



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:59 PM GMT

PDB ID : 4GKO
Title : Crystal structure of the calcium²⁺-bound human IgE-Fc(epsilon)3-4 bound to its B cell receptor derCD23
Authors : Yuan, D.; Sutton, B.J.; Dhaliwal, B.
Deposited on : 2012-08-13
Resolution : 3.30 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

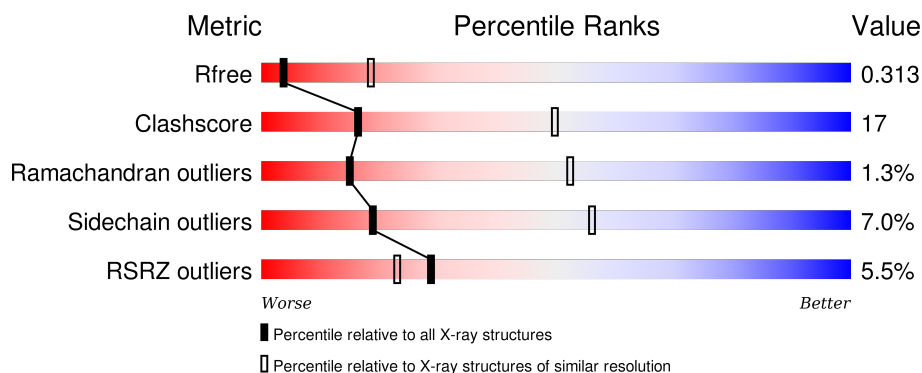
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	223	<div> <div>3%</div> <div>64%</div> <div>26%</div> <div>• • 6%</div> </div>
1	B	223	<div> <div>5%</div> <div>68%</div> <div>23%</div> <div>• 7%</div> </div>
1	C	223	<div> <div>2%</div> <div>56%</div> <div>29%</div> <div>• 12%</div> </div>
1	D	223	<div> <div>4%</div> <div>57%</div> <div>26%</div> <div>• 15%</div> </div>
1	E	223	<div> <div>7%</div> <div>60%</div> <div>17%</div> <div>• 19%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	223	
2	G	143	
2	H	143	
2	I	143	
2	J	143	
2	K	143	
2	L	143	

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
3	NAG	C	601	-	-	X	-
3	MAN	C	604	-	-	X	-
3	NAG	E	601	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16217 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 Ig epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1647	1032	301	308	6			
1	B	207	Total	C	N	O	S	0	0	0
			1642	1029	303	304	6			
1	C	197	Total	C	N	O	S	0	1	0
			1565	981	284	294	6			
1	D	189	Total	C	N	O	S	0	0	0
			1499	944	272	277	6			
1	E	180	Total	C	N	O	S	0	0	0
			1414	882	261	266	5			
1	F	197	Total	C	N	O	S	0	0	0
			1570	980	292	292	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	-	EXPRESSION TAG	UNP P01854
A	326	ASP	-	EXPRESSION TAG	UNP P01854
A	327	PRO	-	EXPRESSION TAG	UNP P01854
A	371	GLN	ASN	CONFLICT	UNP P01854
A	383	GLN	ASN	CONFLICT	UNP P01854
B	325	ALA	-	EXPRESSION TAG	UNP P01854
B	326	ASP	-	EXPRESSION TAG	UNP P01854
B	327	PRO	-	EXPRESSION TAG	UNP P01854
B	371	GLN	ASN	CONFLICT	UNP P01854
B	383	GLN	ASN	CONFLICT	UNP P01854
C	325	ALA	-	EXPRESSION TAG	UNP P01854
C	326	ASP	-	EXPRESSION TAG	UNP P01854
C	327	PRO	-	EXPRESSION TAG	UNP P01854
C	371	GLN	ASN	CONFLICT	UNP P01854
C	383	GLN	ASN	CONFLICT	UNP P01854
D	325	ALA	-	EXPRESSION TAG	UNP P01854
D	326	ASP	-	EXPRESSION TAG	UNP P01854

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Chain	Residue	Modelled	Actual	Comment	Reference
D	327	PRO	-	EXPRESSION TAG	UNP P01854
D	371	GLN	ASN	CONFLICT	UNP P01854
D	383	GLN	ASN	CONFLICT	UNP P01854
E	325	ALA	-	EXPRESSION TAG	UNP P01854
E	326	ASP	-	EXPRESSION TAG	UNP P01854
E	327	PRO	-	EXPRESSION TAG	UNP P01854
E	371	GLN	ASN	CONFLICT	UNP P01854
E	383	GLN	ASN	CONFLICT	UNP P01854
F	325	ALA	-	EXPRESSION TAG	UNP P01854
F	326	ASP	-	EXPRESSION TAG	UNP P01854
F	327	PRO	-	EXPRESSION TAG	UNP P01854
F	371	GLN	ASN	CONFLICT	UNP P01854
F	383	GLN	ASN	CONFLICT	UNP P01854

- Molecule 2 is a protein called Low affinity immunoglobulin epsilon Fc receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	135	Total	C	N	O	S	0	0	0
			1083	680	193	199	11			
2	H	133	Total	C	N	O	S	0	0	0
			1071	672	191	197	11			
2	I	134	Total	C	N	O	S	0	0	0
			1078	677	192	198	11			
2	J	135	Total	C	N	O	S	0	0	0
			1083	680	193	199	11			
2	K	135	Total	C	N	O	S	0	0	0
			1082	679	193	199	11			
2	L	136	Total	C	N	O	S	0	0	0
			1089	683	194	201	11			

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

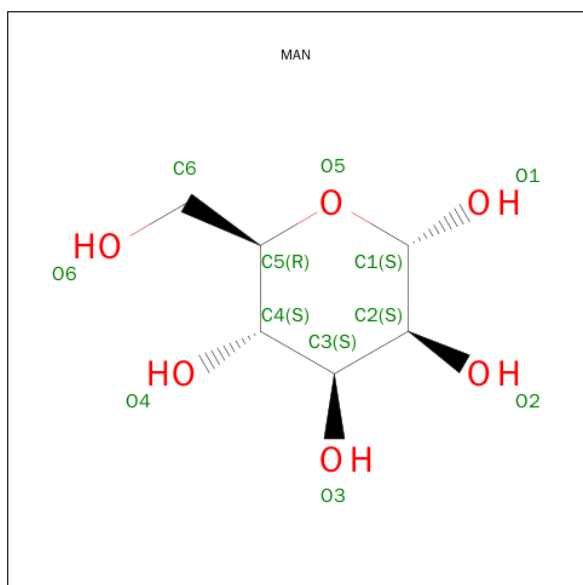
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		
3	B	5	Total	C	N	O	0	0
			61	34	2	25		
3	C	5	Total	C	N	O	0	0
			61	34	2	25		
3	D	5	Total	C	N	O	0	0
			61	34	2	25		

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

- Molecule 4 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Ca	0	0
			1	1		
5	J	1	Total	Ca	0	0
			1	1		
5	K	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		
5	I	1	Total	Ca	0	0
			1	1		

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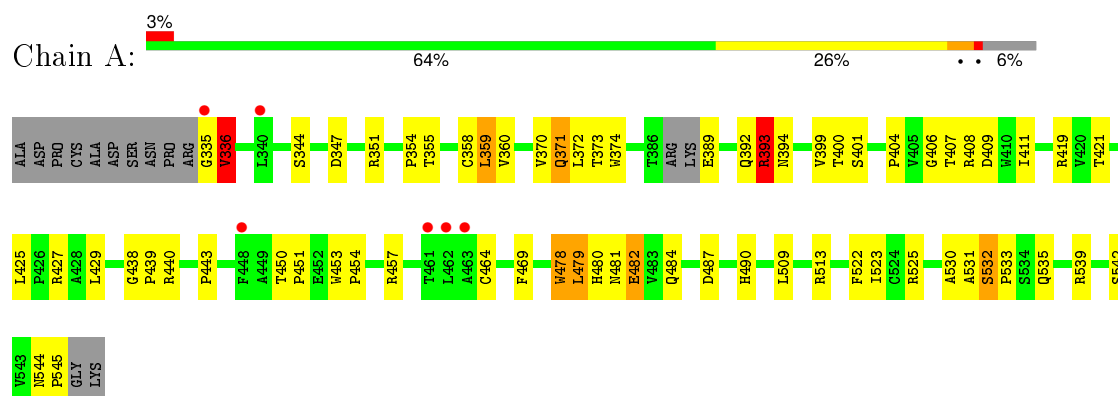
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	1	Total	Ca	0	0
			1	1		

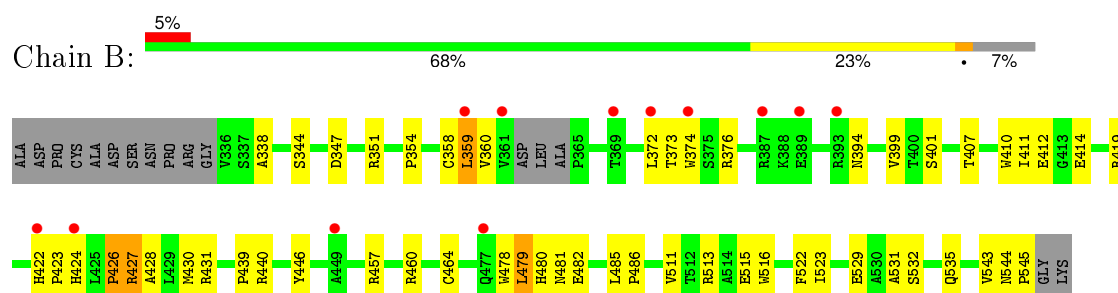
3 Residue-property plots [i](#)

