



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:22 am GMT

PDB ID : 4EZM
Title : Crystal structure of the human IgE-Fc(epsilon)3-4 bound to its B cell receptor derCD23
Authors : Dhaliwal, B.; Yuan, D.; Sutton, B.J.
Deposited on : 2012-05-03
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

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:

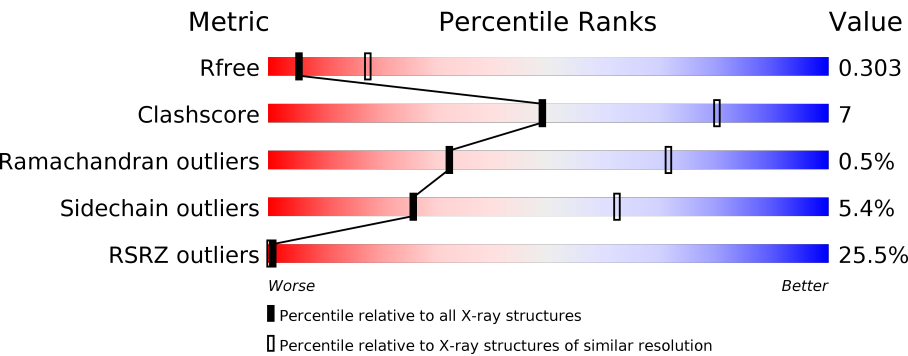
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

1 Overall quality at a glance i

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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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>13%</div><div><div></div><div>82%</div><div>11%</div><div>• 5%</div></div></div>
1	B	223	<div><div>17%</div><div><div></div><div>83%</div><div>10%</div><div>7%</div></div></div>
1	C	223	<div><div>19%</div><div><div></div><div>76%</div><div>10%</div><div>• 12%</div></div></div>
1	D	223	<div><div>20%</div><div><div></div><div>83%</div><div>8%</div><div>• 7%</div></div></div>
1	E	223	<div><div>33%</div><div><div></div><div>75%</div><div>9%</div><div>• 14%</div></div></div>
1	F	223	<div><div>35%</div><div><div></div><div>80%</div><div>11%</div><div>• 7%</div></div></div>

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Mol	Chain	Length	Quality of chain
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	A	601	-	-	-	X
3	NAG	A	602	-	-	-	X
3	NAG	C	601	-	-	-	X
3	NAG	E	601	-	-	-	X
4	MAN	C	607	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16496 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	211	Total	C	N	O	S	0	0	0
			1667	1044	307	310	6			
1	B	208	Total	C	N	O	S	0	0	0
			1650	1033	304	307	6			
1	C	197	Total	C	N	O	S	0	1	0
			1565	981	284	294	6			
1	D	207	Total	C	N	O	S	0	0	0
			1639	1027	302	304	6			
1	E	191	Total	C	N	O	S	0	0	0
			1509	945	276	283	5			
1	F	208	Total	C	N	O	S	0	0	0
			1645	1030	303	306	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	ENGINEERED MUTATION	UNP P01854
A	383	GLN	ASN	ENGINEERED MUTATION	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	ENGINEERED MUTATION	UNP P01854
B	383	GLN	ASN	ENGINEERED MUTATION	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	ENGINEERED MUTATION	UNP P01854
C	383	GLN	ASN	ENGINEERED MUTATION	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	ENGINEERED MUTATION	UNP P01854
D	383	GLN	ASN	ENGINEERED MUTATION	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	ENGINEERED MUTATION	UNP P01854
E	383	GLN	ASN	ENGINEERED MUTATION	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	ENGINEERED MUTATION	UNP P01854
F	383	GLN	ASN	ENGINEERED MUTATION	UNP P01854

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	H	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	I	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	J	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	K	134	Total	C	N	O	S	0	0	0
			1074	675	192	196	11			
2	L	134	Total	C	N	O	S	0	0	0
			1078	677	192	198	11			

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

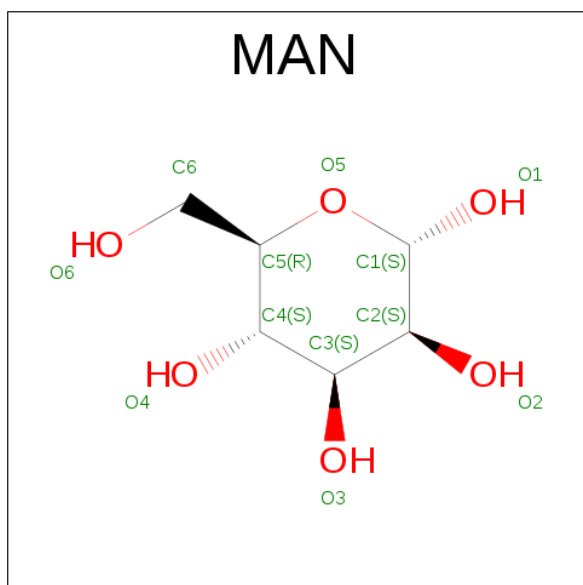
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		
3	B	5	Total	C	N	O	0	0
			61	34	2	25		
3	C	5	Total	C	N	O	0	0
			61	34	2	25		
3	D	5	Total	C	N	O	0	0
			61	34	2	25		

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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		

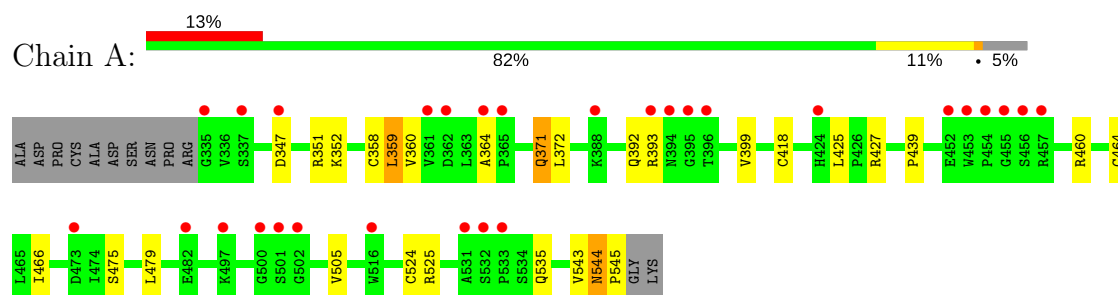
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	O	0	0
			1	1		

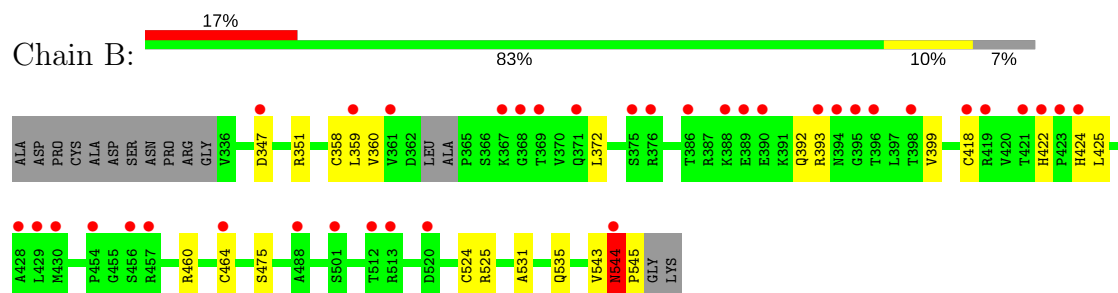
3 Residue-property plots [i](#)

