



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:04 PM BST

PDB ID : 4DEP  
Title : Structure of the IL-1b signaling complex  
Authors : Thomas, C.; Garcia, K.C.  
Deposited on : 2012-01-21  
Resolution : 3.10 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

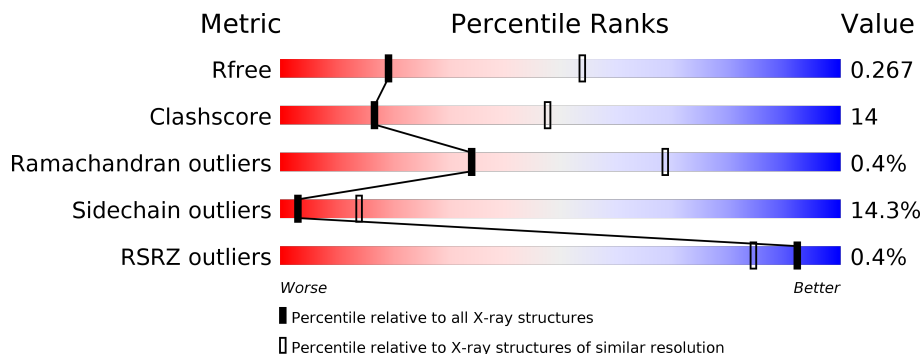
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	158	 % 70% 24% . .
1	D	158	 71% 22% . .
2	B	321	 % 62% 26% 5% 8%
2	E	321	 61% 30% 5% .
3	C	349	 53% 27% . 18%
3	F	349	 54% 26% . 17%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	NAG	F	403	-	-	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11679 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-1 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	151	1167	744	194	221	8	0	0	0
1	D	152	1193	760	197	228	8	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P01584
A	-3	PRO	-	expression tag	UNP P01584
A	-2	LEU	-	expression tag	UNP P01584
A	-1	GLY	-	expression tag	UNP P01584
A	0	SER	-	expression tag	UNP P01584
D	-4	GLY	-	expression tag	UNP P01584
D	-3	PRO	-	expression tag	UNP P01584
D	-2	LEU	-	expression tag	UNP P01584
D	-1	GLY	-	expression tag	UNP P01584
D	0	SER	-	expression tag	UNP P01584

- Molecule 2 is a protein called Interleukin-1 receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	296	2174	1393	370	400	11	0	0	0
2	E	307	2442	1563	415	451	13	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLU	-	expression tag	UNP P14778
B	0	PRO	-	expression tag	UNP P14778

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLU	-	expression tag	UNP P14778
E	0	PRO	-	expression tag	UNP P14778

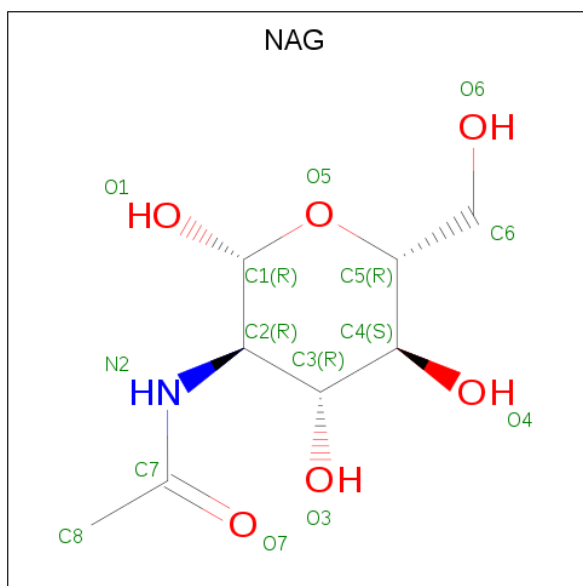
- Molecule 3 is a protein called Interleukin-1 receptor accessory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	287	2260	1451	385	408	16	0	1	0
3	F	289	2240	1440	376	410	14	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLU	-	expression tag	UNP Q9NPH3
C	0	PRO	-	expression tag	UNP Q9NPH3
F	-1	GLU	-	expression tag	UNP Q9NPH3
F	0	PRO	-	expression tag	UNP Q9NPH3

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



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

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

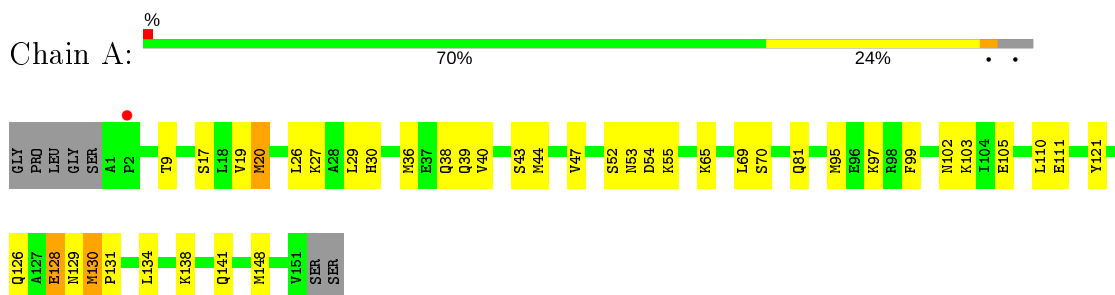
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	O	0	0
			1	1		
5	E	4	Total	O	0	0
			4	4		
5	F	2	Total	O	0	0
			2	2		

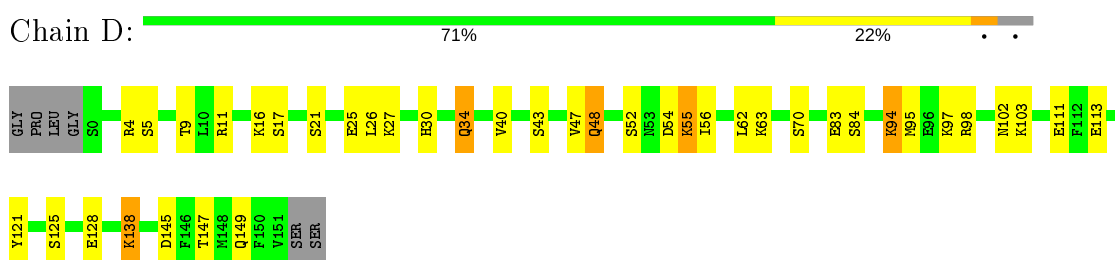
### 3 Residue-property plots [i](#)