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

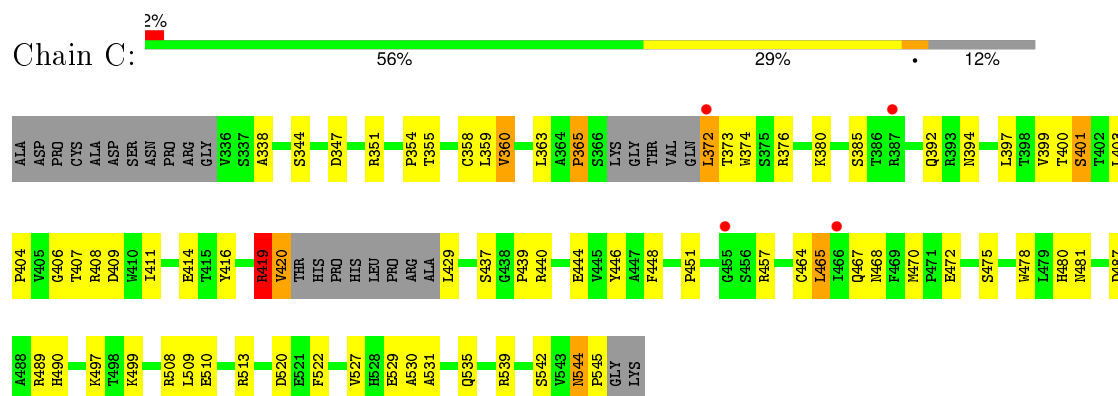
- Molecule 1: Ig epsilon chain C region



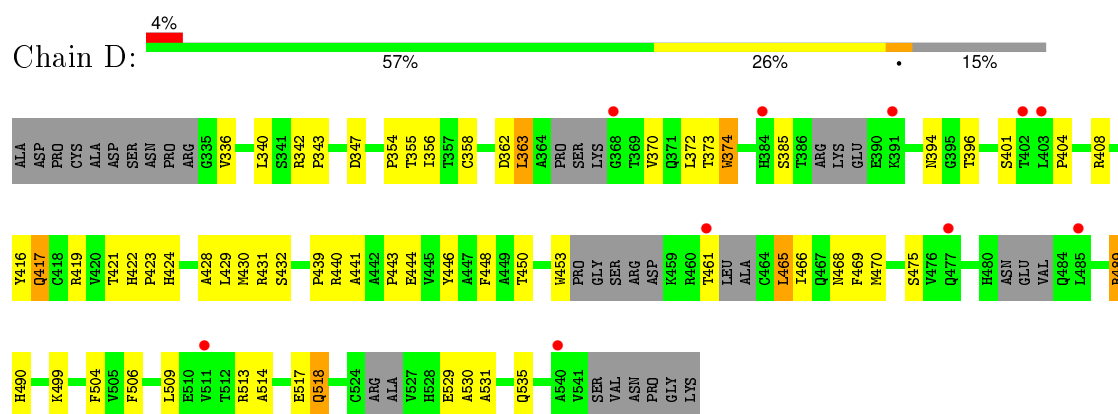
- Molecule 1: Ig epsilon chain C region



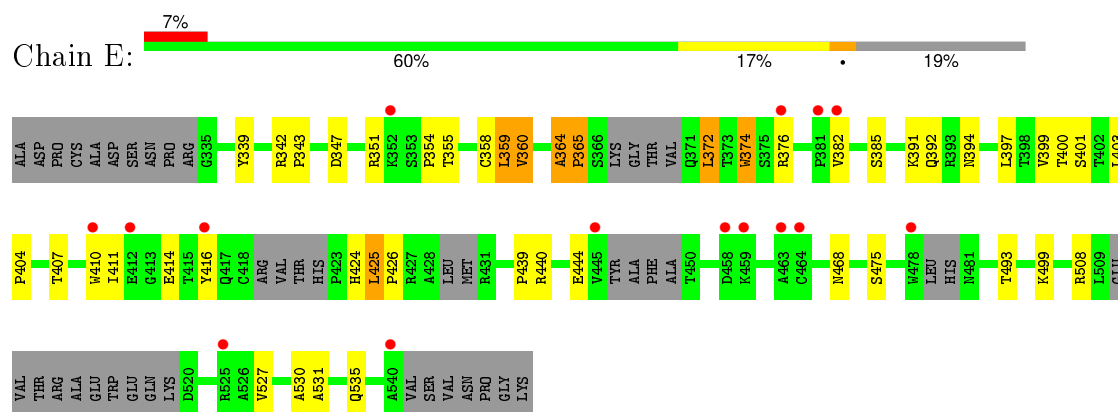
- Molecule 1: Ig epsilon chain C region



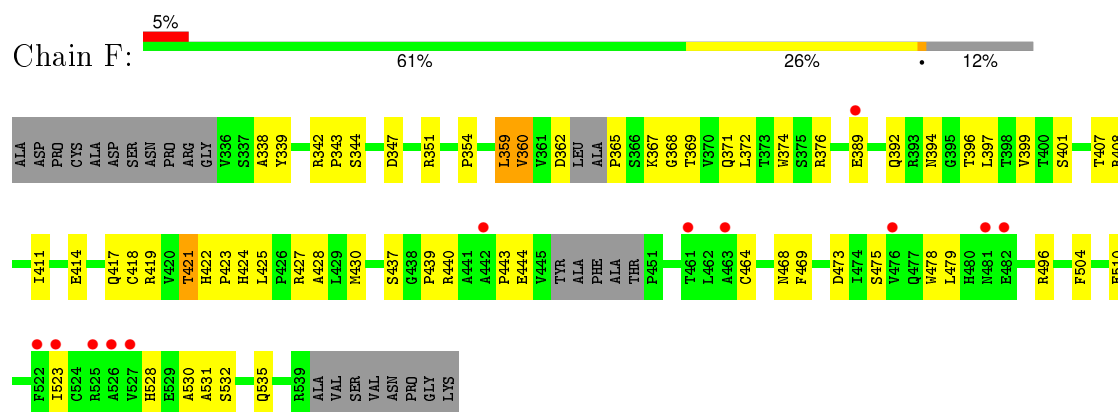
- Molecule 1: Ig epsilon chain C region



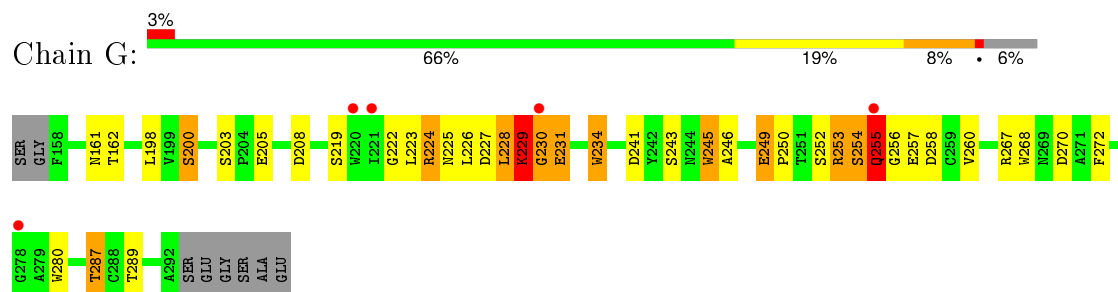
- Molecule 1: Ig epsilon chain C region



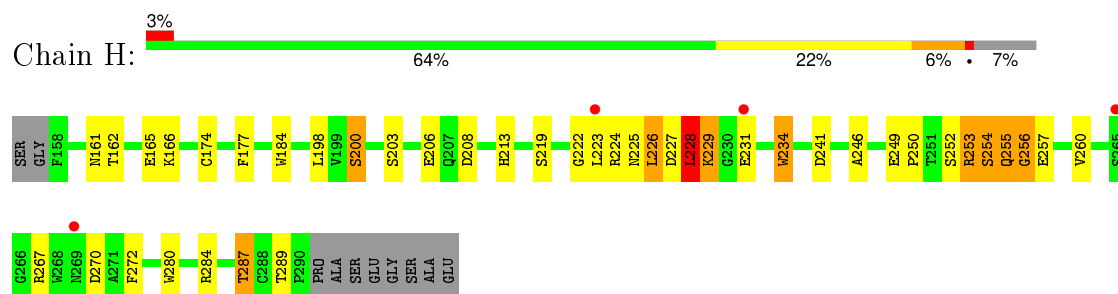
- Molecule 1: Ig epsilon chain C region



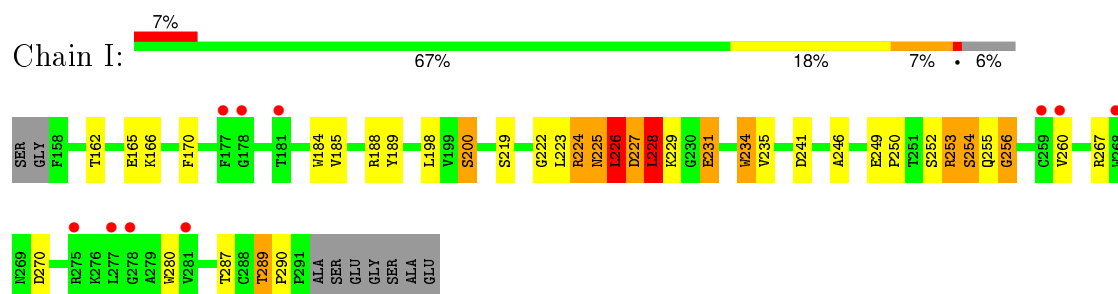
- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



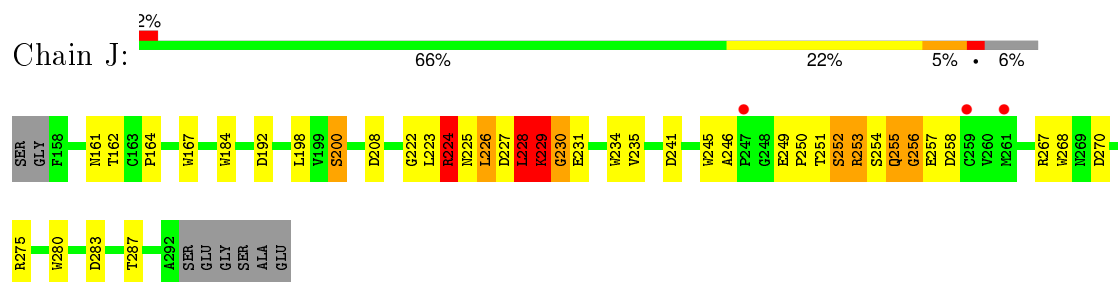
- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



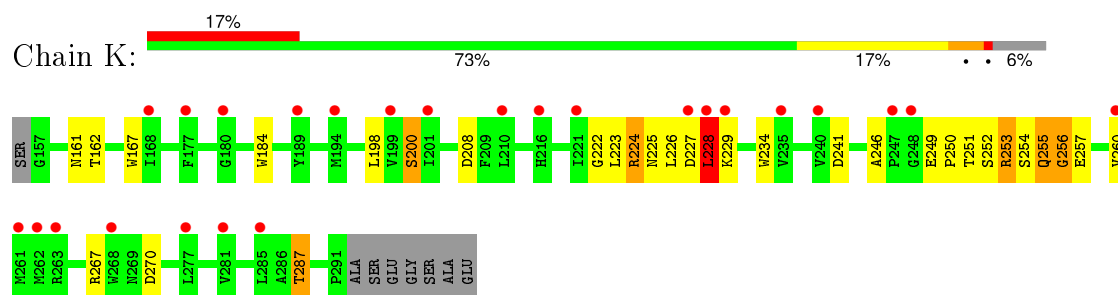
- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



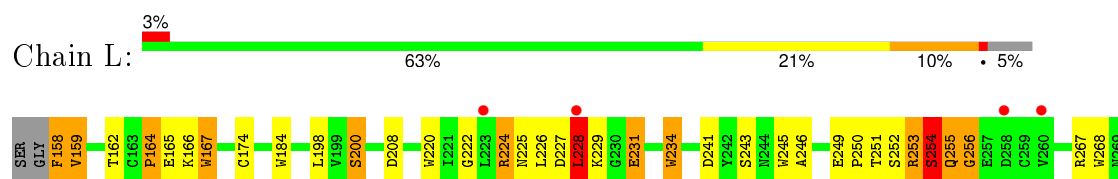
- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



D270	A271	F272	C273	D274	H280	R284	T287	C288	T289	F290	P291	A292	S293	GLU	GLY	SER	ALA	GLU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.83Å 110.13Å 367.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.50 – 3.30 70.54 – 3.30	Depositor EDS
% Data completeness (in resolution range)	85.1 (73.50-3.30) 85.1 (70.54-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.273 , 0.312 0.271 , 0.313	Depositor DCC
R_{free} test set	1684 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	94.9	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 87.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 33653 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16217	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	1.02	2/1689 (0.1%)	1.03	4/2300 (0.2%)
1	B	0.90	2/1684 (0.1%)	0.91	1/2290 (0.0%)
1	C	1.03	0/1605	1.08	8/2182 (0.4%)
1	D	1.03	3/1533 (0.2%)	1.01	2/2079 (0.1%)
1	E	0.81	2/1444 (0.1%)	0.86	0/1955
1	F	0.78	1/1608 (0.1%)	0.84	0/2181
2	G	0.94	3/1117 (0.3%)	0.95	4/1514 (0.3%)
2	H	1.01	3/1104 (0.3%)	0.95	3/1495 (0.2%)
2	I	1.02	2/1112 (0.2%)	1.25	9/1507 (0.6%)
2	J	1.05	3/1117 (0.3%)	1.09	12/1514 (0.8%)
2	K	0.78	1/1116 (0.1%)	0.75	2/1512 (0.1%)
2	L	1.01	4/1123 (0.4%)	0.99	3/1522 (0.2%)
All	All	0.95	26/16252 (0.2%)	0.98	48/22051 (0.2%)

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
2	G	0	1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	ARG	CZ-NH2	9.95	1.46	1.33
2	J	268	TRP	CD2-CE2	7.25	1.50	1.41
2	L	167	TRP	CD2-CE2	6.67	1.49	1.41
1	B	516	TRP	CD2-CE2	6.48	1.49	1.41
2	H	234	TRP	CD2-CE2	6.29	1.48	1.41
2	J	283	ASP	CB-CG	6.27	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	280	TRP	CD2-CE2	6.20	1.48	1.41
2	I	280	TRP	CD2-CE2	6.05	1.48	1.41
2	H	280	TRP	CD2-CE2	6.02	1.48	1.41
2	H	184	TRP	CD2-CE2	5.99	1.48	1.41
1	D	374	TRP	CD2-CE2	5.95	1.48	1.41
2	G	245	TRP	CD2-CE2	5.95	1.48	1.41
2	L	280	TRP	CD2-CE2	5.92	1.48	1.41
2	K	167	TRP	CD2-CE2	5.91	1.48	1.41
1	D	453	TRP	CD2-CE2	5.79	1.48	1.41
2	G	234	TRP	CD2-CE2	5.79	1.48	1.41
1	E	410	TRP	CD2-CE2	5.78	1.48	1.41
1	B	410	TRP	CD2-CE2	5.66	1.48	1.41
1	F	374	TRP	CD2-CE2	5.60	1.48	1.41
2	J	280	TRP	CD2-CE2	5.57	1.48	1.41
2	I	234	TRP	CD2-CE2	5.50	1.48	1.41
2	L	220	TRP	CD2-CE2	5.37	1.47	1.41
2	L	234	TRP	CD2-CE2	5.35	1.47	1.41
1	A	478	TRP	CD2-CE2	5.19	1.47	1.41
1	E	374	TRP	CD2-CE2	5.17	1.47	1.41
1	D	416	TYR	CE1-CZ	5.03	1.45	1.38

