	0/2/19/22	0/1/1/1
5	BMA	F	205	5	-	0/2/19/22	0/1/1/1
3	NAG	F	206	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	207	3	-	0/6/23/26	0/1/1/1
3	BMA	F	208	3	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	205	BMA	C1-C2	2.08	1.57	1.52
3	B	206	NAG	C1-C2	2.09	1.55	1.52
3	B	207	NAG	C1-C2	2.09	1.55	1.52
3	A	206	NAG	C1-C2	2.67	1.56	1.52
2	A	203	BMA	C2-C3	3.07	1.56	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	202	NAG	C2-N2-C7	-2.98	119.22	123.04
4	B	202	NAG	C2-N2-C7	-2.85	119.38	123.04
2	A	202	NAG	C2-N2-C7	-2.74	119.52	123.04
2	A	201	NAG	C2-N2-C7	-2.72	119.54	123.04
5	F	202	NAG	C2-N2-C7	-2.53	119.78	123.04
3	B	206	NAG	C2-N2-C7	-2.47	119.87	123.04
3	A	206	NAG	C2-N2-C7	-2.43	119.92	123.04
4	E	201	NAG	C2-N2-C7	-2.40	119.95	123.04
4	B	201	NAG	C2-N2-C7	-2.37	119.99	123.04
3	A	207	NAG	C2-N2-C7	-2.32	120.05	123.04
3	B	207	NAG	C2-N2-C7	-2.28	120.11	123.04
3	B	206	NAG	C1-O5-C5	2.08	114.89	112.25
3	F	206	NAG	C4-C3-C2	2.16	114.59	111.23
3	A	208	BMA	C1-O5-C5	2.36	115.24	112.25
4	B	205	MAN	C1-O5-C5	2.44	115.34	112.25
3	F	208	BMA	C1-O5-C5	2.55	115.48	112.25
4	E	205	MAN	C1-C2-C3	2.67	112.70	109.54
3	E	206	NAG	C1-O5-C5	2.86	115.88	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	203	BMA	O3-C3-C2	3.13	115.65	110.00
5	F	203	BMA	C1-C2-C3	3.18	113.30	109.54
2	A	205	BMA	C1-C2-C3	4.12	114.42	109.54

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	201	NAG	O7-C7-N2-C2
5	F	201	NAG	O7-C7-N2-C2
5	F	201	NAG	C8-C7-N2-C2

There are no ring outliers.

24 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	NAG	2	0
2	A	202	NAG	2	0
3	A	206	NAG	6	0
3	A	207	NAG	6	0
4	B	201	NAG	2	0
4	B	202	NAG	1	0
4	B	204	BMA	2	0
3	B	206	NAG	4	0
3	B	207	NAG	1	0
3	B	208	BMA	1	0
4	E	201	NAG	1	0
4	E	202	NAG	2	0
4	E	204	BMA	2	0
4	E	205	MAN	3	0
3	E	206	NAG	2	0
3	E	207	NAG	3	0
5	F	201	NAG	4	0
5	F	202	NAG	4	0
5	F	203	BMA	1	0
5	F	204	BMA	1	0
5	F	205	BMA	3	0
3	F	206	NAG	4	0
3	F	207	NAG	3	0
3	F	208	BMA	2	0