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

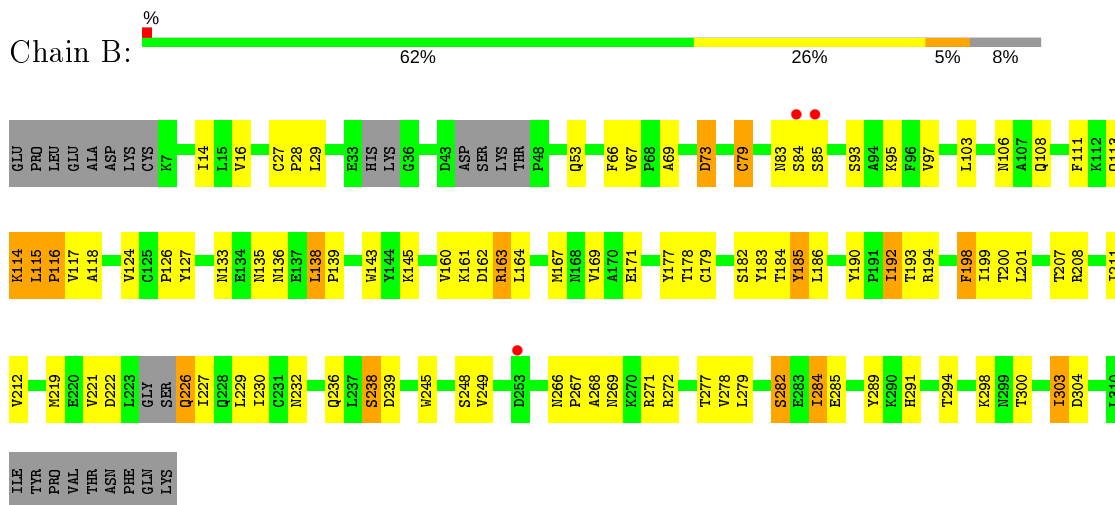
- Molecule 1: Interleukin-1 beta



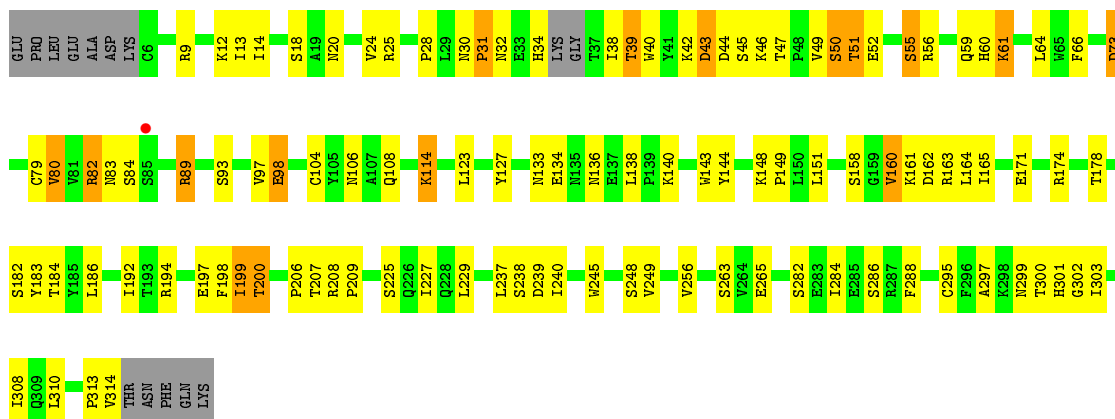
- Molecule 1: Interleukin-1 beta



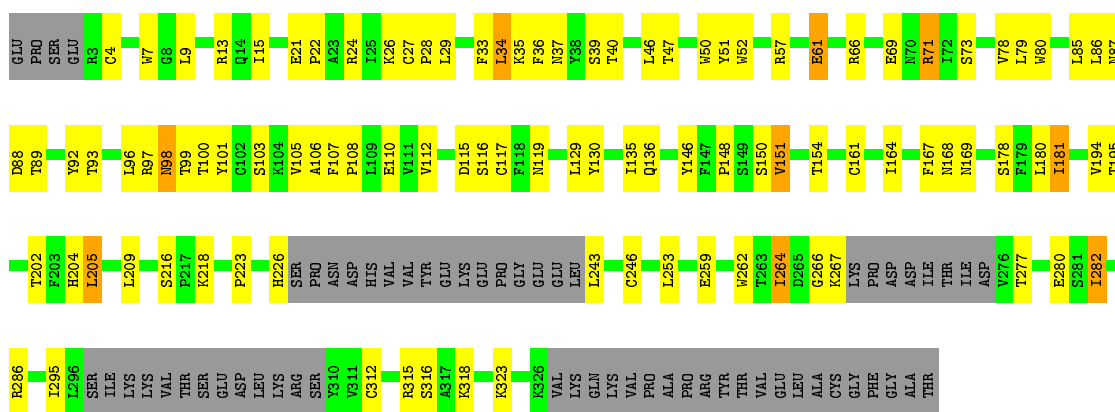
- Molecule 2: Interleukin-1 receptor type 1



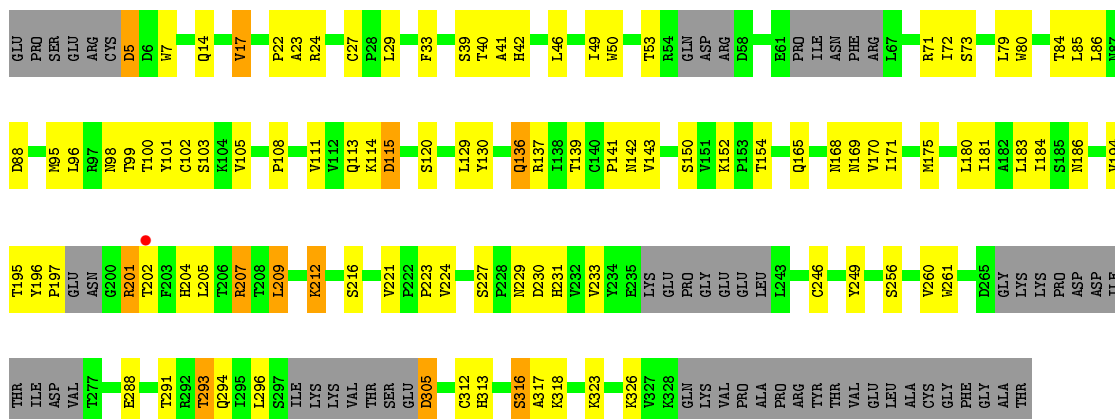
- Molecule 2: Interleukin-1 receptor type 1