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	253	ARG	NE-CZ-NH1	16.64	128.62	120.30
2	I	226	LEU	CA-CB-CG	16.37	152.95	115.30
2	I	226	LEU	CB-CG-CD2	-10.15	93.74	111.00
2	J	230	GLY	N-CA-C	-8.81	91.07	113.10
2	I	226	LEU	CB-CA-C	-8.78	93.52	110.20
2	J	258	ASP	CB-CG-OD1	-8.73	110.44	118.30
1	A	393	ARG	NE-CZ-NH1	8.33	124.47	120.30
2	I	226	LEU	CB-CG-CD1	-8.13	97.19	111.00
2	I	253	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	A	393	ARG	NE-CZ-NH2	-7.89	116.35	120.30
2	H	228	LEU	CA-CB-CG	7.77	133.18	115.30
2	L	228	LEU	CA-CB-CG	7.73	133.08	115.30
2	G	230	GLY	N-CA-C	-7.72	93.81	113.10
2	J	228	LEU	CB-CG-CD1	-7.19	98.78	111.00
2	G	229	LYS	N-CA-C	-7.13	91.75	111.00
1	C	408	ARG	NE-CZ-NH2	-6.89	116.85	120.30
2	J	258	ASP	CB-CG-OD2	6.82	124.44	118.30
2	J	256	GLY	N-CA-C	-6.80	96.10	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	256	GLY	N-CA-C	-6.57	96.68	113.10
1	C	419	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	C	408	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	539	ARG	NE-CZ-NH2	6.24	123.42	120.30
2	J	229	LYS	N-CA-C	-6.18	94.32	111.00
1	C	470	MET	CB-CG-SD	-6.05	94.25	112.40
2	J	224	ARG	NE-CZ-NH1	-5.98	117.31	120.30
2	H	256	GLY	N-CA-C	-5.97	98.19	113.10
2	J	192	ASP	CB-CG-OD1	-5.97	112.93	118.30
2	L	256	GLY	N-CA-C	-5.94	98.26	113.10
2	G	255	GLN	CA-C-N	5.84	127.88	116.20
2	L	228	LEU	CB-CG-CD1	-5.83	101.09	111.00
2	H	226	LEU	CB-CG-CD1	5.81	120.87	111.00
2	J	275	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	I	226	LEU	N-CA-CB	5.77	121.94	110.40
2	K	228	LEU	CA-CB-CG	5.75	128.51	115.30
1	C	465	LEU	CB-CG-CD1	5.73	120.75	111.00
2	J	226	LEU	CB-CG-CD2	-5.57	101.53	111.00
2	J	223	LEU	CB-CG-CD2	-5.52	101.61	111.00
2	K	256	GLY	N-CA-C	-5.36	99.70	113.10
1	C	419	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	487	ASP	CB-CG-OD2	5.33	123.10	118.30
2	G	249	GLU	OE1-CD-OE2	-5.22	117.04	123.30
1	D	489	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	412	GLU	OE1-CD-OE2	-5.17	117.09	123.30
2	J	283	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	487	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	479	LEU	CB-CG-CD1	5.14	119.75	111.00
2	I	188	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	D	466	ILE	CG1-CB-CG2	-5.09	100.21	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	255	GLN	Peptide

5.2 Too-close contacts

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	1647	0	1625	51	0
1	B	1642	0	1629	33	0
1	C	1565	0	1548	77	0
1	D	1499	0	1475	81	0
1	E	1414	0	1394	36	0
1	F	1570	0	1557	48	0
2	G	1083	0	995	52	0
2	H	1071	0	983	36	1
2	I	1078	0	991	32	1
2	J	1083	0	996	43	1
2	K	1082	0	993	36	0
2	L	1089	0	1000	49	1
3	A	61	0	52	5	0
3	B	61	0	52	4	0
3	C	61	0	52	17	0
3	D	61	0	51	2	0
3	E	61	0	52	7	0
3	F	61	0	52	5	0
4	C	22	0	20	7	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
All	All	16217	0	15517	530	2

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 17.

