



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:06 PM GMT

PDB ID : 4KI1
Title : Primitive triclinic crystal form of the human IgE-Fc(epsilon)3-4 bound to its B cell receptor derCD23
Authors : Dhaliwal, B.; Pang, M.O.Y.; Sutton, B.J.; Beavil, A.J.
Deposited on : 2013-05-01
Resolution : 3.20 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

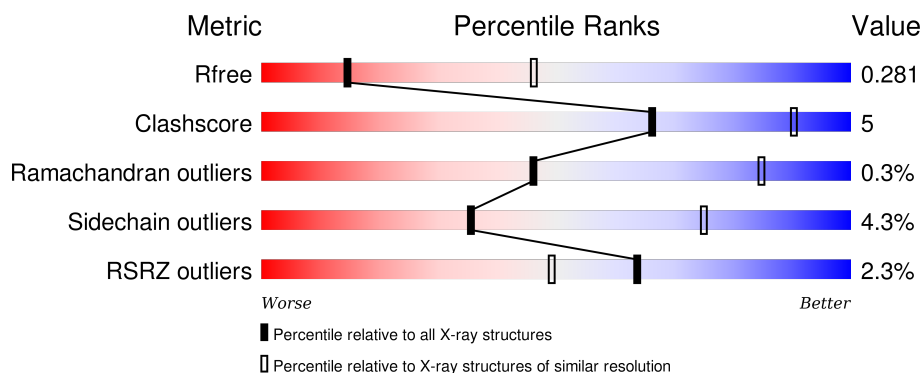
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	
1	B	223	
1	C	223	
1	D	223	
2	E	143	

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Mol	Chain	Length	Quality of chain
2	F	143	
2	G	143	
2	H	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	D	602	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11133 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	208	Total	C	N	O	S	0	0	0
			1650	1033	304	307	6			
1	B	211	Total	C	N	O	S	0	0	0
			1667	1044	307	310	6			
1	C	211	Total	C	N	O	S	0	0	0
			1667	1044	307	310	6			
1	D	208	Total	C	N	O	S	0	0	0
			1650	1033	304	307	6			

There are 20 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
D	327	PRO	-	EXPRESSION TAG	UNP P01854
D	371	GLN	ASN	ENGINEERED MUTATION	UNP P01854
D	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	E	132	Total	C	N	O	S	0	0	0
			1065	670	190	194	11			
2	F	131	Total	C	N	O	S	0	0	0
			1058	665	189	193	11			
2	G	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	H	132	Total	C	N	O	S	0	0	0
			1059	664	190	194	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		

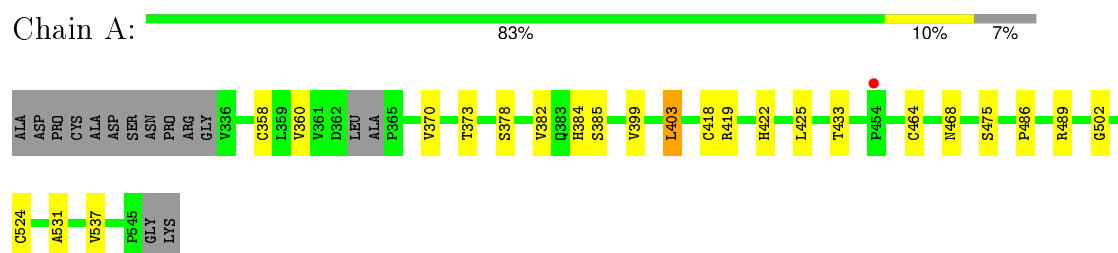
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			1	1		