• Molecule 3: Interleukin-1 receptor accessory protein



• Molecule 3: Interleukin-1 receptor accessory protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.99Å 65.90Å 163.40Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	19.70 – 3.10 19.70 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.70-3.10) 99.4 (19.70-3.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 3.09Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.210 , 0.277 0.203 , 0.267	Depositor DCC
$R_{free}$ test set	2055 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.9	Xtrriage
Anisotropy	0.272	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.70	0/1190	0.72	0/1609
1	D	0.65	0/1216	0.70	0/1640
2	B	0.72	0/2228	0.73	2/3053 (0.1%)
2	E	0.82	0/2504	0.74	1/3410 (0.0%)
3	C	0.66	0/2320	0.71	1/3164 (0.0%)
3	F	0.67	0/2297	0.74	1/3136 (0.0%)
All	All	0.71	0/11755	0.73	5/16012 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	E	0	1
3	C	0	2
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	115	LEU	C-N-CD	-8.68	101.51	120.60
2	E	61	LYS	N-CA-C	-6.07	94.61	111.00
2	B	79	CYS	CA-CB-SG	5.74	124.34	114.00
3	C	34	LEU	CA-CB-CG	-5.23	103.26	115.30
3	F	80	TRP	CB-CA-C	-5.22	99.97	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20	MET	Peptide
3	C	15	ILE	Peptide
3	C	264	ILE	Peptide
2	E	313	PRO	Peptide

## 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	1167	0	1140	25	0
1	D	1193	0	1178	26	0
2	B	2174	0	1914	70	0
2	E	2442	0	2347	86	0
3	C	2260	0	2143	67	0
3	F	2240	0	2075	68	0
4	B	42	0	39	0	0
4	C	56	0	52	1	0
4	E	56	0	52	1	0
4	F	42	0	39	0	0
5	C	1	0	0	0	0
5	E	4	0	0	0	0
5	F	2	0	0	0	0
All	All	11679	0	10979	319	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 14.