All (530) 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)
2:I:226:LEU:O	2:I:228:LEU:N	1.65	1.28
3:C:604:MAN:O6	4:C:607:MAN:C1	1.80	1.26
1:D:417:GLN:CG	1:D:430:MET:SD	2.30	1.20
1:D:417:GLN:HG2	1:D:430:MET:CE	1.72	1.18
1:D:417:GLN:HG2	1:D:430:MET:SD	1.88	1.13
2:L:255:GLN:HE21	2:L:255:GLN:HA	1.02	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:GLN:HG3	1:D:430:MET:SD	1.92	1.08
1:D:417:GLN:HG2	1:D:430:MET:HE1	1.26	1.07
1:E:394:ASN:HD21	3:E:601:NAG:C1	1.67	1.06
2:I:254:SER:HA	2:I:255:GLN:C	1.77	1.05
1:A:371:GLN:HA	1:A:371:GLN:HE21	1.16	1.04
2:H:252:SER:O	2:H:253:ARG:HB2	1.56	1.03
1:D:422:HIS:CD2	1:D:423:PRO:HD2	1.93	1.02
3:C:604:MAN:O3	4:C:606:MAN:C1	2.07	1.01
2:G:226:LEU:HD21	2:G:228:LEU:HD23	1.41	1.01
1:A:439:PRO:HA	2:G:255:GLN:O	1.60	1.01
3:C:604:MAN:O6	4:C:607:MAN:C2	2.11	0.98
2:G:228:LEU:HG	2:G:228:LEU:O	1.60	0.97
2:L:255:GLN:HE21	2:L:255:GLN:CA	1.81	0.93
1:F:394:ASN:HD21	3:F:601:NAG:C1	1.80	0.93
2:L:252:SER:O	2:L:253:ARG:HB2	1.69	0.93
1:C:394:ASN:HD21	3:C:601:NAG:C1	1.82	0.92
1:C:489:ARG:HH11	1:D:499:LYS:NZ	1.67	0.92
2:I:252:SER:O	2:I:253:ARG:HB2	1.67	0.92
2:L:255:GLN:NE2	2:L:255:GLN:HA	1.83	0.90
2:K:252:SER:O	2:K:253:ARG:HB2	1.72	0.90
1:F:439:PRO:HA	2:L:255:GLN:O	1.72	0.90
1:F:422:HIS:HB3	1:F:425:LEU:HB2	1.53	0.90
2:J:228:LEU:O	2:J:228:LEU:HD22	1.71	0.90
2:I:162:THR:HB	2:I:287:THR:HG23	1.54	0.89
1:C:510:GLU:HB2	1:D:499:LYS:HG3	1.55	0.89
1:E:394:ASN:ND2	3:E:601:NAG:C1	2.36	0.89
1:D:408:ARG:NH1	2:J:226:LEU:HD13	1.87	0.89
1:C:489:ARG:HH11	1:D:499:LYS:HZ1	1.20	0.89
1:C:542:SER:HB2	1:C:545:PRO:HG3	1.55	0.89
2:L:249:GLU:OE1	2:L:270:ASP:OD1	1.92	0.88
1:F:422:HIS:CD2	1:F:424:HIS:H	1.90	0.88
1:C:446:TYR:CE2	1:D:450:THR:HB	2.07	0.88
2:H:162:THR:HB	2:H:287:THR:HG23	1.55	0.88
3:C:604:MAN:O6	4:C:607:MAN:H2	1.74	0.87
2:G:249:GLU:OE1	2:G:270:ASP:OD1	1.93	0.87
1:A:531:ALA:O	1:A:535:GLN:HA	1.73	0.87
1:D:394:ASN:HD21	3:D:601:NAG:C1	1.88	0.87
1:A:394:ASN:HD21	3:A:601:NAG:C1	1.88	0.87
1:D:417:GLN:NE2	1:D:432:SER:CB	2.37	0.86
1:E:499:LYS:HB2	1:F:510:GLU:OE1	1.74	0.86
1:C:451:PRO:HD3	1:D:448:PHE:HZ	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:GLN:HE21	1:D:432:SER:CB	1.88	0.86
2:K:254:SER:HA	2:K:255:GLN:C	1.95	0.86
1:B:543:VAL:O	1:B:544:ASN:OD1	1.94	0.86
2:I:249:GLU:OE1	2:I:270:ASP:OD1	1.94	0.85
2:G:254:SER:HB2	2:G:255:GLN:C	1.97	0.85
2:G:252:SER:O	2:G:253:ARG:HB2	1.75	0.85
2:G:254:SER:HB2	2:G:255:GLN:O	1.77	0.84
3:C:604:MAN:O2	4:C:606:MAN:C1	2.26	0.84
1:D:417:GLN:NE2	1:D:432:SER:HB2	1.91	0.84
1:C:499:LYS:HZ3	1:D:489:ARG:HD2	1.43	0.84
2:J:252:SER:O	2:J:253:ARG:HB2	1.78	0.84
1:F:422:HIS:HD2	1:F:424:HIS:H	1.25	0.83
1:E:425:LEU:HD22	1:E:426:PRO:HD2	1.61	0.83
1:A:371:GLN:HA	1:A:371:GLN:NE2	1.94	0.83
2:J:227:ASP:O	2:J:229:LYS:O	1.96	0.83
1:A:371:GLN:HB2	1:A:421:THR:HB	1.61	0.81
1:D:417:GLN:HE21	1:D:432:SER:HB2	1.43	0.81
1:C:499:LYS:NZ	1:D:489:ARG:HD2	1.96	0.81
2:H:255:GLN:HE21	2:H:255:GLN:HA	1.47	0.80
1:D:373:THR:HB	1:D:419:ARG:HB3	1.62	0.80
2:J:254:SER:HA	2:J:255:GLN:C	1.99	0.80
2:G:255:GLN:HA	2:G:255:GLN:HE21	1.46	0.80
1:B:394:ASN:HD21	3:B:601:NAG:C1	1.95	0.80
1:F:394:ASN:ND2	3:F:601:NAG:C1	2.45	0.79
3:C:604:MAN:HO6	4:C:607:MAN:C1	1.95	0.79
2:I:225:ASN:OD1	2:I:227:ASP:N	2.15	0.79
1:E:372:LEU:HD22	1:E:401:SER:HB2	1.66	0.78
1:D:419:ARG:NH1	1:D:430:MET:HB2	2.00	0.77
1:A:371:GLN:CB	1:A:421:THR:HB	2.14	0.77
1:E:392:GLN:NE2	3:E:601:NAG:O6	2.17	0.77
1:D:531:ALA:O	1:D:535:GLN:HA	1.85	0.77
2:K:255:GLN:HA	2:K:255:GLN:HE21	1.49	0.77
1:C:392:GLN:CG	3:C:601:NAG:O6	2.33	0.76
1:C:394:ASN:ND2	3:C:601:NAG:C1	2.48	0.76
1:C:451:PRO:HD3	1:D:448:PHE:CZ	2.21	0.76
2:J:249:GLU:OE1	2:J:270:ASP:OD1	2.04	0.76
2:I:253:ARG:O	2:I:254:SER:HB2	1.86	0.74
1:C:440:ARG:HD2	1:C:530:ALA:HB2	1.68	0.74
2:J:229:LYS:HG3	2:J:231:GLU:HG3	1.69	0.74
1:D:421:THR:HG22	1:D:428:ALA:HB1	1.69	0.74
1:C:359:LEU:HD12	1:C:400:THR:CG2	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:226:LEU:HG	2:H:226:LEU:O	1.85	0.73
1:D:417:GLN:NE2	1:D:432:SER:HB3	2.02	0.73
1:A:542:SER:HB2	1:A:545:PRO:HG3	1.70	0.73
1:C:392:GLN:HG3	3:C:601:NAG:O6	1.87	0.73
1:D:408:ARG:NH1	2:J:226:LEU:CD1	2.51	0.73
2:G:226:LEU:HD21	2:G:228:LEU:CD2	2.19	0.73
2:J:162:THR:HB	2:J:287:THR:HG23	1.69	0.73
1:F:531:ALA:O	1:F:535:GLN:HA	1.89	0.73
2:G:162:THR:HB	2:G:287:THR:HG23	1.71	0.72
1:D:363:LEU:HA	1:D:396:THR:HG22	1.70	0.72
2:L:250:PRO:HB2	2:L:252:SER:OG	1.89	0.72
2:K:254:SER:CA	2:K:255:GLN:C	2.58	0.72
1:C:489:ARG:O	1:D:499:LYS:HE2	1.89	0.72
2:J:229:LYS:HG3	2:J:231:GLU:CG	2.19	0.72
2:G:254:SER:CB	2:G:255:GLN:C	2.58	0.71
2:J:254:SER:HB3	2:J:255:GLN:O	1.91	0.71
1:D:419:ARG:HH12	1:D:430:MET:HB2	1.56	0.71
2:G:229:LYS:HG3	2:G:231:GLU:HG2	1.72	0.71
2:G:229:LYS:HG3	2:G:231:GLU:CG	2.20	0.71
2:G:254:SER:CB	2:G:256:GLY:H	2.04	0.71
2:I:250:PRO:HB2	2:I:252:SER:OG	1.91	0.70
1:F:421:THR:HG23	1:F:428:ALA:HA	1.72	0.70
2:I:254:SER:CA	2:I:255:GLN:C	2.58	0.70
2:L:256:GLY:HA3	2:L:272:PHE:CE2	2.26	0.70
2:K:254:SER:HA	2:K:256:GLY:N	2.06	0.70
2:G:254:SER:CA	2:G:255:GLN:C	2.60	0.70
1:E:392:GLN:CG	3:E:601:NAG:O6	2.40	0.69
2:L:252:SER:O	2:L:253:ARG:CB	2.40	0.69
1:A:480:HIS:CD2	1:A:522:PHE:CE2	2.80	0.69
1:D:372:LEU:HD22	1:D:401:SER:HB2	1.74	0.69
2:G:254:SER:CB	2:G:256:GLY:N	2.55	0.69
1:F:360:VAL:HG13	1:F:399:VAL:HG13	1.72	0.69
1:A:371:GLN:CA	1:A:371:GLN:HE21	1.98	0.69
2:L:255:GLN:NE2	2:L:255:GLN:CA	2.46	0.69
1:D:394:ASN:ND2	3:D:601:NAG:C1	2.56	0.69
1:D:439:PRO:HA	2:J:255:GLN:O	1.91	0.69
2:K:162:THR:HB	2:K:287:THR:HG23	1.73	0.69
2:L:254:SER:HA	2:L:255:GLN:C	2.12	0.68
2:L:256:GLY:HA3	2:L:272:PHE:HE2	1.58	0.68
2:G:226:LEU:CD2	2:G:228:LEU:HD23	2.21	0.68
1:C:360:VAL:HG13	1:C:399:VAL:HG13	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:249:GLU:OE1	2:K:270:ASP:OD1	2.10	0.68
2:J:198:LEU:HB3	2:J:222:GLY:CA	2.24	0.68
1:B:394:ASN:ND2	3:B:601:NAG:C1	2.56	0.68
1:C:392:GLN:NE2	3:C:601:NAG:O6	2.26	0.68
1:D:408:ARG:CZ	2:J:226:LEU:HD13	2.23	0.68
1:C:372:LEU:HD22	1:C:401:SER:HB2	1.75	0.68
1:E:531:ALA:O	1:E:535:GLN:HA	1.95	0.67
2:I:226:LEU:O	2:I:227:ASP:C	2.33	0.67
2:J:251:THR:OG1	2:J:270:ASP:OD1	2.12	0.67
2:L:226:LEU:HG	2:L:226:LEU:O	1.95	0.67
1:A:394:ASN:ND2	3:A:601:NAG:C1	2.56	0.66
1:C:508:ARG:HD2	1:D:504:PHE:CE2	2.30	0.66
1:A:371:GLN:HB3	1:A:421:THR:OG1	1.94	0.66
2:H:254:SER:HA	2:H:255:GLN:C	2.15	0.66
1:A:359:LEU:HD12	1:A:400:THR:CG2	2.26	0.66
2:H:249:GLU:OE1	2:H:270:ASP:OD1	2.13	0.66
1:C:531:ALA:O	1:C:535:GLN:HA	1.96	0.66
2:J:254:SER:CA	2:J:255:GLN:C	2.64	0.66
1:D:340:LEU:HD11	1:D:356:ILE:HD12	1.78	0.66
1:C:510:GLU:OE1	1:D:499:LYS:HB2	1.96	0.65
2:L:246:ALA:HB2	2:L:267:ARG:HB3	1.79	0.65
1:E:392:GLN:HG3	3:E:601:NAG:O6	1.95	0.65
2:G:228:LEU:CG	2:G:228:LEU:O	2.42	0.65
2:K:198:LEU:HB3	2:K:222:GLY:CA	2.26	0.65
1:A:532:SER:OG	1:A:533:PRO:HA	1.97	0.65
1:C:407:THR:O	1:C:411:ILE:HG13	1.96	0.65
2:I:246:ALA:HB2	2:I:267:ARG:HB3	1.79	0.65
2:L:158:PHE:HA	2:L:291:PRO:HG3	1.78	0.65
2:I:184:TRP:CZ2	2:I:224:ARG:HG2	2.32	0.64
1:E:365:PRO:HB3	1:E:397:LEU:HB2	1.78	0.64
1:C:365:PRO:HB3	1:C:397:LEU:HB2	1.78	0.64
1:C:535:GLN:HE22	2:I:228:LEU:HA	1.63	0.64
2:G:226:LEU:HG	2:G:226:LEU:O	1.96	0.64
1:D:429:LEU:HD22	1:D:431:ARG:HH22	1.62	0.64
1:F:422:HIS:HD2	1:F:424:HIS:N	1.96	0.64
2:J:246:ALA:HB2	2:J:267:ARG:HB3	1.80	0.64
1:C:499:LYS:NZ	1:D:489:ARG:HH11	1.96	0.64
1:D:513:ARG:HG2	1:D:517:GLU:OE1	1.98	0.63
2:G:255:GLN:CA	2:G:255:GLN:NE2	2.61	0.63
2:L:291:PRO:O	2:L:292:ALA:HB3	1.97	0.63
2:G:255:GLN:CA	2:G:255:GLN:HE21	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:254:SER:HB3	2:G:256:GLY:H	1.62	0.63
2:L:158:PHE:N	2:L:291:PRO:HG3	2.14	0.63
2:L:158:PHE:N	2:L:291:PRO:CG	2.62	0.63
2:J:254:SER:HA	2:J:256:GLY:N	2.14	0.62
1:A:355:THR:HG22	1:A:404:PRO:HA	1.81	0.62
1:B:407:THR:O	1:B:411:ILE:HG13	1.98	0.62
1:F:419:ARG:HH11	1:F:430:MET:HG3	1.64	0.62
2:G:254:SER:HA	2:G:255:GLN:C	2.18	0.62
1:C:372:LEU:HG	1:C:420:VAL:CG1	2.30	0.62
1:A:359:LEU:HD12	1:A:400:THR:HG22	1.80	0.62
2:J:251:THR:O	2:J:255:GLN:HG3	2.00	0.61
1:B:372:LEU:HD22	1:B:401:SER:HB2	1.82	0.61
2:H:246:ALA:HB2	2:H:267:ARG:HB3	1.82	0.61
2:K:246:ALA:HB2	2:K:267:ARG:HB3	1.81	0.61
1:C:499:LYS:CE	1:D:489:ARG:HH11	2.14	0.61
2:H:255:GLN:NE2	2:H:255:GLN:CA	2.64	0.61
1:D:408:ARG:HH12	2:J:226:LEU:CD1	2.13	0.61
2:J:200:SER:HA	2:J:234:TRP:CE3	2.36	0.61
1:E:439:PRO:HA	2:K:255:GLN:O	2.00	0.61
2:K:255:GLN:CA	2:K:255:GLN:NE2	2.64	0.61
1:B:338:ALA:HB3	1:B:431:ARG:NH1	2.16	0.61
1:A:480:HIS:O	1:A:481:ASN:C	2.38	0.60
1:B:531:ALA:O	1:B:535:GLN:HA	2.00	0.60
2:H:252:SER:O	2:H:253:ARG:CB	2.42	0.60
1:A:371:GLN:CA	1:A:371:GLN:NE2	2.59	0.60
2:H:255:GLN:HE21	2:H:255:GLN:CA	2.15	0.60
2:G:227:ASP:O	2:G:229:LYS:O	2.19	0.60
1:E:392:GLN:HB3	3:E:601:NAG:HO6	1.67	0.60
2:K:255:GLN:CA	2:K:255:GLN:HE21	2.14	0.60
2:I:227:ASP:C	2:I:229:LYS:H	2.04	0.60
2:K:250:PRO:HB2	2:K:252:SER:OG	2.01	0.59
2:H:198:LEU:HB3	2:H:222:GLY:CA	2.32	0.59
2:K:254:SER:OG	2:K:256:GLY:HA2	2.02	0.59
1:D:440:ARG:HD2	1:D:530:ALA:HB2	1.85	0.59
1:A:371:GLN:HB3	1:A:421:THR:CB	2.32	0.59
2:J:226:LEU:O	2:J:226:LEU:HG	2.02	0.59
1:F:440:ARG:NH2	2:L:254:SER:OG	2.36	0.59
1:C:347:ASP:HB3	1:C:354:PRO:HA	1.84	0.59
2:G:255:GLN:H	2:G:255:GLN:NE2	2.00	0.58
2:K:226:LEU:O	2:K:226:LEU:HG	2.02	0.58
1:C:448:PHE:HB3	1:D:448:PHE:CD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:THR:HG22	1:C:404:PRO:HA	1.85	0.58
2:H:270:ASP:O	2:H:270:ASP:OD1	2.21	0.58
2:G:246:ALA:HB2	2:G:267:ARG:HB3	1.85	0.58
2:L:254:SER:HA	2:L:256:GLY:N	2.18	0.58
2:H:254:SER:OG	2:H:256:GLY:HA2	2.04	0.58
1:D:370:VAL:HG13	1:D:421:THR:O	2.04	0.58
1:A:347:ASP:HA	1:A:351:ARG:HB2	1.86	0.57
1:C:499:LYS:HZ1	1:D:489:ARG:NH1	2.02	0.57
2:H:255:GLN:NE2	2:H:255:GLN:HA	2.18	0.57
2:L:270:ASP:OD1	2:L:270:ASP:O	2.22	0.57
1:C:439:PRO:HA	2:I:255:GLN:O	2.03	0.57
2:G:252:SER:O	2:G:253:ARG:CB	2.51	0.57
1:C:520:ASP:O	1:C:542:SER:HB3	2.04	0.57
1:F:339:TYR:CD2	3:F:603:BMA:H3	2.40	0.57
2:I:226:LEU:O	2:I:228:LEU:CA	2.52	0.57
2:K:252:SER:O	2:K:253:ARG:CB	2.48	0.57
1:F:339:TYR:CE2	3:F:603:BMA:H3	2.38	0.57
2:G:250:PRO:HB2	2:G:252:SER:OG	2.04	0.57
1:C:451:PRO:HD2	1:D:446:TYR:CD2	2.40	0.57
2:L:227:ASP:C	2:L:229:LYS:H	2.08	0.57
1:F:473:ASP:O	1:F:528:HIS:HD2	1.88	0.57
2:K:227:ASP:C	2:K:229:LYS:H	2.07	0.56
2:G:254:SER:HB2	2:G:256:GLY:N	2.20	0.56
2:G:254:SER:HA	2:G:256:GLY:N	2.20	0.56
1:A:373:THR:HB	1:A:419:ARG:HB3	1.85	0.56
2:J:164:PRO:O	2:J:167:TRP:HB2	2.05	0.56
1:C:359:LEU:HD12	1:C:400:THR:HG22	1.86	0.56
2:J:228:LEU:CD2	2:J:228:LEU:O	2.49	0.56
2:K:257:GLU:O	2:K:270:ASP:HB2	2.06	0.56
2:L:158:PHE:CA	2:L:291:PRO:HG3	2.35	0.56
2:L:254:SER:CA	2:L:255:GLN:C	2.74	0.56
1:A:392:GLN:HG3	3:A:601:NAG:O6	2.06	0.56
1:C:508:ARG:HD2	1:D:504:PHE:CZ	2.41	0.56
1:C:372:LEU:HA	1:C:419:ARG:O	2.06	0.56
3:C:604:MAN:HO3	4:C:606:MAN:C1	2.19	0.56
1:F:347:ASP:HB3	1:F:354:PRO:HA	1.87	0.56
1:C:372:LEU:HG	1:C:420:VAL:HG13	1.88	0.55
1:B:358:CYS:HB2	1:B:374:TRP:CH2	2.41	0.55
2:I:198:LEU:HB3	2:I:222:GLY:HA2	1.88	0.55
1:D:429:LEU:HD22	1:D:431:ARG:NH2	2.21	0.55
1:C:373:THR:HB	1:C:419:ARG:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:CYS:HB2	1:A:374:TRP:CH2	2.42	0.55
1:E:425:LEU:CD2	1:E:426:PRO:HD2	2.35	0.55
2:J:184:TRP:CH2	2:J:224:ARG:HG2	2.41	0.55
2:H:254:SER:CA	2:H:255:GLN:C	2.75	0.55
2:J:252:SER:O	2:J:253:ARG:CB	2.52	0.55
1:D:443:PRO:HA	1:D:469:PHE:HB3	1.88	0.55
2:H:254:SER:HA	2:H:256:GLY:N	2.22	0.55
1:A:347:ASP:HB3	1:A:354:PRO:HA	1.89	0.55
1:E:355:THR:HG22	1:E:404:PRO:HA	1.90	0.54
1:E:440:ARG:HD2	1:E:530:ALA:HB2	1.88	0.54
2:K:223:LEU:HD23	2:K:260:VAL:HG21	1.90	0.54
2:K:254:SER:CB	2:K:255:GLN:O	2.55	0.54
1:E:372:LEU:HD22	1:E:401:SER:CB	2.35	0.54
2:I:185:VAL:HG22	2:I:189:TYR:CE1	2.43	0.54
1:A:438:GLY:HA2	2:G:272:PHE:CE2	2.43	0.54
2:L:226:LEU:O	2:L:227:ASP:HB2	2.08	0.54
2:J:184:TRP:CZ2	2:J:224:ARG:HG2	2.43	0.54
1:E:360:VAL:HG13	1:E:399:VAL:HG13	1.89	0.54
2:I:198:LEU:HB3	2:I:222:GLY:CA	2.38	0.54
1:B:479:LEU:HB2	1:B:523:ILE:HB	1.89	0.54
1:C:499:LYS:HZ1	1:D:489:ARG:HH11	1.56	0.54
1:B:359:LEU:HD11	3:B:602:NAG:O7	2.08	0.54