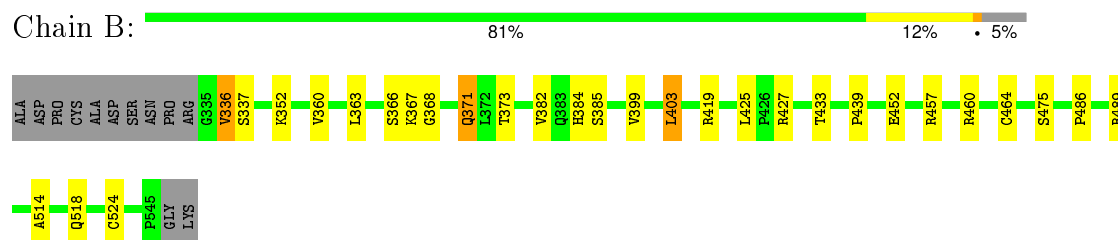
3 Residue-property plots

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

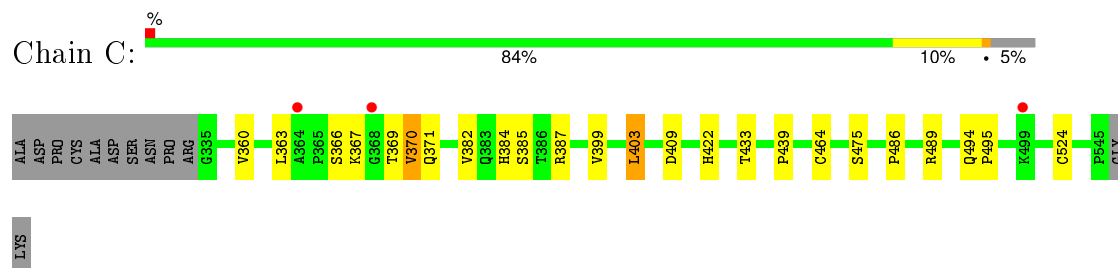
• Molecule 1: IG EPSILON CHAIN C REGION



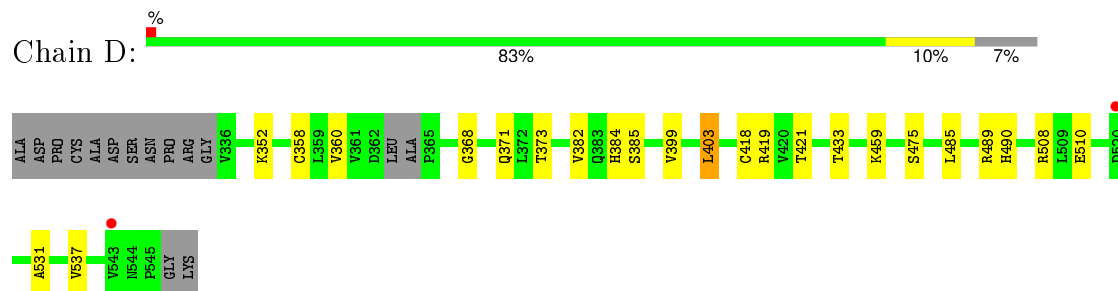
• Molecule 1: IG EPSILON CHAIN C REGION




• Molecule 1: IG EPSILON CHAIN C REGION

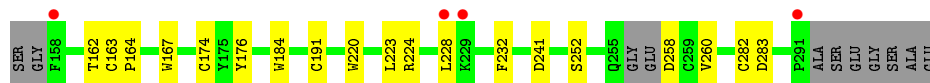


• Molecule 1: IG EPSILON CHAIN C REGION




● Molecule 2: LOW AFFINITY IMMUNOGLOBULIN EPSILON FC RECEPTOR

Chain E: 




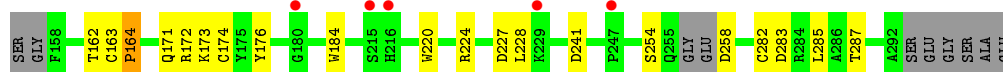
● Molecule 2: LOW AFFINITY IMMUNOGLOBULIN EPSILON FC RECEPTOR

Chain F: 




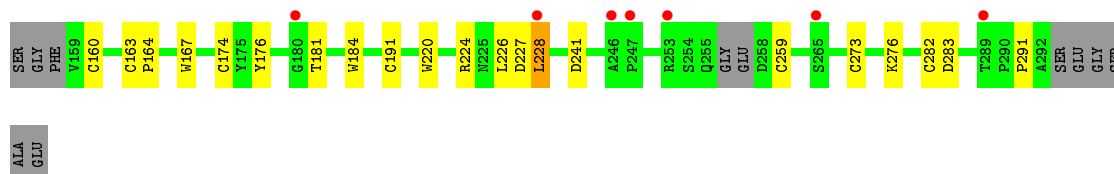
● Molecule 2: LOW AFFINITY IMMUNOGLOBULIN EPSILON FC RECEPTOR