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

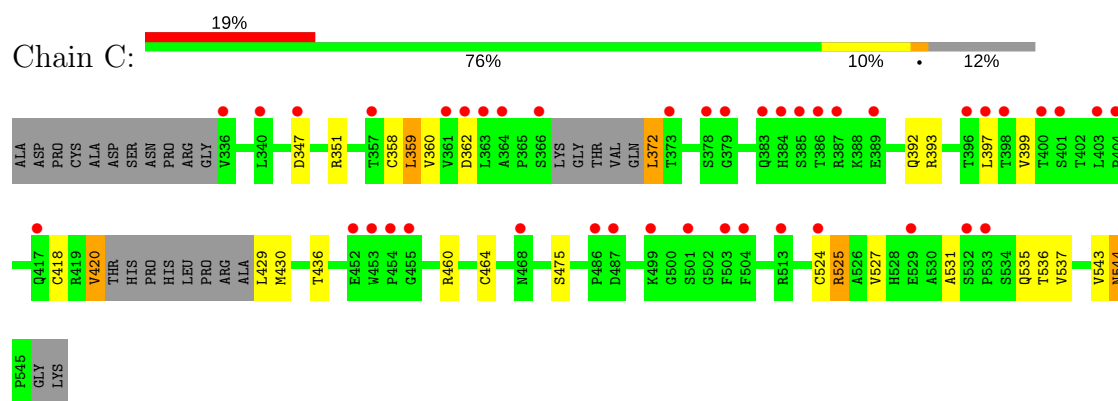
- Molecule 1: Ig epsilon chain C region



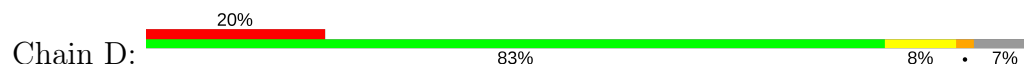
- Molecule 1: Ig epsilon chain C region

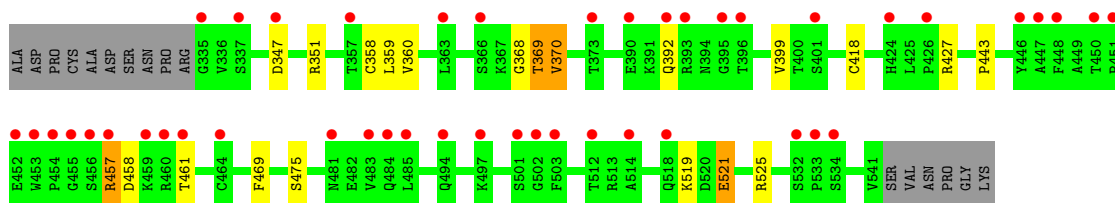


- Molecule 1: Ig epsilon chain C region

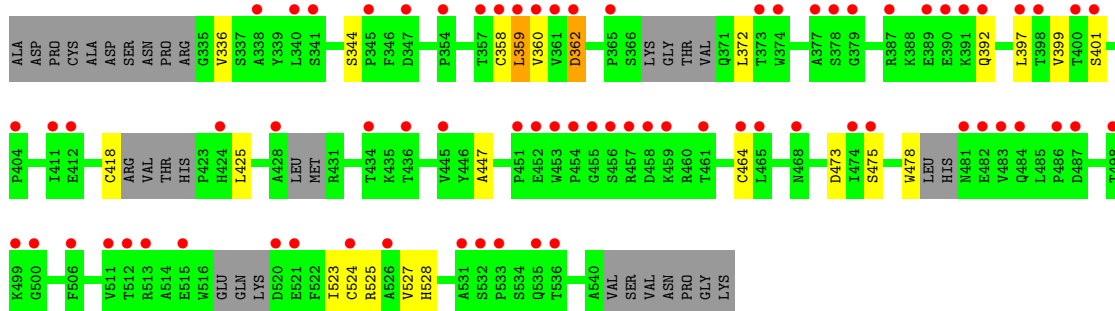
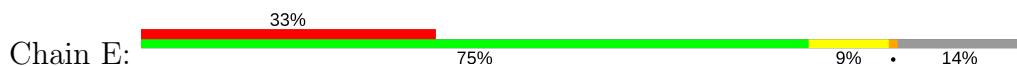


- Molecule 1: Ig epsilon chain C region

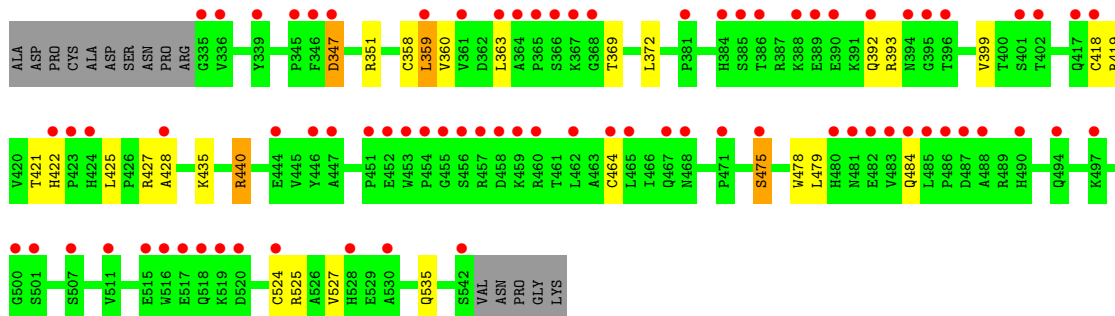
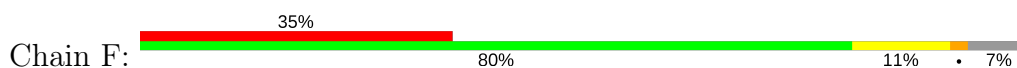




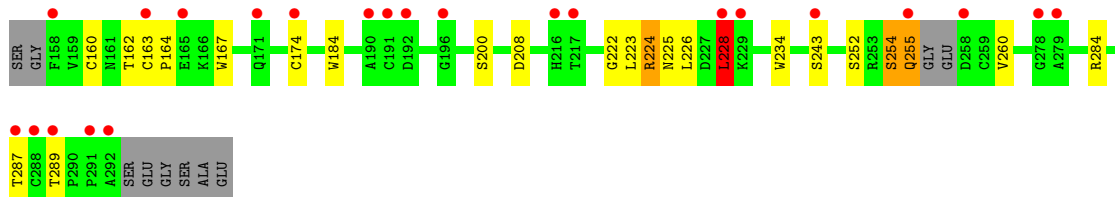
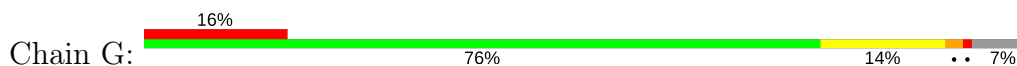
• Molecule 1: Ig epsilon chain C region



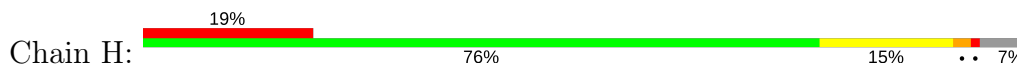
• Molecule 1: Ig epsilon chain C region

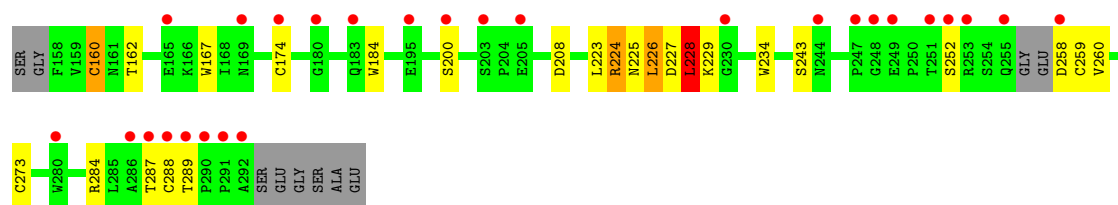


• Molecule 2: Low affinity immunoglobulin epsilon Fc receptor

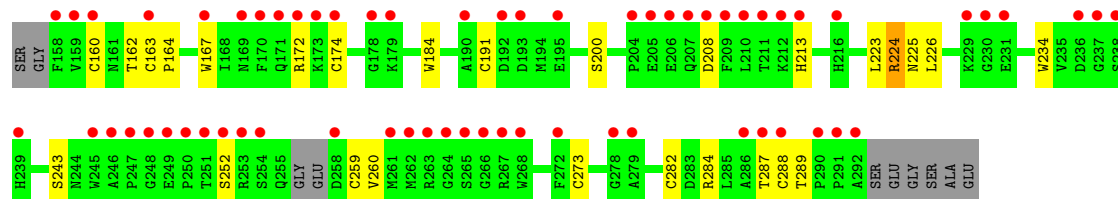
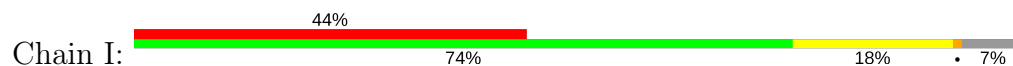


• Molecule 2: Low affinity immunoglobulin epsilon Fc receptor

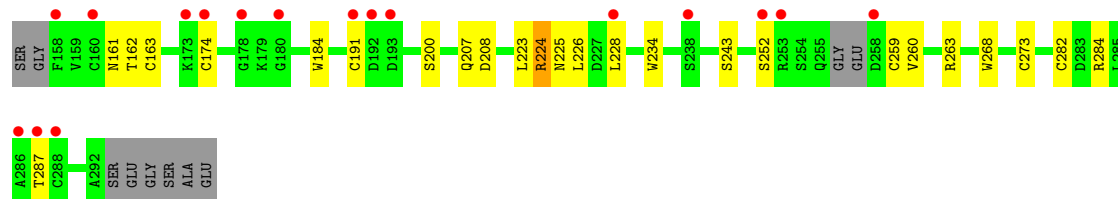
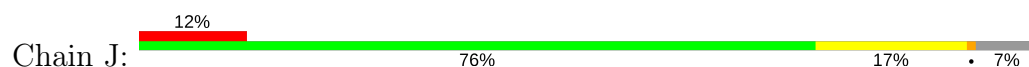




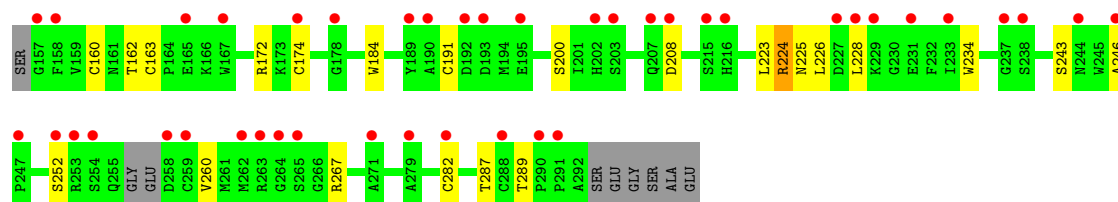
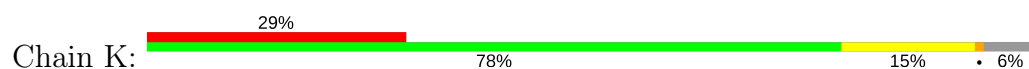
- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