2:H:255:GLN:NE2	2:H:255:GLN:H	2.06	0.53
2:G:253:ARG:O	2:G:254:SER:OG	2.22	0.53
2:G:229:LYS:HG3	2:G:231:GLU:HG3	1.90	0.53
1:D:513:ARG:HG2	1:D:517:GLU:CD	2.29	0.53
2:I:200:SER:HA	2:I:234:TRP:CE3	2.43	0.53
2:K:255:GLN:NE2	2:K:255:GLN:H	2.06	0.53
1:E:347:ASP:HB3	1:E:354:PRO:HA	1.90	0.53
1:F:392:GLN:NE2	3:F:601:NAG:O6	2.40	0.53
1:C:489:ARG:HA	1:D:499:LYS:NZ	2.24	0.53
1:C:489:ARG:NH1	1:D:499:LYS:NZ	2.48	0.53
1:B:373:THR:HB	1:B:419:ARG:HB3	1.90	0.52
2:J:270:ASP:OD1	2:J:270:ASP:O	2.26	0.52
2:K:200:SER:HA	2:K:234:TRP:CE3	2.44	0.52
2:I:184:TRP:CH2	2:I:224:ARG:HG2	2.43	0.52
1:E:358:CYS:HB2	1:E:374:TRP:CH2	2.45	0.52
1:E:407:THR:O	1:E:411:ILE:HG13	2.10	0.52
1:D:444:GLU:CD	1:D:468:ASN:HD22	2.13	0.52
2:G:227:ASP:C	2:G:229:LYS:H	2.13	0.52
2:L:162:THR:HB	2:L:287:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:200:SER:HA	2:L:234:TRP:CE3	2.45	0.52
1:D:408:ARG:HH22	2:J:226:LEU:HD22	1.74	0.52
1:F:372:LEU:HD22	1:F:401:SER:HB2	1.91	0.52
2:G:223:LEU:HD23	2:G:260:VAL:HG21	1.91	0.52
1:B:426:PRO:O	1:B:427:ARG:HG3	2.10	0.52
1:F:360:VAL:CG1	1:F:399:VAL:HG13	2.40	0.51
2:L:158:PHE:N	2:L:291:PRO:HG2	2.25	0.51
1:A:360:VAL:HG13	1:A:399:VAL:HG13	1.92	0.51
1:D:370:VAL:HG13	1:D:422:HIS:HA	1.93	0.51
1:C:499:LYS:HE2	1:D:489:ARG:O	2.10	0.51
1:F:464:CYS:HB2	1:F:478:TRP:CH2	2.45	0.51
2:G:270:ASP:OD1	2:G:270:ASP:O	2.28	0.51
1:A:407:THR:O	1:A:411:ILE:HG13	2.09	0.51
2:L:252:SER:N	2:L:270:ASP:OD2	2.43	0.51
1:B:460:ARG:HG3	1:B:543:VAL:HG11	1.93	0.51
1:B:347:ASP:HA	1:B:351:ARG:HB2	1.93	0.51
1:C:480:HIS:CD2	1:C:522:PHE:CE2	2.97	0.51
2:L:174:CYS:HB2	2:L:284:ARG:HG2	1.92	0.51
2:L:198:LEU:HB3	2:L:222:GLY:CA	2.41	0.51
2:L:229:LYS:HB3	2:L:231:GLU:H	1.76	0.51
2:G:243:SER:HA	2:G:268:TRP:CZ3	2.46	0.51
1:A:440:ARG:HD2	1:A:530:ALA:HB2	1.92	0.51
1:B:440:ARG:HB2	2:H:254:SER:HB3	1.92	0.51
2:G:255:GLN:N	2:G:255:GLN:NE2	2.58	0.51
2:H:227:ASP:C	2:H:229:LYS:H	2.14	0.51
1:C:376:ARG:HD3	1:C:416:TYR:CE2	2.45	0.51
2:I:227:ASP:C	2:I:229:LYS:N	2.65	0.50
2:G:255:GLN:HA	2:G:255:GLN:NE2	2.19	0.50
1:A:490:HIS:HB3	1:A:509:LEU:HD13	1.93	0.50
2:I:250:PRO:C	2:I:252:SER:H	2.14	0.50
1:F:422:HIS:CG	1:F:423:PRO:HD2	2.46	0.50
1:C:480:HIS:O	1:C:481:ASN:HB2	2.11	0.50
2:H:223:LEU:HD23	2:H:260:VAL:HG21	1.93	0.50
2:L:254:SER:HB3	2:L:255:GLN:O	2.12	0.50
1:D:422:HIS:CE1	1:D:424:HIS:H	2.28	0.50
1:F:369:THR:O	1:F:423:PRO:HD3	2.11	0.50
1:E:385:SER:HB3	1:E:403:LEU:HD12	1.94	0.50
2:L:291:PRO:O	2:L:292:ALA:CB	2.59	0.50
1:F:417:GLN:HB3	1:F:430:MET:CE	2.42	0.50
1:B:422:HIS:ND1	1:B:423:PRO:HD2	2.27	0.50
2:H:255:GLN:NE2	2:H:255:GLN:N	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:222:GLY:O	2:I:235:VAL:HG13	2.12	0.50
2:K:270:ASP:OD1	2:K:270:ASP:O	2.30	0.49
2:J:229:LYS:HG3	2:J:231:GLU:HG2	1.91	0.49
2:L:164:PRO:O	2:L:167:TRP:HB2	2.12	0.49
2:K:253:ARG:O	2:K:254:SER:HB2	2.12	0.49
1:C:490:HIS:HB3	1:C:509:LEU:HD13	1.92	0.49
1:C:457:ARG:HG3	1:C:513:ARG:HH21	1.76	0.49
2:L:243:SER:HA	2:L:268:TRP:CZ3	2.48	0.49
2:K:255:GLN:N	2:K:255:GLN:NE2	2.60	0.49
2:K:251:THR:OG1	2:K:270:ASP:OD1	2.30	0.49
1:F:423:PRO:HG2	1:F:424:HIS:HD2	1.77	0.49
1:A:419:ARG:HA	1:A:429:LEU:O	2.13	0.49
1:C:338:ALA:HB2	1:C:429:LEU:HD13	1.94	0.49
2:J:227:ASP:C	2:J:229:LYS:H	2.15	0.49
2:K:253:ARG:HD2	2:K:253:ARG:HA	1.60	0.49
1:C:358:CYS:HB2	1:C:374:TRP:CH2	2.48	0.49
2:L:227:ASP:C	2:L:229:LYS:N	2.66	0.48
2:G:200:SER:HB3	2:G:234:TRP:HB3	1.94	0.48
1:A:371:GLN:CB	1:A:421:THR:CB	2.83	0.48
2:H:200:SER:HA	2:H:234:TRP:CE3	2.48	0.48
1:A:336:VAL:CG2	1:A:425:LEU:HD11	2.44	0.48
1:F:421:THR:CG2	1:F:428:ALA:HA	2.40	0.48
1:A:480:HIS:O	1:A:482:GLU:N	2.46	0.48
1:A:389:GLU:HA	1:A:399:VAL:HA	1.95	0.48
1:F:422:HIS:CD2	1:F:424:HIS:HB2	2.47	0.48
2:J:252:SER:N	2:J:270:ASP:OD2	2.47	0.48
1:A:406:GLY:HA3	1:A:409:ASP:OD2	2.13	0.48
1:C:475:SER:HB2	1:C:527:VAL:HB	1.96	0.48
2:G:223:LEU:HB3	2:G:260:VAL:HB	1.95	0.48
1:C:544:ASN:O	1:C:544:ASN:ND2	2.47	0.48
1:D:440:ARG:HD3	1:D:529:GLU:HG2	1.96	0.47
2:G:256:GLY:HA3	2:G:272:PHE:CE2	2.48	0.47
2:J:227:ASP:C	2:J:229:LYS:N	2.68	0.47
1:D:372:LEU:HD22	1:D:401:SER:CB	2.41	0.47
1:B:424:HIS:CG	1:B:424:HIS:O	2.67	0.47
1:E:376:ARG:HD3	1:E:416:TYR:CE2	2.49	0.47
2:G:200:SER:HA	2:G:234:TRP:CE3	2.49	0.47
2:K:184:TRP:CZ2	2:K:224:ARG:HG2	2.50	0.47
2:I:255:GLN:HB3	2:I:256:GLY:H	1.46	0.47
2:L:250:PRO:C	2:L:252:SER:H	2.17	0.47
1:A:464:CYS:HB2	1:A:478:TRP:CH2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:254:SER:HA	2:I:256:GLY:N	2.25	0.47
1:E:376:ARG:HD2	1:E:414:GLU:OE2	2.13	0.47
1:D:514:ALA:O	1:D:518:GLN:HB3	2.14	0.47
1:B:376:ARG:HD2	1:B:414:GLU:OE2	2.15	0.47
2:G:257:GLU:HG2	2:G:272:PHE:N	2.29	0.47
2:L:159:VAL:HG13	2:L:289:THR:OG1	2.15	0.47
1:D:419:ARG:HH12	1:D:430:MET:CB	2.25	0.47
1:D:408:ARG:HH12	2:J:226:LEU:HD11	1.80	0.46
1:F:408:ARG:CZ	2:L:226:LEU:HD13	2.45	0.46
1:F:347:ASP:HA	1:F:351:ARG:HB2	1.97	0.46
1:E:444:GLU:CD	1:E:468:ASN:HD22	2.19	0.46
2:J:245:TRP:O	2:J:267:ARG:NH1	2.48	0.46
3:C:603:BMA:H61	3:C:604:MAN:H2	1.61	0.46
2:H:250:PRO:HB2	2:H:252:SER:OG	2.16	0.46
2:K:227:ASP:C	2:K:229:LYS:N	2.69	0.46
1:B:360:VAL:HG13	1:B:399:VAL:HG13	1.96	0.46
2:L:165:GLU:O	2:L:166:LYS:HB2	2.14	0.46
1:F:437:SER:HB3	2:L:274:ASP:OD2	2.16	0.46
1:A:393:ARG:H	1:A:393:ARG:HG2	1.52	0.46
1:B:439:PRO:HA	2:H:255:GLN:O	2.16	0.46
1:B:347:ASP:HB3	1:B:354:PRO:HA	1.97	0.46
2:G:254:SER:CA	2:G:256:GLY:N	2.79	0.46
1:D:441:ALA:HB3	1:D:470:MET:HG2	1.96	0.46
2:J:222:GLY:O	2:J:235:VAL:HG13	2.16	0.46
1:C:392:GLN:HB3	3:C:601:NAG:O6	2.16	0.46
1:C:355:THR:HG22	1:C:404:PRO:CA	2.47	0.45
1:F:362:ASP:O	1:F:396:THR:HB	2.16	0.45
1:F:408:ARG:NH2	2:L:226:LEU:HD13	2.30	0.45
2:H:253:ARG:O	2:H:254:SER:HB2	2.15	0.45
2:G:245:TRP:CD2	2:G:250:PRO:HD3	2.52	0.45
1:D:490:HIS:HB3	1:D:509:LEU:HD13	1.98	0.45
1:D:355:THR:HG22	1:D:404:PRO:HA	1.98	0.45
2:H:203:SER:OG	2:H:206:GLU:HB2	2.16	0.45
1:C:392:GLN:HG3	3:C:601:NAG:C6	2.46	0.45
2:J:254:SER:CB	2:J:255:GLN:O	2.62	0.45
1:C:489:ARG:NH1	1:D:499:LYS:HZ1	2.02	0.45
1:C:444:GLU:CD	1:C:468:ASN:HD22	2.20	0.45
1:E:339:TYR:HD1	1:E:359:LEU:HD23	1.82	0.45
1:F:444:GLU:CD	1:F:468:ASN:HD22	2.20	0.45
1:D:422:HIS:CD2	1:D:423:PRO:CD	2.84	0.45
2:K:184:TRP:CH2	2:K:224:ARG:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ARG:HH11	1:A:408:ARG:HG3	1.82	0.45
2:L:251:THR:OG1	2:L:270:ASP:OD1	2.34	0.45
2:H:226:LEU:CG	2:H:226:LEU:O	2.61	0.45
2:G:227:ASP:C	2:G:229:LYS:N	2.70	0.44
1:A:464:CYS:HB2	1:A:478:TRP:CZ2	2.52	0.44
1:A:457:ARG:HG3	1:A:513:ARG:HH21	1.82	0.44
1:C:392:GLN:CD	3:C:601:NAG:O6	2.56	0.44
2:L:174:CYS:HB2	2:L:284:ARG:CG	2.48	0.44
1:B:480:HIS:CD2	1:B:522:PHE:CE2	3.05	0.44
3:B:603:BMA:H61	3:B:604:MAN:H3	1.99	0.44
2:L:245:TRP:CE2	2:L:250:PRO:HD3	2.53	0.44
1:B:481:ASN:O	1:B:482:GLU:HB2	2.18	0.44
2:G:198:LEU:HB3	2:G:222:GLY:CA	2.48	0.44
2:I:231:GLU:HG3	2:I:231:GLU:O	2.17	0.44
2:K:255:GLN:HB3	2:K:256:GLY:H	1.45	0.44
1:E:376:ARG:HG3	1:E:382:VAL:HG12	1.99	0.44
1:E:493:THR:HA	1:F:496:ARG:NH2	2.32	0.44
1:B:464:CYS:HB2	1:B:478:TRP:CZ2	2.52	0.44
1:B:460:ARG:NH1	1:B:543:VAL:HG12	2.33	0.44
1:B:440:ARG:HD3	1:B:529:GLU:OE2	2.18	0.44
1:C:360:VAL:CG1	1:C:399:VAL:HG13	2.46	0.44
2:H:165:GLU:O	2:H:166:LYS:HB2	2.17	0.44
1:C:446:TYR:CD2	1:D:450:THR:HB	2.50	0.44
1:A:479:LEU:HB2	1:A:523:ILE:HB	1.99	0.43
1:E:347:ASP:HA	1:E:351:ARG:HB2	2.00	0.43
1:F:479:LEU:HB2	1:F:523:ILE:HB	2.01	0.43
2:J:250:PRO:C	2:J:252:SER:H	2.21	0.43
1:D:422:HIS:HA	1:D:423:PRO:HD3	1.91	0.43
2:H:226:LEU:O	2:H:228:LEU:N	2.50	0.43
2:G:229:LYS:CG	2:G:231:GLU:HG3	2.48	0.43
1:D:362:ASP:O	1:D:396:THR:HB	2.19	0.43
1:D:347:ASP:HB3	1:D:354:PRO:HA	2.00	0.43
2:G:203:SER:HB2	2:G:205:GLU:OE1	2.19	0.43
1:A:539:ARG:HA	1:A:539:ARG:HD3	1.83	0.43
1:A:451:PRO:HD2	1:B:446:TYR:HD2	1.84	0.43
1:F:376:ARG:HD2	1:F:414:GLU:OE2	2.19	0.43
2:L:222:GLY:O	2:L:234:TRP:HA	2.19	0.43
1:F:365:PRO:HB3	1:F:397:LEU:HB2	2.00	0.43
1:F:440:ARG:HD2	1:F:530:ALA:HB2	2.00	0.43
1:F:423:PRO:HG2	1:F:424:HIS:CD2	2.53	0.43
1:F:418:CYS:O	1:F:430:MET:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:GLY:HA3	1:C:409:ASP:OD2	2.19	0.43
1:C:465:LEU:HD21	1:C:467:GLN:OE1	2.19	0.43
1:C:446:TYR:O	1:C:464:CYS:HA	2.19	0.42
1:C:376:ARG:HD2	1:C:414:GLU:OE2	2.19	0.42
1:C:464:CYS:HB2	1:C:478:TRP:CH2	2.54	0.42
2:H:198:LEU:HB3	2:H:222:GLY:HA3	2.01	0.42
1:A:453:TRP:HA	1:A:454:PRO:HD3	1.88	0.42
2:I:254:SER:CB	2:I:255:GLN:O	2.68	0.42
2:H:250:PRO:C	2:H:252:SER:H	2.23	0.42
2:K:198:LEU:HB3	2:K:222:GLY:HA3	2.00	0.42
2:G:245:TRP:O	2:G:267:ARG:NH1	2.52	0.42
1:C:392:GLN:CB	3:C:601:NAG:O6	2.67	0.42
2:K:254:SER:CB	2:K:255:GLN:C	2.87	0.42
2:J:257:GLU:O	2:J:270:ASP:HB2	2.19	0.42
2:I:289:THR:HA	2:I:290:PRO:HD3	1.84	0.42
1:E:392:GLN:CD	3:E:601:NAG:O6	2.57	0.42
1:B:338:ALA:HB3	1:B:431:ARG:HH11	1.82	0.42
2:J:198:LEU:HB3	2:J:222:GLY:HA3	2.00	0.42
1:C:464:CYS:HB2	1:C:478:TRP:CZ2	2.55	0.42
1:F:389:GLU:HA	1:F:399:VAL:HA	2.00	0.42
1:A:443:PRO:HA	1:A:469:PHE:HB3	2.02	0.42
1:F:407:THR:O	1:F:411:ILE:HG13	2.20	0.42
2:H:254:SER:HG	2:H:256:GLY:HA2	1.84	0.42
1:D:440:ARG:NH2	2:J:254:SER:OG	2.53	0.42
2:J:198:LEU:HB3	2:J:222:GLY:HA2	1.99	0.42
1:C:347:ASP:HA	1:C:351:ARG:HB2	2.02	0.42
2:H:177:PHE:CE2	2:H:213:HIS:HB2	2.54	0.42
1:E:508:ARG:HD2	1:F:504:PHE:CE2	2.54	0.42
1:C:489:ARG:HA	1:D:499:LYS:HZ1	1.85	0.42
1:C:440:ARG:HD3	1:C:529:GLU:OE2	2.20	0.42
2:H:227:ASP:C	2:H:229:LYS:N	2.73	0.42
1:A:479:LEU:HD23	1:A:484:GLN:HA	2.00	0.42
1:D:465:LEU:HD13	1:D:506:PHE:CZ	2.55	0.42
1:C:439:PRO:HA	2:I:254:SER:HB3	2.02	0.42
2:K:254:SER:HB3	2:K:255:GLN:O	2.20	0.42
1:C:499:LYS:HE3	1:D:489:ARG:NH1	2.35	0.42
1:D:342:ARG:HB3	1:D:343:PRO:CD	2.50	0.42
2:H:174:CYS:HB2	2:H:284:ARG:HG2	2.02	0.41
2:H:257:GLU:HG2	2:H:272:PHE:N	2.35	0.41
1:A:335:GLY:C	1:A:336:VAL:HG22	2.40	0.41
2:I:165:GLU:O	2:I:166:LYS:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:417:GLN:HB3	1:F:430:MET:HE2	2.02	0.41
1:B:515:GLU:HB3	1:B:522:PHE:HZ	1.85	0.41
1:E:342:ARG:HB3	1:E:343:PRO:CD	2.50	0.41
2:L:184:TRP:CZ2	2:L:224:ARG:HG2	2.54	0.41
1:E:364:ALA:HA	1:E:365:PRO:HD3	1.84	0.41
1:B:457:ARG:HG3	1:B:513:ARG:HH21	1.86	0.41
1:C:499:LYS:CE	1:D:489:ARG:NH1	2.82	0.41
1:A:336:VAL:HG21	1:A:425:LEU:HD11	2.02	0.41
1:F:443:PRO:HA	1:F:469:PHE:HB3	2.02	0.41
1:E:475:SER:HB2	1:E:527:VAL:HB	2.03	0.41
1:B:543:VAL:C	1:B:544:ASN:OD1	2.58	0.41
1:A:450:THR:HB	1:B:446:TYR:CE2	2.55	0.41
1:F:338:ALA:HA	1:F:359:LEU:O	2.21	0.41
2:G:224:ARG:HA	2:G:258:ASP:O	2.20	0.41
2:I:223:LEU:HD23	2:I:260:VAL:HG21	2.02	0.41
1:F:422:HIS:CB	1:F:425:LEU:HB2	2.37	0.41
1:A:359:LEU:HD11	3:A:602:NAG:O7	2.21	0.41
1:C:467:GLN:OE1	1:D:461:THR:HG21	2.21	0.41
1:C:385:SER:HB3	1:C:403:LEU:HD12	2.03	0.41
1:D:358:CYS:HB2	1:D:374:TRP:CH2	2.55	0.41
2:K:198:LEU:HB3	2:K:222:GLY:HA2	2.01	0.41
1:A:392:GLN:CG	3:A:601:NAG:O6	2.69	0.40
1:B:485:LEU:HA	1:B:486:PRO:HD3	1.96	0.40
2:K:249:GLU:HA	2:K:250:PRO:C	2.42	0.40
1:D:374:TRP:HD1	1:D:385:SER:HG	1.66	0.40
1:E:359:LEU:HD12	1:E:400:THR:CG2	2.51	0.40
1:C:472:GLU:HG2	1:C:472:GLU:H	1.75	0.40
2:L:255:GLN:HB3	2:L:256:GLY:H	1.22	0.40
2:J:255:GLN:HB2	2:J:256:GLY:H	1.49	0.40
1:E:339:TYR:CD1	1:E:359:LEU:HD23	2.56	0.40
1:E:342:ARG:HB3	1:E:343:PRO:HD2	2.04	0.40
1:F:342:ARG:HB3	1:F:343:PRO:CD	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:287:THR:OG1	2:L:287:THR:OG1[4_445]	1.85	0.35
2:H:287:THR:OG1	2:J:287:THR:OG1[3_345]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	205/223 (92%)	189 (92%)	14 (7%)	2 (1%)	19	58
1	B	203/223 (91%)	187 (92%)	14 (7%)	2 (1%)	19	58
1	C	192/223 (86%)	172 (90%)	19 (10%)	1 (0%)	34	71
1	D	175/223 (78%)	165 (94%)	10 (6%)	0	100	100
1	E	166/223 (74%)	155 (93%)	9 (5%)	2 (1%)	16	54
1	F	191/223 (86%)	175 (92%)	15 (8%)	1 (0%)	34	71
2	G	133/143 (93%)	113 (85%)	17 (13%)	3 (2%)	8	39
2	H	131/143 (92%)	112 (86%)	16 (12%)	3 (2%)	8	39
2	I	132/143 (92%)	113 (86%)	15 (11%)	4 (3%)	5	33
2	J	133/143 (93%)	115 (86%)	16 (12%)	2 (2%)	13	49
2	K	133/143 (93%)	114 (86%)	17 (13%)	2 (2%)	13	49
2	L	134/143 (94%)	118 (88%)	13 (10%)	3 (2%)	8	41
All	All	1928/2196 (88%)	1728 (90%)	175 (9%)	25 (1%)	15	52