Chain G: 



● Molecule 2: LOW AFFINITY IMMUNOGLOBULIN EPSILON FC RECEPTOR

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.79Å 63.84Å 163.89Å 100.67° 90.13° 103.49°	Depositor
Resolution (Å)	80.40 – 3.20 80.44 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (80.40-3.20) 78.7 (80.44-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.233 , 0.266 0.264 , 0.281	Depositor DCC
R_{free} test set	1523 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 21.2	EDS
Estimated twinning fraction	0.049 for -h,-k,k+l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 30144 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	11133	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.36	0/1692	0.62	2/2301 (0.1%)
1	B	0.36	0/1710	0.62	2/2328 (0.1%)
1	C	0.41	1/1710 (0.1%)	0.63	2/2328 (0.1%)
1	D	0.35	0/1692	0.66	4/2301 (0.2%)
2	E	0.43	1/1098 (0.1%)	0.59	0/1487
2	F	0.41	1/1090 (0.1%)	0.59	0/1475
2	G	0.43	1/1103 (0.1%)	0.68	2/1494 (0.1%)
2	H	0.41	1/1091 (0.1%)	0.58	0/1478
All	All	0.39	5/11186 (0.0%)	0.62	12/15192 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	164	PRO	N-CD	-6.87	1.38	1.47
2	G	164	PRO	N-CD	-6.08	1.39	1.47
2	F	164	PRO	N-CD	-6.08	1.39	1.47
2	H	164	PRO	N-CD	-5.85	1.39	1.47
1	C	495	PRO	N-CD	-5.04	1.40	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	SER	N-CA-CB	7.06	121.09	110.50
1	B	385	SER	N-CA-CB	7.03	121.04	110.50
2	G	173	LYS	N-CA-CB	6.54	122.37	110.60
2	G	171	GLN	CB-CA-C	6.29	122.98	110.40
1	A	384	HIS	N-CA-C	6.05	127.34	111.00
1	B	384	HIS	N-CA-C	5.95	127.08	111.00
1	C	385	SER	N-CA-CB	5.90	119.35	110.50
1	D	385	SER	N-CA-CB	5.82	119.23	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	384	HIS	N-CA-C	5.50	125.86	111.00
1	D	490	HIS	N-CA-CB	5.40	120.33	110.60
1	C	384	HIS	N-CA-C	5.19	125.02	111.00
1	D	459	LYS	N-CA-C	5.04	124.62	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1650	0	1636	9	0
1	B	1667	0	1655	16	0
1	C	1667	0	1655	14	0
1	D	1650	0	1636	9	0
2	E	1065	0	989	8	1
2	F	1058	0	982	11	0
2	G	1070	0	994	15	0
2	H	1059	0	985	11	1
3	A	61	0	52	0	0
3	B	61	0	52	1	0
3	C	61	0	52	2	0
3	D	61	0	52	1	0
4	B	2	0	0	0	0
4	D	1	0	0	0	0
All	All	11133	0	10740	92	1

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 5.