All (319) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:PHE:C	3:C:34:LEU:HD23	1.49	1.31
3:F:84:THR:O	3:F:85:LEU:HD23	1.19	1.29
3:F:84:THR:C	3:F:85:LEU:HD23	1.58	1.21
2:E:82:ARG:HH11	2:E:82:ARG:HG3	1.09	1.16
2:B:266:ASN:OD1	2:B:267:PRO:HD2	1.44	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:VAL:CB	2:B:289:TYR:HE2	1.61	1.12
3:F:84:THR:O	3:F:85:LEU:CD2	2.05	1.05
2:B:138:LEU:H	2:B:138:LEU:HD12	0.88	1.02
2:B:138:LEU:N	2:B:138:LEU:HD12	1.72	1.01
2:B:138:LEU:CD1	2:B:138:LEU:H	1.74	1.01
3:C:34:LEU:N	3:C:34:LEU:HD23	1.58	0.97
3:C:33:PHE:O	3:C:34:LEU:HD23	1.65	0.96
2:E:82:ARG:HH11	2:E:82:ARG:CG	1.80	0.95
3:C:98:ASN:OD1	4:C:401:NAG:O5	1.81	0.93
2:B:221:VAL:CB	2:B:289:TYR:CE2	2.52	0.91
3:C:33:PHE:CE2	3:C:105:VAL:HG21	2.04	0.91
2:B:266:ASN:OD1	2:B:267:PRO:CD	2.20	0.90
3:C:116:SER:CB	2:E:59:GLN:HE22	1.85	0.90
2:B:162:ASP:OD1	2:B:163:ARG:NH1	2.09	0.85
2:E:82:ARG:NH1	2:E:82:ARG:HG3	1.90	0.85
3:C:34:LEU:CD2	3:C:34:LEU:N	2.34	0.83
3:F:143:VAL:CG1	3:F:143:VAL:O	2.29	0.80
3:C:46:LEU:HB3	3:C:96:LEU:HD22	1.64	0.80
2:B:267:PRO:HD2	2:B:268:ALA:H	1.47	0.79
3:F:71:ARG:HG2	3:F:72:ILE:HG13	1.63	0.79
3:C:266:GLY:O	3:C:267:LYS:CB	2.30	0.79
3:C:26:LYS:O	3:C:28:PRO:HD3	1.84	0.77
3:C:33:PHE:C	3:C:34:LEU:CD2	2.44	0.77
3:C:116:SER:HB3	2:E:59:GLN:HE22	1.51	0.76
1:D:128:GLU:HG2	2:E:127:TYR:CE1	2.21	0.75
3:F:98:ASN:HB2	3:F:101:TYR:HB3	1.68	0.75
3:F:212:LYS:HE3	3:F:288:GLU:HG3	1.70	0.74
1:A:128:GLU:HG2	2:B:127:TYR:CE1	2.23	0.74
3:C:71:ARG:NH2	3:C:88:ASP:OD2	2.21	0.73
2:E:56:ARG:NH2	2:E:73:ASP:OD1	2.21	0.73
3:F:143:VAL:HG12	3:F:143:VAL:O	1.89	0.73
3:C:115:ASP:OD1	3:C:116:SER:N	2.22	0.72
2:B:163:ARG:HH11	2:B:163:ARG:HG2	1.57	0.70
1:D:21:SER:OG	1:D:25:GLU:HG2	1.92	0.70
3:F:229:ASN:HB3	3:F:231:HIS:H	1.56	0.69
2:E:42:LYS:CG	2:E:43:ASP:H	2.05	0.69
2:E:42:LYS:O	2:E:43:ASP:C	2.30	0.69
2:E:45:SER:O	2:E:46:LYS:HB2	1.91	0.69
3:C:57:ARG:NH1	3:C:61:GLU:OE1	2.24	0.69
2:E:45:SER:C	2:E:47:THR:H	1.96	0.69
3:C:33:PHE:HE2	3:C:105:VAL:HG21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:ARG:HH21	2:E:200:THR:HG22	1.58	0.68
3:F:260:VAL:O	3:F:294:GLN:NE2	2.27	0.68
1:A:19:VAL:HG12	1:A:38:GLN:O	1.93	0.68
3:F:139:THR:O	3:F:141:PRO:HD3	1.94	0.67
3:F:33:PHE:CE2	3:F:105:VAL:HG21	2.30	0.67
3:C:46:LEU:CD2	3:C:98:ASN:OD1	2.43	0.67
3:C:116:SER:CB	2:E:59:GLN:NE2	2.58	0.66
1:D:54:ASP:HB2	2:E:300:THR:HG23	1.77	0.66
2:E:34:HIS:HB3	2:E:83:ASN:CB	2.25	0.66
2:E:123:LEU:HD12	2:E:164:LEU:HD23	1.76	0.66
3:F:33:PHE:CZ	3:F:105:VAL:HG21	2.31	0.66
1:A:55:LYS:HD2	1:A:102:ASN:HB3	1.78	0.66
2:E:60:HIS:O	2:E:61:LYS:C	2.30	0.66
3:F:71:ARG:NH2	3:F:85:LEU:HG	2.10	0.66
2:B:226:GLN:HA	2:B:282:SER:HA	1.78	0.66
3:C:21:GLU:OE1	3:C:204[B]:HIS:ND1	2.28	0.65
2:E:30:ASN:OD1	2:E:31:PRO:HD2	1.96	0.65
2:E:45:SER:O	2:E:46:LYS:CB	2.43	0.65
3:F:223:PRO:HG3	3:F:316:SER:HB3	1.78	0.65
2:E:127:TYR:O	2:E:194:ARG:NH2	2.25	0.65
3:C:46:LEU:HD23	3:C:98:ASN:OD1	1.97	0.65
3:F:39:SER:O	3:F:41:ALA:N	2.29	0.65
3:F:130:TYR:O	3:F:136:GLN:NE2	2.30	0.64
2:B:298:LYS:HB2	2:B:303:ILE:HG13	1.78	0.64
2:B:171:GLU:HA	2:B:200:THR:HG21	1.78	0.64
2:B:133:ASN:O	2:B:136:ASN:N	2.30	0.63
3:C:89:THR:HG23	3:C:110:GLU:HA	1.80	0.63
3:F:197:PRO:HA	3:F:201:ARG:O	2.00	0.62
2:B:267:PRO:CD	2:B:268:ALA:H	2.12	0.62
3:C:37:ASN:OD1	3:C:39:SER:N	2.33	0.62
3:F:39:SER:C	3:F:41:ALA:H	2.02	0.62
2:B:83:ASN:O	2:B:85:SER:N	2.32	0.62
2:E:44:ASP:O	2:E:45:SER:C	2.36	0.61
1:A:27:LYS:HA	1:A:131:PRO:HA	1.83	0.61
2:E:44:ASP:O	2:E:46:LYS:HG2	2.01	0.61
3:F:7:TRP:HB3	3:F:33:PHE:CE1	2.36	0.61
1:D:147:THR:HG22	1:D:149:GLN:HE22	1.65	0.60
3:F:169:ASN:ND2	3:F:186:ASN:OD1	2.34	0.60
2:B:73:ASP:OD1	2:B:73:ASP:N	2.30	0.60
2:E:42:LYS:CG	2:E:43:ASP:N	2.64	0.60
1:A:126:GLN:NE2	1:A:141:GLN:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:PHE:HB3	2:B:69:ALA:HB2	1.84	0.60
3:F:169:ASN:HB3	3:F:170:VAL:HG23	1.83	0.60
2:E:42:LYS:HG2	2:E:43:ASP:H	1.66	0.59
1:D:121:TYR:CE2	1:D:138:LYS:HD2	2.37	0.59
3:C:98:ASN:HB2	3:C:101:TYR:HB3	1.84	0.59
1:D:83:GLU:OE1	1:D:98:ARG:NE	2.35	0.59
2:B:163:ARG:NH2	3:C:168:ASN:O	2.36	0.58
4:E:401:NAG:H3	4:E:401:NAG:O7	2.02	0.58
2:E:49:VAL:HG22	2:E:50:SER:H	1.69	0.58
2:B:245:TRP:NE1	2:B:291:HIS:O	2.27	0.58
2:E:45:SER:C	2:E:47:THR:N	2.54	0.57
3:C:9:LEU:HD21	3:C:108:PRO:HG3	1.86	0.57
3:C:130:TYR:O	3:C:136:GLN:NE2	2.36	0.57
3:C:33:PHE:O	3:C:34:LEU:CD2	2.46	0.57
1:D:121:TYR:CZ	1:D:138:LYS:HD2	2.40	0.57
3:F:224:VAL:HB	3:F:249:TYR:HB2	1.86	0.57
1:A:128:GLU:HG2	2:B:127:TYR:CZ	2.39	0.56
3:F:49:ILE:HB	3:F:95:MET:HB3	1.86	0.56
2:B:117:VAL:HA	2:B:169:VAL:HB	1.87	0.56
1:D:4:ARG:HD2	2:E:263:SER:HB3	1.88	0.56
1:A:95:MET:HE3	1:A:99:PHE:HB3	1.87	0.56
1:D:147:THR:HG22	1:D:149:GLN:NE2	2.21	0.56
2:E:162:ASP:OD1	2:E:163:ARG:HD3	2.05	0.56