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	227	ASP
2	L	292	ALA
2	I	170	PHE
2	I	228	LEU
2	K	228	LEU
1	B	428	ALA
1	F	368	GLY
1	A	482	GLU
2	G	161	ASN
2	H	229	LYS
2	I	254	SER
2	J	161	ASN

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Mol	Chain	Res	Type
2	J	230	GLY
2	G	230	GLY
2	G	254	SER
2	H	161	ASN
2	H	228	LEU
2	L	228	LEU
2	L	254	SER
1	C	365	PRO
2	K	161	ASN
1	A	336	VAL
1	B	426	PRO
1	E	364	ALA
1	E	365	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	184/195 (94%)	172 (94%)	12 (6%)	21	59
1	B	184/195 (94%)	176 (96%)	8 (4%)	35	72
1	C	176/195 (90%)	165 (94%)	11 (6%)	22	60
1	D	167/195 (86%)	161 (96%)	6 (4%)	42	76
1	E	159/195 (82%)	153 (96%)	6 (4%)	40	75
1	F	177/195 (91%)	168 (95%)	9 (5%)	29	68
2	G	115/120 (96%)	102 (89%)	13 (11%)	7	30
2	H	114/120 (95%)	101 (89%)	13 (11%)	7	29
2	I	115/120 (96%)	106 (92%)	9 (8%)	16	50
2	J	115/120 (96%)	105 (91%)	10 (9%)	13	45
2	K	115/120 (96%)	106 (92%)	9 (8%)	16	50
2	L	116/120 (97%)	100 (86%)	16 (14%)	4	20
All	All	1737/1890 (92%)	1615 (93%)	122 (7%)	19	56

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	VAL
1	A	344	SER
1	A	359	LEU
1	A	370	VAL
1	A	371	GLN
1	A	372	LEU
1	A	393	ARG
1	A	401	SER
1	A	427	ARG
1	A	525	ARG
1	A	532	SER
1	A	544	ASN
1	B	344	SER
1	B	359	LEU
1	B	427	ARG
1	B	430	MET
1	B	479	LEU
1	B	511	VAL
1	B	532	SER
1	B	545	PRO
1	C	344	SER
1	C	360	VAL
1	C	363	LEU
1	C	372	LEU
1	C	380	LYS
1	C	401	SER
1	C	419	ARG
1	C	420	VAL
1	C	437	SER
1	C	497	LYS
1	C	544	ASN
1	D	336	VAL
1	D	363	LEU
1	D	417	GLN
1	D	465	LEU
1	D	475	SER
1	D	518	GLN
1	E	359	LEU
1	E	360	VAL
1	E	372	LEU
1	E	391	LYS
1	E	424	HIS