All (92) 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:F:163:CYS:SG	2:F:174:CYS:HB3	1.91	1.10
1:C:370:VAL:HG13	1:C:422:HIS:HD2	1.16	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:163:CYS:HB2	2:F:174:CYS:SG	2.05	0.96
2:G:163:CYS:SG	2:G:174:CYS:HB3	2.06	0.96
1:A:464:CYS:HG	1:A:524:CYS:HG	0.95	0.94
1:C:464:CYS:HG	1:C:524:CYS:HG	0.97	0.94
1:A:358:CYS:HG	1:A:418:CYS:HG	1.07	0.92
1:C:370:VAL:HG13	1:C:422:HIS:CD2	2.08	0.87
2:F:163:CYS:SG	2:F:174:CYS:CB	2.62	0.86
1:D:485:LEU:HD22	1:D:489:ARG:NH1	1.95	0.81
2:H:259:CYS:HG	2:H:273:CYS:HG	1.30	0.78
2:F:163:CYS:CB	2:F:174:CYS:SG	2.71	0.78
1:B:367:LYS:HG2	1:B:368:GLY:H	1.49	0.77
1:C:370:VAL:CG1	1:C:422:HIS:HD2	1.96	0.76
1:B:464:CYS:HG	1:B:524:CYS:HG	0.76	0.76
2:G:163:CYS:SG	2:G:174:CYS:CB	2.75	0.75
2:G:163:CYS:HB2	2:G:174:CYS:SG	2.28	0.73
2:H:181:THR:CG2	2:H:276:LYS:HE2	2.22	0.70
2:G:163:CYS:SG	2:G:164:PRO:HD2	2.35	0.66
1:D:358:CYS:HG	1:D:418:CYS:HG	0.68	0.66
2:G:176:TYR:HB3	2:G:282:CYS:HB2	1.77	0.66
2:F:163:CYS:SG	2:F:164:PRO:HD2	2.36	0.66
2:E:223:LEU:HB3	2:E:260:VAL:HB	1.78	0.66
2:G:172:ARG:NH1	2:G:285:LEU:CD2	2.60	0.65
2:G:163:CYS:CB	2:G:174:CYS:SG	2.85	0.64
1:B:367:LYS:HG2	1:B:368:GLY:N	2.12	0.64
1:C:366:SER:OG	1:C:367:LYS:N	2.30	0.64
2:E:223:LEU:HD11	2:E:232:PHE:HB3	1.81	0.63
2:G:172:ARG:HH12	2:G:285:LEU:CD2	2.13	0.62
2:E:163:CYS:HB3	2:E:174:CYS:SG	2.41	0.61
2:G:172:ARG:HH12	2:G:285:LEU:HD21	1.66	0.59
2:F:163:CYS:HG	2:F:174:CYS:HB3	1.65	0.59
1:D:360:VAL:HG13	1:D:399:VAL:HG13	1.85	0.59
1:B:360:VAL:HG13	1:B:399:VAL:HG13	1.86	0.58
1:C:360:VAL:HG13	1:C:399:VAL:HG13	1.86	0.58
1:A:360:VAL:HG13	1:A:399:VAL:HG13	1.86	0.57
1:C:370:VAL:HG23	1:C:387:ARG:HH22	1.69	0.56
2:H:181:THR:HG22	2:H:276:LYS:HE2	1.88	0.55
1:A:422:HIS:HB3	1:A:425:LEU:HB2	1.90	0.54
2:E:167:TRP:HB3	2:E:174:CYS:SG	2.48	0.53
1:C:439:PRO:HA	2:G:254:SER:HA	1.89	0.53
2:H:167:TRP:HB3	2:H:174:CYS:SG	2.49	0.53
2:H:176:TYR:HB3	2:H:282:CYS:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:172:ARG:NH2	2:G:285:LEU:HD22	2.25	0.51
1:B:514:ALA:O	1:B:518:GLN:HG3	2.10	0.51
1:B:363:LEU:HD22	3:B:601:NAG:H83	1.93	0.51
1:C:366:SER:OG	1:C:367:LYS:O	2.29	0.51
2:H:163:CYS:HB3	2:H:174:CYS:SG	2.52	0.50
2:H:181:THR:HG22	2:H:276:LYS:CE	2.42	0.50
1:C:363:LEU:HD22	3:C:601:NAG:H83	1.93	0.50
2:G:163:CYS:SG	2:G:164:PRO:CD	3.00	0.50
2:F:163:CYS:SG	2:F:164:PRO:CD	3.01	0.49
3:D:603:BMA:H61	3:D:604:MAN:H2	1.59	0.48
1:C:494:GLN:HE22	3:C:605:MAN:C3	2.27	0.48
2:F:184:TRP:HD1	2:F:220:TRP:CE3	2.31	0.48
2:G:184:TRP:HD1	2:G:220:TRP:CE3	2.31	0.48
2:E:184:TRP:HD1	2:E:220:TRP:CE3	2.31	0.48
2:H:184:TRP:HD1	2:H:220:TRP:CE3	2.31	0.47
1:B:373:THR:HB	1:B:419:ARG:HB3	1.96	0.47
2:E:191:CYS:HA	2:E:282:CYS:SG	2.54	0.47
1:A:373:THR:HB	1:A:419:ARG:HB3	1.96	0.47
1:B:452:GLU:OE2	1:B:457:ARG:CZ	2.63	0.46
1:B:452:GLU:HB2	1:B:460:ARG:NH2	2.31	0.46
1:C:382:VAL:HB	1:C:403:LEU:HD11	1.99	0.45
1:B:336:VAL:HG13	1:B:337:SER:N	2.31	0.45
1:B:382:VAL:HB	1:B:403:LEU:HD11	1.99	0.45
2:H:181:THR:HG21	2:H:276:LYS:HE2	1.96	0.45
1:D:382:VAL:HB	1:D:403:LEU:HD11	1.98	0.45
1:B:452:GLU:OE2	1:B:457:ARG:NE	2.50	0.44
1:A:382:VAL:HB	1:A:403:LEU:HD11	1.98	0.44
2:F:191:CYS:HA	2:F:282:CYS:SG	2.57	0.44
1:D:373:THR:HB	1:D:419:ARG:HB3	2.00	0.44
2:H:226:LEU:HD23	2:H:228:LEU:HB3	2.01	0.43
1:B:439:PRO:HA	2:F:254:SER:HA	1.99	0.43
1:C:464:CYS:CB	1:C:524:CYS:HG	2.28	0.43
1:D:508:ARG:NH2	1:D:510:GLU:OE2	2.47	0.42
1:B:464:CYS:CB	1:B:524:CYS:HG	2.31	0.42
1:B:486:PRO:HD2	1:B:489:ARG:HG3	2.02	0.42
2:F:162:THR:HB	2:F:287:THR:HG23	2.02	0.42
2:G:162:THR:HB	2:G:287:THR:HG23	2.02	0.42
1:A:468:ASN:HA	1:A:502:GLY:HA3	2.01	0.41
1:D:485:LEU:HD22	1:D:489:ARG:HH11	1.80	0.41
1:C:486:PRO:HD2	1:C:489:ARG:HG3	2.01	0.41
1:D:531:ALA:HB1	1:D:537:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:163:CYS:SG	2:E:174:CYS:HB2	2.61	0.41
1:A:531:ALA:HB1	1:A:537:VAL:HG23	2.03	0.41
2:G:163:CYS:HG	2:G:174:CYS:HB3	1.81	0.41
2:H:191:CYS:HG	2:H:282:CYS:HG	0.67	0.41
1:D:371:GLN:HB2	1:D:421:THR:HB	2.03	0.40
2:E:176:TYR:HB3	2:E:282:CYS:HB2	2.04	0.40
1:A:486:PRO:HD2	1:A:489:ARG:HG3	2.02	0.40
1:B:336:VAL:CG1	1:B:337:SER:N	2.80	0.40