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	172/175 (98%)	0.41	8 (4%) 35 34	26, 61, 129, 150	0
1	B	162/175 (92%)	0.58	15 (9%) 11 8	40, 73, 138, 150	0
1	E	171/175 (97%)	1.75	57 (33%) 0 0	69, 124, 150, 150	0
1	F	172/175 (98%)	0.50	17 (9%) 9 7	44, 78, 137, 150	0
All	All	677/700 (96%)	0.81	97 (14%) 4 3	26, 82, 149, 150	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	25	GLU	7.7
1	B	193	LEU	7.5
1	E	80	LEU	7.3
1	E	146	LEU	7.1
1	E	141	HIS	6.7
1	F	26	ILE	6.5
1	E	145	VAL	6.3
1	E	142	VAL	5.9
1	E	157	LYS	5.9
1	E	133	LEU	5.7
1	E	90	LEU	5.7
1	E	155	SER	5.5
1	B	194	PRO	5.5
1	E	154	LEU	5.4
1	F	144	ALA	5.4
1	E	176	TYR	5.3
1	E	158	LEU	5.2
1	E	82	LYS	5.0
1	A	26	ILE	4.9
1	E	77	ILE	4.9
1	E	193	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	26	ILE	4.6
1	E	143	GLU	4.6
1	F	142	VAL	4.5
1	F	138	ILE	4.5
1	F	134	MET	4.4
1	E	93	LEU	4.4
1	E	27	TRP	4.3
1	A	25	GLU	4.3
1	E	136	VAL	4.3
1	A	30	THR	4.2
1	F	88	ARG	4.2
1	E	129	VAL	4.1
1	E	79	ARG	4.1
1	E	73	ARG	3.9
1	F	30	THR	3.8
1	B	153	GLY	3.7
1	E	161	PRO	3.6
1	A	24	LEU	3.6
1	E	138	ILE	3.5
1	B	192	GLU	3.5
1	B	141	HIS	3.5
1	E	191	CYS	3.5
1	A	23	ASN	3.5
1	E	29	LEU	3.5
1	B	37	LEU	3.4
1	B	85	VAL	3.4
1	E	134	MET	3.4
1	E	64	ILE	3.2
1	E	175	LEU	3.2
1	F	136	VAL	3.2
1	E	85	VAL	3.1
1	E	96	LEU	3.0
1	F	192	GLU	3.0
1	F	141	HIS	2.9
1	E	122	VAL	2.9
1	E	71	VAL	2.9
1	E	53	TYR	2.9
1	B	188	TRP	2.8
1	E	183	SER	2.8
1	E	81	GLN	2.8
1	F	158	LEU	2.8
1	E	95	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	88	ARG	2.7
1	B	40	TYR	2.7
1	E	135	ASP	2.7
1	F	27	TRP	2.6
1	F	23	ASN	2.6
1	B	142	VAL	2.6
1	E	72	LEU	2.6
1	E	41	LEU	2.6
1	A	155	SER	2.6
1	E	78	THR	2.5
1	E	38	THR	2.4
1	E	159	VAL	2.4
1	E	140	PRO	2.4
1	E	184	PRO	2.4
1	E	86	SER	2.4
1	E	89	GLU	2.3
1	B	90	LEU	2.3
1	E	84	HIS	2.3
1	A	141	HIS	2.2
1	E	92	TYR	2.2
1	F	77	ILE	2.2
1	F	24	LEU	2.2
1	E	118	TYR	2.2
1	B	36	ASP	2.2
1	E	111	GLU	2.2
1	F	137	GLU	2.1
1	E	31	GLN	2.1
1	B	155	SER	2.1
1	E	164	LEU	2.1
1	F	147	SER	2.1
1	B	134	MET	2.0
1	B	143	GLU	2.0
1	E	65	ALA	2.0
1	A	194	PRO	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	F	206	14/15	0.89	0.36	2.31	129,136,137,138	0
5	NAG	F	201	14/15	0.89	0.23	0.79	91,95,98,98	0
3	NAG	A	206	14/15	0.91	0.20	0.40	143,149,149,149	0
3	NAG	E	206	14/15	0.74	0.33	0.35	150,150,150,150	0
3	NAG	B	206	14/15	0.86	0.24	0.34	129,134,134,134	0
4	NAG	E	201	14/15	0.86	0.30	-0.87	112,116,119,119	0
2	NAG	A	201	14/15	0.97	0.15	-0.99	69,70,72,73	0
4	NAG	B	201	14/15	0.94	0.15	-1.04	80,84,87,87	0
4	NAG	E	202	14/15	0.84	0.25	-	122,122,122,122	0
4	BMA	B	204	11/12	0.50	0.36	-	150,150,150,150	0
4	BMA	E	204	11/12	0.52	0.34	-	150,150,150,150	0
4	BMA	E	203	11/12	0.51	0.28	-	150,150,150,150	0
2	NAG	A	202	14/15	0.94	0.13	-	57,63,70,81	0
5	BMA	F	204	11/12	0.62	0.38	-	150,150,150,150	0
3	NAG	A	207	14/15	0.71	0.39	-	150,150,150,150	0
3	BMA	B	208	11/12	0.56	0.40	-	147,148,148,148	0
3	NAG	F	207	14/15	0.81	0.46	-	149,149,149,149	0
5	BMA	F	203	11/12	0.78	0.17	-	148,148,148,148	0
3	NAG	E	207	14/15	0.62	0.34	-	150,150,150,150	0
5	NAG	F	202	14/15	0.87	0.17	-	90,94,98,101	0
2	BMA	A	205	11/12	0.82	0.13	-	125,129,131,133	0
5	BMA	F	205	11/12	0.81	0.25	-	150,150,150,150	0
3	BMA	F	208	11/12	0.21	0.57	-	150,150,150,150	0
2	MAN	A	204	11/12	0.67	0.21	-	149,150,150,150	0
2	BMA	A	203	11/12	0.90	0.11	-	104,112,119,125	0
4	NAG	B	202	14/15	0.85	0.17	-	98,102,105,105	0
4	BMA	B	203	11/12	0.58	0.23	-	147,147,147,147	0
4	MAN	B	205	11/12	0.60	0.42	-	150,150,150,150	0
3	BMA	A	208	11/12	0.53	0.33	-	150,150,150,150	0
3	NAG	B	207	14/15	0.60	0.30	-	150,150,150,150	0
3	BMA	E	208	11/12	0.66	0.35	-	150,150,150,150	0
4	MAN	E	205	11/12	0.45	0.39	-	150,150,150,150	0

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.