3:F:39:SER:C	3:F:41:ALA:N	2.58	0.56
3:C:33:PHE:CZ	3:C:105:VAL:HG21	2.41	0.55
3:F:230:ASP:HA	3:F:326:LYS:HD2	1.89	0.55
3:F:27:CYS:SG	3:F:29:LEU:HB2	2.47	0.55
2:E:163:ARG:NH2	3:F:168:ASN:O	2.38	0.55
1:D:103:LYS:HE2	2:E:238:SER:O	2.08	0.54
1:A:110:LEU:HD11	1:A:148:MET:HB2	1.89	0.54
2:B:117:VAL:HG13	2:B:201:LEU:O	2.07	0.54
3:C:223:PRO:HG3	3:C:316:SER:HB3	1.89	0.54
1:D:25:GLU:OE2	2:E:30:ASN:ND2	2.41	0.54
2:B:67:VAL:HG11	2:B:185:TYR:HD2	1.73	0.54
1:A:105:GLU:HG3	1:A:110:LEU:HG	1.89	0.54
2:B:212:VAL:HB	2:B:232:ASN:HB3	1.89	0.54
3:C:181:ILE:HG22	3:C:181:ILE:O	2.08	0.54
2:E:143:TRP:HA	2:E:178:THR:O	2.07	0.54
2:B:117:VAL:O	2:B:118:ALA:HB3	2.06	0.53
2:B:53:GLN:NE2	2:B:186:LEU:HD21	2.22	0.53
2:B:83:ASN:O	2:B:84:SER:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:SER:HB3	1:D:27:LYS:HD2	1.90	0.53
2:B:163:ARG:CG	2:B:163:ARG:NH1	2.71	0.53
3:C:115:ASP:HB3	3:C:119:ASN:H	1.72	0.53
2:E:206:PRO:HB3	2:E:301:HIS:CE1	2.44	0.53
2:E:225:SER:O	2:E:284:ILE:HG12	2.08	0.53
2:B:229:LEU:HD23	2:B:279:LEU:HD23	1.90	0.53
3:C:259:GLU:OE1	3:C:315:ARG:NH1	2.42	0.53
1:D:56:ILE:HD13	2:E:240:ILE:HG23	1.91	0.53
1:D:128:GLU:HG2	2:E:127:TYR:CZ	2.44	0.52
3:F:22:PRO:HG2	3:F:196:TYR:OH	2.08	0.52
3:C:46:LEU:HD13	3:C:96:LEU:HD13	1.91	0.52
1:D:47:VAL:HG11	1:D:95:MET:HG3	1.92	0.52
2:E:239:ASP:CB	2:E:299:ASN:HB3	2.38	0.52
3:F:14:GLN:HB3	3:F:108:PRO:HG2	1.91	0.52
2:E:82:ARG:NH1	2:E:82:ARG:CG	2.51	0.52
3:F:17:VAL:HG21	3:F:23:ALA:HB2	1.91	0.52
3:C:71:ARG:HH22	3:C:88:ASP:CG	2.12	0.52
3:C:180:LEU:HD12	3:C:180:LEU:N	2.25	0.51
1:D:34:GLN:NE2	2:E:108:GLN:O	2.42	0.51
2:E:31:PRO:O	2:E:32:ASN:OD1	2.29	0.51
2:B:163:ARG:NH1	2:B:163:ARG:HG2	2.25	0.51
3:F:169:ASN:HD22	3:F:186:ASN:HD21	1.57	0.51
3:F:71:ARG:NH2	3:F:88:ASP:OD2	2.44	0.51
3:C:98:ASN:HB3	3:C:100:THR:H	1.76	0.51
3:C:148:PRO:HG2	3:C:151:VAL:HG12	1.93	0.50
3:F:169:ASN:HD22	3:F:186:ASN:ND2	2.09	0.50
3:C:33:PHE:CE2	3:C:105:VAL:CG2	2.89	0.50
2:E:160:VAL:O	2:E:161:LYS:HB2	2.10	0.50
2:B:143:TRP:CE3	2:B:164:LEU:HD22	2.47	0.50
2:E:158:SER:HB2	2:E:165:ILE:HB	1.93	0.50
3:F:49:ILE:O	3:F:95:MET:N	2.45	0.50
3:F:154:THR:HB	3:F:195:THR:OG1	2.12	0.50
1:A:30:HIS:ND1	2:B:126:PRO:HB3	2.27	0.49
2:E:51:THR:OG1	2:E:51:THR:O	2.30	0.49
2:B:124:VAL:HG22	2:B:163:ARG:HD3	1.94	0.49
2:E:14:ILE:HG12	2:E:93:SER:HB2	1.94	0.49
1:A:47:VAL:HG11	1:A:95:MET:HG3	1.93	0.49
2:B:14:ILE:HG22	2:B:14:ILE:O	2.11	0.49
2:E:143:TRP:CE2	2:E:164:LEU:HB2	2.47	0.49
2:B:97:VAL:HG21	2:B:106:ASN:HD22	1.76	0.49
3:F:142:ASN:O	3:F:207:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:141:PRO:HG3	3:F:209:LEU:HD23	1.93	0.49
3:C:93:THR:OG1	3:C:106:ALA:HB2	2.11	0.49
3:C:36:PHE:HB2	3:C:40:THR:OG1	2.13	0.49
2:E:237:LEU:HD11	2:E:265:GLU:HG3	1.95	0.49
3:C:7:TRP:CD2	3:C:33:PHE:CD1	3.01	0.49
1:D:83:GLU:CD	1:D:98:ARG:HE	2.16	0.49
2:B:114:LYS:O	2:B:115:LEU:HD23	2.12	0.49
2:B:163:ARG:HH11	2:B:163:ARG:CG	2.19	0.48
2:B:183:TYR:HB2	2:B:192:ILE:HD11	1.94	0.48
2:E:30:ASN:OD1	2:E:31:PRO:CD	2.61	0.48
3:F:115:ASP:N	3:F:115:ASP:OD1	2.46	0.48
2:E:183:TYR:HB2	2:E:192:ILE:HD11	1.95	0.48
3:C:29:LEU:HA	3:C:33:PHE:HB2	1.95	0.48
2:B:135:ASN:O	2:B:136:ASN:CB	2.61	0.48
3:F:230:ASP:OD2	3:F:323:LYS:HD3	2.13	0.48
2:B:138:LEU:HB3	2:B:139:PRO:HD2	1.95	0.48
2:B:222:ASP:O	2:B:289:TYR:OH	2.30	0.48
2:E:40:TRP:CE2	2:E:79:CYS:HB3	2.48	0.48
2:B:143:TRP:CH2	2:B:179:CYS:HB3	2.49	0.48
2:B:115:LEU:HA	2:B:116:PRO:HD3	1.49	0.47
3:F:50:TRP:CZ2	3:F:79:LEU:HB2	2.48	0.47
1:A:103:LYS:HD2	1:A:110:LEU:CD2	2.44	0.47
1:A:111:GLU:OE1	1:A:138:LYS:NZ	2.35	0.47
1:D:48:GLN:HB3	1:D:94:LYS:HE2	1.97	0.47
3:F:316:SER:C	3:F:318:LYS:H	2.18	0.47
1:D:26:LEU:HD21	1:D:62:LEU:HD21	1.97	0.47
2:E:13:ILE:HD12	2:E:13:ILE:O	2.13	0.47
3:C:116:SER:HB3	2:E:59:GLN:NE2	2.22	0.47
3:C:21:GLU:HG2	3:C:204[B]:HIS:CE1	2.49	0.47
3:F:143:VAL:HG11	3:F:175:MET:HE1	1.97	0.47
3:C:209:LEU:O	3:C:209:LEU:HD12	2.14	0.47
3:C:282:ILE:HG13	3:C:282:ILE:H	1.58	0.47
2:B:226:GLN:N	2:B:282:SER:O	2.48	0.47
1:A:44:MET:HB3	1:A:44:MET:HE2	1.80	0.47
2:B:111:PHE:CD2	2:B:126:PRO:HG2	2.50	0.47
2:E:133:ASN:O	2:E:134:GLU:O	2.32	0.47
2:B:267:PRO:CD	2:B:268:ALA:N	2.76	0.46
3:F:143:VAL:HG13	3:F:143:VAL:O	2.11	0.46
2:E:160:VAL:HG21	3:F:180:LEU:HD21	1.97	0.46
3:F:46:LEU:HD21	3:F:101:TYR:HD2	1.79	0.46
3:C:246:CYS:HB2	3:C:262:TRP:CZ2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:133:ASN:O	2:E:134:GLU:C	2.51	0.46
2:E:30:ASN:O	2:E:32:ASN:N	2.36	0.46
3:F:71:ARG:HH21	3:F:85:LEU:HG	1.79	0.46
3:C:29:LEU:HD23	3:C:33:PHE:CD2	2.51	0.46
1:A:29:LEU:HD12	2:B:127:TYR:OH	2.15	0.46
3:C:168:ASN:OD1	3:C:169:ASN:N	2.48	0.46
3:C:85:LEU:N	3:C:88:ASP:OD2	2.31	0.46
3:F:246:CYS:O	3:F:293:THR:HA	2.15	0.46
3:F:84:THR:C	3:F:85:LEU:CD2	2.54	0.46
2:B:115:LEU:HB2	2:B:198:PHE:CE1	2.51	0.46