All (1) 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:E:162:THR:CG2	2:H:276:LYS:NZ[1_666]	1.97	0.23

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	204/223 (92%)	194 (95%)	10 (5%)	0	100	100
1	B	209/223 (94%)	200 (96%)	8 (4%)	1 (0%)	34	78
1	C	209/223 (94%)	200 (96%)	8 (4%)	1 (0%)	34	78
1	D	204/223 (92%)	193 (95%)	10 (5%)	1 (0%)	34	78
2	E	128/143 (90%)	122 (95%)	6 (5%)	0	100	100
2	F	127/143 (89%)	119 (94%)	8 (6%)	0	100	100
2	G	129/143 (90%)	122 (95%)	7 (5%)	0	100	100
2	H	128/143 (90%)	121 (94%)	6 (5%)	1 (1%)	24	69
All	All	1338/1464 (91%)	1271 (95%)	63 (5%)	4 (0%)	46	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	368	GLY
1	B	371	GLN
1	C	371	GLN
2	H	291	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	185/195 (95%)	180 (97%)	5 (3%)	52	85
1	B	186/195 (95%)	177 (95%)	9 (5%)	31	72
1	C	186/195 (95%)	180 (97%)	6 (3%)	46	81
1	D	185/195 (95%)	181 (98%)	4 (2%)	60	87
2	E	114/120 (95%)	108 (95%)	6 (5%)	28	69
2	F	113/120 (94%)	104 (92%)	9 (8%)	15	52
2	G	114/120 (95%)	108 (95%)	6 (5%)	28	69
2	H	113/120 (94%)	107 (95%)	6 (5%)	28	69
All	All	1196/1260 (95%)	1145 (96%)	51 (4%)	35	75