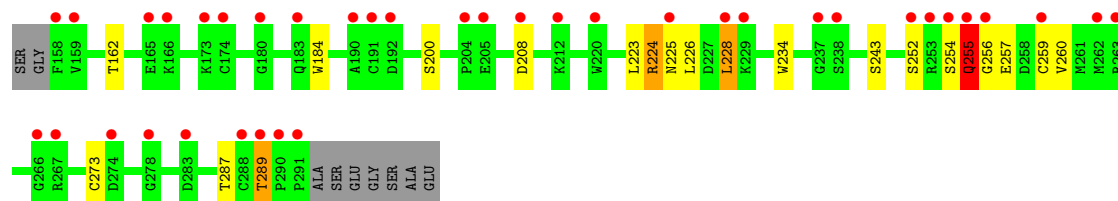
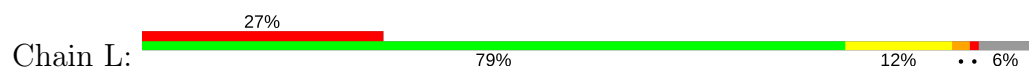
- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



- Molecule 2: Low affinity immunoglobulin epsilon Fc receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.89Å 110.75Å 376.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 3.10 29.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.87-3.10) 98.7 (29.87-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 3.11Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.264 , 0.283 0.282 , 0.303	Depositor DCC
R_{free} test set	2437 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	98.7	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	16496	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.47	1/1710 (0.1%)	0.72	7/2328 (0.3%)
1	B	0.39	0/1692	0.65	1/2301 (0.0%)
1	C	0.37	0/1605	0.64	0/2182
1	D	0.40	0/1681	0.76	4/2287 (0.2%)
1	E	0.37	0/1544	0.61	0/2094
1	F	0.37	0/1687	0.62	0/2295
2	G	0.42	0/1103	0.69	1/1494 (0.1%)
2	H	0.43	0/1103	0.70	0/1494
2	I	0.40	0/1103	0.68	0/1494
2	J	0.41	0/1103	0.68	0/1494
2	K	0.39	0/1107	0.68	0/1499
2	L	0.39	0/1112	0.75	3/1507 (0.2%)
All	All	0.40	1/16550 (0.0%)	0.68	16/22469 (0.1%)

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	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	545	PRO	N-CD	10.62	1.62	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	THR	CB-CA-C	13.29	147.49	111.60
2	L	256	GLY	N-CA-C	10.56	139.50	113.10
1	D	369	THR	N-CA-C	-8.64	87.67	111.00
1	A	364	ALA	N-CA-C	-6.86	92.48	111.00
1	A	371	GLN	N-CA-C	6.16	127.64	111.00
1	B	544	ASN	N-CA-C	5.97	127.12	111.00
2	G	254	SER	N-CA-C	-5.96	94.91	111.00
1	A	544	ASN	N-CA-C	5.83	126.75	111.00
1	A	545	PRO	CA-N-CD	-5.61	103.65	111.50
2	L	289	THR	N-CA-CB	5.60	120.94	110.30
1	D	369	THR	C-N-CA	5.57	135.62	121.70
1	A	544	ASN	C-N-CD	-5.56	108.36	120.60
2	L	255	GLN	CB-CA-C	-5.38	99.63	110.40
1	A	545	PRO	N-CA-C	5.25	125.75	112.10
1	A	364	ALA	CB-CA-C	5.19	117.89	110.10
1	D	368	GLY	C-N-CA	5.18	134.64	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	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	1667	0	1656	15	0
1	B	1650	0	1637	12	0
1	C	1565	0	1552	19	0
1	D	1639	0	1629	16	0
1	E	1509	0	1483	20	0
1	F	1645	0	1633	25	0
2	G	1070	0	994	20	0
2	H	1070	0	994	18	0
2	I	1070	0	994	17	0
2	J	1070	0	994	12	0
2	K	1074	0	996	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1078	0	999	14	0
3	A	61	0	52	5	0
3	B	61	0	52	4	0
3	C	61	0	52	9	0
3	D	61	0	52	4	0
3	E	61	0	52	6	0
3	F	61	0	52	5	0
4	C	22	0	20	3	0
5	J	1	0	0	0	0
All	All	16496	0	15893	192	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 7.