3:C:46:LEU:HD21	3:C:98:ASN:OD1	2.15	0.45
2:E:133:ASN:O	2:E:136:ASN:N	2.49	0.45
3:F:227:SER:O	3:F:246:CYS:HA	2.16	0.45
1:D:30:HIS:N	1:D:128:GLU:OE2	2.49	0.45
2:B:16:VAL:HG22	2:B:95:LYS:HB3	1.98	0.45
2:E:209:PRO:HB2	2:E:297:ALA:HB1	1.98	0.45
2:E:20:ASN:ND2	2:E:98:GLU:OE2	2.49	0.45
2:E:133:ASN:OD1	2:E:133:ASN:C	2.55	0.45
2:E:52:GLU:O	2:E:55:SER:HB2	2.16	0.45
2:E:60:HIS:O	2:E:61:LYS:CB	2.62	0.45
1:D:16:LYS:HE3	1:D:125:SER:O	2.17	0.45
2:B:160:VAL:O	2:B:161:LYS:C	2.53	0.45
1:D:26:LEU:HD22	1:D:40:VAL:HG21	1.99	0.45
2:E:49:VAL:HG22	2:E:50:SER:N	2.31	0.45
2:E:245:TRP:CZ2	2:E:288:PHE:HA	2.52	0.45
1:D:113:GLU:HG3	1:D:121:TYR:CE1	2.51	0.45
3:F:183:LEU:HD23	3:F:183:LEU:HA	1.76	0.45
2:B:236:GLN:HB2	2:B:239:ASP:OD1	2.17	0.44
2:E:208:ARG:HG2	2:E:302:GLY:HA3	1.99	0.44
2:E:56:ARG:HH21	2:E:73:ASP:CG	2.21	0.44
3:F:7:TRP:CD2	3:F:33:PHE:HD1	2.36	0.44
1:D:55:LYS:HD2	1:D:102:ASN:HB3	1.98	0.44
3:F:184:ILE:HA	3:F:184:ILE:HD13	1.62	0.44
3:F:85:LEU:HD23	3:F:85:LEU:N	2.09	0.44
1:A:36:MET:O	1:A:39:GLN:HG3	2.18	0.44
2:B:269:ASN:O	2:B:271:ARG:N	2.51	0.44
3:C:22:PRO:HD2	3:C:205:LEU:HD13	2.00	0.44
3:C:253:LEU:HD22	3:C:318:LYS:HG3	1.98	0.44
2:B:28:PRO:HD2	2:B:79:CYS:SG	2.58	0.44
2:B:183:TYR:O	2:B:190:TYR:N	2.42	0.44
3:F:305:ASP:N	3:F:305:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:160:VAL:O	2:E:161:LYS:C	2.49	0.44
2:E:45:SER:CB	2:E:47:THR:H	2.31	0.44
1:A:105:GLU:OE1	2:B:238:SER:HB2	2.18	0.44
3:F:17:VAL:O	3:F:111:VAL:HA	2.18	0.43
1:D:9:THR:HB	1:D:149:GLN:HB2	2.00	0.43
3:F:141:PRO:O	3:F:207:ARG:HD3	2.18	0.43
2:B:138:LEU:CB	2:B:139:PRO:HD2	2.48	0.43
3:F:261:TRP:CZ2	3:F:313:HIS:HB3	2.53	0.43
1:A:20:MET:HE1	1:A:65:LYS:NZ	2.34	0.43
2:E:239:ASP:HB2	2:E:299:ASN:HB3	2.00	0.43
2:E:39:THR:O	2:E:79:CYS:HA	2.18	0.43
3:C:146:TYR:CG	3:C:205:LEU:HD21	2.53	0.42
1:A:54:ASP:OD2	3:C:286:ARG:NH1	2.49	0.42
2:B:113:GLN:C	2:B:114:LYS:HG2	2.39	0.42
2:B:115:LEU:HB2	2:B:198:PHE:HE1	1.84	0.42
3:C:26:LYS:O	3:C:28:PRO:CD	2.63	0.42
3:C:50:TRP:CH2	3:C:79:LEU:HB2	2.54	0.42
2:E:227:ILE:HD11	2:E:310:LEU:HD11	2.01	0.42
3:F:7:TRP:CG	3:F:33:PHE:CD1	3.07	0.42
3:F:139:THR:O	3:F:141:PRO:CD	2.65	0.42
3:C:116:SER:HB2	2:E:59:GLN:NE2	2.34	0.42
3:C:92:TYR:HB2	3:C:107:PHE:CZ	2.55	0.42
2:E:40:TRP:CD2	2:E:79:CYS:HB3	2.55	0.42
2:B:145:LYS:HD2	2:B:177:TYR:CZ	2.55	0.42
3:C:164:ILE:HG23	3:C:167:PHE:CD2	2.55	0.42
2:E:171:GLU:O	2:E:174:ARG:HG3	2.19	0.42
2:E:60:HIS:ND1	2:E:61:LYS:N	2.68	0.42
3:C:246:CYS:HB2	3:C:262:TRP:CE2	2.55	0.42
3:F:256:SER:HA	3:F:317:ALA:HB2	2.00	0.42
1:A:130:MET:HG3	1:A:131:PRO:HD2	2.00	0.42
3:C:7:TRP:HB3	3:C:33:PHE:CE1	2.55	0.41
2:E:140:LYS:HB2	2:E:140:LYS:HE3	1.54	0.41
2:E:24:VAL:O	2:E:25:ARG:HD3	2.20	0.41
1:A:70:SER:N	1:A:81:GLN:O	2.41	0.41
2:B:53:GLN:HE22	2:B:186:LEU:HD21	1.85	0.41
2:B:266:ASN:HA	2:B:267:PRO:HD3	1.73	0.41
2:E:144:TYR:N	2:E:178:THR:O	2.52	0.41
2:E:40:TRP:N	2:E:59:GLN:OE1	2.50	0.41
3:C:24:ARG:HD2	3:C:80:TRP:CZ2	2.56	0.41
2:E:114:LYS:HE2	2:E:199:ILE:HD11	2.03	0.41
2:E:148:LYS:HA	2:E:149:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:243:LEU:HD23	3:C:243:LEU:HA	1.87	0.41
3:C:51:TYR:CZ	3:C:93:THR:HG21	2.56	0.41
1:A:121:TYR:CZ	1:A:138:LYS:HD2	2.55	0.41
1:A:26:LEU:HD22	1:A:40:VAL:HG21	2.01	0.41
2:B:14:ILE:HG12	2:B:93:SER:HB2	2.03	0.41
3:C:180:LEU:N	3:C:180:LEU:CD1	2.83	0.41
2:E:64:LEU:HG	2:E:66:PHE:CE1	2.56	0.41
3:F:5:ASP:HB2	3:F:102:CYS:O	2.21	0.41
2:E:144:TYR:CD1	2:E:144:TYR:N	2.89	0.41
3:F:205:LEU:HD12	3:F:205:LEU:HA	1.87	0.41
3:F:71:ARG:HG2	3:F:72:ILE:CG1	2.42	0.41
2:B:211:ILE:HG13	2:B:304:ASP:HB3	2.02	0.41
1:A:103:LYS:HD2	1:A:110:LEU:HD23	2.02	0.41
2:B:103:LEU:HA	2:B:103:LEU:HD23	1.85	0.41
2:B:162:ASP:OD1	2:B:162:ASP:N	2.45	0.40
2:E:160:VAL:HG11	3:F:171:ILE:HD12	2.03	0.40
2:E:80:VAL:HB	2:E:89:ARG:HB2	2.02	0.40
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.88	0.40
2:E:97:VAL:HB	2:E:106:ASN:ND2	2.37	0.40
2:B:284:ILE:HG22	2:B:285:GLU:N	2.35	0.40
1:D:54:ASP:HB2	2:E:300:THR:CG2	2.47	0.40
2:B:207:THR:OG1	2:B:236:GLN:OE1	2.38	0.40
2:B:97:VAL:O	2:B:97:VAL:HG23	2.21	0.40
3:C:27:CYS:HA	3:C:28:PRO:HD2	1.70	0.40
3:F:29:LEU:HA	3:F:33:PHE:HB2	2.04	0.40
3:F:46:LEU:HB3	3:F:96:LEU:HD22	2.04	0.40
3:F:96:LEU:HD23	3:F:96:LEU:HA	1.75	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	149/158 (94%)	139 (93%)	9 (6%)	1 (1%)	22	57
1	D	150/158 (95%)	146 (97%)	4 (3%)	0	100	100
2	B	288/321 (90%)	268 (93%)	19 (7%)	1 (0%)	41	73
2	E	304/321 (95%)	284 (93%)	19 (6%)	1 (0%)	41	73
3	C	280/349 (80%)	251 (90%)	28 (10%)	1 (0%)	34	69
3	F	275/349 (79%)	247 (90%)	26 (10%)	2 (1%)	22	57
All	All	1446/1656 (87%)	1335 (92%)	105 (7%)	6 (0%)	34	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	40	THR
1	A	97	LYS
3	C	181	ILE
2	B	116	PRO
2	E	28	PRO
3	F	181	ILE