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Mol	Chain	Res	Type
1	E	425	LEU
1	F	344	SER
1	F	359	LEU
1	F	360	VAL
1	F	367	LYS
1	F	371	GLN
1	F	421	THR
1	F	427	ARG
1	F	475	SER
1	F	532	SER
2	G	200	SER
2	G	208	ASP
2	G	219	SER
2	G	224	ARG
2	G	225	ASN
2	G	228	LEU
2	G	229	LYS
2	G	231	GLU
2	G	241	ASP
2	G	253	ARG
2	G	255	GLN
2	G	287	THR
2	G	289	THR
2	H	200	SER
2	H	208	ASP
2	H	219	SER
2	H	224	ARG
2	H	225	ASN
2	H	228	LEU
2	H	231	GLU
2	H	241	ASP
2	H	253	ARG
2	H	254	SER
2	H	255	GLN
2	H	287	THR
2	H	289	THR
2	I	200	SER
2	I	219	SER
2	I	224	ARG
2	I	225	ASN
2	I	226	LEU
2	I	228	LEU

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Mol	Chain	Res	Type
2	I	231	GLU
2	I	241	ASP
2	I	289	THR
2	J	200	SER
2	J	208	ASP
2	J	224	ARG
2	J	225	ASN
2	J	228	LEU
2	J	229	LYS
2	J	241	ASP
2	J	252	SER
2	J	253	ARG
2	J	255	GLN
2	K	200	SER
2	K	208	ASP
2	K	224	ARG
2	K	225	ASN
2	K	228	LEU
2	K	241	ASP
2	K	253	ARG
2	K	255	GLN
2	K	287	THR
2	L	158	PHE
2	L	159	VAL
2	L	164	PRO
2	L	200	SER
2	L	208	ASP
2	L	224	ARG
2	L	225	ASN
2	L	228	LEU
2	L	231	GLU
2	L	241	ASP
2	L	253	ARG
2	L	254	SER
2	L	255	GLN
2	L	287	THR
2	L	289	THR
2	L	293	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	GLN
1	A	394	ASN
1	A	468	ASN
1	A	480	HIS
1	B	394	ASN
1	B	468	ASN
1	C	392	GLN
1	C	394	ASN
1	C	468	ASN
1	C	544	ASN
1	D	394	ASN
1	D	417	GLN
1	D	422	HIS
1	D	468	ASN
1	D	490	HIS
1	D	518	GLN
1	E	392	GLN
1	E	394	ASN
1	E	468	ASN
1	F	392	GLN
1	F	394	ASN
1	F	422	HIS
1	F	424	HIS
1	F	468	ASN
1	F	481	ASN
2	G	171	GLN
2	G	225	ASN
2	G	239	HIS
2	G	255	GLN
2	G	269	ASN
2	H	213	HIS
2	H	225	ASN
2	H	255	GLN
2	I	171	GLN
2	J	171	GLN
2	J	225	ASN
2	J	255	GLN
2	K	171	GLN
2	K	255	GLN
2	K	269	ASN
2	L	171	GLN
2	L	255	GLN
2	L	269	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 ⓘ

30 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	$\# Z > 2$
3	NAG	A	601	3	14,14,15	0.54	0	15,19,21	0.60	0
3	NAG	A	602	3	14,14,15	0.54	0	15,19,21	1.91	4 (26%)
3	BMA	A	603	3	11,11,12	0.82	0	14,15,17	1.93	6 (42%)
3	MAN	A	604	3	11,11,12	0.79	0	14,15,17	1.57	3 (21%)
3	MAN	A	605	3	11,11,12	0.76	0	14,15,17	1.63	3 (21%)
3	NAG	B	601	3	14,14,15	0.54	0	15,19,21	0.59	0
3	NAG	B	602	3	14,14,15	0.57	0	15,19,21	1.07	1 (6%)
3	BMA	B	603	3	11,11,12	0.32	0	14,15,17	1.37	2 (14%)
3	MAN	B	604	3	11,11,12	0.68	0	14,15,17	1.51	4 (28%)
3	MAN	B	605	3	11,11,12	0.60	0	14,15,17	1.76	4 (28%)
3	NAG	C	601	3	14,14,15	0.53	0	15,19,21	0.59	0
3	NAG	C	602	3	14,14,15	0.55	0	15,19,21	1.00	0
3	BMA	C	603	3	11,11,12	0.56	0	14,15,17	2.23	5 (35%)
3	MAN	C	604	3	11,11,12	1.58	2 (18%)	14,15,17	3.77	8 (57%)
3	MAN	C	605	3	11,11,12	0.82	0	14,15,17	1.83	4 (28%)
3	NAG	D	601	3	14,14,15	0.55	0	15,19,21	0.59	0
3	NAG	D	602	3	14,14,15	0.82	0	15,19,21	1.67	4 (26%)
3	BMA	D	603	3	11,11,12	0.59	0	14,15,17	2.13	6 (42%)
3	MAN	D	604	3	11,11,12	0.49	0	14,15,17	1.77	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	D	605	3	11,11,12	1.44	2 (18%)	14,15,17	2.39	6 (42%)
3	NAG	E	601	3	14,14,15	0.53	0	15,19,21	0.59	0
3	NAG	E	602	3	14,14,15	0.50	0	15,19,21	1.07	0
3	BMA	E	603	3	11,11,12	0.97	1 (9%)	14,15,17	1.83	4 (28%)
3	MAN	E	604	3	11,11,12	0.58	0	14,15,17	1.89	4 (28%)
3	MAN	E	605	3	11,11,12	0.81	0	14,15,17	1.42	2 (14%)
3	NAG	F	601	3	14,14,15	0.53	0	15,19,21	0.59	0
3	NAG	F	602	3	14,14,15	0.53	0	15,19,21	1.09	1 (6%)
3	BMA	F	603	3	11,11,12	0.88	0	14,15,17	1.78	4 (28%)
3	MAN	F	604	3	11,11,12	0.60	0	14,15,17	1.71	4 (28%)
3	MAN	F	605	3	11,11,12	0.80	0	14,15,17	1.51	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	601	3	-	0/6/23/26	0/1/1/1
3	NAG	A	602	3	-	0/6/23/26	0/1/1/1
3	BMA	A	603	3	-	0/2/19/22	0/1/1/1
3	MAN	A	604	3	-	0/2/19/22	0/1/1/1
3	MAN	A	605	3	-	0/2/19/22	0/1/1/1
3	NAG	B	601	3	-	0/6/23/26	0/1/1/1
3	NAG	B	602	3	-	0/6/23/26	0/1/1/1
3	BMA	B	603	3	-	0/2/19/22	0/1/1/1
3	MAN	B	604	3	-	0/2/19/22	0/1/1/1
3	MAN	B	605	3	-	0/2/19/22	0/1/1/1
3	NAG	C	601	3	-	0/6/23/26	0/1/1/1
3	NAG	C	602	3	-	0/6/23/26	0/1/1/1
3	BMA	C	603	3	-	0/2/19/22	0/1/1/1
3	MAN	C	604	3	-	0/2/19/22	0/1/1/1
3	MAN	C	605	3	-	0/2/19/22	0/1/1/1
3	NAG	D	601	3	-	0/6/23/26	0/1/1/1
3	NAG	D	602	3	-	0/6/23/26	0/1/1/1
3	BMA	D	603	3	-	0/2/19/22	0/1/1/1
3	MAN	D	604	3	-	0/2/19/22	0/1/1/1
3	MAN	D	605	3	-	0/2/19/22	0/1/1/1
3	NAG	E	601	3	-	0/6/23/26	0/1/1/1
3	NAG	E	602	3	-	0/6/23/26	0/1/1/1
3	BMA	E	603	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	E	604	3	-	0/2/19/22	0/1/1/1
3	MAN	E	605	3	-	0/2/19/22	0/1/1/1
3	NAG	F	601	3	-	0/6/23/26	0/1/1/1
3	NAG	F	602	3	-	0/6/23/26	0/1/1/1
3	BMA	F	603	3	-	0/2/19/22	0/1/1/1
3	MAN	F	604	3	-	0/2/19/22	0/1/1/1
3	MAN	F	605	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)
3	D	605	MAN	O4-C4	-2.03	1.38	1.43
3	C	604	MAN	O6-C6	2.14	1.51	1.42
3	E	603	BMA	O5-C1	2.50	1.47	1.43
3	D	605	MAN	C2-C3	3.39	1.57	1.52
3	C	604	MAN	O3-C3	4.05	1.52	1.43

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	MAN	O2-C2-C3	-6.61	96.82	110.12
3	C	604	MAN	O3-C3-C2	-5.37	100.29	110.00
3	D	605	MAN	C2-C3-C4	-4.77	102.93	111.04
3	D	604	MAN	O5-C1-C2	-4.64	103.34	110.86
3	A	602	NAG	O7-C7-C8	-4.36	114.06	122.06
3	E	604	MAN	O5-C1-C2	-4.27	103.93	110.86
3	F	603	BMA	O3-C3-C4	-4.24	100.80	110.34
3	D	605	MAN	O2-C2-C1	-4.14	100.90	109.21
3	C	603	BMA	C6-C5-C4	-4.14	102.81	113.02
3	E	603	BMA	O3-C3-C4	-3.89	101.59	110.34
3	F	604	MAN	O5-C1-C2	-3.86	104.60	110.86
3	D	603	BMA	O3-C3-C4	-3.66	102.10	110.34
3	A	604	MAN	O5-C1-C2	-3.61	105.00	110.86
3	B	605	MAN	O5-C1-C2	-3.58	105.05	110.86
3	D	604	MAN	O4-C4-C3	-3.32	102.86	110.34
3	D	605	MAN	C3-C4-C5	-3.25	104.53	110.20
3	E	603	BMA	O2-C2-C3	-3.24	103.61	110.12
3	E	605	MAN	O5-C1-C2	-3.23	105.61	110.86
3	A	605	MAN	C3-C4-C5	-3.20	104.62	110.20
3	C	604	MAN	O2-C2-C1	-3.19	102.82	109.21
3	D	605	MAN	O5-C1-C2	-3.02	105.95	110.86
3	B	605	MAN	C3-C4-C5	-2.95	105.06	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	BMA	O3-C3-C4	-2.88	103.86	110.34
3	E	604	MAN	O2-C2-C3	-2.87	104.36	110.12
3	C	605	MAN	C3-C4-C5	-2.86	105.21	110.20
3	F	605	MAN	C1-C2-C3	-2.83	106.20	109.54
3	B	605	MAN	C2-C3-C4	-2.82	106.26	111.04
3	A	603	BMA	O2-C2-C3	-2.81	104.47	110.12
3	B	604	MAN	O5-C1-C2	-2.75	106.39	110.86
3	C	605	MAN	C1-O5-C5	-2.72	108.80	112.25
3	B	603	BMA	O3-C3-C4	-2.63	104.41	110.34
3	A	603	BMA	O3-C3-C4	-2.63	104.41	110.34
3	A	604	MAN	O2-C2-C3	-2.63	104.83	110.12
3	C	605	MAN	O5-C1-C2	-2.60	106.64	110.86
3	C	605	MAN	C2-C3-C4	-2.59	106.64	111.04
3	C	604	MAN	O4-C4-C3	-2.58	104.52	110.34
3	D	602	NAG	C3-C4-C5	-2.57	105.71	110.20
3	F	605	MAN	C3-C4-C5	-2.40	106.02	110.20
3	A	603	BMA	C6-C5-C4	-2.38	107.14	113.02
3	F	605	MAN	C2-C3-C4	-2.35	107.05	111.04
3	D	603	BMA	O4-C4-C3	-2.30	105.15	110.34
3	B	605	MAN	C1-C2-C3	-2.29	106.83	109.54
3	D	603	BMA	C1-O5-C5	-2.28	109.35	112.25
3	B	604	MAN	O4-C4-C3	-2.27	105.22	110.34
3	A	605	MAN	C2-C3-C4	-2.23	107.25	111.04
3	E	605	MAN	C1-C2-C3	-2.18	106.96	109.54
3	F	604	MAN	O4-C4-C3	-2.15	105.49	110.34
3	D	603	BMA	C6-C5-C4	-2.14	107.74	113.02
3	C	604	MAN	C1-O5-C5	-2.12	109.56	112.25
3	D	603	BMA	O2-C2-C1	-2.10	105.00	109.21
3	F	603	BMA	C6-C5-C4	-2.07	107.91	113.02
3	F	603	BMA	O6-C6-C5	2.04	118.08	111.33
3	E	604	MAN	C3-C4-C5	2.07	113.80	110.20
3	D	605	MAN	O3-C3-C2	2.08	113.76	110.00
3	E	603	BMA	O6-C6-C5	2.16	118.48	111.33
3	A	605	MAN	O3-C3-C4	2.19	115.28	110.34
3	A	603	BMA	C1-O5-C5	2.27	115.12	112.25
3	F	604	MAN	C1-O5-C5	2.32	115.19	112.25
3	B	602	NAG	C2-N2-C7	2.51	126.26	123.04
3	A	602	NAG	C2-N2-C7	2.60	126.38	123.04
3	D	602	NAG	C2-N2-C7	2.61	126.39	123.04
3	E	603	BMA	O5-C5-C6	2.63	113.04	107.35
3	B	604	MAN	C3-C4-C5	2.68	114.86	110.20
3	F	603	BMA	O5-C5-C6	2.72	113.23	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	MAN	O5-C5-C6	2.76	113.32	107.35
3	B	604	MAN	C1-O5-C5	2.78	115.78	112.25
3	D	602	NAG	O3-C3-C2	2.83	114.73	109.11
3	F	602	NAG	C2-N2-C7	2.85	126.70	123.04
3	E	604	MAN	C1-O5-C5	2.88	115.90	112.25
3	D	605	MAN	O2-C2-C3	2.88	115.90	110.12
3	A	602	NAG	O5-C5-C6	2.94	113.72	107.35
3	A	603	BMA	O5-C5-C6	2.99	113.81	107.35
3	A	603	BMA	C3-C4-C5	2.99	115.42	110.20
3	C	603	BMA	O5-C5-C6	3.10	114.05	107.35
3	B	603	BMA	O5-C5-C6	3.22	114.32	107.35
3	A	602	NAG	C8-C7-N2	3.25	122.32	116.11
3	A	604	MAN	C3-C4-C5	3.32	115.99	110.20
3	F	604	MAN	C3-C4-C5	3.40	116.13	110.20
3	D	602	NAG	O5-C5-C6	3.41	114.72	107.35
3	C	603	BMA	C1-O5-C5	3.59	116.80	112.25
3	C	603	BMA	C3-C4-C5	3.73	116.69	110.20
3	C	604	MAN	C3-C4-C5	4.43	117.91	110.20
3	D	603	BMA	O5-C5-C6	4.83	117.81	107.35
3	C	604	MAN	C1-C2-C3	8.25	119.30	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NAG	4	0
3	A	602	NAG	1	0
3	B	601	NAG	2	0
3	B	602	NAG	1	0
3	B	603	BMA	1	0
3	B	604	MAN	1	0
3	C	601	NAG	9	0
3	C	603	BMA	1	0
3	C	604	MAN	8	0
3	D	601	NAG	2	0
3	E	601	NAG	7	0
3	F	601	NAG	3	0
3	F	603	BMA	2	0