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	370	VAL
1	A	378	SER
1	A	403	LEU
1	A	433	THR
1	A	475	SER
1	B	336	VAL
1	B	352	LYS
1	B	366	SER
1	B	371	GLN
1	B	403	LEU

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Mol	Chain	Res	Type
1	B	425	LEU
1	B	427	ARG
1	B	433	THR
1	B	475	SER
1	C	369	THR
1	C	370	VAL
1	C	403	LEU
1	C	409	ASP
1	C	433	THR
1	C	475	SER
1	D	352	LYS
1	D	403	LEU
1	D	433	THR
1	D	475	SER
2	E	224	ARG
2	E	228	LEU
2	E	241	ASP
2	E	252	SER
2	E	258	ASP
2	E	283	ASP
2	F	224	ARG
2	F	225	ASN
2	F	227	ASP
2	F	228	LEU
2	F	231	GLU
2	F	241	ASP
2	F	253	ARG
2	F	258	ASP
2	F	283	ASP
2	G	224	ARG
2	G	227	ASP
2	G	228	LEU
2	G	241	ASP
2	G	258	ASP
2	G	283	ASP
2	H	160	CYS
2	H	224	ARG
2	H	227	ASP
2	H	228	LEU
2	H	241	ASP
2	H	283	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	392	GLN
1	C	422	HIS
1	C	494	GLN
2	E	183	GLN
2	E	269	ASN
2	F	183	GLN
2	F	269	ASN
2	G	269	ASN
2	H	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 ⓘ

20 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	1,3	14,14,15	0.23	0	15,19,21	0.52	0
3	NAG	A	602	3	14,14,15	0.25	0	15,19,21	0.53	0
3	BMA	A	603	3	11,11,12	0.35	0	14,15,17	0.59	0
3	MAN	A	604	3	11,11,12	0.37	0	14,15,17	1.28	1 (7%)
3	MAN	A	605	3	11,11,12	0.38	0	14,15,17	0.79	1 (7%)
3	NAG	B	601	1,3	14,14,15	0.24	0	15,19,21	0.50	0
3	NAG	B	602	3	14,14,15	0.26	0	15,19,21	0.53	0
3	BMA	B	603	3	11,11,12	0.30	0	14,15,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	B	604	3	11,11,12	0.37	0	14,15,17	1.25	1 (7%)
3	MAN	B	605	3	11,11,12	0.34	0	14,15,17	0.87	1 (7%)
3	NAG	C	601	1,3	14,14,15	0.26	0	15,19,21	0.52	0
3	NAG	C	602	3	14,14,15	0.25	0	15,19,21	0.55	0
3	BMA	C	603	3	11,11,12	0.35	0	14,15,17	0.98	1 (7%)
3	MAN	C	604	3	11,11,12	0.43	0	14,15,17	1.13	2 (14%)
3	MAN	C	605	3	11,11,12	0.35	0	14,15,17	0.76	1 (7%)
3	NAG	D	601	1,3	14,14,15	0.24	0	15,19,21	0.50	0
3	NAG	D	602	3	14,14,15	0.27	0	15,19,21	0.54	0
3	BMA	D	603	3	11,11,12	0.29	0	14,15,17	0.98	1 (7%)
3	MAN	D	604	3	11,11,12	0.41	0	14,15,17	1.06	2 (14%)
3	MAN	D	605	3	11,11,12	0.30	0	14,15,17	0.87	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	601	1,3	-	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	1/1/1/1
3	MAN	A	605	3	-	0/2/19/22	0/1/1/1
3	NAG	B	601	1,3	-	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	1/1/1/1
3	MAN	B	605	3	-	0/2/19/22	0/1/1/1
3	NAG	C	601	1,3	-	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	1,3	-	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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	BMA	C1-C2-C3	2.21	112.15	109.54
3	D	604	MAN	C1-C2-C3	2.22	112.16	109.54
3	C	605	MAN	C1-O5-C5	2.28	115.14	112.25
3	A	605	MAN	C1-O5-C5	2.30	115.17	112.25
3	C	604	MAN	C1-C2-C3	2.42	112.41	109.54
3	D	603	BMA	C1-O5-C5	2.63	115.59	112.25
3	B	605	MAN	C1-O5-C5	2.66	115.63	112.25
3	D	605	MAN	C1-O5-C5	2.68	115.66	112.25
3	D	604	MAN	C1-O5-C5	3.17	116.27	112.25
3	C	604	MAN	C1-O5-C5	3.37	116.52	112.25
3	B	604	MAN	C1-O5-C5	4.43	117.86	112.25
3	A	604	MAN	C1-O5-C5	4.51	117.97	112.25