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	128/143 (90%)	119 (93%)	9 (7%)	15	45
1	D	133/143 (93%)	117 (88%)	16 (12%)	5	20
2	B	204/292 (70%)	171 (84%)	33 (16%)	2	10
2	E	265/292 (91%)	226 (85%)	39 (15%)	3	13
3	C	243/320 (76%)	203 (84%)	40 (16%)	2	10
3	F	235/320 (73%)	199 (85%)	36 (15%)	2	12
All	All	1208/1510 (80%)	1035 (86%)	173 (14%)	3	14

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	17	SER
1	A	43	SER
1	A	52	SER
1	A	53	ASN
1	A	128	GLU
1	A	129	ASN
1	A	130	MET
1	A	134	LEU
2	B	27	CYS
2	B	29	LEU
2	B	73	ASP
2	B	108	GLN
2	B	114	LYS
2	B	138	LEU
2	B	163	ARG
2	B	167	MET
2	B	178	THR
2	B	182	SER
2	B	184	THR
2	B	185	TYR
2	B	192	ILE
2	B	193	THR
2	B	194	ARG
2	B	198	PHE
2	B	199	ILE
2	B	208	ARG
2	B	219	MET
2	B	226	GLN
2	B	227	ILE
2	B	230	ILE
2	B	238	SER
2	B	248	SER
2	B	249	VAL
2	B	272	ARG
2	B	277	THR
2	B	278	VAL
2	B	282	SER
2	B	284	ILE
2	B	294	THR
2	B	300	THR
2	B	303	ILE
3	C	4	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	13	ARG
3	C	35	LYS
3	C	47	THR
3	C	52	TRP
3	C	61	GLU
3	C	66	ARG
3	C	69	GLU
3	C	71	ARG
3	C	73	SER
3	C	78	VAL
3	C	86	LEU
3	C	87	ASN
3	C	97	ARG
3	C	98	ASN
3	C	99	THR
3	C	103	SER
3	C	112	VAL
3	C	117	CYS
3	C	129	LEU
3	C	135	ILE
3	C	150	SER
3	C	151	VAL
3	C	154	THR
3	C	161	CYS
3	C	178	SER
3	C	194	VAL
3	C	195	THR
3	C	202	THR
3	C	205	LEU
3	C	216	SER
3	C	218	LYS
3	C	226	HIS
3	C	264	ILE
3	C	277	THR
3	C	280	GLU
3	C	282	ILE
3	C	295	ILE
3	C	312	CYS
3	C	323	LYS
1	D	5	SER
1	D	11	ARG
1	D	17	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	34	GLN
1	D	43	SER
1	D	48	GLN
1	D	52	SER
1	D	55	LYS
1	D	63	LYS
1	D	70	SER
1	D	84	SER
1	D	94	LYS
1	D	97	LYS
1	D	111	GLU
1	D	138	LYS
1	D	145	ASP
2	E	9	ARG
2	E	12	LYS
2	E	18	SER
2	E	31	PRO
2	E	38	ILE
2	E	39	THR
2	E	43	ASP
2	E	50	SER
2	E	51	THR
2	E	55	SER
2	E	73	ASP
2	E	80	VAL
2	E	82	ARG
2	E	84	SER
2	E	89	ARG
2	E	98	GLU
2	E	104	CYS
2	E	114	LYS
2	E	138	LEU
2	E	151	LEU
2	E	160	VAL
2	E	182	SER
2	E	184	THR
2	E	186	LEU
2	E	197	GLU
2	E	198	PHE
2	E	199	ILE
2	E	200	THR
2	E	207	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	E	229	LEU
2	E	248	SER
2	E	249	VAL
2	E	256	VAL
2	E	282	SER
2	E	286	SER
2	E	295	CYS
2	E	303	ILE
2	E	308	ILE
2	E	314	VAL
3	F	5	ASP
3	F	17	VAL
3	F	24	ARG
3	F	42	HIS
3	F	53	THR
3	F	73	SER
3	F	86	LEU
3	F	99	THR
3	F	100	THR
3	F	103	SER
3	F	113	GLN
3	F	114	LYS
3	F	115	ASP
3	F	120	SER
3	F	129	LEU
3	F	136	GLN
3	F	137	ARG
3	F	150	SER
3	F	152	LYS
3	F	165	GLN
3	F	194	VAL
3	F	201	ARG
3	F	202	THR
3	F	204	HIS
3	F	207	ARG
3	F	209	LEU
3	F	212	LYS
3	F	216	SER
3	F	221	VAL
3	F	233	VAL
3	F	291	THR
3	F	293	THR