All (192) 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:H:167:TRP:HB3	2:H:174:CYS:SG	1.43	1.57
1:E:478:TRP:CZ3	1:E:524:CYS:SG	2.15	1.37
2:I:163:CYS:SG	2:I:167:TRP:HB2	1.68	1.33
2:G:163:CYS:SG	2:G:167:TRP:HB2	1.72	1.27
2:H:167:TRP:CB	2:H:174:CYS:SG	2.25	1.22
1:E:478:TRP:CH2	1:E:524:CYS:SG	2.36	1.19
2:I:163:CYS:SG	2:I:167:TRP:CB	2.31	1.18
2:G:163:CYS:SG	2:G:167:TRP:CB	2.31	1.17
3:C:604:MAN:O6	4:C:607:MAN:H2	1.45	1.16
1:F:464:CYS:SG	1:F:478:TRP:CH2	2.53	1.00
2:H:259:CYS:HG	2:H:273:CYS:HG	1.07	0.97
1:E:478:TRP:CE3	1:E:524:CYS:SG	2.58	0.95
1:E:392:GLN:HG3	3:E:601:NAG:O6	1.67	0.94
1:C:392:GLN:NE2	3:C:601:NAG:O6	2.02	0.93
1:F:358:CYS:HG	1:F:418:CYS:HG	1.10	0.93
1:A:358:CYS:HG	1:A:418:CYS:HG	1.06	0.91
1:D:358:CYS:HG	1:D:418:CYS:HG	1.14	0.91
2:G:163:CYS:SG	2:G:167:TRP:HB3	2.09	0.90
2:I:191:CYS:HG	2:I:282:CYS:HG	1.21	0.89
1:D:369:THR:O	1:D:370:VAL:HG23	1.72	0.88
1:A:464:CYS:HG	1:A:524:CYS:HG	1.11	0.86
1:C:392:GLN:HG3	3:C:601:NAG:O6	1.75	0.86
1:E:392:GLN:NE2	3:E:601:NAG:O6	2.08	0.86
1:F:392:GLN:NE2	3:F:601:NAG:O6	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:GLN:CG	3:E:601:NAG:O6	2.25	0.84
1:F:440:ARG:NH1	2:L:255:GLN:O	2.10	0.84
2:L:254:SER:O	2:L:255:GLN:HB2	1.79	0.83
2:I:259:CYS:HG	2:I:273:CYS:HG	1.06	0.83
1:E:358:CYS:HG	1:E:418:CYS:HG	1.22	0.82
2:I:163:CYS:SG	2:I:167:TRP:HB3	2.16	0.82
1:C:544:ASN:O	1:C:544:ASN:ND2	2.13	0.82
1:D:392:GLN:NE2	3:D:601:NAG:O6	2.13	0.81
1:C:392:GLN:CG	3:C:601:NAG:O6	2.30	0.79
1:A:392:GLN:HG3	3:A:601:NAG:O6	1.81	0.79
1:B:392:GLN:NE2	3:B:601:NAG:O6	2.14	0.79
3:C:604:MAN:O6	4:C:607:MAN:C2	2.30	0.78
2:J:259:CYS:HG	2:J:273:CYS:HG	1.28	0.78
1:F:392:GLN:HG3	3:F:601:NAG:O6	1.82	0.78
2:K:191:CYS:HG	2:K:282:CYS:HG	1.28	0.78
1:C:464:CYS:HG	1:C:524:CYS:HG	1.32	0.77
1:C:544:ASN:CG	1:C:544:ASN:O	2.23	0.75
1:A:392:GLN:CG	3:A:601:NAG:O6	2.36	0.73
3:C:604:MAN:HO6	4:C:607:MAN:H2	1.52	0.73
2:H:160:CYS:HG	2:H:288:CYS:HG	1.28	0.73
1:D:521:GLU:HG3	1:F:421:THR:HG21	1.72	0.71
2:J:191:CYS:HG	2:J:282:CYS:HG	1.27	0.71
1:B:392:GLN:HG3	3:B:601:NAG:O6	1.92	0.70
1:E:464:CYS:SG	1:E:478:TRP:CH2	2.84	0.70
1:F:392:GLN:CG	3:F:601:NAG:O6	2.38	0.70
2:G:163:CYS:SG	2:G:164:PRO:HD2	2.31	0.70
1:D:392:GLN:HG3	3:D:601:NAG:O6	1.94	0.67
2:L:259:CYS:HG	2:L:273:CYS:HG	1.40	0.66
1:B:358:CYS:HG	1:B:418:CYS:HG	1.42	0.66
2:H:167:TRP:CG	2:H:174:CYS:SG	2.89	0.65
1:C:392:GLN:HE21	3:C:601:NAG:C6	2.10	0.65
1:C:543:VAL:O	1:C:544:ASN:OD1	2.16	0.64
1:B:392:GLN:CG	3:B:601:NAG:O6	2.46	0.64
1:E:478:TRP:CZ2	1:E:524:CYS:SG	2.92	0.63
2:H:167:TRP:CE3	2:H:174:CYS:SG	2.90	0.63
1:D:392:GLN:CG	3:D:601:NAG:O6	2.48	0.62
2:I:160:CYS:HG	2:I:288:CYS:HG	1.22	0.62
2:H:167:TRP:HB3	2:H:174:CYS:HG	1.55	0.62
2:L:254:SER:O	2:L:255:GLN:CB	2.48	0.62
1:D:392:GLN:HE21	3:D:601:NAG:C6	2.15	0.60
1:F:392:GLN:HE21	3:F:601:NAG:C6	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:252:SER:HB2	2:G:255:GLN:HA	1.84	0.59
1:E:392:GLN:HE21	3:E:601:NAG:C6	2.15	0.59
1:F:440:ARG:NH1	2:L:257:GLU:H	2.01	0.59
2:G:163:CYS:SG	2:G:164:PRO:CD	2.93	0.57
1:C:531:ALA:O	1:C:535:GLN:HA	2.05	0.57
1:E:475:SER:HB2	1:E:527:VAL:HB	1.86	0.56
2:J:162:THR:HB	2:J:287:THR:HG23	1.88	0.56
1:B:392:GLN:HE21	3:B:601:NAG:C6	2.16	0.56
1:E:359:LEU:HD11	3:E:602:NAG:O7	2.05	0.55
2:K:246:ALA:HA	2:K:267:ARG:HE	1.71	0.55
1:F:464:CYS:SG	1:F:478:TRP:HH2	2.18	0.55
2:I:162:THR:HB	2:I:287:THR:HG23	1.88	0.55
2:K:226:LEU:HG	2:K:226:LEU:O	2.07	0.55
1:A:360:VAL:HG13	1:A:399:VAL:HG13	1.89	0.55
1:B:464:CYS:HG	1:B:524:CYS:HG	0.59	0.55
2:H:162:THR:HB	2:H:287:THR:HG23	1.89	0.55
2:G:162:THR:HB	2:G:287:THR:HG23	1.88	0.54
2:J:174:CYS:HB2	2:J:284:ARG:HG2	1.90	0.54
1:F:464:CYS:SG	1:F:478:TRP:CZ2	2.92	0.54
1:B:360:VAL:HG13	1:B:399:VAL:HG13	1.90	0.54
2:I:163:CYS:SG	2:I:164:PRO:HD2	2.48	0.54
2:L:162:THR:HB	2:L:287:THR:HG23	1.90	0.54
1:E:336:VAL:HG12	1:E:362:ASP:HA	1.90	0.53
2:G:184:TRP:CH2	2:G:224:ARG:HG2	2.44	0.53
2:J:226:LEU:HG	2:J:226:LEU:O	2.08	0.53
2:L:226:LEU:HG	2:L:226:LEU:O	2.09	0.53
2:G:174:CYS:HB2	2:G:284:ARG:HG2	1.91	0.53
2:K:162:THR:HB	2:K:287:THR:HG23	1.89	0.53
1:C:360:VAL:HG13	1:C:399:VAL:HG13	1.91	0.52
1:D:360:VAL:HG13	1:D:399:VAL:HG13	1.91	0.52
1:F:360:VAL:HG13	1:F:399:VAL:HG13	1.91	0.52
1:E:360:VAL:HG13	1:E:399:VAL:HG13	1.91	0.52
2:J:184:TRP:CZ2	2:J:224:ARG:HG2	2.45	0.52
2:I:226:LEU:HG	2:I:226:LEU:O	2.09	0.52
1:F:347:ASP:HA	1:F:351:ARG:HB2	1.90	0.52
2:G:184:TRP:CZ2	2:G:224:ARG:HG2	2.45	0.51
1:D:443:PRO:HB3	1:D:469:PHE:HB3	1.91	0.51
1:C:359:LEU:HD11	3:C:602:NAG:O7	2.10	0.51
2:K:184:TRP:CH2	2:K:224:ARG:HG2	2.45	0.51
2:L:184:TRP:CH2	2:L:224:ARG:HG2	2.46	0.51
2:G:226:LEU:O	2:G:226:LEU:HG	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:226:LEU:O	2:H:226:LEU:HG	2.10	0.51
1:A:460:ARG:HG3	1:A:543:VAL:HG13	1.92	0.51
1:C:475:SER:HB2	1:C:527:VAL:HB	1.92	0.51
1:A:535:GLN:OE1	2:G:228:LEU:HG	2.10	0.51
2:K:184:TRP:CZ2	2:K:224:ARG:HG2	2.46	0.51
1:F:358:CYS:CB	1:F:418:CYS:HG	2.23	0.50
1:C:460:ARG:HG3	1:C:543:VAL:HG13	1.92	0.50
1:F:359:LEU:HD11	3:F:602:NAG:O7	2.11	0.50
2:H:223:LEU:HB3	2:H:260:VAL:HB	1.93	0.50
2:I:184:TRP:CZ2	2:I:224:ARG:HG2	2.47	0.50
1:D:358:CYS:CB	1:D:418:CYS:HG	2.25	0.50
1:F:479:LEU:HG	1:F:484:GLN:HA	1.93	0.50
2:G:163:CYS:HG	2:G:174:CYS:HB3	1.76	0.50
2:J:184:TRP:CH2	2:J:224:ARG:HG2	2.47	0.49
1:D:347:ASP:HA	1:D:351:ARG:HB2	1.94	0.49
1:B:460:ARG:HG3	1:B:543:VAL:HG13	1.94	0.49
2:L:184:TRP:CZ2	2:L:224:ARG:HG2	2.47	0.49
1:F:440:ARG:HH12	2:L:257:GLU:H	1.59	0.49
1:D:519:LYS:HD3	1:F:419:ARG:HH22	1.78	0.49
2:K:160:CYS:HB2	2:K:172:ARG:HG2	1.94	0.49
1:D:519:LYS:HA	1:F:419:ARG:HH22	1.77	0.48
1:B:347:ASP:HA	1:B:351:ARG:HB2	1.95	0.48
1:C:358:CYS:CB	1:C:418:CYS:HG	2.26	0.48
2:G:252:SER:C	2:G:254:SER:H	2.17	0.48
1:D:369:THR:O	1:D:370:VAL:CG2	2.54	0.48
1:F:478:TRP:CE2	1:F:524:CYS:SG	2.99	0.48
2:K:163:CYS:CB	2:K:174:CYS:HG	2.16	0.48
2:I:160:CYS:HB2	2:I:172:ARG:HG2	1.96	0.48
1:A:392:GLN:CD	3:A:601:NAG:HO6	2.14	0.48
2:I:184:TRP:CH2	2:I:224:ARG:HG2	2.48	0.48
2:K:163:CYS:HA	2:K:174:CYS:SG	2.54	0.48
1:C:392:GLN:CD	3:C:601:NAG:O6	2.52	0.47
2:H:167:TRP:HE3	2:H:174:CYS:SG	2.36	0.47
1:D:519:LYS:HE3	1:F:428:ALA:H	1.79	0.47
1:E:447:ALA:CB	1:E:464:CYS:SG	3.02	0.47
1:A:439:PRO:HA	2:G:254:SER:HA	1.96	0.47
2:L:200:SER:HA	2:L:234:TRP:CE3	2.50	0.47
1:F:535:GLN:OE1	2:L:228:LEU:HG	2.14	0.47
2:I:174:CYS:HB2	2:I:284:ARG:HG2	1.96	0.47
2:K:200:SER:HA	2:K:234:TRP:CE3	2.50	0.47
2:G:200:SER:HA	2:G:234:TRP:CE3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:163:CYS:SG	2:I:174:CYS:SG	3.13	0.47
2:H:174:CYS:HB3	2:H:284:ARG:HG2	1.97	0.47
1:F:435:LYS:HE3	2:L:257:GLU:HG3	1.97	0.46
2:H:184:TRP:CH2	2:H:224:ARG:HG2	2.50	0.46
2:I:200:SER:HA	2:I:234:TRP:CE3	2.50	0.46
2:H:227:ASP:C	2:H:229:LYS:H	2.18	0.46
2:J:200:SER:HA	2:J:234:TRP:CE3	2.50	0.46
1:E:392:GLN:CD	3:E:601:NAG:O6	2.54	0.46
2:H:226:LEU:H	2:H:229:LYS:HG3	1.81	0.46
2:G:163:CYS:SG	2:G:174:CYS:SG	3.14	0.45
2:J:207:GLN:OE1	2:J:268:TRP:NE1	2.48	0.45
2:H:167:TRP:HB2	2:H:174:CYS:SG	2.44	0.45
1:E:447:ALA:HB2	1:E:464:CYS:SG	2.56	0.45
1:D:457:ARG:HA	1:D:457:ARG:NE	2.32	0.44
1:A:358:CYS:CB	1:A:418:CYS:HG	2.31	0.44
1:B:544:ASN:HA	1:B:545:PRO:HD2	1.74	0.44
1:C:347:ASP:HA	1:C:351:ARG:HB2	1.99	0.44
1:A:392:GLN:OE1	3:A:601:NAG:O6	2.23	0.44
1:E:362:ASP:HB3	1:E:397:LEU:O	2.18	0.44
2:J:163:CYS:CB	2:J:174:CYS:SG	3.06	0.44
2:K:163:CYS:CB	2:K:174:CYS:SG	3.04	0.44
2:I:163:CYS:SG	2:I:164:PRO:CD	3.06	0.43
1:C:525:ARG:HD2	1:C:536:THR:HG21	2.01	0.43
1:B:422:HIS:HB3	1:B:425:LEU:HB3	2.01	0.42
2:G:222:GLY:O	2:G:234:TRP:HA	2.19	0.42
1:F:422:HIS:HB3	1:F:425:LEU:HD13	2.00	0.42
2:J:163:CYS:HG	2:J:174:CYS:HG	0.42	0.42
1:A:347:ASP:HA	1:A:351:ARG:HB2	2.01	0.42
2:L:223:LEU:HB3	2:L:260:VAL:HB	2.02	0.42
1:A:460:ARG:HG3	1:A:543:VAL:CG1	2.50	0.42
1:A:359:LEU:HD11	3:A:602:NAG:O7	2.20	0.41
1:B:531:ALA:O	1:B:535:GLN:HA	2.19	0.41
1:C:531:ALA:HB1	1:C:537:VAL:HG23	2.01	0.41
2:G:254:SER:O	2:G:255:GLN:OE1	2.39	0.41
2:G:223:LEU:HB3	2:G:260:VAL:HB	2.02	0.41
1:E:478:TRP:CD2	1:E:524:CYS:SG	3.09	0.41
2:K:223:LEU:HB3	2:K:260:VAL:HB	2.03	0.41
2:I:223:LEU:HB3	2:I:260:VAL:HB	2.02	0.41
2:H:226:LEU:O	2:H:228:LEU:N	2.54	0.41
1:C:372:LEU:HA	1:C:420:VAL:HG13	2.04	0.40
1:E:473:ASP:O	1:E:528:HIS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:223:LEU:HB3	2:J:260:VAL:HB	2.03	0.40
1:F:475:SER:HB2	1:F:527:VAL:HB	2.03	0.40
2:H:200:SER:HA	2:H:234:TRP:CE3	2.57	0.40
1:A:466:ILE:HD13	1:A:505:VAL:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/223 (94%)	198 (95%)	10 (5%)	1 (0%)	32	71
1	B	204/223 (92%)	190 (93%)	13 (6%)	1 (0%)	32	71
1	C	192/223 (86%)	183 (95%)	8 (4%)	1 (0%)	32	71
1	D	205/223 (92%)	193 (94%)	11 (5%)	1 (0%)	32	71
1	E	179/223 (80%)	171 (96%)	8 (4%)	0	100	100
1	F	206/223 (92%)	200 (97%)	5 (2%)	1 (0%)	32	71
2	G	129/143 (90%)	113 (88%)	15 (12%)	1 (1%)	22	62
2	H	129/143 (90%)	118 (92%)	9 (7%)	2 (2%)	11	43
2	I	129/143 (90%)	113 (88%)	16 (12%)	0	100	100
2	J	129/143 (90%)	116 (90%)	12 (9%)	1 (1%)	22	62
2	K	130/143 (91%)	118 (91%)	12 (9%)	0	100	100
2	L	132/143 (92%)	118 (89%)	14 (11%)	0	100	100
All	All	1973/2196 (90%)	1831 (93%)	133 (7%)	9 (0%)	32	71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	370	VAL
2	H	228	LEU
1	A	393	ARG
1	B	393	ARG
1	F	393	ARG
1	C	393	ARG
2	G	228	LEU
2	H	226	LEU
2	J	161	ASN