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	604	MAN	C1-C2-C3-C4-C5-O5
3	A	604	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	NAG	1	0
3	C	601	NAG	1	0
3	C	605	MAN	1	0
3	D	603	BMA	1	0
3	D	604	MAN	1	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	208/223 (93%)	0.19	1 (0%) 91 87	40, 66, 105, 125	0
1	B	211/223 (94%)	0.15	0 100 100	40, 67, 100, 112	0
1	C	211/223 (94%)	0.11	3 (1%) 78 65	40, 67, 95, 114	0
1	D	208/223 (93%)	0.15	2 (0%) 84 75	39, 64, 105, 131	0
2	E	132/143 (92%)	0.36	4 (3%) 54 39	58, 89, 115, 135	0
2	F	131/143 (91%)	0.62	9 (6%) 20 11	86, 103, 136, 169	0
2	G	133/143 (93%)	0.40	5 (3%) 44 29	47, 78, 97, 117	0
2	H	132/143 (92%)	0.50	7 (5%) 30 17	71, 102, 136, 148	0
All	All	1366/1464 (93%)	0.27	31 (2%) 64 49	39, 76, 118, 169	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	289	THR	7.3
2	F	229	LYS	4.7
2	H	247	PRO	4.7
2	H	253	ARG	4.6
1	A	454	PRO	3.5
2	F	290	PRO	3.5
1	C	368	GLY	3.0
2	F	247	PRO	2.9
2	H	246	ALA	2.9
2	F	162	THR	2.8
2	H	265	SER	2.8
2	E	228	LEU	2.8
2	E	291	PRO	2.7
1	D	520	ASP	2.7
2	F	180	GLY	2.7
2	E	158	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	180	GLY	2.7
2	H	289	THR	2.6
1	C	364	ALA	2.5
2	G	229	LYS	2.4
2	G	247	PRO	2.4
2	E	229	LYS	2.3
2	F	248	GLY	2.3
2	G	216	HIS	2.3
2	G	215	SER	2.2
1	C	499	LYS	2.2
2	F	253	ARG	2.2
2	G	180	GLY	2.1
2	H	228	LEU	2.1
1	D	543	VAL	2.1
2	F	241	ASP	2.1

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	D	602	14/15	0.92	0.36	3.75	100,101,105,106	0
3	NAG	C	601	14/15	0.87	0.36	1.99	93,96,101,104	0
3	NAG	A	602	14/15	0.95	0.30	1.91	90,92,95,95	0
3	NAG	B	602	14/15	0.88	0.33	1.02	93,95,97,97	0
3	NAG	C	602	14/15	0.91	0.23	-1.10	89,91,94,94	0
3	NAG	B	601	14/15	0.89	0.18	-1.18	87,89,92,92	0
3	MAN	A	605	11/12	0.57	0.41	-	108,109,109,110	0
3	BMA	D	603	11/12	0.77	0.23	-	108,110,112,115	0
3	NAG	D	601	14/15	0.87	0.19	-	92,96,100,102	0
3	MAN	C	604	11/12	0.82	0.27	-	92,93,93,93	0
3	MAN	B	604	11/12	0.78	0.23	-	99,101,102,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MAN	A	604	11/12	0.82	0.25	-	99,102,104,105	0
3	NAG	A	601	14/15	0.87	0.25	-	88,90,93,95	0
3	MAN	D	604	11/12	0.69	0.41	-	115,116,117,118	0
3	MAN	B	605	11/12	0.75	0.42	-	105,106,107,109	0
3	MAN	D	605	11/12	0.76	0.35	-	119,120,124,125	0
3	BMA	B	603	11/12	0.82	0.22	-	99,100,102,103	0
3	BMA	C	603	11/12	0.79	0.30	-	93,93,95,97	0
3	BMA	A	603	11/12	0.85	0.21	-	97,100,101,104	0
3	MAN	C	605	11/12	0.71	0.31	-	99,100,102,102	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.