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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	MAN	C	606	-	11,11,12	1.91	4 (36%)	14,15,17	6.17	7 (50%)
4	MAN	C	607	-	11,11,12	1.93	4 (36%)	14,15,17	2.59	6 (42%)

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	MAN	C	606	-	-	0/2/19/22	0/1/1/1
4	MAN	C	607	-	-	0/2/19/22	1/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	606	MAN	O2-C2	2.31	1.48	1.43
4	C	606	MAN	C4-C3	2.35	1.58	1.52
4	C	607	MAN	C2-C3	2.70	1.56	1.52
4	C	607	MAN	O5-C1	2.73	1.48	1.43
4	C	607	MAN	C4-C5	2.94	1.59	1.53
4	C	607	MAN	O5-C5	3.25	1.50	1.43
4	C	606	MAN	C1-C2	3.37	1.60	1.52
4	C	606	MAN	C4-C5	3.47	1.60	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	606	MAN	C1-C2-C3	-14.09	92.88	109.54
4	C	606	MAN	C1-O5-C5	-3.15	108.26	112.25
4	C	606	MAN	O4-C4-C3	-2.47	104.77	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	606	MAN	C3-C4-C5	-2.12	106.50	110.20
4	C	607	MAN	O4-C4-C5	2.10	114.81	109.24
4	C	607	MAN	O2-C2-C3	2.37	114.89	110.12
4	C	607	MAN	O5-C5-C6	3.11	114.08	107.35
4	C	607	MAN	O2-C2-C1	3.58	116.37	109.21
4	C	607	MAN	O3-C3-C4	4.73	120.99	110.34
4	C	606	MAN	C6-C5-C4	4.74	124.70	113.02
4	C	607	MAN	C1-O5-C5	5.79	119.60	112.25
4	C	606	MAN	O3-C3-C4	6.58	125.16	110.34
4	C	606	MAN	O2-C2-C1	15.53	140.35	109.21

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	607	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	606	MAN	3	0
4	C	607	MAN	4	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	209/223 (93%)	-0.01	6 (2%) 55 49	94, 119, 157, 195	0
1	B	207/223 (92%)	0.40	12 (5%) 26 21	99, 125, 208, 246	0
1	C	197/223 (88%)	0.25	4 (2%) 68 62	91, 122, 180, 240	0
1	D	189/223 (84%)	0.40	10 (5%) 30 24	99, 142, 228, 268	0
1	E	180/223 (80%)	0.40	15 (8%) 14 11	140, 176, 225, 256	0
1	F	197/223 (88%)	0.50	12 (6%) 25 20	120, 154, 222, 232	0
2	G	135/143 (94%)	0.15	5 (3%) 45 38	124, 156, 195, 239	0
2	H	133/143 (93%)	-0.00	4 (3%) 54 47	105, 128, 152, 182	0
2	I	134/143 (93%)	0.40	10 (7%) 17 14	90, 141, 200, 225	0
2	J	135/143 (94%)	0.00	3 (2%) 65 59	90, 125, 156, 179	0
2	K	135/143 (94%)	0.88	25 (18%) 2 1	175, 231, 352, 467	0
2	L	136/143 (95%)	0.08	4 (2%) 55 49	104, 126, 159, 196	0
All	All	1987/2196 (90%)	0.29	110 (5%) 29 23	90, 139, 229, 467	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	522	PHE	7.5
1	D	384	HIS	6.4
2	K	262	MET	5.8
1	B	361	VAL	5.7
1	D	511	VAL	5.4
2	G	220	TRP	5.3
1	E	463	ALA	5.2
1	E	458	ASP	4.9
2	K	247	PRO	4.8
1	F	527	VAL	4.5
1	B	393	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
2	K	248	GLY	4.2
2	L	258	ASP	4.2
2	K	261	MET	4.0
2	K	268	TRP	4.0
2	K	216	HIS	4.0
1	D	368	GLY	4.0
1	F	482	GLU	4.0
1	B	387	ARG	3.9
1	D	540	ALA	3.7
1	F	526	ALA	3.6
2	I	277	LEU	3.6
2	I	268	TRP	3.6
1	F	481	ASN	3.5
1	D	403	LEU	3.4
2	L	223	LEU	3.4
1	E	382	VAL	3.3
1	A	463	ALA	3.3
2	K	210	LEU	3.3
1	E	445	VAL	3.2
1	E	352	LYS	3.2
2	J	259	CYS	3.2
2	I	178	GLY	3.2
1	A	335	GLY	3.1
1	E	376	ARG	3.1
2	G	255	GLN	3.1
1	D	461	THR	3.1
1	B	372	LEU	3.0
2	I	181	THR	2.9
1	C	387	ARG	2.9
2	I	260	VAL	2.8
1	E	459	LYS	2.8
2	K	221	ILE	2.7
1	E	525	ARG	2.7
1	E	478	TRP	2.7
1	B	374	TRP	2.7
2	I	281	VAL	2.7
1	E	412	GLU	2.6
2	G	230	GLY	2.6
2	K	240	VAL	2.6
1	F	461	THR	2.6
1	F	389	GLU	2.5
1	B	422	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
2	K	260	VAL	2.5
2	K	281	VAL	2.5
1	B	449	ALA	2.5
2	I	259	CYS	2.5
2	K	235	VAL	2.5
2	K	189	TYR	2.4
2	H	265	SER	2.4
2	K	180	GLY	2.4
1	F	525	ARG	2.4
1	A	462	LEU	2.4
1	F	476	VAL	2.4
2	K	201	ILE	2.4
1	C	455	GLY	2.4
1	F	442	ALA	2.4
2	L	228	LEU	2.4
2	H	231	GLU	2.4
2	K	227	ASP	2.4
1	A	340	LEU	2.4
1	E	464	CYS	2.3
2	K	285	LEU	2.3
2	I	275	ARG	2.3
1	B	389	GLU	2.3
1	A	461	THR	2.3
2	I	177	PHE	2.3
1	B	477	GLN	2.3
2	G	278	GLY	2.3
1	B	359	LEU	2.3
1	D	402	THR	2.2
2	K	228	LEU	2.2
2	K	263	ARG	2.2
1	F	523	ILE	2.2
1	D	485	LEU	2.2
2	H	223	LEU	2.2
2	I	278	GLY	2.2
1	C	372	LEU	2.2
1	D	391	LYS	2.2
2	J	247	PRO	2.2
1	F	463	ALA	2.1
2	K	177	PHE	2.1
1	E	540	ALA	2.1
2	K	199	VAL	2.1
2	H	269	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	477	GLN	2.1
1	B	424	HIS	2.1
2	K	168	ILE	2.1
1	C	466	ILE	2.1
2	G	221	ILE	2.1
1	A	448	PHE	2.1
2	K	277	LEU	2.1
1	B	369	THR	2.0
1	E	410	TRP	2.0
2	L	260	VAL	2.0
1	E	381	PRO	2.0
1	E	416	TYR	2.0
2	K	194	MET	2.0
2	K	229	LYS	2.0
2	J	261	MET	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](#)

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	NAG	C	601	14/15	0.79	0.25	1.56	146,152,164,184	0
3	NAG	A	601	14/15	0.81	0.25	0.60	136,142,158,159	0
3	NAG	C	602	14/15	0.84	0.22	0.17	137,149,162,165	0
3	NAG	D	601	14/15	0.86	0.22	-0.17	140,144,149,153	0
3	NAG	F	601	14/15	0.89	0.17	-0.55	170,179,203,213	0
3	NAG	E	601	14/15	0.87	0.17	-0.67	160,163,169,170	0
3	NAG	B	601	14/15	0.78	0.20	-0.68	197,214,222,233	0
3	NAG	F	602	14/15	0.90	0.17	-0.73	164,180,191,195	0
3	NAG	B	602	14/15	0.83	0.17	-0.81	175,193,202,202	0
3	NAG	D	602	14/15	0.94	0.16	-1.97	121,125,131,131	0
3	MAN	D	604	11/12	0.91	0.26	-	127,135,144,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MAN	B	604	11/12	0.76	0.29	-	197,213,228,250	0
3	BMA	D	603	11/12	0.94	0.17	-	132,135,143,153	0
3	BMA	A	603	11/12	0.94	0.18	-	131,140,149,160	0
3	MAN	A	604	11/12	0.85	0.32	-	139,148,174,219	0
3	MAN	A	605	11/12	0.89	0.31	-	157,162,166,175	0
3	MAN	B	605	11/12	0.84	0.23	-	173,186,197,201	0
3	MAN	F	604	11/12	0.86	0.36	-	148,159,170,180	0
3	MAN	E	604	11/12	0.91	0.20	-	156,163,174,181	0
3	MAN	C	604	11/12	0.88	0.21	-	123,131,144,153	0
3	BMA	B	603	11/12	0.90	0.17	-	167,195,218,224	0
3	BMA	C	603	11/12	0.91	0.16	-	135,141,147,150	0
3	MAN	C	605	11/12	0.86	0.34	-	161,172,197,198	0
3	BMA	E	603	11/12	0.94	0.14	-	150,157,167,175	0
3	NAG	E	602	14/15	0.92	0.16	-	155,161,177,180	0
3	MAN	E	605	11/12	0.92	0.25	-	149,156,165,170	0
3	NAG	A	602	14/15	0.87	0.23	-	140,148,153,155	0
3	MAN	F	605	11/12	0.91	0.24	-	152,164,174,179	0
3	BMA	F	603	11/12	0.90	0.16	-	157,162,168,169	0
3	MAN	D	605	11/12	0.84	0.33	-	126,144,170,194	0

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(\AA^2)	Q<0.9
5	CA	I	301	1/1	0.89	0.28	0.68	242,242,242,242	0
5	CA	G	301	1/1	0.91	0.13	-1.06	224,224,224,224	0
4	MAN	C	607	11/12	0.84	0.13	-1.11	111,125,127,128	0
5	CA	H	301	1/1	0.97	0.05	-	117,117,117,117	0
5	CA	K	301	1/1	0.84	0.14	-	232,232,232,232	0
4	MAN	C	606	11/12	0.70	0.27	-	155,175,185,193	0
5	CA	L	301	1/1	0.95	0.29	-	222,222,222,222	0
5	CA	J	301	1/1	0.91	0.15	-	222,222,222,222	0

6.5 Other polymers [i](#)

There are no such residues in this entry.