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	186/195 (95%)	176 (95%)	10 (5%)	26	62
1	B	185/195 (95%)	179 (97%)	6 (3%)	44	78
1	C	176/195 (90%)	166 (94%)	10 (6%)	24	60
1	D	182/195 (93%)	174 (96%)	8 (4%)	33	69
1	E	167/195 (86%)	159 (95%)	8 (5%)	30	67
1	F	183/195 (94%)	174 (95%)	9 (5%)	29	66
2	G	114/120 (95%)	106 (93%)	8 (7%)	18	52
2	H	114/120 (95%)	105 (92%)	9 (8%)	14	47
2	I	114/120 (95%)	107 (94%)	7 (6%)	22	58
2	J	114/120 (95%)	107 (94%)	7 (6%)	22	58
2	K	114/120 (95%)	107 (94%)	7 (6%)	22	58
2	L	115/120 (96%)	108 (94%)	7 (6%)	22	58
All	All	1764/1890 (93%)	1668 (95%)	96 (5%)	26	62

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	352	LYS
1	A	359	LEU

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Mol	Chain	Res	Type
1	A	371	GLN
1	A	372	LEU
1	A	425	LEU
1	A	427	ARG
1	A	475	SER
1	A	479	LEU
1	A	525	ARG
1	A	544	ASN
1	B	359	LEU
1	B	372	LEU
1	B	424	HIS
1	B	475	SER
1	B	525	ARG
1	B	544	ASN
1	C	359	LEU
1	C	362	ASP
1	C	372	LEU
1	C	397	LEU
1	C	420	VAL
1	C	429	LEU
1	C	430	MET
1	C	436	THR
1	C	525	ARG
1	C	544	ASN
1	D	359	LEU
1	D	427	ARG
1	D	457	ARG
1	D	458	ASP
1	D	461	THR
1	D	475	SER
1	D	521	GLU
1	D	525	ARG
1	E	344	SER
1	E	359	LEU
1	E	362	ASP
1	E	372	LEU
1	E	401	SER
1	E	425	LEU
1	E	523	ILE
1	E	525	ARG
1	F	347	ASP
1	F	359	LEU

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Mol	Chain	Res	Type
1	F	363	LEU
1	F	369	THR
1	F	372	LEU
1	F	427	ARG
1	F	440	ARG
1	F	475	SER
1	F	525	ARG
2	G	160	CYS
2	G	208	ASP
2	G	224	ARG
2	G	225	ASN
2	G	228	LEU
2	G	243	SER
2	G	255	GLN
2	G	289	THR
2	H	160	CYS
2	H	208	ASP
2	H	224	ARG
2	H	225	ASN
2	H	228	LEU
2	H	243	SER
2	H	252	SER
2	H	258	ASP
2	H	289	THR
2	I	208	ASP
2	I	213	HIS
2	I	224	ARG
2	I	225	ASN
2	I	243	SER
2	I	252	SER
2	I	289	THR
2	J	208	ASP
2	J	224	ARG
2	J	225	ASN
2	J	228	LEU
2	J	243	SER
2	J	252	SER
2	J	263	ARG
2	K	208	ASP
2	K	224	ARG
2	K	225	ASN
2	K	228	LEU