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Mol	Chain	Res	Type
3	F	296	LEU
3	F	305	ASP
3	F	312	CYS
3	F	316	SER

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

Mol	Chain	Res	Type
1	A	39	GLN
2	B	53	GLN
2	B	106	ASN
2	B	309	GLN
1	D	66	ASN
3	F	169	ASN

### 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 monosaccharides 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
4	NAG	C	402	3	14,14,15	0.60	0	17,19,21	0.93	0
4	NAG	E	401	2	14,14,15	0.61	0	17,19,21	1.07	2 (11%)
4	NAG	B	401	2	14,14,15	0.50	0	17,19,21	1.10	2 (11%)
4	NAG	E	402	2	14,14,15	0.69	0	17,19,21	1.03	2 (11%)
4	NAG	C	401	3	14,14,15	0.60	0	17,19,21	1.08	2 (11%)
4	NAG	F	402	3	14,14,15	0.51	0	17,19,21	0.66	0
4	NAG	B	402	2	14,14,15	0.53	0	17,19,21	0.95	2 (11%)
4	NAG	F	401	3	14,14,15	0.56	0	17,19,21	1.05	0
4	NAG	E	404	2	14,14,15	0.65	0	17,19,21	1.46	1 (5%)
4	NAG	E	403	2	14,14,15	0.44	0	17,19,21	1.57	3 (17%)
4	NAG	F	403	3	14,14,15	0.61	0	17,19,21	1.07	2 (11%)
4	NAG	C	403	3	14,14,15	0.83	0	17,19,21	1.15	2 (11%)
4	NAG	C	404	3	14,14,15	0.52	0	17,19,21	0.67	0
4	NAG	B	403	2	14,14,15	0.61	0	17,19,21	1.06	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	402	3	-	5/6/23/26	0/1/1/1
4	NAG	E	401	2	-	1/6/23/26	0/1/1/1
4	NAG	B	401	2	-	4/6/23/26	0/1/1/1
4	NAG	E	402	2	-	1/6/23/26	0/1/1/1
4	NAG	C	401	3	-	0/6/23/26	0/1/1/1
4	NAG	F	402	3	-	4/6/23/26	0/1/1/1
4	NAG	B	402	2	-	2/6/23/26	0/1/1/1
4	NAG	F	401	3	-	2/6/23/26	0/1/1/1
4	NAG	E	404	2	-	1/6/23/26	0/1/1/1
4	NAG	E	403	2	-	0/6/23/26	0/1/1/1
4	NAG	F	403	3	-	1/6/23/26	0/1/1/1
4	NAG	C	403	3	-	0/6/23/26	0/1/1/1
4	NAG	C	404	3	-	0/6/23/26	0/1/1/1
4	NAG	B	403	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	E	404	NAG	C1-O5-C5	4.99	118.95	112.19
4	E	403	NAG	C2-N2-C7	-4.13	117.02	122.90
4	B	403	NAG	C1-O5-C5	-3.21	107.84	112.19
4	C	401	NAG	C1-O5-C5	-3.21	107.85	112.19
4	E	401	NAG	C1-O5-C5	-3.18	107.89	112.19
4	F	403	NAG	C1-O5-C5	-3.16	107.92	112.19
4	E	402	NAG	C2-N2-C7	-2.96	118.69	122.90
4	B	401	NAG	C1-O5-C5	2.83	116.03	112.19
4	B	402	NAG	C2-N2-C7	-2.59	119.22	122.90
4	E	402	NAG	C1-O5-C5	2.36	115.39	112.19
4	B	402	NAG	C1-O5-C5	2.36	115.38	112.19
4	C	403	NAG	O5-C5-C6	2.25	110.73	107.20
4	E	403	NAG	O5-C5-C6	2.15	110.57	107.20
4	B	401	NAG	O5-C5-C6	2.12	110.53	107.20
4	F	403	NAG	O5-C1-C2	-2.07	108.03	111.29
4	C	401	NAG	O5-C1-C2	-2.06	108.03	111.29
4	E	401	NAG	O5-C1-C2	-2.05	108.05	111.29
4	C	403	NAG	O5-C5-C4	-2.05	105.85	110.83
4	E	403	NAG	C1-O5-C5	2.04	114.96	112.19
4	B	403	NAG	O5-C1-C2	-2.01	108.11	111.29

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	402	NAG	C3-C2-N2-C7
4	C	402	NAG	C8-C7-N2-C2
4	C	402	NAG	O7-C7-N2-C2
4	E	401	NAG	C3-C2-N2-C7
4	F	402	NAG	C8-C7-N2-C2
4	F	402	NAG	O7-C7-N2-C2
4	B	402	NAG	C8-C7-N2-C2
4	B	402	NAG	O7-C7-N2-C2
4	F	402	NAG	O5-C5-C6-O6
4	F	402	NAG	C4-C5-C6-O6
4	B	403	NAG	C1-C2-N2-C7
4	B	401	NAG	C8-C7-N2-C2
4	B	401	NAG	O5-C5-C6-O6
4	C	402	NAG	C4-C5-C6-O6
4	B	401	NAG	O7-C7-N2-C2
4	B	401	NAG	C4-C5-C6-O6
4	F	401	NAG	C4-C5-C6-O6
4	F	401	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	E	404	NAG	O5-C5-C6-O6
4	F	403	NAG	C1-C2-N2-C7
4	C	402	NAG	O5-C5-C6-O6
4	E	402	NAG	C4-C5-C6-O6
4	B	403	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	NAG	1	0
4	C	401	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	151/158 (95%)	-0.39	1 (0%) 87 75	41, 62, 87, 96	0
1	D	152/158 (96%)	-0.62	0 100 100	24, 38, 65, 73	0
2	B	296/321 (92%)	-0.24	3 (1%) 82 67	42, 71, 93, 116	0
2	E	307/321 (95%)	-0.53	1 (0%) 94 88	20, 43, 71, 90	0
3	C	287/349 (82%)	-0.49	0 100 100	27, 46, 73, 83	0
3	F	289/349 (82%)	-0.45	1 (0%) 94 88	24, 55, 83, 95	0
All	All	1482/1656 (89%)	-0.44	6 (0%) 92 84	20, 53, 84, 116	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	85	SER	2.5
2	B	253	ASP	2.3
2	E	85	SER	2.3
1	A	2	PRO	2.1
3	F	202	THR	2.0
2	B	84	SER	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	F	403	14/15	0.75	0.48	94,101,110,113	0
4	NAG	C	401	14/15	0.84	0.28	64,69,75,79	0
4	NAG	C	404	14/15	0.85	0.37	81,92,104,106	0
4	NAG	B	403	14/15	0.85	0.31	67,79,83,85	0
4	NAG	E	404	14/15	0.89	0.34	42,67,83,87	0
4	NAG	F	401	14/15	0.89	0.33	55,76,89,93	0
4	NAG	F	402	14/15	0.90	0.33	57,84,92,93	0
4	NAG	E	401	14/15	0.90	0.21	28,51,59,67	0
4	NAG	B	402	14/15	0.92	0.27	62,75,82,83	0
4	NAG	C	402	14/15	0.93	0.24	29,50,61,66	0
4	NAG	C	403	14/15	0.94	0.16	42,59,67,68	0
4	NAG	B	401	14/15	0.95	0.19	56,72,78,78	0
4	NAG	E	402	14/15	0.96	0.15	29,43,48,60	0
4	NAG	E	403	14/15	0.97	0.13	28,36,44,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.