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Mol	Chain	Res	Type
2	K	243	SER
2	K	252	SER
2	K	289	THR
2	L	208	ASP
2	L	224	ARG
2	L	225	ASN
2	L	228	LEU
2	L	243	SER
2	L	252	SER
2	L	289	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	392	GLN
1	B	481	ASN
1	C	392	GLN
1	C	544	ASN
1	D	392	GLN
1	E	392	GLN
1	F	392	GLN
2	G	213	HIS
2	G	225	ASN
2	G	255	GLN
2	G	269	ASN
2	H	213	HIS
2	H	269	ASN
2	I	225	ASN
2	I	269	ASN
2	J	213	HIS
2	J	225	ASN
2	J	269	ASN
2	K	213	HIS
2	K	225	ASN
2	K	269	ASN
2	L	213	HIS
2	L	225	ASN
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	0.51	0	15,19,21	1.25	1 (6%)
3	NAG	A	602	3	14,14,15	0.56	0	15,19,21	1.35	2 (13%)
3	BMA	A	603	3	11,11,12	0.71	0	13,15,17	1.53	2 (15%)
3	MAN	A	604	3	11,11,12	0.63	0	13,15,17	1.70	3 (23%)
3	MAN	A	605	3	11,11,12	0.58	0	13,15,17	1.70	3 (23%)
3	NAG	B	601	3	14,14,15	0.50	0	15,19,21	1.25	1 (6%)
3	NAG	B	602	3	14,14,15	0.56	0	15,19,21	1.35	2 (13%)
3	BMA	B	603	3	11,11,12	0.70	0	13,15,17	1.54	2 (15%)
3	MAN	B	604	3	11,11,12	0.62	0	13,15,17	1.69	3 (23%)
3	MAN	B	605	3	11,11,12	0.60	0	13,15,17	1.70	3 (23%)
3	NAG	C	601	3	14,14,15	0.51	0	15,19,21	1.25	1 (6%)
3	NAG	C	602	3	14,14,15	0.55	0	15,19,21	1.35	2 (13%)
3	BMA	C	603	3	11,11,12	0.70	0	13,15,17	1.53	2 (15%)
3	MAN	C	604	3	11,11,12	0.62	0	13,15,17	1.69	3 (23%)
3	MAN	C	605	3	11,11,12	0.60	0	13,15,17	1.69	3 (23%)
3	NAG	D	601	3	14,14,15	0.51	0	15,19,21	1.25	1 (6%)
3	NAG	D	602	3	14,14,15	0.55	0	15,19,21	1.35	2 (13%)
3	BMA	D	603	3	11,11,12	0.70	0	13,15,17	1.54	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	D	604	3	11,11,12	0.63	0	13,15,17	1.69	3 (23%)
3	MAN	D	605	3	11,11,12	0.60	0	13,15,17	1.69	3 (23%)
3	NAG	E	601	3	14,14,15	0.51	0	15,19,21	1.25	1 (6%)
3	NAG	E	602	3	14,14,15	0.56	0	15,19,21	1.35	2 (13%)
3	BMA	E	603	3	11,11,12	0.70	0	13,15,17	1.54	2 (15%)
3	MAN	E	604	3	11,11,12	0.62	0	13,15,17	1.69	3 (23%)
3	MAN	E	605	3	11,11,12	0.60	0	13,15,17	1.69	3 (23%)
3	NAG	F	601	3	14,14,15	0.51	0	15,19,21	1.24	1 (6%)
3	NAG	F	602	3	14,14,15	0.56	0	15,19,21	1.35	2 (13%)
3	BMA	F	603	3	11,11,12	0.70	0	13,15,17	1.53	2 (15%)
3	MAN	F	604	3	11,11,12	0.62	0	13,15,17	1.70	3 (23%)
3	MAN	F	605	3	11,11,12	0.60	0	13,15,17	1.69	3 (23%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	603	BMA	O3-C3-C4	-3.29	103.20	110.36
3	A	603	BMA	O3-C3-C4	-3.29	103.21	110.36
3	B	603	BMA	O3-C3-C4	-3.28	103.21	110.36
3	D	603	BMA	O3-C3-C4	-3.28	103.22	110.36
3	A	605	MAN	O5-C1-C2	-3.27	105.67	110.79
3	C	603	BMA	O3-C3-C4	-3.27	103.25	110.36
3	F	603	BMA	O3-C3-C4	-3.26	103.25	110.36
3	A	604	MAN	O5-C1-C2	-3.25	105.70	110.79
3	F	605	MAN	O5-C1-C2	-3.25	105.70	110.79
3	F	604	MAN	O5-C1-C2	-3.25	105.70	110.79
3	D	605	MAN	O5-C1-C2	-3.23	105.72	110.79
3	B	605	MAN	O5-C1-C2	-3.23	105.72	110.79
3	C	604	MAN	O5-C1-C2	-3.22	105.74	110.79
3	D	604	MAN	O5-C1-C2	-3.22	105.74	110.79
3	E	605	MAN	O5-C1-C2	-3.22	105.74	110.79
3	E	604	MAN	O5-C1-C2	-3.22	105.75	110.79
3	B	604	MAN	O5-C1-C2	-3.21	105.77	110.79
3	C	605	MAN	O5-C1-C2	-3.19	105.78	110.79
3	C	603	BMA	C6-C5-C4	-3.00	105.99	113.00
3	F	603	BMA	C6-C5-C4	-2.99	105.99	113.00
3	B	603	BMA	C6-C5-C4	-2.99	106.01	113.00
3	E	603	BMA	C6-C5-C4	-2.98	106.03	113.00
3	D	603	BMA	C6-C5-C4	-2.98	106.03	113.00
3	A	603	BMA	C6-C5-C4	-2.97	106.04	113.00
3	C	601	NAG	O5-C1-C2	-2.83	107.54	111.47
3	E	601	NAG	O5-C1-C2	-2.82	107.54	111.47
3	B	601	NAG	O5-C1-C2	-2.82	107.55	111.47
3	D	601	NAG	O5-C1-C2	-2.82	107.55	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAG	O5-C1-C2	-2.81	107.56	111.47
3	F	601	NAG	O5-C1-C2	-2.80	107.58	111.47
3	B	605	MAN	C3-C4-C5	-2.79	105.30	110.22
3	A	605	MAN	C3-C4-C5	-2.78	105.31	110.22
3	D	605	MAN	C3-C4-C5	-2.78	105.33	110.22
3	F	605	MAN	C3-C4-C5	-2.77	105.34	110.22
3	C	605	MAN	C3-C4-C5	-2.76	105.35	110.22
3	E	605	MAN	C3-C4-C5	-2.76	105.36	110.22
3	B	604	MAN	O4-C4-C3	-2.70	104.48	110.36
3	D	604	MAN	O4-C4-C3	-2.70	104.49	110.36
3	C	604	MAN	O4-C4-C3	-2.69	104.50	110.36
3	A	604	MAN	O4-C4-C3	-2.69	104.51	110.36
3	E	604	MAN	O4-C4-C3	-2.68	104.52	110.36
3	F	604	MAN	O4-C4-C3	-2.68	104.52	110.36
3	C	605	MAN	C2-C3-C4	-2.33	106.81	110.88
3	A	605	MAN	C2-C3-C4	-2.32	106.83	110.88
3	B	605	MAN	C2-C3-C4	-2.31	106.85	110.88
3	D	605	MAN	C2-C3-C4	-2.31	106.85	110.88
3	E	605	MAN	C2-C3-C4	-2.31	106.85	110.88
3	F	605	MAN	C2-C3-C4	-2.29	106.88	110.88
3	E	602	NAG	O7-C7-C8	-2.04	118.34	122.06
3	D	602	NAG	O7-C7-C8	-2.04	118.35	122.06
3	C	602	NAG	O7-C7-C8	-2.02	118.37	122.06
3	A	602	NAG	O7-C7-C8	-2.01	118.40	122.06
3	B	602	NAG	O7-C7-C8	-2.01	118.41	122.06
3	F	602	NAG	O7-C7-C8	-2.00	118.41	122.06
3	E	602	NAG	C1-O5-C5	2.77	115.99	112.17
3	D	602	NAG	C1-O5-C5	2.78	116.00	112.17
3	C	602	NAG	C1-O5-C5	2.78	116.00	112.17
3	F	602	NAG	C1-O5-C5	2.79	116.01	112.17
3	B	602	NAG	C1-O5-C5	2.80	116.02	112.17
3	A	602	NAG	C1-O5-C5	2.83	116.07	112.17
3	D	604	MAN	C3-C4-C5	3.05	115.58	110.22
3	E	604	MAN	C3-C4-C5	3.05	115.59	110.22
3	C	604	MAN	C3-C4-C5	3.07	115.62	110.22
3	A	604	MAN	C3-C4-C5	3.07	115.64	110.22
3	B	604	MAN	C3-C4-C5	3.08	115.65	110.22
3	F	604	MAN	C3-C4-C5	3.11	115.69	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 33 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	4	0
3	C	601	NAG	5	0
3	C	602	NAG	1	0
3	C	604	MAN	3	0
3	D	601	NAG	4	0
3	E	601	NAG	5	0
3	E	602	NAG	1	0
3	F	601	NAG	4	0
3	F	602	NAG	1	0

5.6 Ligand geometry [i](#)

2 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	MAN	C	606	-	11,11,12	1.42	2 (18%)	13,15,17	1.97	7 (53%)
4	MAN	C	607	-	11,11,12	1.60	3 (27%)	13,15,17	1.32	2 (15%)

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	1/1/1/1
4	MAN	C	607	-	-	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)
4	C	606	MAN	C1-C2	2.03	1.57	1.52
4	C	607	MAN	C4-C3	2.15	1.57	1.52
4	C	607	MAN	O5-C5	2.22	1.48	1.43
4	C	607	MAN	C4-C5	2.43	1.58	1.53
4	C	606	MAN	C4-C5	2.50	1.58	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	606	MAN	C3-C4-C5	-2.50	105.81	110.22
4	C	606	MAN	C1-C2-C3	2.02	112.21	109.65
4	C	606	MAN	O4-C4-C5	2.08	114.52	109.28
4	C	607	MAN	O5-C1-C2	2.09	114.07	110.79
4	C	606	MAN	C6-C5-C4	2.20	118.15	113.00
4	C	606	MAN	O3-C3-C4	2.45	115.68	110.36
4	C	606	MAN	O5-C1-C2	2.68	114.99	110.79
4	C	607	MAN	O3-C3-C4	2.85	116.57	110.36
4	C	606	MAN	C1-O5-C5	3.38	116.83	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	606	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	607	MAN	3	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	211/223 (94%)	1.04	29 (13%) 3 1	58, 83, 128, 143	0
1	B	208/223 (93%)	1.07	37 (17%) 2 1	55, 84, 162, 190	0
1	C	197/223 (88%)	1.23	42 (21%) 1 0	70, 100, 137, 178	0
1	D	207/223 (92%)	1.28	45 (21%) 1 0	65, 93, 144, 186	0
1	E	191/223 (85%)	2.16	73 (38%) 0 0	103, 134, 192, 213	0
1	F	208/223 (93%)	1.93	79 (37%) 0 0	97, 125, 172, 194	0
2	G	133/143 (93%)	1.04	23 (17%) 2 1	68, 91, 140, 176	0
2	H	133/143 (93%)	1.13	27 (20%) 1 0	66, 98, 129, 153	0
2	I	133/143 (93%)	2.47	63 (47%) 0 0	109, 140, 171, 197	0
2	J	133/143 (93%)	0.89	17 (12%) 4 2	62, 85, 120, 158	0
2	K	134/143 (93%)	1.65	42 (31%) 0 0	92, 122, 148, 168	0
2	L	134/143 (93%)	1.59	38 (28%) 1 0	91, 122, 155, 183	0
All	All	2022/2196 (92%)	1.45	515 (25%) 1 0	55, 109, 161, 213	0

All (515) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	292	ALA	23.0
2	I	264	GLY	12.7
1	E	456	SER	10.5
2	I	173	LYS	9.8
1	E	515	GLU	9.8
1	A	395	GLY	9.7
1	F	500	GLY	9.6
1	E	532	SER	9.4
2	I	291	PRO	9.2
1	D	454	PRO	9.2
2	H	292	ALA	8.8

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Mol	Chain	Res	Type	RSRZ
2	I	205	GLU	8.5
1	D	452	GLU	8.2
1	E	424	HIS	8.2
1	A	501	SER	8.0
2	I	193	ASP	8.0
1	F	480	HIS	7.9
1	D	335	GLY	7.8
2	K	264	GLY	7.8
2	I	265	SER	7.7
1	C	533	PRO	7.6
2	K	259	CYS	7.6
1	D	533	PRO	7.5
1	B	369	THR	7.5
1	F	542	SER	7.5
1	E	359	LEU	7.2
1	D	459	LYS	7.2
1	E	452	GLU	7.1
1	D	483	VAL	7.1
1	F	464	CYS	7.1
1	F	396	THR	7.1
2	K	247	PRO	7.0
1	E	531	ALA	7.0
2	G	288	CYS	6.9
2	I	158	PHE	6.9
2	I	178	GLY	6.8
1	F	487	ASP	6.7
1	F	424	HIS	6.7
2	I	216	HIS	6.7
2	L	253	ARG	6.6
1	E	358	CYS	6.6
1	B	395	GLY	6.5
2	K	178	GLY	6.5
2	L	205	GLU	6.5
1	E	484	GLN	6.5
1	F	486	PRO	6.4
1	D	366	SER	6.4
2	L	252	SER	6.2
2	I	231	GLU	6.2
1	E	434	THR	6.1
1	F	481	ASN	6.1
1	C	373	THR	6.0
1	E	457	ARG	5.9

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Mol	Chain	Res	Type	RSRZ
1	F	454	PRO	5.9
2	H	252	SER	5.8
1	F	455	GLY	5.8
1	D	456	SER	5.8
1	F	483	VAL	5.7
1	B	424	HIS	5.7
1	C	417	GLN	5.7
1	E	390	GLU	5.7
2	J	193	ASP	5.6
1	A	394	ASN	5.6
2	H	289	THR	5.6
1	F	501	SER	5.5
1	C	378	SER	5.5
2	I	250	PRO	5.5
1	A	393	ARG	5.5
1	E	487	ASP	5.5
2	L	291	PRO	5.5
1	B	419	ARG	5.5
1	B	418	CYS	5.5
2	I	174	CYS	5.4
2	I	172	ARG	5.4
2	K	253	ARG	5.4
1	C	347	ASP	5.4
2	L	256	GLY	5.4
1	E	458	ASP	5.4
2	G	289	THR	5.3
1	F	335	GLY	5.3
2	K	174	CYS	5.3
1	E	454	PRO	5.3
1	A	533	PRO	5.3
2	I	279	ALA	5.3
1	A	454	PRO	5.2
1	F	402	THR	5.2
1	F	368	GLY	5.2
2	L	266	GLY	5.2
1	C	363	LEU	5.2
1	C	501	SER	5.2
2	K	165	GLU	5.1
2	G	228	LEU	5.1
1	C	336	VAL	5.1
1	B	454	PRO	5.1
1	E	428	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
2	K	229	LYS	5.1
1	E	378	SER	5.1
1	E	377	ALA	5.1
1	E	392	GLN	5.0
1	A	482	GLU	5.0
1	B	393	ARG	5.0
1	F	451	PRO	4.9
2	J	174	CYS	4.9
2	L	254	SER	4.9
2	K	238	SER	4.9
2	L	191	CYS	4.9
1	F	456	SER	4.9
1	D	393	ARG	4.9
2	L	190	ALA	4.8
1	C	389	GLU	4.8
2	L	255	GLN	4.8
1	F	390	GLU	4.8
2	I	249	GLU	4.7
1	F	347	ASP	4.7
1	E	499	LYS	4.7
2	G	192	ASP	4.7
2	K	216	HIS	4.7
2	G	216	HIS	4.7
2	I	272	PHE	4.7
1	F	365	PRO	4.6
1	B	347	ASP	4.6
2	K	193	ASP	4.6
1	D	424	HIS	4.6
2	G	278	GLY	4.6
1	B	394	ASN	4.5
1	E	533	PRO	4.5
1	C	379	GLY	4.5
1	E	373	THR	4.5
1	F	519	LYS	4.5
2	L	278	GLY	4.5
1	D	460	ARG	4.5
2	H	253	ARG	4.5
1	A	531	ALA	4.5
1	E	361	VAL	4.5
1	F	361	VAL	4.5
1	E	451	PRO	4.5
1	F	459	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
2	L	263	ARG	4.4
1	C	453	TRP	4.4
1	E	482	GLU	4.4
2	I	167	TRP	4.4
2	I	263	ARG	4.4
2	L	159	VAL	4.4
1	F	418	CYS	4.4
2	J	287	THR	4.3
1	D	457	ARG	4.3
1	E	512	THR	4.3
1	B	386	THR	4.3
2	I	229	LYS	4.3
1	E	464	CYS	4.3
2	I	248	GLY	4.3
1	C	397	LEU	4.3
2	K	263	ARG	4.3
2	L	289	THR	4.2
1	F	363	LEU	4.2
2	K	190	ALA	4.2
1	F	389	GLU	4.2
1	C	383	GLN	4.2
1	B	512	THR	4.2
1	E	340	LEU	4.2
1	B	501	SER	4.2
1	F	516	TRP	4.2
1	D	512	THR	4.2
1	F	345	PRO	4.2
1	E	341	SER	4.2
1	D	392	GLN	4.2
1	F	417	GLN	4.1
1	E	459	LYS	4.1
1	A	456	SER	4.1
1	E	486	PRO	4.1
1	A	532	SER	4.1
1	E	468	ASN	4.1
1	D	455	GLY	4.1
2	I	251	THR	4.1
2	I	207	GLN	4.1
2	I	266	GLY	4.0
1	F	524	CYS	4.0
1	C	487	ASP	4.0
2	L	212	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	335	GLY	4.0
2	I	236	ASP	4.0
2	L	288	CYS	4.0
1	F	460	ARG	4.0
2	I	290	PRO	4.0
1	E	453	TRP	3.9
2	H	291	PRO	3.9
1	C	364	ALA	3.9
1	A	453	TRP	3.9
2	G	165	GLU	3.9
1	F	485	LEU	3.9
1	B	396	THR	3.9
2	K	228	LEU	3.9
2	K	192	ASP	3.9
1	E	389	GLU	3.9
1	E	481	ASN	3.9
2	K	262	MET	3.9
1	D	373	THR	3.8
1	C	454	PRO	3.8
1	E	511	VAL	3.8
1	D	481	ASN	3.8
2	K	271	ALA	3.8
2	I	163	CYS	3.8
1	E	400	THR	3.8
1	E	401	SER	3.8
1	A	424	HIS	3.7
1	E	357	THR	3.7
1	D	401	SER	3.7
1	D	518	GLN	3.7
2	G	229	LYS	3.7
2	I	160	CYS	3.7
2	L	229	LYS	3.7
2	H	203	SER	3.7
2	K	258	ASP	3.6
1	F	458	ASP	3.6
1	C	503	PHE	3.6
2	G	279	ALA	3.6
1	A	455	GLY	3.6
2	K	157	GLY	3.6
1	E	338	ALA	3.6
2	H	174	CYS	3.6
1	B	457	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	452	GLU	3.6
2	J	238	SER	3.6
1	F	490	HIS	3.6
1	E	498	THR	3.5
1	E	520	ASP	3.5
2	K	246	ALA	3.5
1	C	532[A]	SER	3.5
1	F	511	VAL	3.5
1	E	536	THR	3.5
1	E	354	PRO	3.5
2	L	225	ASN	3.5
1	E	465	LEU	3.5
2	I	238	SER	3.5
1	F	446	TYR	3.5
1	E	535	GLN	3.5
1	F	482	GLU	3.5
2	L	173	LYS	3.5
2	L	165	GLU	3.5
2	L	238	SER	3.4
2	J	288	CYS	3.4
2	I	171	GLN	3.4
2	K	282	CYS	3.4
1	D	532	SER	3.4
1	C	384	HIS	3.4
1	F	517	GLU	3.4
1	F	392	GLN	3.4
1	F	385	SER	3.4
2	I	288	CYS	3.4
1	E	404	PRO	3.3
2	G	191	CYS	3.3
2	I	212	LYS	3.3
2	L	180	GLY	3.3
2	I	246	ALA	3.3
1	B	423	PRO	3.3
2	H	183	GLN	3.3
1	C	386	THR	3.3
2	L	237	GLY	3.3
1	A	364	ALA	3.3
1	E	391	LYS	3.3
2	G	292	ALA	3.3
2	H	169	ASN	3.2
2	L	158	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	452	GLU	3.2
1	F	364	ALA	3.2
1	B	371	GLN	3.2
1	A	365	PRO	3.2
1	F	346	PHE	3.2
1	F	465	LEU	3.2
1	A	361	VAL	3.2
1	B	389	GLU	3.2
1	C	499	LYS	3.2
1	E	362	ASP	3.2
1	F	452	GLU	3.2
1	A	347	ASP	3.2
1	A	388	LYS	3.2
2	L	192	ASP	3.2
2	L	204	PRO	3.2
1	E	374	TRP	3.2
1	C	385	SER	3.2
2	G	287	THR	3.2
2	K	231	GLU	3.1
2	K	252	SER	3.1
1	A	396	THR	3.1
1	E	500	GLY	3.1
1	B	421	THR	3.1
2	K	233	ILE	3.1
2	J	286	ALA	3.1
2	K	189	TYR	3.1
2	L	259	CYS	3.1
1	F	444	GLU	3.1
2	H	286	ALA	3.1
1	B	428	ALA	3.1
1	F	395	GLY	3.1
2	H	205	GLU	3.1
1	C	401	SER	3.1
1	F	497	LYS	3.1
1	D	503	PHE	3.1
1	E	506	PHE	3.0
1	F	494	GLN	3.0
1	D	464	CYS	3.0
1	F	367	LYS	3.0
2	K	207	GLN	3.0
1	A	516	TRP	3.0
2	I	210	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	I	258	ASP	3.0
2	H	230	GLY	3.0
1	A	502	GLY	3.0
1	D	497	LYS	3.0
2	I	159	VAL	3.0
2	L	228	LEU	3.0
1	E	513	ARG	3.0
2	H	251	THR	3.0
1	B	422	HIS	3.0
1	F	471	PRO	3.0
2	H	247	PRO	3.0
1	E	455	GLY	3.0
1	B	398	THR	3.0
2	H	288	CYS	3.0
1	D	451	PRO	3.0
1	E	347	ASP	2.9
2	K	208	ASP	2.9
1	F	339	TYR	2.9
2	L	267	ARG	2.9
1	D	461	THR	2.9
2	K	288	CYS	2.9
2	I	190	ALA	2.9
2	H	248	GLY	2.9
2	K	203	SER	2.9
1	A	337	SER	2.8
1	B	456	SER	2.8
2	H	255	GLN	2.8
2	J	180	GLY	2.8
2	J	191	CYS	2.8
1	F	359	LEU	2.8
1	C	400	THR	2.8
2	I	206	GLU	2.8
1	D	484	GLN	2.8
1	D	447	ALA	2.8
2	H	165	GLU	2.8
2	H	287	THR	2.8
1	C	361	VAL	2.8
2	I	209	PHE	2.8
1	F	388	LYS	2.8
2	J	253	ARG	2.8
2	J	252	SER	2.8
1	A	362	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	362	ASP	2.8
2	J	158	PHE	2.7
1	E	461	THR	2.7
1	F	528	HIS	2.7
1	F	507	SER	2.7
1	C	387	ARG	2.7
1	F	518	GLN	2.7
2	I	278	GLY	2.7
1	F	515	GLU	2.7
2	G	291	PRO	2.7
2	I	254	SER	2.7
2	I	230	GLY	2.7
1	A	457	ARG	2.7
2	I	179	LYS	2.7
2	K	215	SER	2.7
1	F	386	THR	2.7
2	I	211	THR	2.7
2	K	237	GLY	2.7
2	K	279	ALA	2.7
1	B	390	GLU	2.7
1	B	359	LEU	2.6
1	D	347	ASP	2.6
1	F	468	ASN	2.6
2	I	286	ALA	2.6
2	I	245	TRP	2.6
1	F	520	ASP	2.6
1	C	455	GLY	2.6
1	F	394	ASN	2.6
1	F	428	ALA	2.6
2	H	290	PRO	2.6
2	L	174	CYS	2.6
1	F	488	ALA	2.6
1	E	436	THR	2.6
1	B	361	VAL	2.6
2	H	195	GLU	2.6
1	F	366	SER	2.6
1	A	473	ASP	2.6
1	B	488	ALA	2.6
1	B	367	LYS	2.6
1	D	534	SER	2.6
2	I	252	SER	2.6
2	H	180	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	237	GLY	2.6
1	E	387	ARG	2.6
2	L	262	MET	2.6
1	D	446	TYR	2.6
1	D	395	GLY	2.6
2	J	178	GLY	2.6
1	E	365	PRO	2.6
1	F	381	PRO	2.5
1	D	357	THR	2.5
1	B	388	LYS	2.5
1	B	430	MET	2.5
1	E	524	CYS	2.5
1	D	485	LEU	2.5
2	J	192	ASP	2.5
1	F	467	GLN	2.5
1	F	484	GLN	2.5
2	J	173	LYS	2.5
2	G	217	THR	2.5
1	E	397	LEU	2.5
2	G	243	SER	2.5
2	I	208	ASP	2.5
2	I	169	ASN	2.5
2	K	291	PRO	2.5
2	L	283	ASP	2.5
1	C	403	LEU	2.5
2	G	190	ALA	2.5
1	E	360	VAL	2.5
2	H	249	GLU	2.5
2	I	213	HIS	2.5
1	E	398	THR	2.4
1	F	475	SER	2.4
1	D	426	PRO	2.4
2	K	202	HIS	2.4
2	I	262	MET	2.4
1	D	501	SER	2.4
1	D	514	ALA	2.4
2	K	167	TRP	2.4
1	B	464	CYS	2.4
2	K	254	SER	2.4
2	I	192	ASP	2.4
1	E	445	VAL	2.4
1	F	401	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	258	ASP	2.4
2	I	268	TRP	2.4
2	K	265	SER	2.4
1	C	524	CYS	2.4
2	J	160	CYS	2.4
1	E	379	GLY	2.3
2	G	196	GLY	2.3
2	H	258	ASP	2.3
2	J	228	LEU	2.3
1	E	483	VAL	2.3
2	I	267	ARG	2.3
1	B	520	ASP	2.3
1	D	502	GLY	2.3
1	F	423	PRO	2.3
2	H	244	ASN	2.3
1	F	336	VAL	2.3
1	F	453	TRP	2.3
2	H	280	TRP	2.3
1	E	521	GLU	2.3
2	K	227	ASP	2.3
1	B	513	ARG	2.3
2	L	290	PRO	2.3
1	D	337	SER	2.3
1	C	504	PHE	2.2
1	D	448	PHE	2.2
1	E	475	SER	2.2
1	C	513	ARG	2.2
2	L	208	ASP	2.2
1	D	396	THR	2.2
2	G	171	GLN	2.2
1	C	404	PRO	2.2
2	I	253	ARG	2.2
2	I	170	PHE	2.2
2	K	158	PHE	2.2
2	L	166	LYS	2.2
1	E	474	ILE	2.2
1	B	375	SER	2.2
1	D	453	TRP	2.2
1	E	526	ALA	2.2
1	F	530	ALA	2.2
1	D	390	GLU	2.2
2	I	239	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
2	G	163	CYS	2.2
2	I	247	PRO	2.2
1	A	500	GLY	2.2
2	L	220	TRP	2.1
1	F	447	ALA	2.1
1	B	376	ARG	2.1
2	L	274	ASP	2.1
1	C	366	SER	2.1
2	K	244	ASN	2.1
1	D	494	GLN	2.1
2	L	183	GLN	2.1
1	E	345	PRO	2.1
1	F	422	HIS	2.1
1	C	357	THR	2.1
2	J	258	ASP	2.1
1	D	450	THR	2.1
1	B	368	GLY	2.1
2	I	195	GLU	2.1
1	C	340	LEU	2.1
1	E	412	GLU	2.1
2	K	195	GLU	2.1
1	F	457	ARG	2.1
2	G	174	CYS	2.1
2	H	200	SER	2.1
1	B	429	LEU	2.1
2	G	158	PHE	2.1
1	C	468	ASN	2.1
1	A	497	LYS	2.0
1	C	529	GLU	2.0
1	C	396	THR	2.0
2	I	287	THR	2.0
2	I	261	MET	2.0
1	D	363	LEU	2.0
1	C	398	THR	2.0
1	C	486	PRO	2.0
2	K	290	PRO	2.0
1	F	384	HIS	2.0
1	E	411	ILE	2.0
1	F	462	LEU	2.0
1	B	544	ASN	2.0
2	G	255	GLN	2.0
2	I	204	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	E	601	14/15	0.67	0.80	1.63	158,160,162,164	0
3	NAG	A	602	14/15	0.88	0.51	0.75	146,148,151,152	0
3	NAG	C	601	14/15	0.40	0.59	0.62	148,155,161,164	0
3	NAG	A	601	14/15	0.72	0.44	-0.25	142,147,153,157	0
3	NAG	C	602	14/15	0.87	0.31	-0.80	135,137,142,143	0
3	NAG	D	601	14/15	0.79	0.31	-0.88	139,144,146,147	0
3	NAG	F	602	14/15	0.83	0.40	-0.97	147,150,151,151	0
3	NAG	B	602	14/15	0.84	0.31	-1.10	120,124,127,128	0
3	NAG	D	602	14/15	0.90	0.28	-1.22	103,105,106,107	0
3	NAG	E	602	14/15	0.76	0.21	-1.58	132,134,136,136	0
3	MAN	A	605	11/12	0.82	0.38	-	163,165,168,169	0
3	NAG	B	601	14/15	0.52	0.50	-	185,189,195,198	0
3	MAN	D	605	11/12	0.88	0.21	-	156,157,159,159	0
3	MAN	F	605	11/12	0.85	0.16	-	147,149,151,151	0
3	MAN	A	604	11/12	0.72	0.34	-	153,154,155,156	0
3	BMA	E	603	11/12	0.78	0.21	-	150,152,153,153	0
3	BMA	D	603	11/12	0.89	0.21	-	105,106,107,108	0
3	BMA	B	603	11/12	0.89	0.19	-	123,126,128,128	0
3	MAN	E	605	11/12	0.78	0.24	-	153,155,156,157	0
3	BMA	F	603	11/12	0.87	0.25	-	137,139,139,139	0
3	BMA	C	603	11/12	0.85	0.17	-	139,143,145,146	0
3	MAN	F	604	11/12	0.65	0.36	-	154,155,156,157	0
3	MAN	C	604	11/12	0.73	0.31	-	142,142,144,144	0
3	MAN	C	605	11/12	0.68	0.41	-	164,166,168,169	0
3	NAG	F	601	14/15	0.84	0.29	-	142,147,151,153	0
3	BMA	A	603	11/12	0.90	0.21	-	141,143,145,146	0
3	MAN	B	604	11/12	0.81	0.28	-	155,156,157,157	0
3	MAN	B	605	11/12	0.78	0.32	-	155,157,160,161	0
3	MAN	D	604	11/12	0.74	0.34	-	146,148,149,150	0
3	MAN	E	604	11/12	0.75	0.38	-	138,139,140,141	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(Å ²)	Q<0.9
4	MAN	C	607	11/12	0.43	0.84	3.13	122,122,126,128	0
4	MAN	C	606	11/12	0.57	0.53	-	127,128,130,131	0

6.5 Other polymers [i](#)

There are no such residues in this entry.